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PRENTICE HALL

Analysis, Synthesis, and Design of Chemical Processes

Fourth Edition

Richard Turton • Richard C. Bailie • Wallace B. Whiting
Joseph A. Shaeiwitz • Debangsu Bhattacharyya





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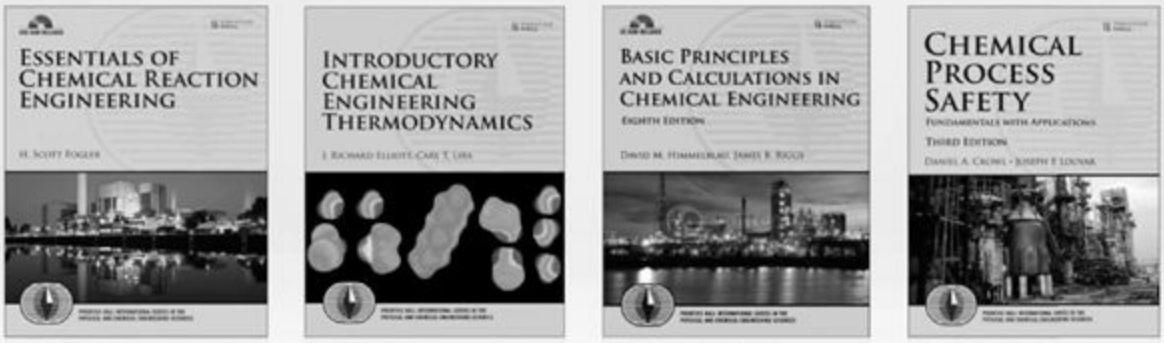
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C.5.2 Cumene Production Reactions
C.5.3 Process Description
C.5.4 Recent Problems in Unit 800
C.5.5 Other Information
C.5.6 Assignment
C.5.7 Report Format
C.5.8 Process Calculations
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Preface

This book represents the culmination of many years of teaching experience in the senior design course at West Virginia University (WVU) and University of Nevada, Reno. Although the program at WVU has evolved over the past 35 years and is still evolving, it is fair to say that the current program has gelled over the past 25 years as a concerted effort by the authors to integrate design throughout the undergraduate curriculum in chemical engineering.

We view design as the focal point of chemical engineering practice. Far more than the development of a set of specifications for a new chemical plant, design is the creative activity through which engineers continuously improve the operations of facilities to create products that enhance the quality of life. Whether developing the grassroots plant, proposing and guiding process modifications, or troubleshooting and implementing operational strategies for existing equipment, engineering design requires a broad spectrum of knowledge and intellectual skills to be able to analyze the big picture and the minute details and, most important, to know when to concentrate on each.

Our vehicle for helping students develop and hone their design skills is process design rather than plant design, covering synthesis of the entire chemical process through topics relating to the preliminary sizing of equipment, flowsheet optimization, economic evaluation of projects, and the operation of chemical processes. The purpose of this text is to assist chemical engineering students in making the transition from solving well-posed problems in a specific subject to integrating all the knowledge that they have gained in their undergraduate education and applying this information to solving open-ended process problems. Many of the nuts-and-bolts issues regarding plant design (for example, what schedule pipe to use for a given stream or what corrosion allowance to use for a vessel in a certain service) are not covered. Although such issues are clearly important to the practicing engineer, several excellent handbooks and textbooks are available to address such problems, and these are cited in the text where applicable.

In the fourth edition, we have rearranged some of the material from previous editions, and we have added two new chapters on advanced concepts in steady-state simulation (Chapter 16) and dynamic simulation of processes (Chapter 17). We have also added extensive material on the choice of thermodynamics package to use for modeling processes containing electrolyte solutions and solids (Chapter 13) and a brief introduction to logic control (Chapter 18). Additional pedagogical material has been added to each chapter to outline the key concepts and major lessons to be learned from each chapter.

We continue to emphasize the importance of understanding, analyzing, and synthesizing chemical processes and process flow diagrams. To this end, we have expanded Appendix B to include an additional four (making a total of 15) preliminary designs of chemical processes. All the projects have been moved to the CD accompanying the text, along with the chapters on outcomes assessment, written and oral communications, and a written report case study and the projects from Appendix C of the first edition.

The arrangement of chapters into the six sections of the book is similar to that adopted in the second edition. These sections are as follows:

- Section I—Conceptualization and Analysis of Chemical Processes
- Section II—Engineering Economic Analysis of Chemical Processes

- Section III—Synthesis and Optimization of Chemical Processes
- Section IV—Analysis of Process Performance
- Section V—The Impact of Chemical Engineering Design on Society
- Section VI—Interpersonal and Communication Skills

In Section I, the student is introduced first to the principal diagrams that are used to describe a chemical process. Next, the evolution and generation of different process configurations are covered. Key concepts used in evaluating batch processes are included in Chapter 3, and the concepts of product design are given in Chapter 4. Finally, the analysis of existing processes is covered. In Section II, the information needed to assess the economic feasibility of a process is covered. This includes the estimation of fixed capital investment and manufacturing costs, the concepts of the time value of money and financial calculations, and finally the combination of these costs into profitability measures for the process. Section III covers the synthesis of a chemical process. The minimum information required to simulate a process is given, as are the basics of using a process simulator. The choice of the appropriate thermodynamic model to use in a simulation is covered, and the choice of separation operations is covered. Process optimization (including an introduction to optimization of batch processes) and heat integration techniques are covered in this section. In addition, new material on advanced concepts using steady-state process simulators (Chapter 16) and the use of dynamic simulators (Chapter 17) has been added, and the chapter on process regulation has been expanded and rounds out Section III. In Section IV, the analysis of the performance of existing processes and equipment is covered. The material in Section 4 is substantially different from that found in most textbooks. We consider equipment that is already built and operating and analyze how the operation can be changed, how an operating problem may be solved, and how to analyze what has occurred in the process to cause an observed change. In Section V, the impact of chemical engineering design on society is covered. The role of the professional engineer in society is addressed. Separate chapters addressing ethics and professionalism, health, safety, and the environment, and green engineering are included. Finally, in Section VI, the interpersonal skills required by the engineer to function as part of a team and to communicate both orally and in written form are covered (on the CD). An entire chapter (on the CD) is devoted to addressing some of the common mistakes that students make in written reports.

Finally, three appendices are included. Appendix A gives a series of cost charts for equipment. This information is embedded in the CAPCOST program for evaluating fixed capital investments and process economics. Appendix B gives the preliminary design information for 15 chemical processes: dimethyl ether, ethylbenzene, styrene, drying oil, maleic anhydride, ethylene oxide, formalin, batch manufacture of amino acids, acrylic acid, acetone, heptenes production, shift reaction, acid-gas removal by a physical solvent, the removal of H_2S from a gas stream using the Claus process, and finally coal gasification. Appendix B is now located on the CD accompanying the book. This information is used in many of the end-of-chapter problems in the book. These processes can also be used as the starting point for more detailed analyses—for example, optimization studies. Other projects, given in Appendix C, are also included on the CD book. The reader (faculty and students) is also referred to our Web site at www.che.cemr.wvu.edu/publications/projects/, where a variety of design projects for sophomore-through senior-level chemical engineering courses is provided. There is also a link to another Web site that contains environmentally related design projects.

For a one-semester design course, we recommend including the following core:

- Section I—Chapters 1 through 6
- Section III—Chapters 11, 12, and 13
- Section V—Chapters 25 and 26

For programs in which engineering economics is not a prerequisite to the design course, Section II (Chapters 7–10) should also be included. If students have previously covered engineering economics, Chapters 14 and 15 covering optimization and pinch technology could be substituted.

For the second term of a two-term sequence, we recommend Chapters 19 through 23 (and Chapters 14 and 15 if not included in the first design course) plus a design project. Alternatively, advanced simulation techniques in Chapters 16 and 17 could be covered. If time permits, we also recommend Chapter 18 (Regulation and Control of Chemical Processes with Applications Using Commercial Software) and Chapter 24 (Process Troubleshooting and Debottlenecking) because these tend to solidify as well as extend the concepts of Chapters 19 through 23, that is, what an entry-level process engineer will encounter in the first few years of employment at a chemical process facility. For an environmental emphasis, Chapter 27 could be substituted for Chapters 18 and 24; however, it is recommended that supplementary material be included.

We have found that the most effective way both to enhance and to examine student progress is through oral presentations in addition to the submission of written reports. During these oral presentations, individual students or a student group defends its results to a faculty panel, much as a graduate student defends a thesis or dissertation.

Because design is at its essence a creative, dynamic, challenging, and iterative activity, we welcome feedback on and encourage experimentation with this design textbook. We hope that students and faculty will find the excitement in teaching and learning engineering design that has sustained us over the years.

Finally, we would like to thank those people who have been instrumental to the successful completion of this book. Many thanks are given to all undergraduate chemical engineering students at West Virginia University over the years, particularly the period 1992–2011. In particular, we would like to thank Joe Stoffa, who was responsible for developing the spreadsheet version of CAPCOST, and Mary Metzger and John Ramsey, who were responsible for collecting and correlating equipment cost information for this edition. We also acknowledge the many colleagues who have provided, both formally and informally, feedback about this text. Finally, RT would like to thank his wife, Becky; JAS would like to thank his wife, Terry; and DB would like to thank his parents, Sambhunath and Gayatri, wife Pampa, and son Swagat for their continued support, love, and patience during the preparation of this fourth edition.

R.T.
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List of Nomenclature

Symbol	Definition	SI Units
A	Equipment Cost Attribute	
A	Area	m^2
A	Absorption Factor	
A	Annuity Value	\$/time
$A/F, i, n$	Sinking Fund Factor	
$A/P, i, n$	Capital Recovery Factor	
A_b	Bubbling Area	m^2
A_c	Cross-Sectional Area	m^2
a	Interfacial Area	m^2
a	Mean Ionic Diameter of an Electrolyte	m
a'	Interface Area per Unit Volume	m^2/m^3
BV	Book Value	\$
C	Molar Density	mol/m^3
C	Equipment Cost	\$
C or c	Molar Concentration	$kmol/m^3$
CA	Corrosion Allowance	m
CBM	Bare Module Cost	\$
COM	Cost of Manufacture	\$/time
cop	Coefficient of Performance	
C_p	Heat Capacity	kJ/kg°C or kJ/kmol°C
CCP	Cumulative Cash Position	\$
CCR	Cumulative Cash Ratio	
D	Diffusivity	m^2/s
D	Diameter	m
D	Amount Allowed for Depreciation	\$
D	Distillate Product Flowrate	kmol/time
d	Yearly Depreciation Allowance	\$/yr
$DCFROR$	Discounted Cash Flow Rate of Return	
DMC	Direct Manufacturing Cost	\$/time

$DPBP$	Discounted Payback Period	years
$\bar{D}$	Average Diffusivity	m^2/s
D_0	Diffusivity at Infinite Dilution	m^2/s
$\boldsymbol{d}$	Vector of Disturbance Inputs	
d_s	Average Solvent Density	kg/m^3
e	Elementary Charge	Columb
E	Money Earned	$
E	Weld Efficiency	
E_{act} or E	Activation Energy	kJ/kmol
$EAOC$	Equivalent Annual Operating Cost	$/yr
ECC	Equivalent Capitalized Cost	$
F	Faraday's Constant	Columb/kmol
f_q	Quantity Factors for Trays	
F	Future Value	$
F	Molar Flowrate	kmol/s
F	Equipment Module Cost Factor	
F	Correction for Multipass Heat Exchangers	
F	Future Value	$
F_d	Drag Force	N/m^2 or kPa
f	Friction Factor	
f	Rate of Inflation	
$F/A, i, n$	Uniform Series Compound Amount Factor	
FCI	Fixed Capital Investment	$
$F/P, i, n$	Single Payment Compound Amount Factor	
FMC	Fixed Manufacturing Costs	$/time
F_{Lang}	Lang Factor	
f_i	Fugacity of Pure Component i	bar or kPa
$\hat{f}_i$	Fugacity of Component i in Mixture	bar or kPa
$\boldsymbol{f}$	System of Equations (vector)	
G	Gibbs Free Energy	kJ

G	Gas Flowrate	kg/s, kmol/s
GE	General Expenses	\$/time
H	Henry's Law Constant	bar or kPa in Equation (13.5), but can be different elsewhere
h	Individual Heat Transfer Coefficient	W/m^2K
H	Enthalpy or Specific Enthalpy	kJ or kJ/kg
H	Height	m
h_f	Froth Height in a Tray	m
$\boldsymbol{I}$	Identity Matrix	
I	Ionic Concentration	$kmol/m^3$
I_x	Ionic Strength on a Mole Fraction Basis	
I	Cost Index	
i	Compound Interest	
i'	Effective Interest Rate Including Inflation	
$INPV$	Incremental Net Present Value	\$
$IPBP$	Incremental Payback Period	years
$\boldsymbol{J}$	Jacobian Matrix	
k	Thermal Conductivity	W/m K
k_o	Preexponential Factor for Reaction Rate Constant	Depends on molecularity of reaction
K_p	Equilibrium Constant	Depends on reaction stoichiometry
k_{reac} or k_i	Reaction Rate Constant	Depends on molecularity of reaction
K_c	Proportional Gain	
K_{cu}	Ultimate Controller Gain	
K_{eq}	Equilibrium Constant of a Chemical Reaction	
K_i	Vapor-Liquid Equilibrium Ratio of Species i	

k_B	Boltzmann Constant	kJ/K
k_m	Average Mass Transfer Coefficient	m/s
L	Lean Stream Flowrate	kg/s
L	Liquid Flowrate	kg/s or kmol/s
$\dot{m}$	Flowrate	kg/s
m	Partition Coefficient (y/x)	
M	Mass	kg
m	Molality	kmol/kg
n	Life of Equipment	years
n	Years of Investment	years
n	Number of Batches	
n_c	Number of Campaigns	
N	Number of Streams	
N	Number of Trays, Stages, or Shells	
N	Molar Flowrate	kmol/s
NPSH	Net Positive Suction Head	m of liquid
NPV	Net Present Value	$
N_{toG}	Number of Transfer Units	
N	Molar Hold-up	kmol
OBJ, OF	Objective Function	usually $ or $/time
p	Price	$
P	Dimensionless Temperature Approach	
P	Pressure	bar or kPa
P	Present Value	$
P^*	Vapor Pressure	bar or kPa
P/A, i, n	Uniform Series Present Worth Factor	
PBP	Payback Period	year
PC	Project Cost	$
P/F, i, n	Single Payment Present Worth Factor	
PVR	Present Value Ratio	
P(x)	Probability Density Function of x	
P_u	Ultimate Period of Oscillation	s
Q *or* q	Rate of Heat Transfer	W or MJ/h

Q	Quantity	
$\dot{Q}$	Heat Transfer Rate	W or MJ/h
r	Radius	m
r	Reaction Rate	kmol/m^3 or kmol/kg cat s
r	Rate of Production	kg/h
R	Gas Constant	kJ/kmol K
R	Ratio of Heat Capabilities	
R	Residual Funds Needed	$
R	Reflux Ratio	
Re	Reynolds Number	
R	Rich Stream Flowrate	kg/s
Rand	Random Number	
ROROI	Rate of Return on Investment	
ROROII	Rate of Return on Incremental Investment	
S	Entropy	kJ/K
S	Salvage Value	$
S	Maximum Allowable Working Pressure	bar
S	Salt Concentration Factor	
S	Sensitivity	
SF	Stream Factor	
T_m	Melting Temperature	K
t	Thickness of Wall	m
t	Time	s, min, h, yr
T	Total Time for a Batch	s, min, h, yr
T	Temperature	K, R, °C, or °F
U	Internal Energy	kJ
$\boldsymbol{u}$	Vector of Manipulated Inputs	
u	Flow Velocity	m/s
U	Overall Heat Transfer Coefficient	W/m^{2}K
v	Molar Volume	m^3/mol
V	Volume	m^3

V	Vapor Flow Rate	kmol/h
v_{react}	Specific Volume of Reactor	m^3/kg of product
v_p	Velocity	m/s
$\dot{v}$	Volumetric Flowrate	m^3/s
W	Weight	kg
W	Total Moles of a Component	kmol
W or WS	Work	kJ/kg
WC	Working Capital	$
$\boldsymbol{X}$	Matrix of Independent Variables	
$\boldsymbol{x}$	Vector of Variables	
X	Conversion	
X	Base-Case Ratio	
x	Mole or Mass Fraction	
y	Mole or Mass Fraction	
YOC	Yearly Operating Cost	$/yr
YS	Yearly Cash Flow (Savings)	$/yr
z	Valence of Ions	
z	Solids Mole Fraction	
z	Distance	m

Greek Symbols

α	Multiplication Cost Factor	
α	Relative Volatility	
α	NRTL Non-randomness Factor	
δ	Thickness of the Ion-Free Layer below	
ε	Void Fraction	
ε	Pump Efficiency	
ε	Tolerance, Error	
ε_{ij}	Lennard-Jones Energy Parameter between Species i and j	kJ/kmol
ε_r	Relative Permittivity of the Solvent	
ε'_r	Relative Permittivity of the Vapor Phase	
ε_s	Permittivity of the Solvent	$Columb^2$/kJ m

ϕ	Fugacity Coefficient	
$\hat{\phi}$	Fugacity Coefficient in Mixture	
ϕ^*	Fugacity Coefficient of Saturated Vapor	
γ	Activity Coefficient	
γ^∞	Activity Coefficient in the Mixture at Infinite Dilution	
$\gamma_\pm$	Mean Ionic Activity Coefficient	
κ	Inverse of Debye-Hückel length	1/m
η	Selectivity	
λ	Heat of Vaporization	kJ/kg
λ	Eigenvalue	
λ	Heat of Vaporization/Condensation	kJ/kg
$\boldsymbol{\lambda}$	Lagrangian Multiplier Vector	
λ_0	Thermal Conductivity of Pure Solvent	W/−m K
μ	Viscosity	kg/m s
μ_c	Chemical Potential	kJ
μ_0	Viscosity of Pure Solvent	kg/m s
$\boldsymbol{\theta}$	Parameter Vector	
θ	Rates of Species Concentration to that of Limiting Reactant	s\
σ	Statistical Variance	
σ	Collision Diameter	m
σ	Surface Tension	N/m
ξ	Selectivity	
ρ	Density	kg/m^3
Θ	Cycle Time	s
τ	Space Time	s
$\boldsymbol{\tau}$	NRTL Binary Interaction Energy Parameter	
τ_D	Derivative Time Constant	s
τ_I	Integral Time	s
Ω	Collision Integral	

Subscripts

1	Base Time
2	Desired Time
a	Required Attribute
ACT	Actual
Aux	Auxiliary Buildings
a, a′	Anion
b	Base Attribute
BM	Bare Module
c, c′	Cation
c	Cold
clean	Cleaning
Cont	Contingency
cycle	Cycle
d	Without Depreciation
D, d	Demand
E	Contractor Engineering Expenses
eff	Effective Interest
eq	Equivalent
el	Electrolyte(s)
eq	Metal in the Equipment
Fee	Contractor Fee
FTT	Transportation, etc.
GR	Grass Roots
h	Hot
i	Species
i	Index
in	Inlet
k	Year
L	Installation Labor
L	Lean Streams
L	Without Land Cost

LF	Long-Range Force
m	Molality Scale
m	Molecular Species
m	Heating/Cooling Medium
m	Number of Years
M	Materials for Installation
M	Material Cost Factor
max	Maximum
MC	Matching Costs
min	Minimum
n	Index for Time Instant
nom	Nominal Interest
out	Outlet
O or *OH*	Construction Overhead
Off	Offsites and Utilities
OL	Operating Labor
opt	Optimum
p	Production
P	Equipment at Manufacturer's Site (Purchased)
P	Pressure Cost Factor
P&I	Piping and Instrumentation
R	Rich Stream
RM	Raw Materials
rev	Reversible
rxn, r	Reaction
s	All Non-Water Solvents
s	Simple Interest
S	Supply
Site	Site Development
SF	Short-Range Force
TM	Total Module
UT	Utilities
WT	Waste Treatment

w	Water
$+$	Cation
$-$	Anion

Superscripts

DB	Double Declining Balance Depreciation
E or ex	Excess Property
L	Lower Limit
l	Liquid
o	Cost for Ambient Pressure Using Carbon Steel
s	Solid
SL	Straight Line Depreciation
SOYD	Sum of the Years Depreciation
U	Upper Limit
v	Vapor
∞	Aqueous Infinite Dilution
$'$	Includes Effect of Inflation on Interest

Additional Nomenclature

Table 1.2	Convention for Specifying Process Equipment
Table 1.3	Convention for Specifying Process Streams
Table 1.7	Abbreviations for Equipment and Materials of Construction
Table 1.10	Convention for Specifying Instrumentation and Control Systems

Note: In this book, matrices are denoted by boldface, uppercase, italicized letters and vectors are denoted by boldface, lowercase, italicized letters.

Section I: Conceptualization and Analysis of Chemical Processes

The purpose of this section of the book is to introduce the tools necessary to understand, interpret, synthesize, and create chemical processes. The basis of interpreting chemical processes lies with understanding the principal diagrams that are routinely used to describe chemical processes, most important of which is the process flow diagram (PFD). Although PFDs are unique for each chemical product, they possess many of the same characteristics and attributes. Moreover, the conditions (pressure, temperature, and concentration) at which different equipment operate are unique to the chemical product and processing route chosen. In order for process engineers to understand a given process or to be able to synthesize and optimize a new process, they must be able to apply the principles outlined in this section.

Chapter 1: Diagrams for Understanding Chemical Processes

The technical diagrams commonly used by chemical engineers are presented. These diagrams include the block flow diagram (BFD), the process flow diagram (PFD), and the piping and instrumentation diagram (P&ID). A standard method for presenting a PFD is given and illustrated using a process to produce benzene via the catalytic hydrodealkylation of toluene. The 3-D topology of chemical processes is introduced, and some basic information on the spacing and elevation of equipment is presented. These concepts are further illustrated in the Virtual Plant Tour AVI file on the CD accompanying the textbook. Finally, operator training (OTS) and the 3-D immersive training (ITS) simulators are discussed and their role in training and educating engineers is covered.

Chapter 2: The Structure and Synthesis of Process Flow Diagrams

The evolutionary process of design is investigated. This evolution begins with the process concept diagram that shows the *input/output* structure of all processes. From this simple starting point, the engineer can estimate the gross profit margins of competing processes and of processes that use different chemical synthesis routes to produce the same product. In this chapter, it is shown that all processes have a similar input/output structure whereby raw materials enter a process and are reacted to form products and by-products. These products are separated from unreacted feed, which is usually recycled. The product streams are then purified to yield products that are acceptable to the marketplace. All equipment in a process can be categorized into one of the six elements of the generic block flow process diagram. The process of process design continues by building preliminary flowsheets from these basic functional elements that are common to all processes.

Chapter 3: Batch Processing

In this chapter, key issues relating to the production of chemical products using batch processes are explored. The major difference between continuous and batch processes is that unsteady-state operations are normal to batch plants whereas steady state is the norm for continuous processes. The chapter starts with an example illustrating typical calculations required to design a sequence of batch operations to produce a given product. The remainder of the chapter is devoted to how best to sequence the different operations required to produce multiple chemical products using a fixed amount of equipment. The concepts of Gantt charts,

cycle times, batch campaigning, intermediate and final product storage, and parallel operations are covered.

Chapter 4: Chemical Product Design

Chemical product design is defined to include application of chemical engineering principles to the development of new devices, development of new chemicals, development of new processes to produce these new chemicals, and development of marketable technology. The design hierarchy for chemical product design is presented. The necessity of considering customer needs in chemical product design and the need to develop interdisciplinary teams are discussed.

Chapter 5: Tracing Chemicals through the Process Flow Diagram

In order to gain a better understanding of a PFD, it is often necessary to follow the flow of key chemical components through the diagram. This chapter presents two different methods to accomplish this. The tracing of chemicals through the process reinforces our understanding of the role that each piece of equipment plays. In most cases, the major chemical species can be followed throughout the flow diagram using simple logic without referring to the flow summary table.

Chapter 6: Understanding Process Conditions

Once the connectivity or topology of the PFD has been understood, it is necessary to understand why a piece of equipment is operated at a given pressure and temperature. The idea of conditions of special concern is introduced. These conditions are either expensive to implement (due to special materials of construction and/or the use of thick-walled vessels) or use expensive utilities. The reasons for using these conditions are introduced and explained.

Chapter 1. Diagrams for Understanding Chemical Processes

What You Will Learn

- Different types of chemical process diagrams
- How these diagrams represent different scales of process views
- One consistent method for drawing process flow diagrams
- The information to be included in a process flow diagram
- The purpose of operator training simulators and recent advances in 3-D representation of different chemical processes

The chemical process industry (CPI) is involved in the production of a wide variety of products that improve the quality of our lives and generate income for companies and their stockholders. In general, chemical processes are complex, and chemical engineers in industry encounter a variety of chemical process flow diagrams. These processes often involve substances of high chemical reactivity, high toxicity, and high corrosivity operating at high pressures and temperatures. These characteristics can lead to a variety of potentially serious consequences, including explosions, environmental damage, and threats to people's health. It is essential that errors or omissions resulting from missed communication between persons and/or groups involved in the design and operation do not occur when dealing with chemical processes. Visual information is the clearest way to present material and is least likely to be misinterpreted. For these reasons, it is essential that chemical engineers be able to formulate appropriate process diagrams and be skilled in analyzing and interpreting diagrams prepared by others.

The most effective way of communicating information about a process is through the use of flow diagrams.

This chapter presents and discusses the more common flow diagrams encountered in the chemical process industry. These diagrams evolve from the time a process is conceived in the laboratory through the design, construction, and the many years of plant operation. The most important of these diagrams are described and discussed in this chapter.

The following narrative is taken from Kauffman [1] and describes a representative case history related to the development of a new chemical process. It shows how teams of engineers work together to provide a plant design and introduces the types of diagrams that will be explored in this chapter.

> *The research and development group at ABC Chemicals Company worked out a way to produce alpha-beta souptol (ABS). Process engineers assigned to work with the development group have pieced together a continuous process for making ABS in commercial quantities and have tested key parts of it. This work involved hundreds of* ***block flow diagrams,*** *some more complex than others. Based on information derived from these block flow diagrams, a decision was made to proceed with this process.*
>
> *A process engineering team from ABC's central office carries out the detailed process*

*calculations, material and energy balances, equipment sizing, etc. Working with their drafting department, they produced a series of **PFDs (Process Flow Diagrams)** for the process. As problems arise and are solved, the team may revise and redraw the PFDs. Often the work requires several rounds of drawing, checking, and revising.*

Specialists in distillation, process control, kinetics, and heat transfer are brought in to help the process team in key areas. Some are company employees and others are consultants.

*Since ABC is only a moderate-sized company, it does not have sufficient staff to prepare the 120 **P&IDs (Piping and Instrumentation Diagrams)** needed for the new ABS plant. ABC hires a well-known engineering and construction firm **(E&C Company)**, DEFCo, to do this work for them. The company assigns two of the ABC process teams to work at DEFCo to coordinate the job. DEFCo's process engineers, specialists, and drafting department prepare the P&IDs. They do much of the detailed engineering (pipe sizes, valve specifications, etc.) as well as the actual drawing. The job may take two to six months. Every drawing is reviewed by DEFCo's project team and by ABC's team. If there are disagreements, the engineers and specialists from the companies must resolve them.*

Finally, all the PFDs and the P&IDs are completed and approved. ABC can now go ahead with the construction. They may extend their contract with DEFCo to include this phase, or they may go out for construction bids from a number of sources.

This narrative describes a typical sequence of events taking a project from its initial stages through plant construction. If DEFCo had carried out the construction, ABC could go ahead and take over the plant or DEFCo could be contracted to carry out the start-up and to commission the plant. Once satisfactory performance specifications have been met, ABC would take over the operation of the plant and commercial production would begin.

From conception of the process to the time the plant starts up, two or more years will have elapsed and millions of dollars will have been spent with no revenue from the plant. The plant must operate successfully for many years to produce sufficient income to pay for all plant operations and to repay the costs associated with designing and building the plant. During this operating period, many unforeseen changes are likely to take place. The quality of the raw materials used by the plant may change, product specifications may be raised, production rates may need to be increased, the equipment performance will decrease because of wear, the development of new and better catalysts will occur, the costs of utilities will change, new environmental regulations may be introduced, or improved equipment may appear on the market.

As a result of these unplanned changes, plant operations must be modified. Although the operating information on the original process diagrams remains informative, the actual performance taken from the operating plant will be different. The current operating conditions will appear on updated versions of the various process diagrams, which will act as a primary basis for understanding the changes taking place in the plant. These process diagrams are essential to an engineer who has been asked to diagnose operating problems, solve problems in operations, debottleneck systems for increased capacity, and predict the effects of making changes in operating conditions. All these activities are essential in order to maintain profitable plant operation.

In this chapter, the focus is on three diagrams that are important to chemical engineers: block flow, process flow, and piping and instrumentation diagrams. Of these three diagrams, the most useful to

chemical engineers is the PFD. The understanding of the PFD represents a central goal of this textbook.

1.1. Block Flow Diagram (BFD)

Block flow diagrams were introduced early in the chemical engineering curriculum. In the first course in material and energy balances, often an initial step was to convert a word problem into a simple block diagram. This diagram consisted of a series of blocks representing different equipment or unit operations that were connected by input and output streams. Important information such as operating temperatures, pressures, conversions, and yield was included on the diagram along with flowrates and some chemical compositions. However, the diagram did not include any details of equipment within any of the blocks.

The block flow diagram can take one of two forms. First, a block flow diagram may be drawn for a single process. Alternatively, a block flow diagram may be drawn for a complete chemical complex involving many different chemical processes. These two types of diagrams are differentiated by calling the first a block flow process diagram and the second a block flow plant diagram.

1.1.1. Block Flow Process Diagram

An example of a block flow process diagram is shown in Figure 1.1, and the process illustrated is described below.

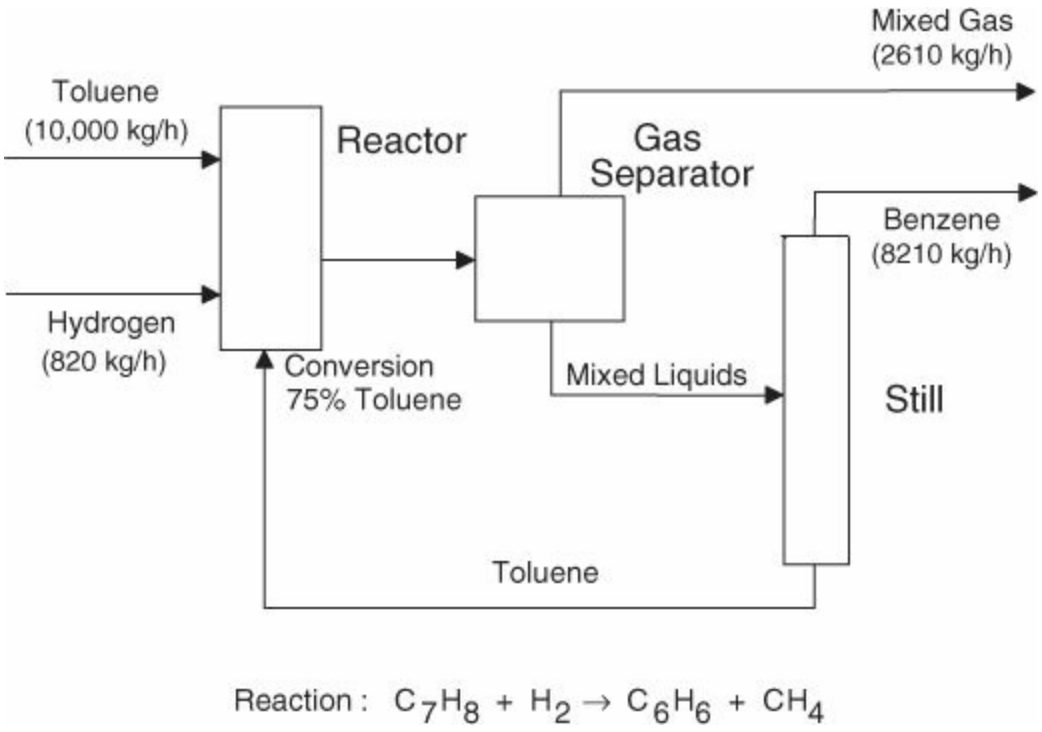


Figure 1.1. Block Flow Process Diagram for the Production of Benzene

Toluene and hydrogen are converted in a reactor to produce benzene and methane. The reaction does not go to completion, and excess toluene is required. The noncondensable gases are separated and discharged. The benzene product and the unreacted toluene are then separated by distillation. The toluene is then recycled back to the reactor and the benzene removed in the product stream.

This block flow diagram gives a clear overview of the production of benzene, unobstructed by the many details related to the process. Each block in the diagram represents a process function and may, in reality, consist of several pieces of equipment. The general format and conventions used in

preparing block flow process diagrams are presented in Table 1.1.

Table 1.1. Conventions and Format Recommended for Laying Out a Block Flow Process Diagram

1. Operations shown by blocks.
2. Major flow lines shown with arrows giving direction of flow.
3. Flow goes from left to right whenever possible.
4. Light stream (gases) toward top with heavy stream (liquids and solids) toward bottom.
5. Critical information unique to process supplied.
6. If lines cross, then the horizontal line is continuous and the vertical line is broken (hierarchy for all drawings in this book).
7. Simplified material balance provided.

Although much information is missing from Figure 1.1, it is clear that such a diagram is very useful for "getting a feel" for the process. Block flow process diagrams often form the starting point for developing a PFD. They are also very helpful in conceptualizing new processes and explaining the main features of the process without getting bogged down in the details.

1.1.2. Block Flow Plant Diagram

An example of a block flow plant diagram for a complete chemical complex is illustrated in Figure 1.2. This block flow plant diagram is for a coal to higher alcohol fuels plant. Clearly, this is a complicated process in which there are a number of alcohol fuel products produced from a feedstock of coal. Each block in this diagram represents a complete chemical process (compressors and turbines are also shown as trapezoids), and a block flow process diagram could be drawn for each block in Figure 1.2. The advantage of a diagram such as Figure 1.2 is that it allows a complete picture of what this plant does and how all the different processes interact to be obtained. On the other hand, in order to keep the diagram relatively uncluttered, only limited information is available about each process unit. The conventions for drawing block flow plant diagrams are similar to Table 1.1.

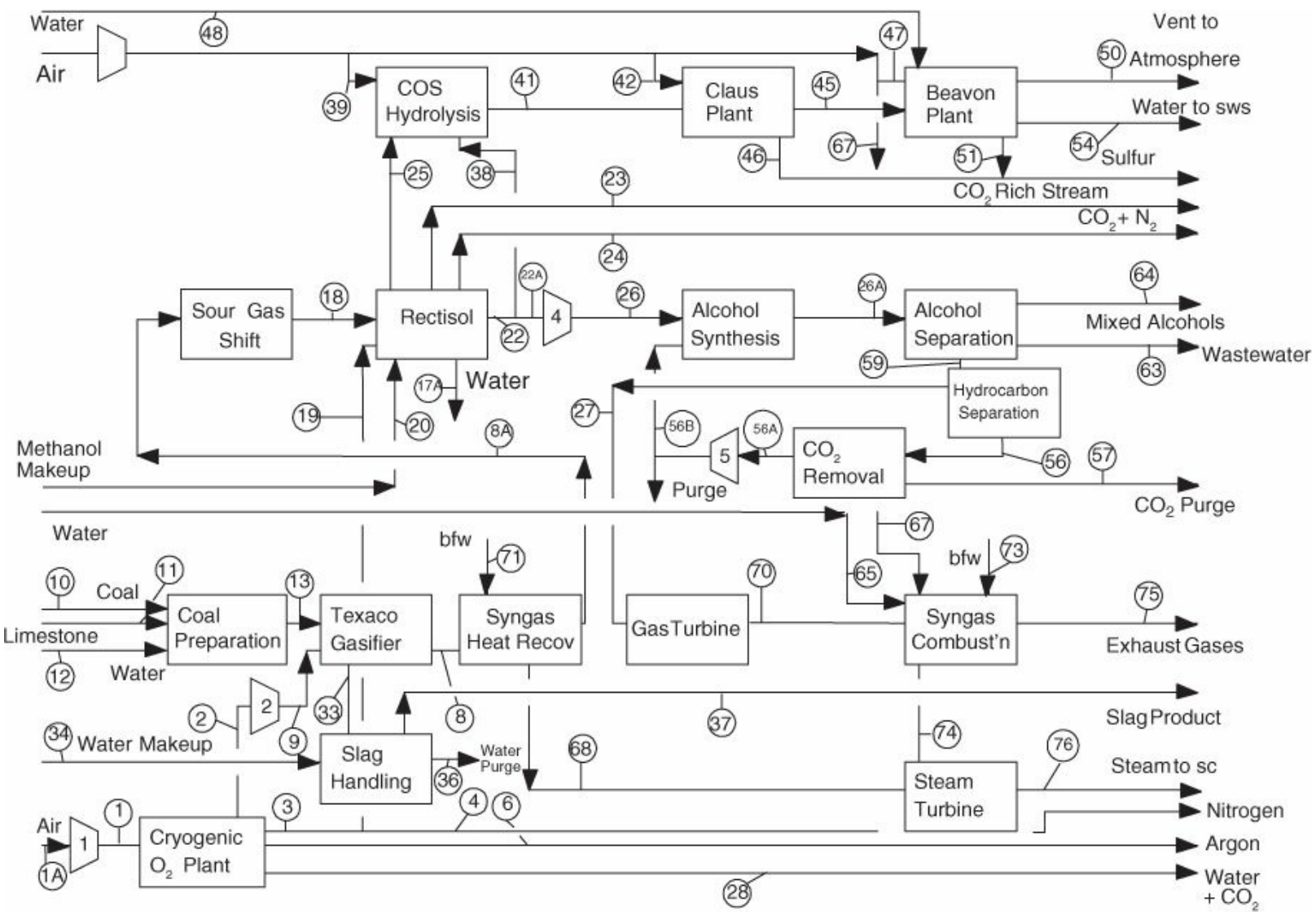


Figure 1.2. Block Flow Plant Diagram of a Coal to Higher Alcohol Fuels Process

Both types of block flow diagrams are useful for explaining the overall operation of chemical plants. For example, consider that you have just joined a large chemical manufacturing company that produces a wide range of chemical products from the site to which you have been assigned. You would most likely be given a *block flow plant diagram* to orient you to the products and important areas of operation. Once assigned to one of these areas, you would again likely be provided with a *block flow process diagram* describing the operations in your particular area.

In addition to the orientation function described earlier, block flow diagrams are used to sketch out and screen potential process alternatives. Thus, they are used to convey information necessary to make early comparisons and eliminate competing alternatives without having to make detailed and costly comparisons.

1.2. Process Flow Diagram (PFD)

The process flow diagram (PFD) represents a quantum step up from the BFD in terms of the amount of information that it contains. The PFD contains the bulk of the chemical engineering data necessary for the design of a chemical process. For all of the diagrams discussed in this chapter, there are no universally accepted standards. The PFD from one company will probably contain slightly different information from the PFD for the same process from another company. Having made this point, it is fair to say that most PFDs convey very similar information. A typical commercial PFD will contain the following information:

1. All the major pieces of equipment in the process will be represented on the diagram along with a description of the equipment. Each piece of equipment will have assigned a unique equipment number and a descriptive name.
2. All process flow streams will be shown and identified by a number. A description of the process conditions and chemical composition of each stream will be included. These data will be either displayed directly on the PFD or included in an accompanying flow summary table.
3. All utility streams supplied to major equipment that provides a process function will be shown.
4. Basic control loops, illustrating the control strategy used to operate the process during normal operations, will be shown.

It is clear that the PFD is a complex diagram requiring a substantial effort to prepare. It is essential that it should remain uncluttered and be easy to follow, to avoid errors in presentation and interpretation. Often PFDs are drawn on large sheets of paper (for example, size D: 24 in × 36 in), and several connected sheets may be required for a complex process. Because of the page size limitations associated with this text, complete PFDs cannot be presented here. Consequently, certain liberties have been taken in the presentation of the PFDs in this text. Specifically, certain information will be presented in accompanying tables, and only the essential process information will be included on the PFD. The resulting PFDs will retain clarity of presentation, but the reader must refer to the flow summary and equipment summary tables in order to extract all the required information about the process.

Before the various aspects of the PFD are discussed, it should be noted that the PFD and the process that is described in this chapter will be used throughout the book. The process is the hydrodealkylation of toluene to produce benzene. This is a well-studied and well-understood commercial process still used today. The PFD presented in this chapter for this process is technically feasible but is in no way optimized. In fact, many improvements to the process technology and economic performance can be made. Many of these improvements will become evident when the appropriate material is presented. This allows the techniques provided throughout this text to be applied both to identify technical and economic problems in the process and to make the necessary process improvements. Therefore, throughout the text, weak spots in the design, potential improvements, and a path toward an optimized process flow diagram will be identified.

The basic information provided by a PFD can be categorized into one of the following:

1. Process topology
2. Stream information
3. Equipment information

Each aspect of the PFD will be considered separately. After each of the three topics has been addressed, all the information will be gathered and presented in the form of a PFD for the benzene process.

1.2.1. Process Topology

Figure 1.3 is a skeleton process flow diagram for the production of benzene (see also the block flow process diagram in Figure 1.1). This skeleton diagram illustrates the location of the major pieces of equipment and the connections that the process streams make between equipment. The location of and interaction between equipment and process streams are referred to as the process topology.

V-101 Toluene Storage Drum | P-101A/B Toluene Feed Pumps | E-101 Feed Preheater | H-101 Feed Heater | R-101 Reactor | C-101A/B Recycle Gas Compressor | E-102 Reactor Effluent Cooler | V-102 High-Pres. Phase Sep. | V-103 Low-Pres. Phase Sep. | E-103 Tower Feed Heater | E-106 Benzene Reboiler | T-101 Benzene Column | E-104 Benzene Condenser | V-104 Reflux Drum | P-102A/B Reflux Pumps | E-105 Product Cooler

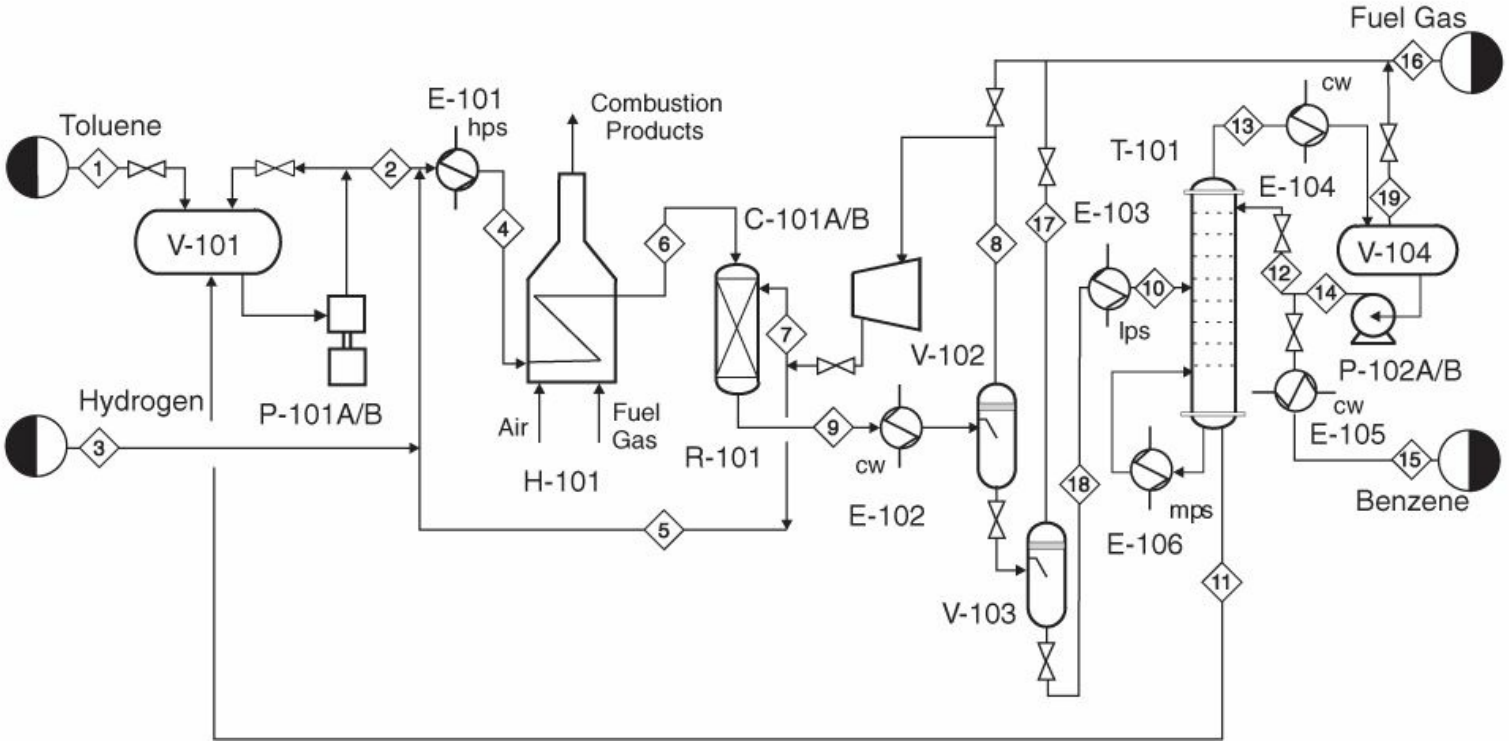


Figure 1.3. Skeleton Process Flow Diagram (PFD) for the Production of Benzene via the Hydrodealkylation of Toluene

Equipment is represented symbolically by "icons" that identify specific unit operations. Although the American Society of Mechanical Engineers (ASME) [2] publishes a set of symbols to use in preparing flowsheets, it is not uncommon for companies to use in-house symbols. A comprehensive set of symbols is also given by Austin [3]. Whatever set of symbols is used, there is seldom a problem in identifying the operation represented by each icon. Figure 1.4 contains a list of the symbols used in process diagrams presented in this text. This list covers more than 90% of those needed in fluid (gas or liquid) processes.

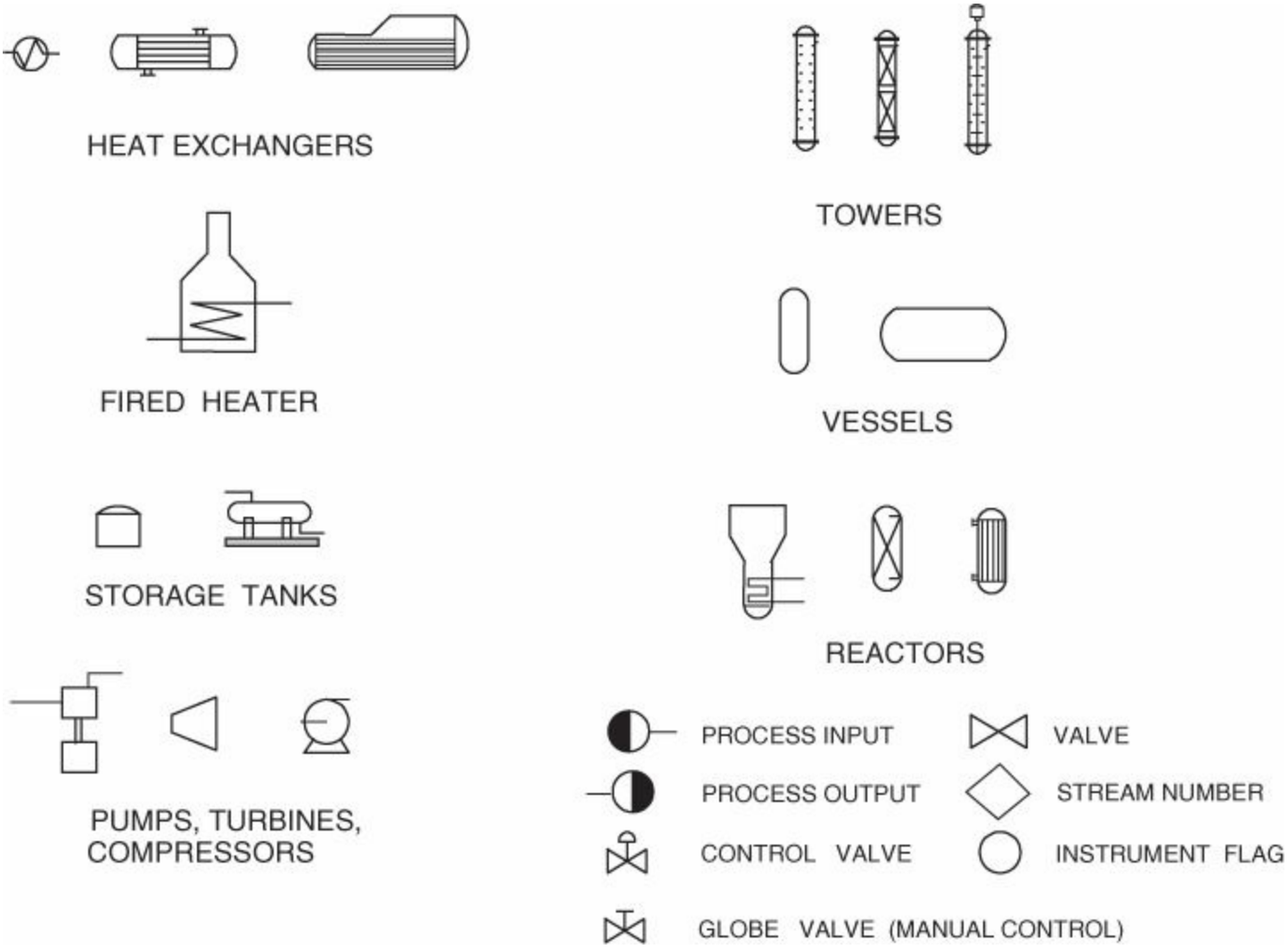


Figure 1.4. Symbols for Drawing Process Flow Diagrams

Figure 1.3 shows that each major piece of process equipment is identified by a number on the diagram. A list of the equipment numbers along with a brief descriptive name for the equipment is printed along the top of the diagram. The location of these equipment numbers and names roughly corresponds to the horizontal location of the corresponding piece of equipment. The convention for formatting and identifying the process equipment is given in Table 1.2.

Table 1.2. Conventions Used for Identifying Process Equipment

Process Equipment	General Format XX-YZZ A/B
	XX are the identification letters for the equipment classification
	C - Compressor or Turbine
	E - Heat Exchanger
	H - Fired Heater
	P - Pump
	R - Reactor
	T - Tower
	TK - Storage Tank
	V - Vessel
	Y designates an area within the plant
	ZZ is the number designation for each item in an equipment class
	A/B identifies parallel units or backup units not shown on a PFD
Supplemental Information	Additional description of equipment given on top of PFD

Table 1.2 provides the information necessary for the identification of the process equipment icons shown in a PFD. As an example of how to use this information, consider the unit operation P-101A/B and what each number or letter means.

P-101A/B identifies the equipment as a pump.

P-**1**01A/B indicates that the pump is located in area 100 of the plant.

P-1**01**A/B indicates that this specific pump is number 01 in unit 100.

P-101**A/B** indicates that a backup pump is installed. Thus, there are two identical pumps, P-101A and P-101B. One pump will be operating while the other is idle.

The 100 area designation will be used for the benzene process throughout this text. Other processes presented in the text will carry other area designations. Along the top of the PFD, each piece of process equipment is assigned a descriptive name. From Figure 1.3 it can be seen that Pump P-101 is called the "toluene feed pump." This name will be commonly used in discussions about the process and is synonymous with P-101.

During the life of the plant, many modifications will be made to the process; often it will be necessary to replace or eliminate process equipment. When a piece of equipment wears out and is replaced by a new unit that provides essentially the same process function as the old unit, then it is not uncommon for the new piece of equipment to inherit the old equipment's name and number (often an additional letter suffix will be used, e.g., H-101 might become H-101A). On the other hand, if a significant process modification takes place, then it is usual to use new equipment numbers and names. Example 1.1, taken from Figure 1.3, illustrates this concept.

Example 1.1.

Operators report frequent problems with E-102, which are to be investigated. The PFD for the plant's 100 area is reviewed, and E-102 is identified as the "Reactor Effluent Cooler." The process stream entering the cooler is a mixture of condensable and noncondensable gases at 654°C that are partially condensed to form a two-phase mixture. The coolant is water at 30°C. These conditions characterize

a complex heat transfer problem. In addition, operators have noticed that the pressure drop across E-102 fluctuates wildly at certain times, making control of the process difficult. Because of the frequent problems with this exchanger, it is recommended that E-102 be replaced by two separate heat exchangers. The first exchanger cools the effluent gas and generates steam needed in the plant. The second exchanger uses cooling water to reach the desired exit temperature of 38°C. These exchangers are to be designated as E-107 (reactor effluent boiler) and E-108 (reactor effluent condenser).

The E-102 designation is retired and not reassigned to the new equipment. There can be no mistake that E-107 and E-108 are new units in this process and that E-102 no longer exists.

1.2.2. Stream Information

Referring back to Figure 1.3, it can be seen that each of the process streams is identified by a number in a diamond box located on the stream. The direction of the stream is identified by one or more arrowheads. The process stream numbers are used to identify streams on the PFD, and the type of information that is typically given for each stream is discussed in the next section.

Also identified in Figure 1.3 are utility streams. Utilities are needed services that are available at the plant. Chemical plants are provided with a range of central utilities that include electricity, compressed air, cooling water, refrigerated water, steam, condensate return, inert gas for blanketing, chemical sewer, wastewater treatment, and flares. A list of the common services is given in Table 1.3, which also provides a guide for the identification of process streams.

Table 1.3. Conventions for Identifying Process and Utility Streams

Process Streams	
All conventions shown in Table 1.1 apply.	
Diamond symbol located in flow lines.	
Numerical identification (unique for that stream) inserted in diamond.	
Flow direction shown by arrows on flow lines.	
Utility Streams	
lps	Low-Pressure Steam: 3–5 barg (sat)*
mps	Medium-Pressure Steam: 10–15 barg (sat)*
hps	High-Pressure Steam: 40–50 barg (sat)*
htm	Heat Transfer Media (Organic): to 400°C
cw	Cooling Water: From Cooling Tower 30°C Returned at Less than 45°C†
wr	River Water: From River 25°C Returned at Less than 35°C
rw	Refrigerated Water: In at 5°C Returned at Less than 15°C
rb	Refrigerated Brine: In at –45°C Returned at Less than 0°C
cs	Chemical Wastewater with High COD
ss	Sanitary Wastewater with High BOD, etc.
el	Electric Heat (Specify 220, 440, 660V Service)
bfw	Boiler Feed Water
ng	Natural Gas
fg	Fuel Gas
fo	Fuel Oil
fw	Fire Water

*These pressures are set during the preliminary design stages and typical values vary within the ranges shown.

†Above 45°C, significant scaling occurs.

Each utility is identified by the initials provided in Table 1.3. As an example, locate E-102 in Figure 1.3. The notation, cw, associated with the nonprocess stream flowing into E-102 indicates that cooling water is used as a coolant.

Electricity used to power motors and generators is an additional utility that is not identified directly on the PFD or in Table 1.3 but is treated separately. Most of the utilities shown are related to equipment that adds or removes heat within the process in order to control temperatures. This is common for most chemical processes.

From the PFD in Figure 1.3, the identification of the process streams is clear. For small diagrams containing only a few operations, the characteristics of the streams such as temperatures, pressures, compositions, and flowrates can be shown directly on the figure, adjacent to the stream. This is not practical for a more complex diagram. In this case, only the stream number is provided on the diagram. This indexes the stream to information on a flow summary or stream table, which is often provided below the process flow diagram. In this text the flow summary table is provided as a separate attachment to the PFD.

The stream information that is normally given in a flow summary table is given in Table 1.4. It is

divided into two groups—required information and optional information—that may be important to specific processes. The flow summary table, for Figure 1.3, is given in Table 1.5 and contains all the required information listed in Table 1.4.

Table 1.4. Information Provided in a Flow Summary

Required Information
Stream Number
Temperature (°C)
Pressure (bar)
Vapor Fraction
Total Mass Flowrate (kg/h)
Total Mole Flowrate (kmol/h)
Individual Component Flowrates (kmol/h)
Optional Information
Component Mole Fractions
Component Mass Fractions
Individual Component Flowrates (kg/h)
Volumetric Flowrates (m^3/h)
Significant Physical Properties
Density
Viscosity
Other
Thermodynamic Data
Heat Capacity
Stream Enthalpy
K-values
Stream Name

Table 1.5. Flow Summary Table for the Benzene Process Shown in Figure 1.3 (and Figure 1.5)

Stream Number	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19
Temperature (°C)	25	59	25	225	41	600	41	38	654	90	147	112	112	112	38	38	38	38	112
Pressure (bar)	1.90	25.8	25.5	25.2	25.5	25.0	25.5	23.9	24.0	2.6	2.8	3.3	2.5	3.3	2.3	2.5	2.8	2.9	2.5
Vapor Fraction	0.0	0.0	1.00	1.0	1.0	1.0	1.0	1.0	1.0	0.0	0.0	0.0	1.0	0.0	0.0	1.0	1.0	0.0	1.0
Mass Flow (tonne/h)	10.0	13.3	0.82	20.5	6.41	20.5	0.36	9.2	20.9	11.6	3.27	14.0	22.7	22.7	8.21	2.61	0.07	11.5	0.01
Mole Flow (kmol/h)	108.7	144.2	301.0	1204.4	758.8	1204.4	42.6	1100.8	1247.0	142.2	35.7	185.2	291.6	290.7	105.6	304.2	4.06	142.2	0.90
Component Flowrates (kmol/h)																			
Hydrogen	0.0	0.0	286.0	735.4	449.4	735.4	25.2	651.9	652.6	0.02	0.0	0.0	0.02	0.0	0.0	178.0	0.67	0.02	0.02
Methane	0.0	0.0	15.0	317.3	302.2	317.3	16.95	438.3	442.3	0.88	0.0	0.0	0.88	0.0	0.0	123.05	3.10	0.88	0.88
Benzene	0.0	1.0	0.0	7.6	6.6	7.6	0.37	9.55	116.0	106.3	1.1	184.3	289.46	289.46	105.2	2.85	0.26	106.3	0.0
Toluene	108.7	143.2	0.0	144.0	0.7	144.0	0.04	1.05	36.0	35.0	34.6	0.88	1.22	1.22	0.4	0.31	0.03	35.0	0.0

With information from the PFD (Figure 1.3) and the flow summary table (Table 1.5), problems regarding material balances and other problems are easily analyzed. Example 1.2 and Example 1.3 are provided to offer experience in working with information from the PFD.

Example 1.2.

Check the overall material balance for the benzene process shown in Figure 1.3. From the figure,

identify the input streams as Stream 1 (toluene feed) and Stream 3 (hydrogen feed) and the output streams as Stream 15 (product benzene) and Stream 16 (fuel gas). From the flow summary table, these flows are listed as (units are in $(10^3$ kg)/h):

Input:		Output:	
Stream 3	0.82	Stream 15	8.21
Stream 1	10.00	Stream 16	2.61
Total	10.82×10^3 kg/h	Total	10.82×10^3 kg/h

Balance is achieved since Output = Input.

Example 1.3.

Determine the conversion per pass of toluene to benzene in R-101 in Figure 1.3. Conversion is defined as

ε = (benzene produced)/(total toluene introduced)

From the PFD, the input streams to R-101 are shown as Stream 6 (reactor feed) and Stream 7 (recycle gas quench), and the output stream is Stream 9 (reactor effluent stream). From the information in Table 1.5 (units are kmol/h):

Toluene introduced = 144 (Stream 6) + 0.04 (Stream 7) = 144.04 kmol/h

Benzene produced = 116 (Stream 9) – 7.6 (Stream 6) – 0.37 (Stream 7)

= 108.03 kmol/h

$$\varepsilon = 108.03/144.04 = 0.75$$

Alternatively, the following can be written:

Moles of benzene produced = Toluene in – Toluene out = 144.04 – 36.00

= 108.04 kmol/h

$$\varepsilon = 108.04/144.04 = 0.75$$

1.2.3. Equipment Information

The final element of the PFD is the equipment summary. This summary provides the information necessary to estimate the costs of equipment and furnish the basis for the detailed design of equipment. Table 1.6 provides the information needed for the equipment summary for most of the equipment encountered in fluid processes.

Table 1.6. Equipment Descriptions for PFD and P&IDs

Equipment Type
Description of Equipment
Towers
Size (height and diameter), Pressure, Temperature Number and Type of Trays Height and Type of Packing Materials of Construction
Heat Exchangers
Type: Gas-Gas, Gas-Liquid, Liquid-Liquid, Condenser, Vaporizer Process: Duty, Area, Temperature, and Pressure for both streams Number of Shell and Tube Passes Materials of Construction: Tubes and Shell
Tanks and Vessels
Height, Diameter, Orientation, Pressure, Temperature, Materials of Construction
Pumps
Flow, Discharge Pressure, Temperature, ΔP, Driver Type, Shaft Power, Materials of Construction
Compressors
Actual Inlet Flowrate, Temperature, Pressure, Driver Type, Shaft Power, Materials of Construction
Heaters (Fired)
Type, Tube Pressure, Tube Temperature, Duty, Fuel, Material of Construction
Other
Provide Critical Information

The information presented in Table 1.6 is used in preparing the equipment summary portion of the PFD for the benzene process. The equipment summary for the benzene process is presented in Table 1.7, and details of how to estimate and choose various equipment parameters are discussed in Chapter 11.

Table 1.7. Equipment Summary for Toluene Hydrodealkylation PFD

Heat Exchangers	E-101	E-102	E-103	E-104	E-105	E-106
Type	Fl.H.	Fl.H.	MDP	Fl.H.	MDP	Fl.H.
Area (m^2)	36	763	11	35	12	80
Duty (MJ/h)	15,190	46,660	1055	8335	1085	9045
Shell						
Temp. (°C)	225	654	160	112	112	185
Pres. (bar)	26	24	6	3	3	11
Phase	Vap.	Par. Cond.	Cond.	Cond.	l	Cond.
MOC	316SS	316SS	CS	CS	CS	CS
Tube						
Temp. (°C)	258	40	90	40	40	147
Pres. (bar)	42	3	3	3	3	3
Phase	Cond.	l	l	l	l	Vap.
MOC	316SS	316SS	CS	CS	CS	CS
Vessels/Tower/ Reactors	**V-101**	**V-102**	**V-103**	**V-104**	**T-101**	**R-101**
Temperature (°C)	55	38	38	112	147	660
Pressure (bar)	2.0	24	3.0	2.5	3.0	25
Orientation	Horizontal	Vertical	Vertical	Horizontal	Vertical	Vertical
MOC	CS	CS	CS	CS	CS	316SS
Size						

Height/Length (m)	5.9	3.5	3.5	3.9	29	14.2
Diameter (m)	1.9	1.1	1.1	1.3	1.5	2.3
Internals		s.p.	s.p.		42 sieve trays 316SS	Catalyst packed bed-10m

Pumps/Compressors	P-101 (A/B)	P-102 (A/B)	C-101 (A/B)	Heater	H-101
Flow (kg/h)	13,000	22,700	6770	Type	Fired
Fluid Density (kg/m^3)	870	880	8.02	MOC	316SS
Power (shaft) (kW)	14.2	3.2	49.1	Duty (MJ/h)	27,040
Type/Drive	Recip./ Electric	Centrf./ Electric	Centrf./ Electric	Radiant Area (m^2)	106.8
Efficiency (Fluid Power/Shaft Power)	0.75	0.50	0.75	Convective Area (m^2)	320.2
MOC	CS	CS	CS	Tube P (bar)	26.0
Temp. (in) (°C)	55	112	38		
Pres. (in) (bar)	1.2	2.2	23.9		
Pres. (out) (bar)	27.0	4.4	25.5		

Key:

MOC	Materials of construction	Par	Partial
316SS	Stainless steel type 316	F.H.	Fixed head
CS	Carbon steel	Fl.H.	Floating head
Vap	Stream being vaporized	Rbl	Reboiler
Cond	Stream being condensed	s.p.	Splash plate
Recipr.	Reciprocating	l	Liquid
Centrf.	Centrifugal	MDP	Multiple double pipe

1.2.4. Combining Topology, Stream Data, and Control Strategy to Give a PFD

Up to this point, the amount of process information displayed on the PFD has been kept to a minimum. A more representative example of a PFD for the benzene process is shown in Figure 1.5. This diagram includes all of the elements found in Figure 1.3, some of the information found in Table 1.5, plus additional information on the major control loops used in the process.

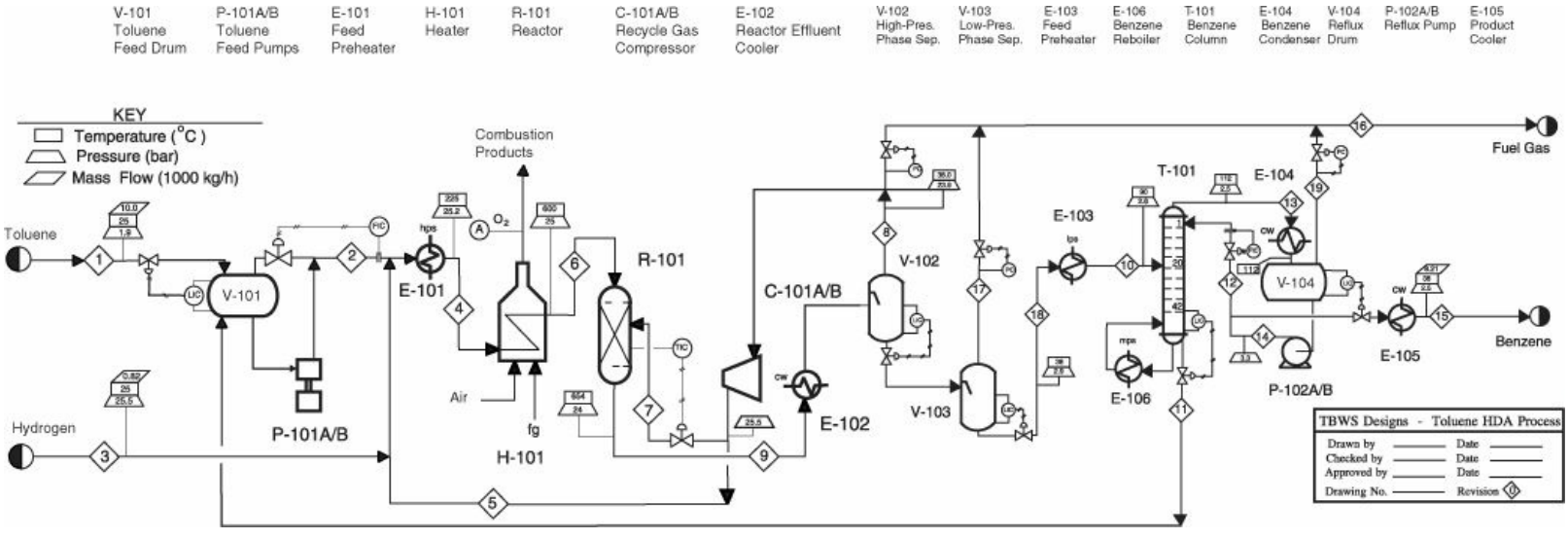


Figure 1.5. Benzene Process Flow Diagram (PFD) for the Production of Benzene via the Hydrodealkylation of Toluene

Stream information is added to the diagram by attaching "information flags." The shape of the flags indicates the specific information provided on the flag. Figure 1.6 illustrates all the flags used in this text. These information flags play a dual role. They provide information needed in the plant design leading to plant construction and in the analysis of operating problems during the life of the plant. Flags are mounted on a staff connected to the appropriate process stream. More than one flag may be mounted on a staff. Example 1.4 illustrates the different information displayed on the PFD.

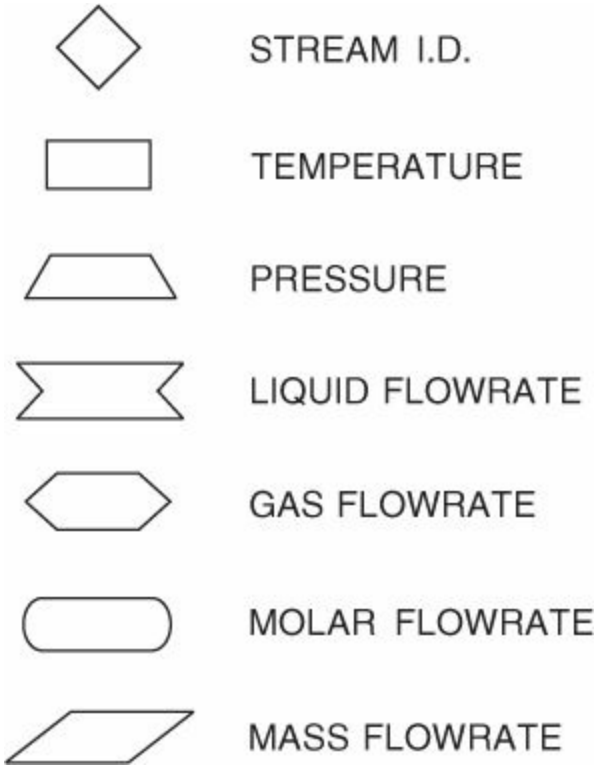


Figure 1.6. Symbols for Stream Identification

Example 1.4.

Locate Stream 1 in Figure 1.5 and note that immediately following the stream identification diamond a staff is affixed. This staff carries three flags containing the following stream data:

1. Temperature of 25°C
2. Pressure of 1.9 bar
3. Mass flowrate of 10.0×10^3 kg/h

The units for each process variable are indicated in the key provided at the left-hand side of Figure 1.5.

With the addition of the process control loops and the information flags, the PFD starts to become cluttered. Therefore, in order to preserve clarity, it is necessary to limit what data are presented with these information flags. Fortunately, flags on a PFD are easy to add, remove, and change, and even temporary flags may be provided from time to time.

The information provided on the flags is also included in the flow summary table. However, often it is far more convenient when analyzing the PFD to have certain data directly on the diagram.

Not all process information is of equal importance. General guidelines for what data should be

included in information flags on the PFD are difficult to define. However, at a minimum, information critical to the safety and operation of the plant should be given. This includes temperatures and pressures associated with the reactor, flowrates of feed and product streams, and stream pressures and temperatures that are substantially higher than the rest of the process. Additional needs are process specific. Examples 1.5–1.7 illustrate where and why information should be included directly on a PFD.

Example 1.5.

Acrylic acid is temperature sensitive and polymerizes at 90°C when present in high concentration. It is separated by distillation and leaves from the bottom of the tower. In this case, a temperature and pressure flag would be provided for the stream leaving the reboiler.

Example 1.6.

In the benzene process, the feed to the reactor is substantially hotter than the rest of the process and is crucial to the operation of the process. In addition, the reaction is exothermic, and the reactor effluent temperature must be carefully monitored. For this reason Stream 6 (entering) and Stream 9 (leaving) have temperature flags.

Example 1.7.

The pressures of the streams to and from R-101 in the benzene process are also important. The difference in pressure between the two streams gives the pressure drop across the reactor. This, in turn, gives an indication of any maldistribution of gas through the catalyst beds. For this reason, pressure flags are also included on Streams 6 and 9.

Of secondary importance is the fact that flags are useful in reducing the size of the flow summary table. For pumps, compressors, and heat exchangers, the mass flows are the same for the input and output streams, and complete entries in the stream table are not necessary. If the input (or output) stream is included in the stream table, and a flag is added to provide the temperature (in the case of a heat exchanger) or the pressure (in the case of a pump) for the other stream, then there is no need to present this stream in the flow summary table. Example 1.8 illustrates this point.

Example 1.8.

Follow Stream 13 leaving the top of the benzene column in the benzene PFD given in Figure 1.5 and in Table 1.5. This stream passes through the benzene condenser, E-104, into the reflux drum, V-104. The majority of this stream then flows into the reflux pump, P-102, and leaves as Stream 14, while the remaining noncondensables leave the reflux drum in Stream 19. The mass flowrate and component flowrates of all these streams are given in Table 1.5. The stream leaving E-104 is not included in the stream table. Instead, a flag giving the temperature (112°C) was provided on the diagram (indicating condensation without subcooling). An additional flag, showing the pressure following the pump, is also shown. In this case the entry for Stream 14 could be omitted from the stream table, because it is simply the sum of Streams 12 and 15, and no information would be lost.

More information could be included in Figure 1.5 had space for the diagram not been limited by text format. It is most important that the PFD remain uncluttered and easy to follow in order to avoid errors and misunderstandings. Adding additional material to Figure 1.5 risks sacrificing clarity.

The flow table presented in Table 1.5, the equipment summary presented in Table 1.7, and Figure 1.5 taken together constitute all the information contained on a commercially produced PFD.

The PFD is the first comprehensive diagram drawn for any new plant or process. It provides all of the information needed to understand the chemical process. In addition, sufficient information is given on the equipment, energy, and material balances to establish process control protocol and to prepare cost estimates to determine the economic viability of the process.

Many additional drawings are needed to build the plant. All the process information required can be taken from this PFD. As described in the narrative at the beginning of this chapter, the development of the PFD is most often carried out by the operating company. Subsequent activities in the design of the plant are often contracted out.

The value of the PFD does not end with the construction of the plant. It remains the document that best describes the process, and it is used in the training of operators and new engineers. It is consulted regularly to diagnose operating problems that arise and to predict the effects of changes on the process.

1.3. Piping and Instrumentation Diagram (P&ID)

The piping and instrumentation diagram (P&ID), also known as mechanical flow diagram (MFD), provides information needed by engineers to begin planning for the construction of the plant. The P&ID includes every mechanical aspect of the plant except the information given in Table 1.8. The general conventions used in drawing P&IDs are given in Table 1.9.

Table 1.8. Exclusions from Piping and Instrumentation Diagram

1. Operating Conditions *T*, *P*
2. Stream Flows
3. Equipment Locations
4. Pipe Routing
   a. Pipe Lengths
   b. Pipe Fittings
5. Supports, Structures, and Foundations

Table 1.9. Conventions in Constructing Piping and Instrumentation Diagrams

For Equipment—Show Every Piece Including
Spare Units Parallel Units Summary Details of Each Unit
For Piping—Include All Lines Including Drains and Sample Connections, and Specify
Size (Use Standard Sizes) Schedule (Thickness) Materials of Construction Insulation (Thickness and Type)
For Instruments—Identify
Indicators Recorders Controllers Show Instrument Lines
For Utilities—Identify
Entrance Utilities Exit Utilities Exit to Waste Treatment Facilities

Each PFD will require many P&IDs to provide the necessary data. Figure 1.7 is a representative P&ID for the distillation section of the benzene process shown in Figure 1.5. The P&ID presented in Figure 1.7 provides information on the piping, and this is included as part of the diagram. As an alternative, each pipe can be numbered, and the specifics of every line can be provided in a separate table accompanying this diagram. When possible, the physical size of the larger-sized unit operations is reflected by the size of the symbol in the diagram.

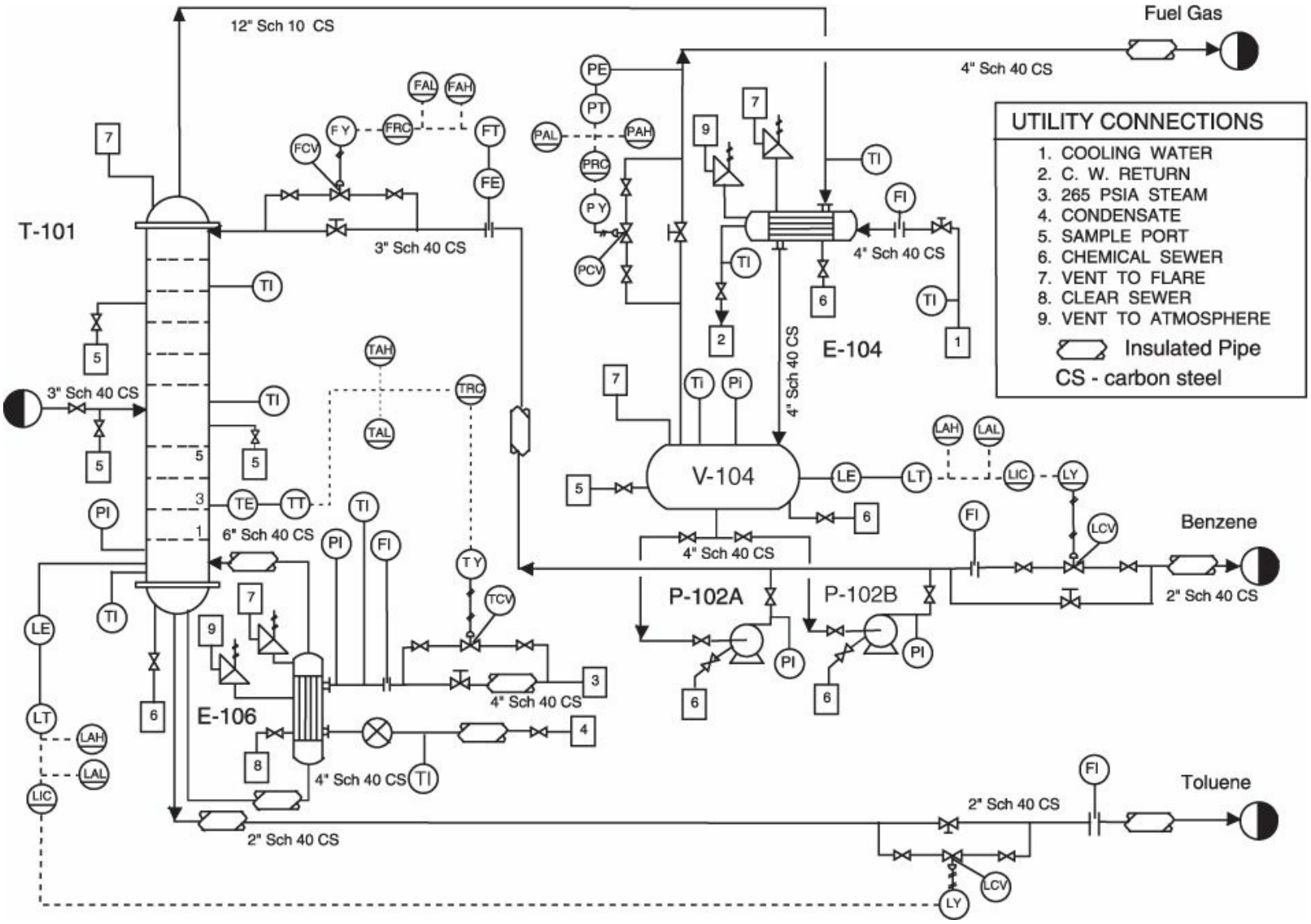


Figure 1.7. Piping and Instrumentation Diagram for Benzene Distillation (adapted from Kauffman, D., *Flow Sheets and Diagrams, AIChE Modular Instruction, Series G: Design of Equipment*, series editor J. Beckman, AIChE, New York, 1986, vol. 1, Chapter G.1.5, AIChE copyright © 1986 AIChE, all rights reserved)

Utility connections are identified by a numbered box in the P&ID. The number within the box identifies the specific utility. The key identifying the utility connections is shown in a table on the P&ID.

All process information that can be measured in the plant is shown on the P&ID by circular flags. This includes the information to be recorded and used in process control loops. The circular flags on the diagram indicate where the information is obtained in the process and identify the measurements taken and how the information is dealt with. Table 1.10 summarizes the conventions used to identify information related to instrumentation and control. Example 1.9 illustrates the interpretation of instrumentation and control symbols.

Table 1.10. Conventions Used for Identifying Instrumentation on P&IDs (ISA standard ISA-S5-1, [4])

Location of Instrumentation	
◯	Instrument Located in Plant
⊖	Instrument Located on Front of Panel in Control Room
⊖ (dashed)	Instrument Located on Back of Panel in Control Room

Meanings of Identification Letters (XYY)		
	First Letter (X)	*Second or Third Letter (Y)*
A	Analysis	Alarm
B	Burner Flame	
C	Conductivity	Control
D	Density or Specific Gravity	
E	Voltage	Element
F	Flowrate	
H	Hand (Manually Initiated)	High
I	Current	Indicate
J	Power	
K	Time or Time Schedule	Control Station
L	Level	Light or Low
M	Moisture or Humidity	Middle or Intermediate
O		Orifice
P	Pressure or Vacuum	Point
Q	Quantity or Event	
R	Radioactivity or Ratio	Record or print
S	Speed or Frequency	Switch
T	Temperature	Transmit
V	Viscosity	Valve, Damper, or Louver
W	Weight	Well
Y		Relay or Compute
Z	Position	Drive

Identification of Instrument Connections	
———	Capillary
—//—	Pneumatic
.....	Electrical

Example 1.9.

Consider the benzene product line leaving the right-hand side of the P&ID in Figure 1.7. The flowrate of this stream is controlled by a control valve that receives a signal from a level measuring element placed on V-104. The sequence of instrumentation is as follows:

A level sensing element (LE) is located on the reflux drum V-104. A level transmitter (LT) also located on V-104 sends an electrical signal (designated by a dashed line) to a level indicator and controller (LIC). This LIC is located in the control room on the control panel or console (as indicated by the horizontal line under LIC) and can be observed by the operators. From the LIC, an electrical signal is sent to an instrument (LY) that computes the correct valve position and in turn sends a pneumatic signal (designated by a solid line with cross hatching) to activate the control valve (LCV). In order to warn operators of potential problems, two alarms are placed in the control room. These are a high-level alarm (LAH) and a low-level alarm (LAL), and they receive the same signal from the level transmitter as does the controller.

This control loop is also indicated on the PFD of Figure 1.5. However, the details of all the instrumentation are condensed into a single symbol (LIC), which adequately describes the essential process control function being performed. The control action that takes place is not described explicitly in either drawing. However, it is a simple matter to infer that if there is an increase in the level of liquid in V-104, the control valve will open slightly and the flow of benzene product will increase, tending to lower the level in V-104. For a decrease in the level of liquid, the valve will close slightly.

The details of the other control loops in Figures 1.5 and 1.7 are left to problems at the end of this chapter. It is worth mentioning that in virtually all cases of process control in chemical processes, the final control element is a valve. Thus, all control logic is based on the effect that a change in a given flowrate has on a given variable. The key to understanding the control logic is to identify which flowrate is being manipulated to control which variable. Once this has been done, it is a relatively simple matter to see in which direction the valve should change in order to make the desired change in the control variable. The response time of the system and type of control action used—for example, proportional, integral, or differential—are left to the instrument engineers and are not covered in this text.

The final control element in nearly all chemical process control loops is a valve.

The P&ID is the last stage of process design and serves as a guide for those who will be responsible for the final design and construction. Based on this diagram,

1. Mechanical engineers and civil engineers will design and install pieces of equipment.
2. Instrument engineers will specify, install, and check control systems.
3. Piping engineers will develop plant layout and elevation drawings.
4. Project engineers will develop plant and construction schedules.

Before final acceptance, the P&IDs serve as a checklist against which each item in the plant is checked.

The P&ID is also used to train operators. Once the plant is built and is operational, there are limits to what operators can do. About all that can be done to correct or alter performance of the plant is to open, close, or change the position of a valve. Part of the training would pose situations and require the operators to be able to describe what specific valve should be changed, how it should be changed, and what to observe in order to monitor the effects of the change. Plant simulators (similar to flight simulators) are sometimes involved in operator training. These programs are sophisticated,

realtime process simulators that show a trainee operator how quickly changes in controlled variables propagate through the process. It is also possible for such programs to display scenarios of process upsets so that operators can get training in recognizing and correcting such situations. These types of programs are very useful and cost-effective in initial operator training. However, the use of P&IDs is still very important in this regard.

The P&ID is particularly important for the development of start-up procedures when the plant is not under the influence of the installed process control systems. An example of a start-up procedure is given in Example 1.10.

Example 1.10.

Consider the start-up of the distillation column shown in Figure 1.7. What sequence would be followed? The procedure is beyond the scope of this text, but it would be developed from a series of questions such as

a. What valve should be opened first?

b. What should be done when the temperature of … reaches …?

c. To what value should the controller be set?

d. When can the system be put on automatic control?

These last three sections have followed the development of a process from a simple BFD through the PFD and finally to the P&ID. Each step showed additional information. This can be seen by following the progress of the distillation unit as it moves through the three diagrams described.

1. **Block Flow Diagram (BFD) (see Figure 1.1):** The column was shown as a part of one of the three process blocks.
2. **Process Flow Diagram (PFD) (see Figure 1.5):** The column was shown as the following set of individual equipment: a tower, condenser, reflux drum, reboiler, reflux pumps, and associated process controls.
3. **Piping and Instrumentation Diagram (P&ID) (see Figure 1.7):** The column was shown as a comprehensive diagram that includes additional details such as pipe sizes, utility streams, sample taps, numerous indicators, and so on. It is the only unit operation on the diagram.

The value of these diagrams does not end with the start-up of the plant. The design values on the diagram are changed to represent the actual values determined under normal operating conditions. These conditions form a “base case” and are used to compare operations throughout the life of the plant.

1.4. Additional Diagrams

During the planning and construction phases of a new project, many additional diagrams are needed. Although these diagrams do not possess additional process information, they are essential to the successful completion of the project. Computers are being used more and more to do the tedious work associated with all of these drawing details. The creative work comes in the development of the concepts provided in the BFD and the process development required to produce the PFD. The computer can help with the drawings but cannot create a new process. Computers are valuable in many aspects of the design process where the size of equipment to do a specific task is to be

determined. Computers may also be used when considering performance problems that deal with the operation of existing equipment. However, they are severely limited in dealing with diagnostic problems that are required throughout the life of the plant.

The diagrams presented here are in both American Engineering and SI units. The most noticeable exception is in the sizing of piping, where pipes are specified in inches and pipe schedule. This remains the way they are produced and purchased in the United States. A process engineer today must be comfortable with SI, conventional metric, and American (formerly British, who now use SI exclusively) Engineering units.

These additional diagrams are discussed briefly below.

A **utility flowsheet** may be provided that shows all the headers for utility inputs and outputs available along with the connections needed to the process. It provides information on the flows and characteristics of the utilities used by the plant.

Vessel sketches, logic ladder diagrams, wiring diagrams, site plans, structural support diagrams, and many other drawings are routinely used but add little to our understanding of the basic chemical processes that take place.

Additional drawings are necessary to locate all of the equipment in the plant. **Plot plans** and **elevation diagrams** are provided that locate the placement and elevation of all of the major pieces of equipment such as towers, vessels, pumps, heat exchangers, and so on. When constructing these drawings, it is necessary to consider and to provide for access for repairing equipment, removing tube bundles from heat exchangers, replacement of units, and so on. What remains to be shown is the addition of the structural support and piping.

Piping isometrics are drawn for every piece of pipe required in the plant. These drawings are 3-D sketches of the pipe run, indicating the elevations and orientation of each section of pipe. In the past, it was also common for comprehensive plants to build a **scale model** so the system could be viewed in three dimensions and modified to remove any potential problems. Over the past thirty years, scale models have been replaced by three-dimensional **computer aided design (CAD)** programs that are capable of representing the plant as-built in three dimensions. They provide an opportunity to view the local equipment topology from any angle at any location inside the plant. One can actually "walk through" the plant and preview what will be seen when the plant is built. The ability to "view" the plant before construction will be made even more realistic with the help of **virtual reality** software. With this new tool, it is possible not only to walk through the plant but also to "touch" the equipment, turn valves, climb to the top of distillation columns, and so on. In the next section, the information needed to complete a preliminary plant layout design is reviewed, and the logic used to locate the process units in the plant and how the elevations of different equipment are determined are briefly explained.

1.5. Three-Dimensional Representation of a Process

As mentioned earlier, the major design work products, both chemical and mechanical, are recorded on two-dimensional diagrams (PFD, P&ID, etc.). However, when it comes to the construction of the plant, there are many issues that require a three-dimensional representation of the process. For example, the location of shell-and-tube exchangers must allow for tube bundle removal for cleaning and repair. Locations of pumps must allow for access for maintenance and replacement. For compressors, this access may also require that a crane be able to remove and replace a damaged

drive. Control valves must be located at elevations that allow operator access. Sample ports and instrumentation must also be located conveniently. For anyone who has toured a moderate-to-large chemical facility, the complexity of the piping and equipment layout is immediately apparent. Even for experienced engineers, the review of equipment and piping topology is far easier to accomplish in 3-D than 2-D. Due to the rapid increase in computer power and advanced software, such representations are now done routinely using the computer. In order to "build" an electronic representation of the plant in 3-D, all the information in the previously mentioned diagrams must be accessed and synthesized. This in itself is a daunting task, and a complete accounting of this process is well beyond the scope of this text. However, in order to give the reader a flavor of what can now be accomplished using such software, a brief review of the principles of plant layout design will be given. A more detailed account involving a virtual plant tour of the dimethyl ether (DME) plant (Appendix B.1) is given on the CD accompanying this book.

For a complete, detailed analysis of the plant layout, all equipment sizes, piping sizes, PFDs, P&IDs, and all other information should be known. However, for this description, a preliminary plant layout based on information given in the PFD of Figure B.1.1 is considered. Using this figure and the accompanying stream tables and equipment summary table (Tables B.1.1 and B.1.3), the following steps are followed:

1. *The PFD is divided into logical subsystems.* For the DME process, there are three logical subsections, namely, the feed and reactor section, the DME purification section, and the methanol separation and recycle section. These sections are shown as dotted lines on Figure 1.8.

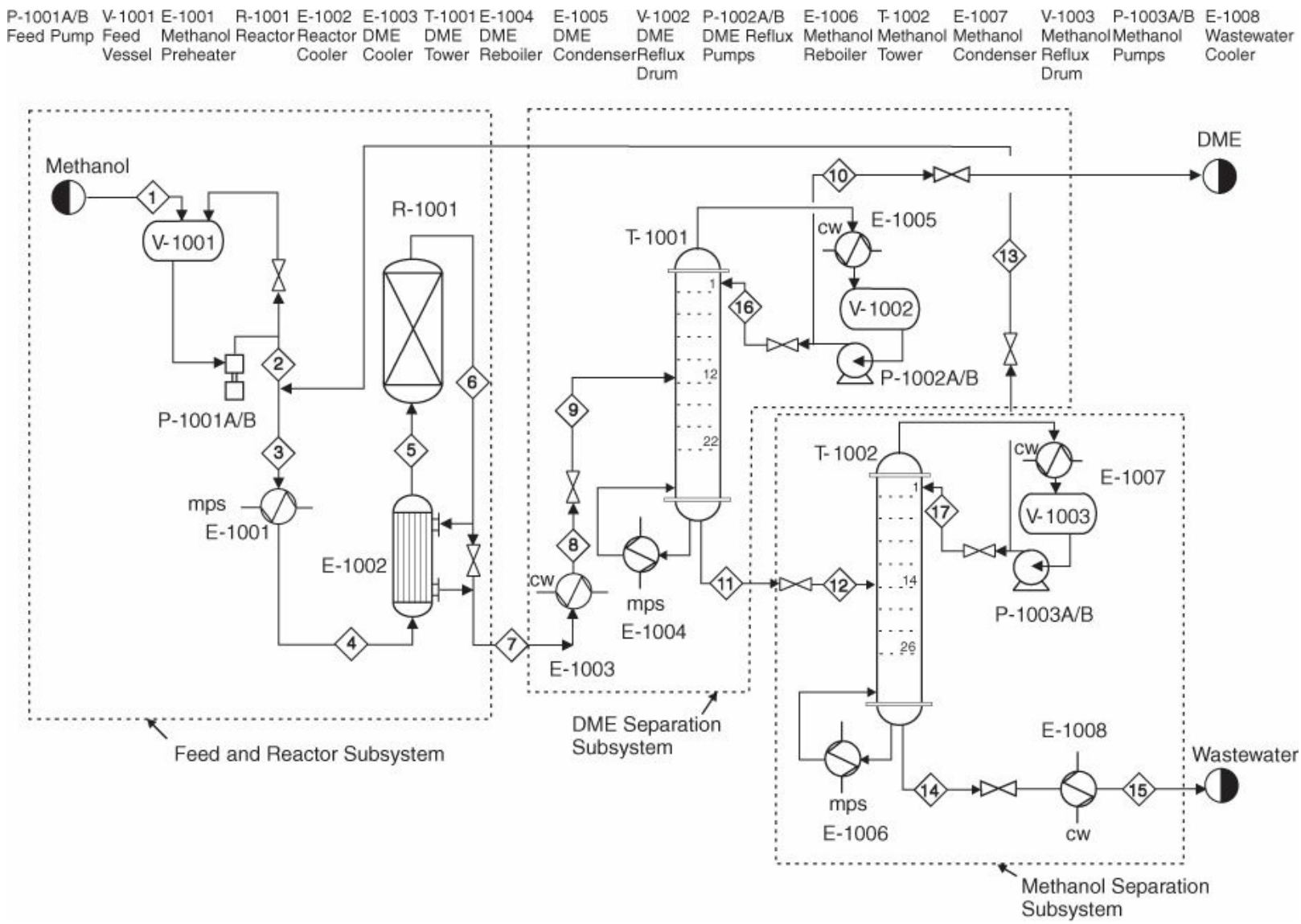


Figure 1.8. Subsystems for Preliminary Plan Layout for DME Process

2. *For each subsystem, a preliminary plot plan is created.* The topology of the plot plan depends on many factors, the most important of which are discussed below.

   In general, the layout of the plot plan can take one of two basic configurations: the grade-level, horizontal, in-line arrangement and the structure-mounted vertical arrangement [5]. The grade-level, horizontal, in-line arrangement will be used for the DME facility. In this arrangement, the process equipment units are aligned on either side of a pipe rack that runs through the middle of the process unit. The purpose of the pipe rack is to carry piping for utilities, product, and feed to and from the process unit. Equipment is located on either side of the pipe rack, which allows for easy access. In addition, vertical mounting of equipment is usually limited to a single level. This arrangement generally requires a larger "footprint" and, hence, more land than does the structure-mounted vertical arrangement. The general arrangement for these layout types is shown in Figure 1.9.

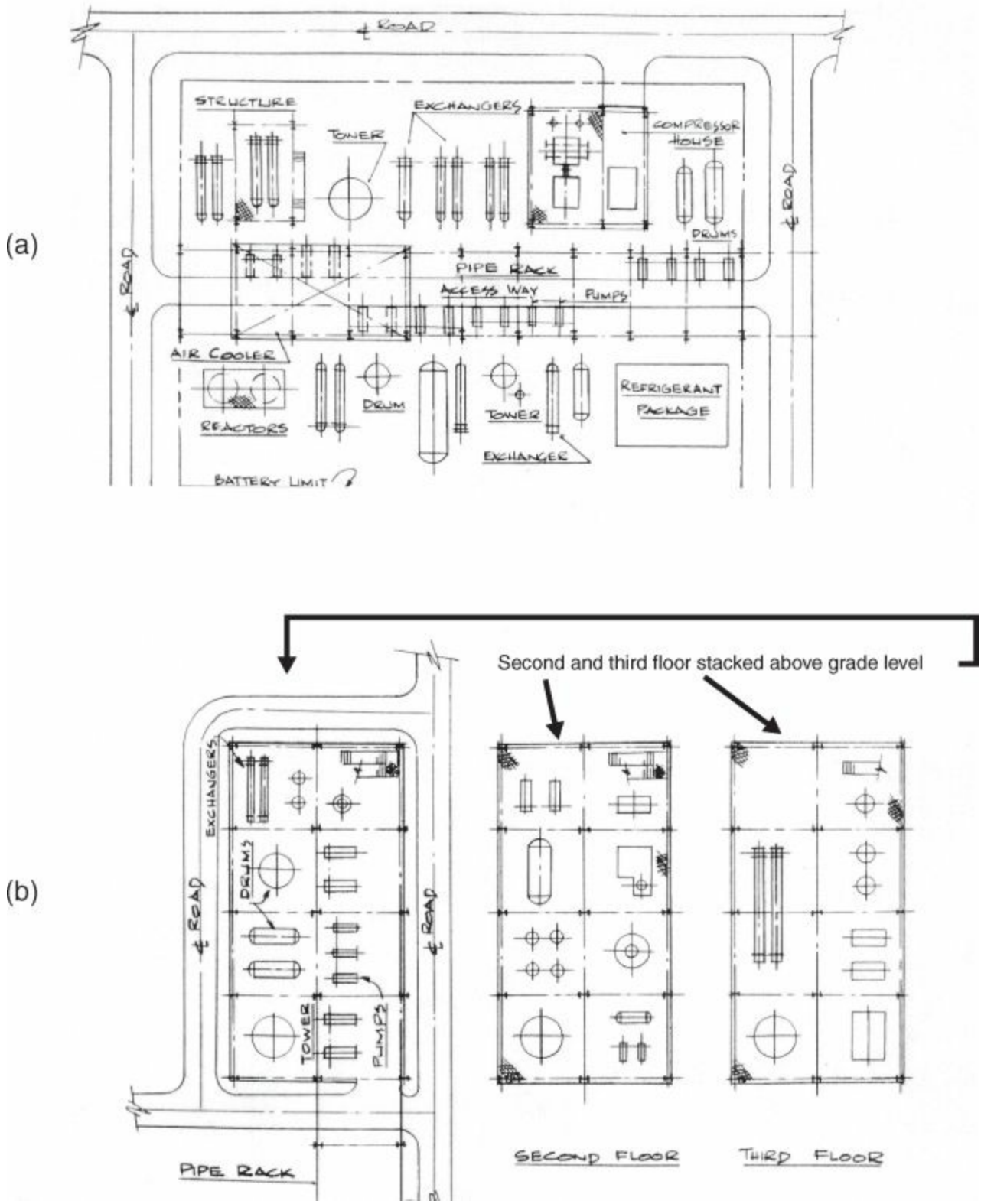


Figure 1.9. Different Types of Plant Layout: (a) Grade-Mounted, Horizontal, In-line Arrangement, and (b) Structure-Mounted Vertical Arrangement (*Source: Process Plant Layout and Piping Design*, by E. Bausbacher and R. Hunt, © 1994, reprinted by permission of Pearson Education, Inc., Upper Saddle River, NJ)

The minimum spacing between equipment should be set early on in the design. These distances are set for safety purposes and should be set with both local and national codes in mind. A comprehensive list of the recommended minimum distances between process equipment is given by Bausbacher and Hunt [5]. The values for some basic process equipment are listed in Table 1.11.

Table 1.11. Recommended Minimum Spacing (in Feet) between Process Equipment for

Refinery, Chemical, and Petrochemical Plants

	Pumps	Compressors	Reactors	Towers and Vessels	Exchangers
Pumps	M	25	M	M	M
Compressors		M	30	M	M
Reactors			M	15	M
Towers				M	M
Exchangers					M

M = minimum for maintenance access

Source: Process Plant Layout and Piping Design, by E. Bausbacher and R. Hunt, © 1994, reprinted by permission of Pearson Education, Inc., Upper Saddle River, NJ

The sizing of process equipment should be completed and the approximate location on the plot plan determined. Referring to Table B.1.3 for equipment specifications gives some idea of key equipment sizes. For example, the data given for the reflux drums V-202 and V-203, reactor R-201, and towers T-201 and T-202 are sufficient to sketch these units on the plot plan. However, pump sizes must be obtained from vendors or previous jobs, and additional calculations for heat exchangers must be done to estimate their required footprint on the plot plan. Calculations to illustrate the estimation of equipment footprints are given in Example 1.11.

Example 1.11.

Estimate the footprint for E-202 in the DME process.

From Table B.1.3 the following information can be found:

Floating-Head Shell-and-Tube design

Area = 171 m^2

Hot Side—Temperatures: in at 364°C and out at 281°C

Cold Side—Temperatures: in at 154°C and out at 250°C

Choose a two-shell pass and four-tube pass exchanger

Area per shell = 171/2 = 85.5 m^2

Using 12 ft, 1-in OD tubes, 293 tubes per shell are needed

Assuming the tubes are laid out on a 1¼-in square pitch, a 27-in ID shell is required.

Assume that the front and rear heads (where the tube fluid turns at the end of the exchanger) are 30 in in diameter and require 2 ft each (including flanges), and that the two shells are stacked on top of each other. The footprint of the exchanger is given in Figure E1.11.

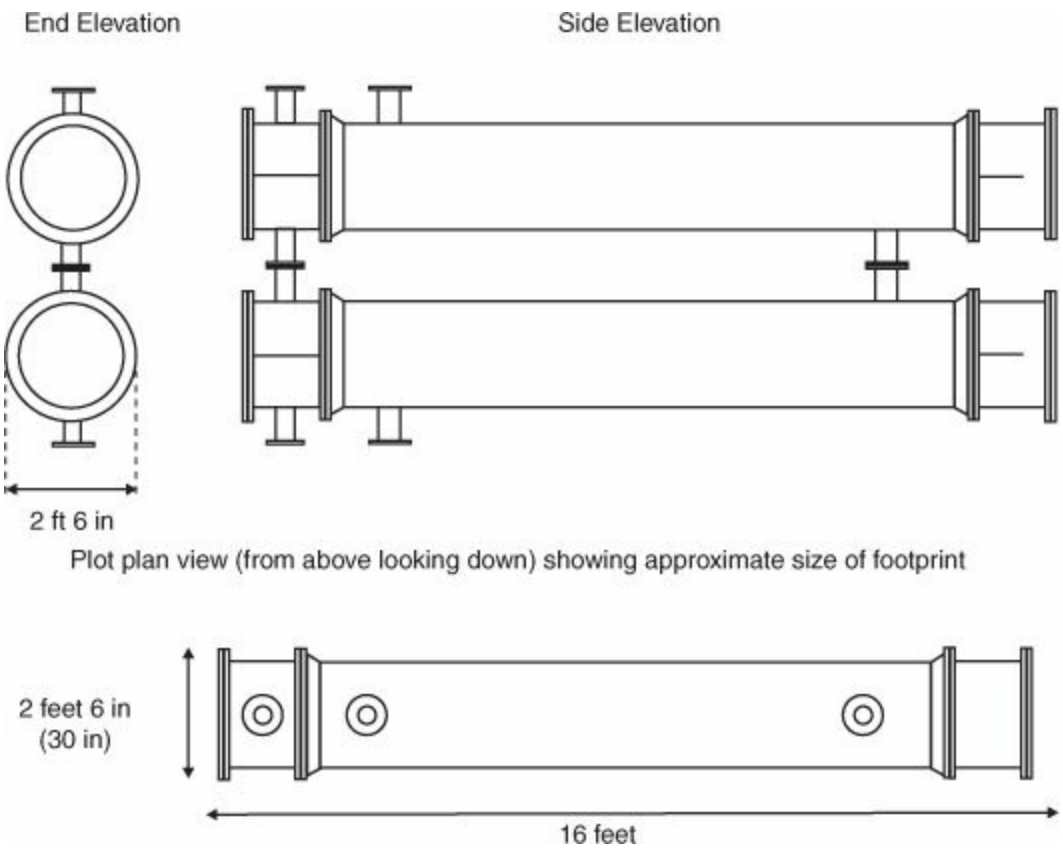


Figure E1.11. Approximate Dimensions and Footprint of Exchanger E-202

Next, the size of the major process lines must be determined. In order to estimate these pipe sizes, it is necessary to make use of some heuristics. A heuristic is a simple algorithm or hint that allows an approximate answer to be calculated. The preliminary design of a piece of equipment might well use many such heuristics, and some of these might conflict with each other. Like any simplifying procedure, the result from a heuristic must be reviewed carefully. For preliminary purposes, the heuristics from Chapter 11 can be used to estimate approximate pipe sizes. Example 1.12 illustrates the heuristic for calculating pipe size.

Example 1.12.

Consider the suction line to P-202 A/B; what should be the pipe diameter?

From Table 11.8, 1(b) for liquid pump suction, the recommended liquid velocity and pipe diameter are related by $u = (1.3 + D\ (\text{in})/6)$ ft/s.

From Table B.1.1, the mass flowrate of the stream entering P-202, $\dot{m}$ = Stream 16 + Stream 10 = 2170 + 5970 = 8140 kg/h and the density is found to be 800 kg/m^3.

The volumetric flowrate is 8140/800 = 10.2 m^3/h = 0.00283 m^3/s= 0.0998 ft^3/s.

The procedure is to calculate the velocity in the suction line and compare it to the heuristic. Using this approach, the following table is constructed:

Nominal Pipe Diameter (inch)	Velocity (ft/s) = Vol Flow/Flow Area	Velocity (h/s) from $u = (1.3 + D/6)$
1.0	18.30	1.47
1.5	8.13	1.55
2.0	4.58	1.63
3.0	2.03	1.80
4.0	1.14 ⟷	1.97

Therefore, the pipe diameter that satisfies both the heuristic and the continuity equation lies between 3 and 4 in. Taking a conservative estimate, a 4-in suction line is chosen for P-202.

The next step to consider is the placement of equipment within the plot plan. This placement must be made considering the required access for maintenance of the equipment and also the initial installation. Although this step may seem elementary, there are many cases [5] where the incorrect placement of equipment subsequently led to considerable cost overruns and major problems both during the construction of the plant and during maintenance operations. Consider the example shown in Figure 1.10(a), where two vessels, a tower, and a heat exchanger are shown in the plot plan. Clearly, V-1 blocks the access to the exchanger's tube bundle, which often requires removal to change leaking tubes or to remove scale on the outside of the tubes. With this arrangement, the exchanger would have to be lifted up vertically and placed somewhere where there was enough clearance so that the tube bundle could be removed. However, the second vessel, V-2, and the tower T-1 are located such that crane access is severely limited and a very tall (and expensive) crane would be required. The relocation of these same pieces of equipment, as shown in Figure 1.10(b), alleviates both these problems. There are too many considerations of this type to cover in detail in this text, and the reader is referred to Bausbacher and Hunt [5] for more in-depth coverage of these types of problems. Considering the DME facility, a possible arrangement for the feed and reactor subsection is shown in Figure 1.11.

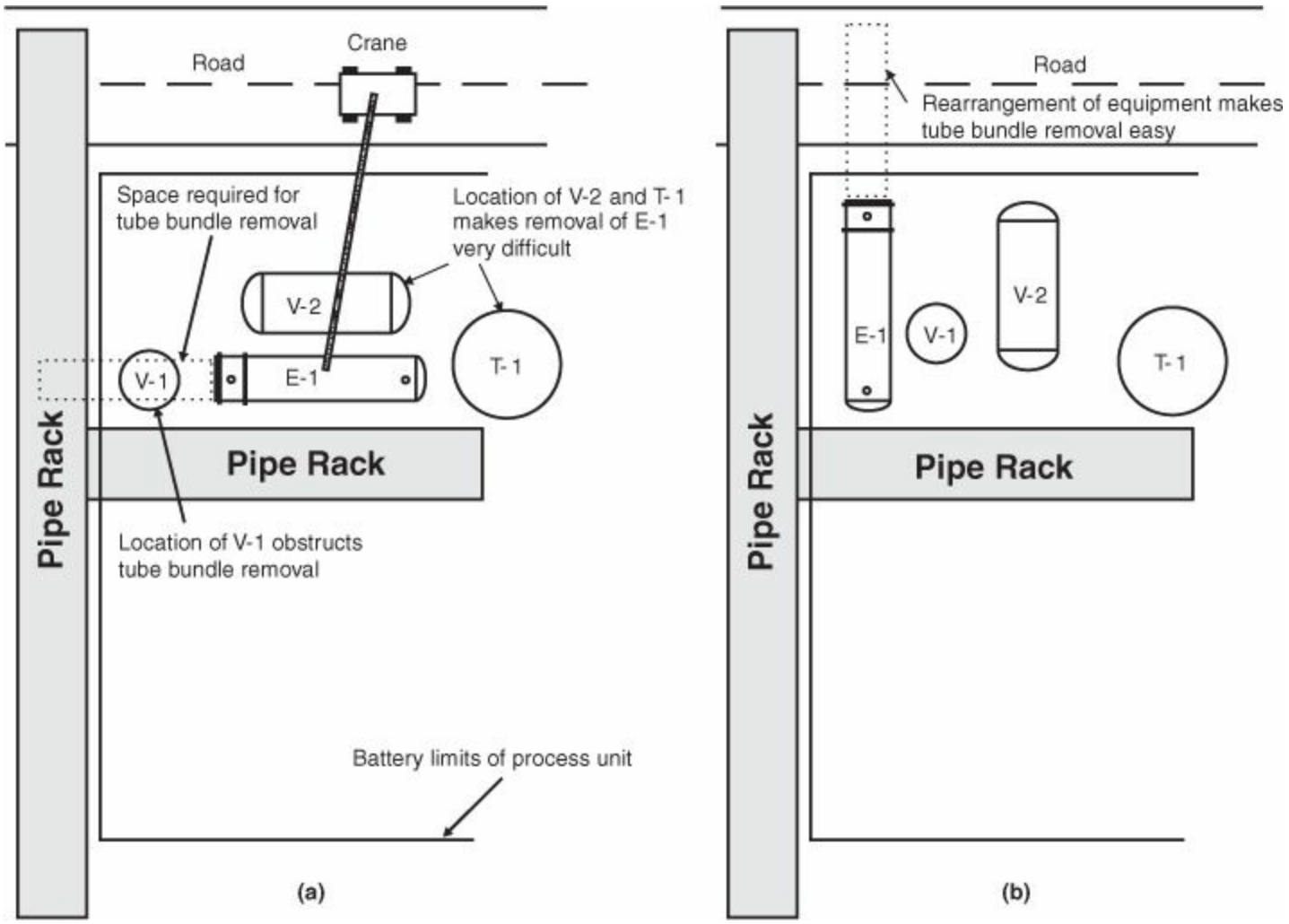


Figure 1.10. The Effect of Equipment Location on the Ease of Access for Maintenance, Installation, and Removal

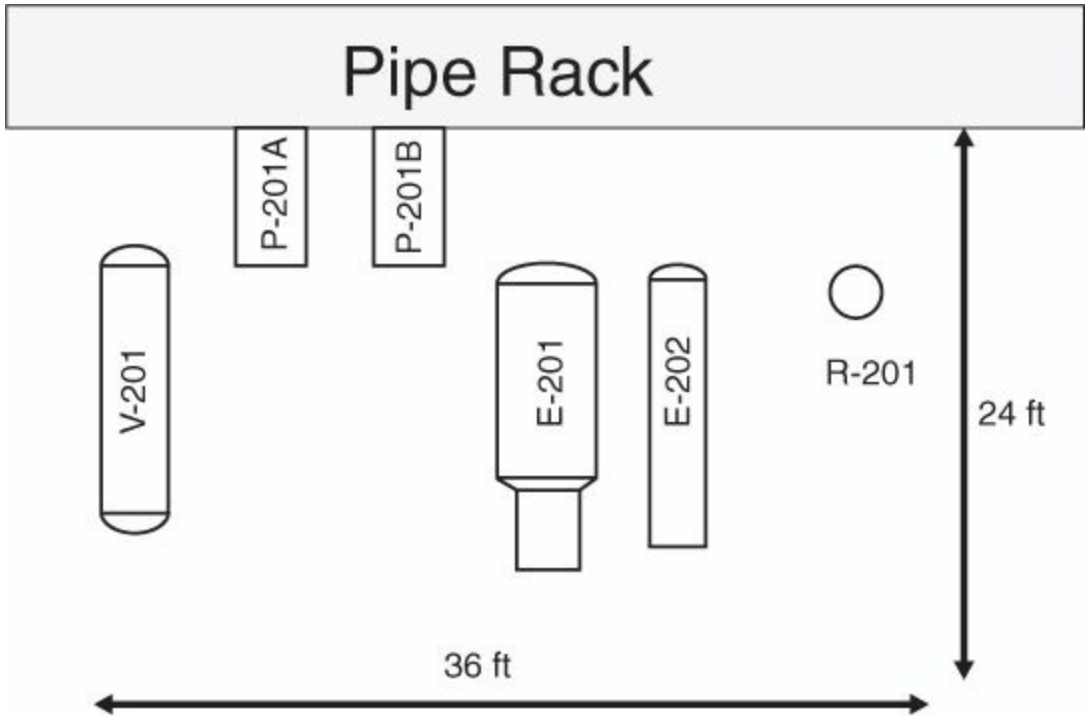


Figure 1.11. Possible Equipment Arrangement for the Reactor and Feed Section of DME Facility, Unit 200

3. *The elevation of all major equipment is established.* In general, equipment located at grade (ground) level is easier to access and maintain and is cheaper to install. However, there are

circumstances that dictate that equipment be elevated in order to provide acceptable operation. For example, the bottoms product of a distillation column is a liquid at its bubble point. If this liquid is fed to a pump, then, as the pressure drops in the suction line due to friction, the liquid boils and causes the pumps to cavitate. To alleviate this problem, it is necessary to elevate the bottom of the column relative to the pump inlet, in order to increase the Net Positive Suction Head Available (for more detail about $NPSH_A$ see Chapter 21). This can be done by digging a pit below grade for the pump or by elevating the tower. Pump pits have a tendency to accumulate denser-than-air gases, and maintenance of equipment in such pits is dangerous due to the possibility of suffocation and poisoning (if the gas is poisonous). For this reason, towers are generally elevated between 3 and 5 m (10 and 15 ft) above ground level by using a "skirt." This is illustrated in Figure 1.12. Another reason for elevating a distillation column is also illustrated in Figure 1.12. Often a thermosiphon reboiler is used. These reboilers use the difference in density between the liquid fed to the reboiler and the two-phase mixture (saturated liquid-vapor) that leaves the reboiler to "drive" the circulation of bottoms liquid through the reboiler. In order to obtain an acceptable driving force for this circulation, the static head of the liquid must be substantial, and a 3–5 m height differential between the liquid level in the column and the liquid inlet to the reboiler is typically sufficient. Examples showing when equipment elevation is required are given in Table 1.12.

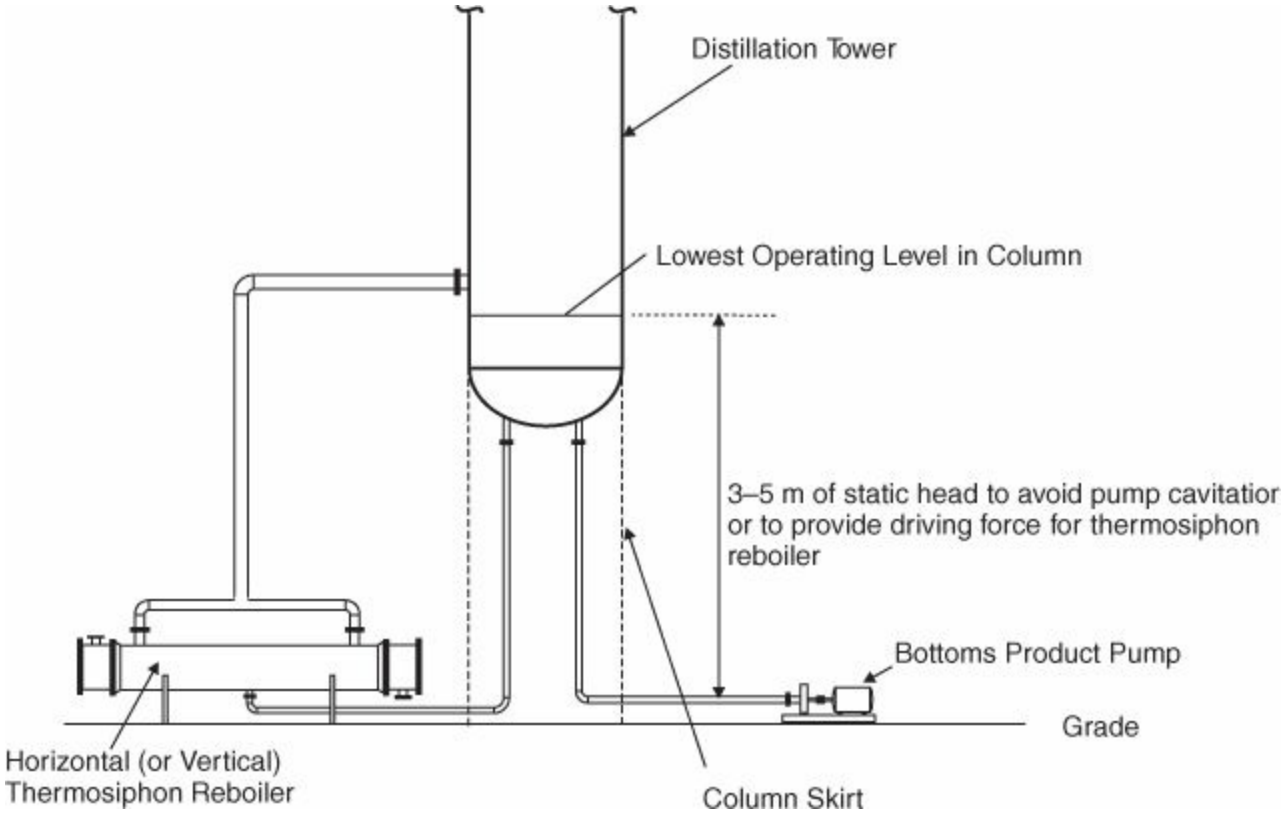


Figure 1.12. Sketch Illustrating Reasons for Elevating Distilling Column

Table 1.12. Reasons for Elevating Equipment

Equipment to Be Elevated	Reason for Elevation
Columns or vessels	When the NPSH available is too low to avoid cavitation in the discharge pump, equipment must be elevated.
Columns	To provide driving head for thermosiphon re-boilers.
Any equipment containing suspended solids or slurries	To provide gravity flow of liquids containing solids that avoids the use of problematic slurry pumps.
Contact barometric condensers	This equipment is used to produce vacuum by expanding high-pressure steam through an ejector. The condensables in the vapor are removed by direct contact with a cold-water spray. The tail pipe of such a condenser is sealed with a 34-foot leg of water.
Critical fire-water tank (or cooling water holding tank)	In some instances, flow of water is absolutely critical, for example, in firefighting or critical cooling operations. The main water supply tank for these operations may be elevated to provide enough water pressure to eliminate the need for feed pumps.

4. *Major process and utility piping are sketched in.* The final step in this preliminary plant layout is to sketch in where the major process (and utility) pipes (lines) go. Again, there are no set rules to do this. However, the most direct route between equipment that avoids clashes with other equipment and piping is usually desirable. It should be noted that utility lines originate and usually terminate in headers located on the pipe rack. When process piping must be run from one side of the process to another, it may be convenient to run the pipe on the pipe rack. All control valves, sampling ports, and major instrumentation must be located conveniently for the operators. This usually means that they should be located close to grade or a steel access platform. This is also true for equipment isolation valves.

1.6. The 3-D Plant Model

The best way to see how all the above elements fit together is to view the Virtual Plant Tour AVI file on the CD that accompanies this text. The quality and level of detail that 3-D software is capable of giving depend on the system used and the level of detailed engineering that is used to produce the model. Figures 1.13–1.15 were generated for the DME facility using the PDMS software package from Cadcentre, Inc. (These figures and the Virtual_Plant_Tour.AVI file are presented here with permission of Cadcentre, Inc.) In Figure 1.13, an isometric view of the DME facility is shown. All major process equipment, major process and utility piping, and basic steel structures are shown. The pipe rack is shown running through the center of the process, and steel platforms are shown where support of elevated process equipment is required. The distillation sections are shown to the rear of the figure on the far side of the pipe rack. The reactor and feed section is shown on the near side of the pipe rack. The elevation of the process equipment is better illustrated in Figure 1.14, where the piping and structural steel have been removed. The only elevated equipment apparent from this figure are the overhead condensers and reflux drums for the distillation columns. The overhead condensers

are located vertically above their respective reflux drums to allow for the gravity flow of condensate from the exchangers to the drums. Figure 1.15 shows the arrangement of process equipment and piping for the feed and reactor sections. The layout of equipment corresponds to that shown in Figure 1.11. It should be noted that the control valve on the discharge of the methanol feed pumps is located close to grade level for easy access.

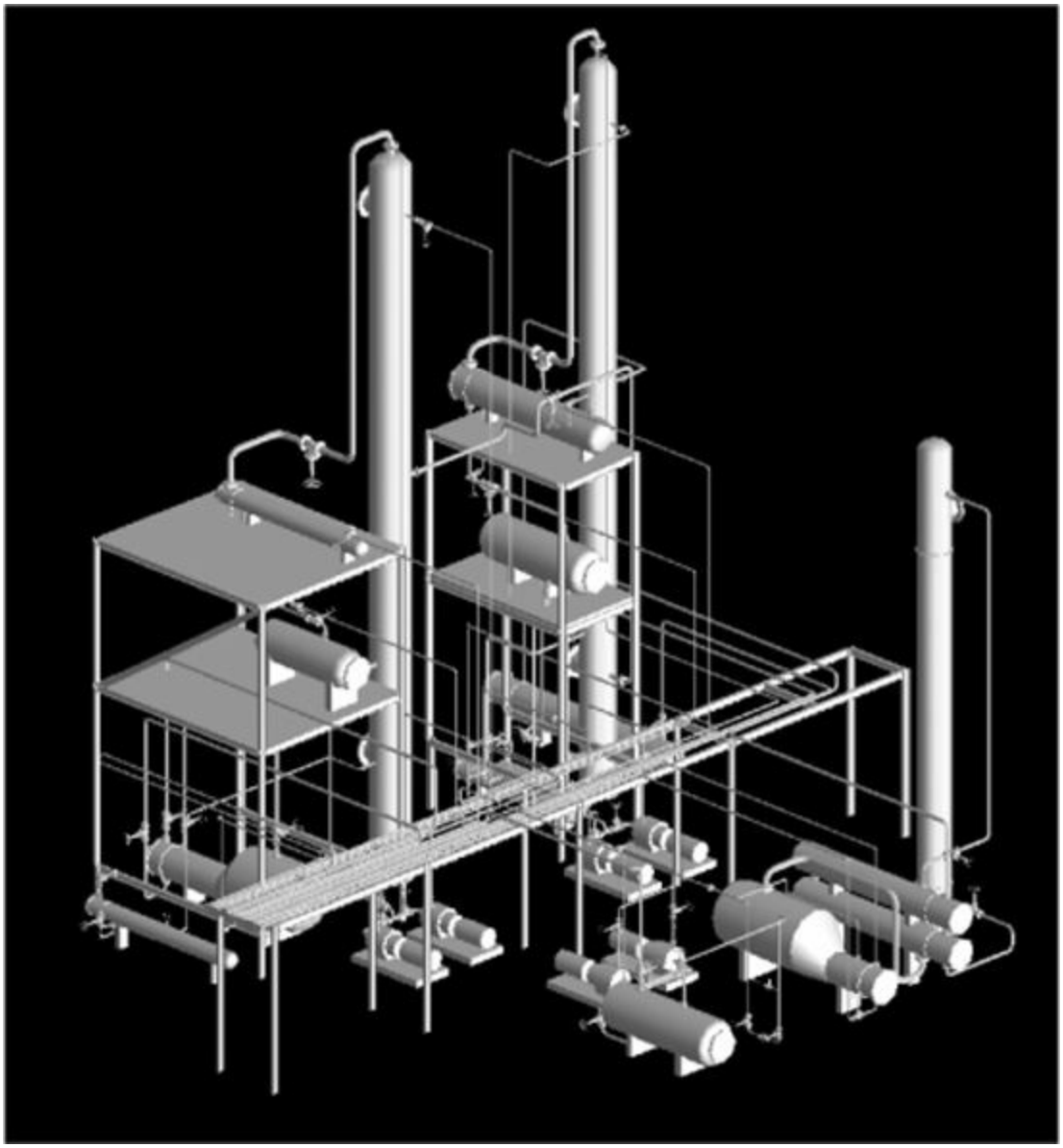


Figure 1.13. Isometric View of Preliminary 3-D Plant Layout Model for DME Process (Reproduced by Permission of Cadcentre, an Aveva Group Company, from their Vantage/PDMS Software)

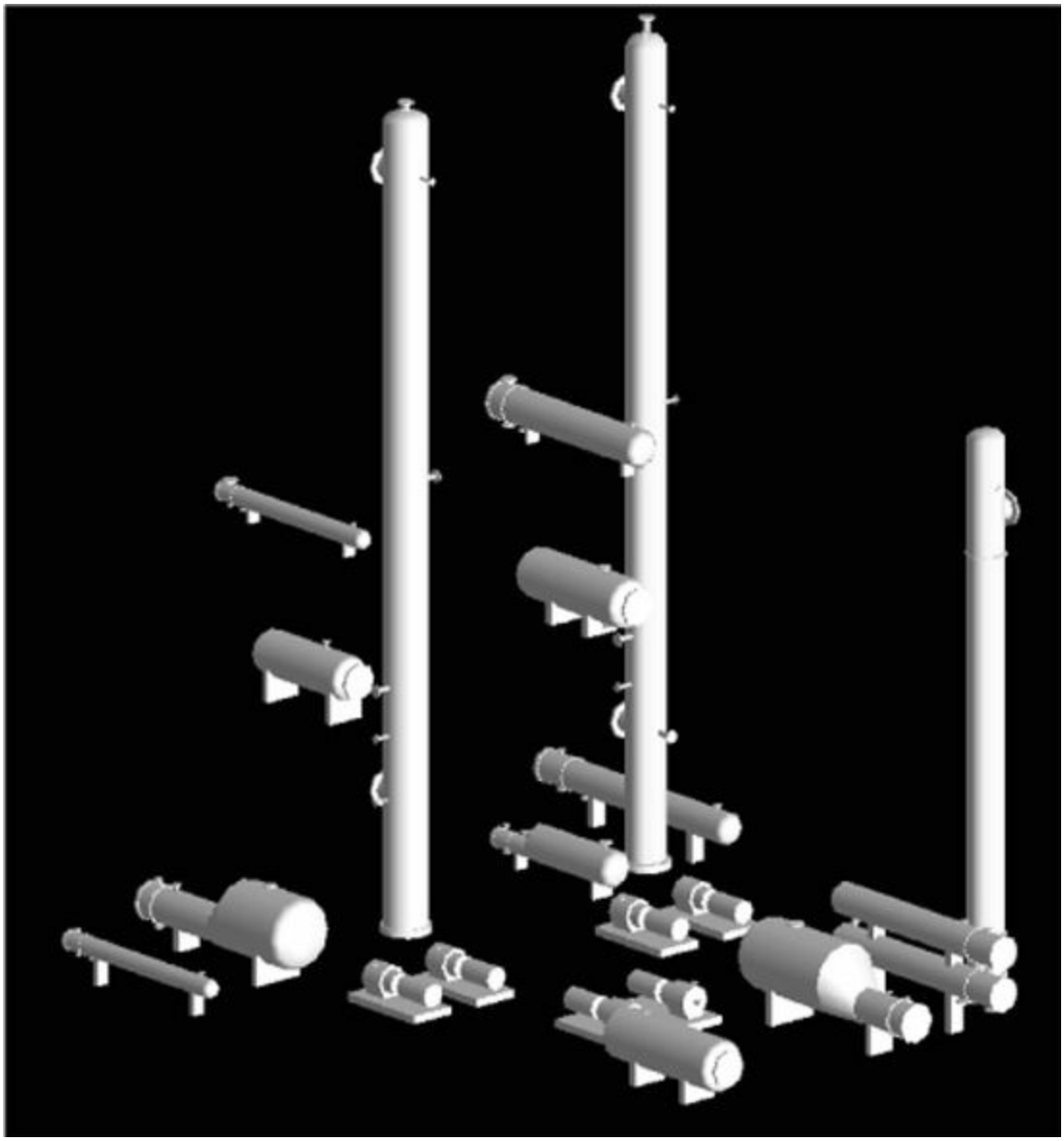


Figure 1.14. 3-D Representation of Preliminary Equipment Layout for the DME Process (Reproduced by Permission of Cadcentre, an Aveva Group Company, from their Vantage/PDMS Software)

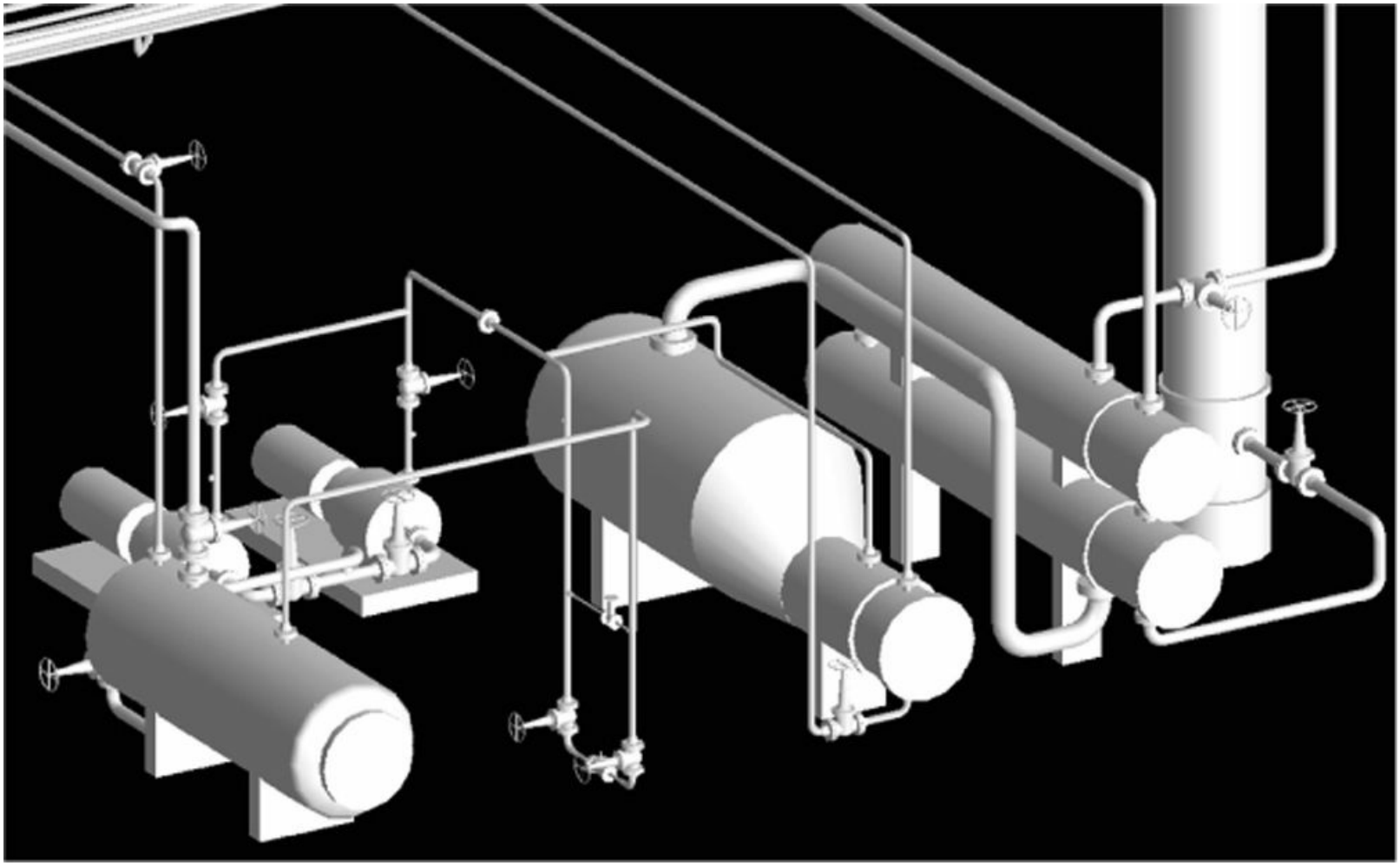


Figure 1.15. 3-D Representation of the Reactor and Feed Sections of the DME Process Model (Reproduced by Permission of Cadcentre, an Aveva Group Company, from their Vantage/PDMS Software)

1.7. Operator and 3-D Immersive Training Simulators

1.7.1. Operator Training Simulators (OTS)

Up to this point in the chapter, the different elements and diagrams used in the specification and description of a process have been covered. The means by which the material balances, energy balances, and design calculations for the various unit operations, required to specify all the design conditions, have been carried out has not been covered. Indeed, the simulation of chemical processes using programs such as CHEMCAD, Aspen Plus, PRO/II, HYSIS, and others is not addressed until much later, in Chapter 13. Nevertheless, it should be clear that extensive simulation of the process will be required to determine and to specify all of the conditions needed in the design. Typically, these simulations are carried out under steady-state conditions and represent a single design operating point, or possibly are made for several different operating points. The steady-state simulation of the process is clearly very important from the standpoint of defining the design conditions and specifying the equipment parameters, such as vessel sizes, heat-exchanger areas and duties, pipe sizes, and so on. However, once the plant has been built, started up, and commissioned, it is rare that the process will operate at that design condition for any given period of time. Moreover, how the process can be started up or run at, for example, 65% or 110% of design capacity is not evident from the original design. Nevertheless, the plant will be run at off-design conditions throughout its life. In order to help operators and engineers understand how to start up and shut down the process, deal with

emergencies, or operate at off-design conditions, an operator training simulator (OTS) may be built.

The foundation of an OTS is a dynamic simulation (model) of the process to which a human machine interface (HMI) is connected. The HMI, in its simplest form, is a pictorial representation of the process that communicates with the dynamic model, and through it, process variables are displayed. The HMI also displays all the controls for the process; an operator can control the process by changing these controls. An example of an HMI is shown in Figure 1.16. This particular example shows a portion of an acid-gas recovery (AGR) unit for an OTS developed by the Department of Energy to simulate an IGCC (Integrated Gasification Combined Cycle) coal-fed power plant. Process variables calculated by the dynamic model are displayed in boxes throughout the HMI. Operators can monitor the change in these variables with time just as they would in a control room situation. The only difference is that the process is simulated rather than actually operating. In general terms, the OTS functions for an operator just as a flight simulator does for a pilot or astronaut. Therefore, operators and engineers can gain operational experience and understanding about a process or plant through the OTS but with the added benefit that any mistakes or errors can be identified and corrected during training sessions without exposing personnel to any risks that might occur if training were to be done on the actual plant.

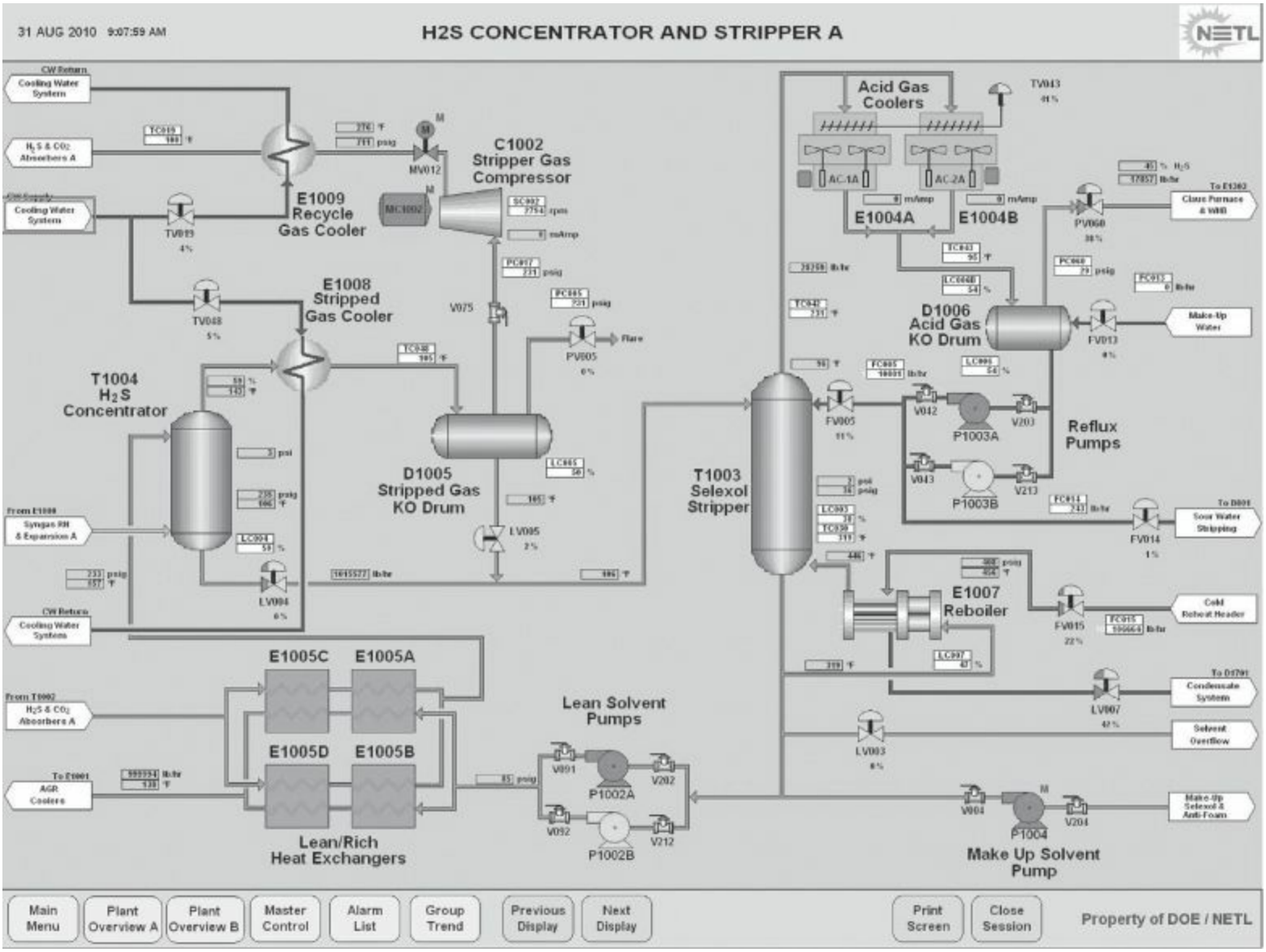


Figure 1.16. Example of an HMI Interface for an OTS (Reproduced by Permission of the DOE's National Energy Technical Laboratory and Invensys Systems Inc., Property and Copyright of Invensys plc, UK)

The starting point for developing an OTS is the steady-state simulation, the equipment information, and instrumentation and control data. In general, the P&IDs are used as the starting point for the generation of the HMI since they contain all the necessary information for the controls and instrumentation. The dynamic model is developed so that the steady-state design condition will be simulated when all the inputs (feeds) are at their design values. Details of how dynamic simulators are used in process design are included in Chapter 17. Needless to say, the development of a fully functioning dynamic model for a process that accurately reflects all the controls and valves in the process is a substantial task that takes a team of engineers many months to accomplish.

1.7.2. 3-D Immersive Training Simulators (ITS)

In Section 1.6, the concept of a 3-D plant model was introduced. Such models are "constructed" in an "electronic" environment using precise design data on the size, location and elevation (x-, y-, and z-coordinates), and orientation of each piece of equipment. In addition, the piping arrangement and location of valves, nozzles, instruments, sample ports, drains, and so forth are all specified. Such a representation allows the engineer and operator to evaluate the accessibility of critical process components and to obtain a feel for how the plant will look (and operate) when constructed. The engineer may access this information through either a 2-D viewer or a 3-D virtual environment (for example, using 3-D goggles). However, no matter how the information is viewed, the resulting images are essentially static and are generally of low to medium fidelity. Therefore, when viewing a 3-D plant model, it will always be clear to the viewer that it is just a model, and that the representation of the 3-D object is crude.

The visual enhancement of 3-D models using sophisticated imaging software and overlaying photorealistic images on top of a skeleton of the 3-D representation are now not only possible but commonplace for higher-end video games. Computer-generated graphics are now so advanced that, as any movie fan will attest, it is often difficult to determine what is "real" and what is animated. This technology is now being applied to develop 3-D immersive training simulators (ITS) for chemical plants. As can be seen from Figure 1.17, the quality and realism captured by computer-generated graphics are truly amazing. Furthermore, the use of avatars to represent plant operators makes it possible for a user to navigate through, interact with, and be truly immersed in the virtual plant.

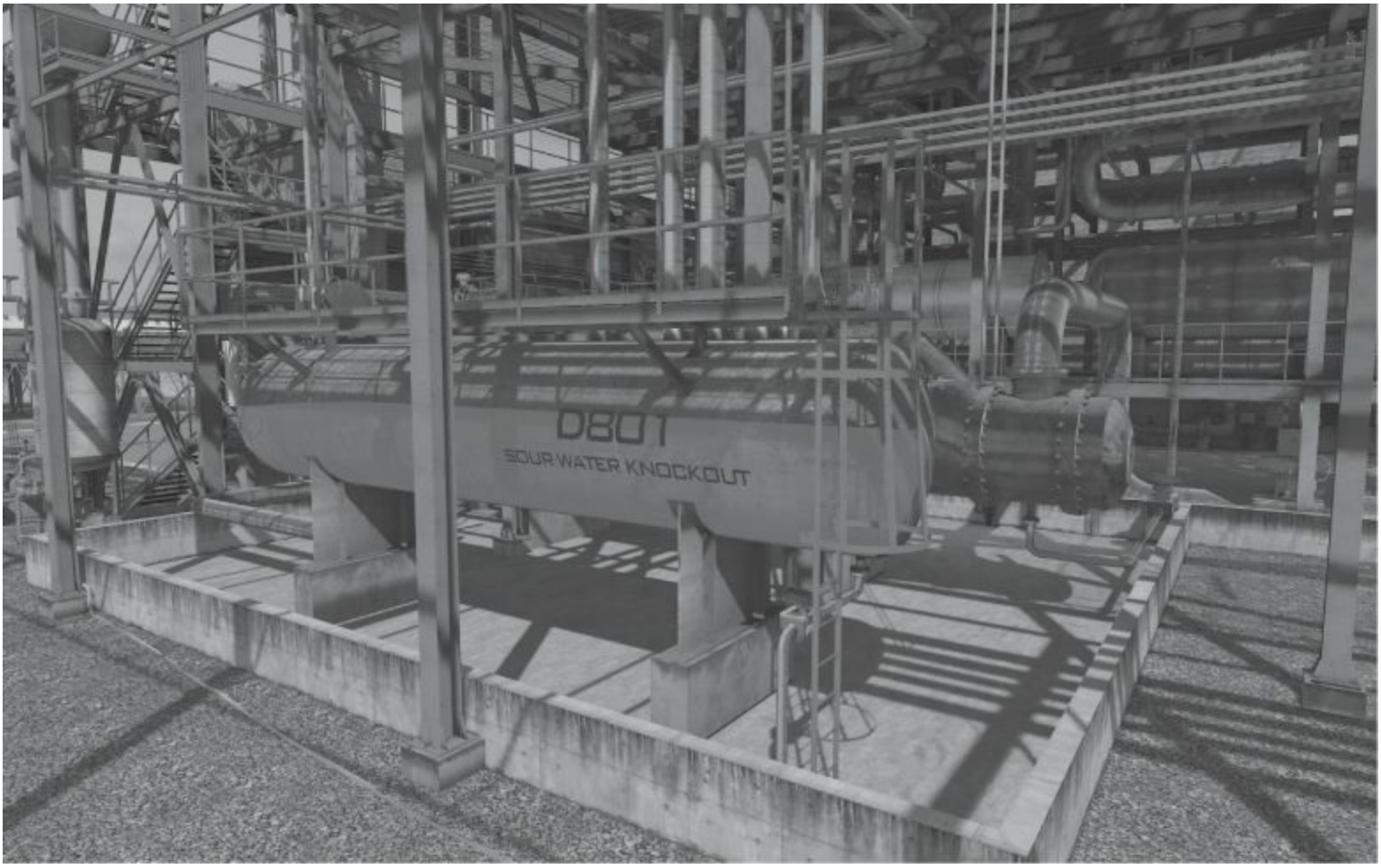


Figure 1.17. An Example of a Computer-Generated Image of a Horizontal Drum (Reproduced by Permission of the DOE's National Energy Technical Laboratory and Invensys Systems Inc., Property and Copyright of Invensys plc, UK)

1.7.3. Linking the ITS with an OTS

The potential for education and training of engineers, operators, and students using both the OTS and ITS appears to be limitless. Indeed, these two systems can be linked together such that they can communicate, and the real-time operation of the process, both in the control room and outside in the plant, can be simulated in the virtual environment. Consider the following scenario that might occur during the start-up of a chemical process:

> *Feed to a distillation column from an on-site storage drum has begun. The feed pump has been started and the flow through the pump has been confirmed from the HMI display in the control room. The liquid feed flows into the top of the tower, and the liquid levels on the distillation trays start to increase. The process appears to be working as described in the start-up manual that the operator is following. However, approximately 30 minutes after the start of the feed pumps, a low-level alarm sounds on the on-site storage drum. The operator monitors the level in the drum from the control room and determines that it is continuing to fall and will cause the feed pump to vapor lock (cavitate) if the situation is not remedied. In reviewing the start-up procedure, the operator determines that there is a remote function valve (one that cannot be operated remotely from the control room) that connects the on-site storage drum to the off-site storage tank, and that this valve may have been closed inadvertently. She then contacts an operator in the field by walkie-talkie and asks him to check the status of the remote function valve. The field operator walks to the*

storage drum, identifies the tag name on the valve, and confirms that the valve is indeed closed. The control room operator then instructs the field operator to open the valve, which he does. The control room operator then confirms that the level in the drum has started to go back up and thanks the field operator for his help.

This scenario might well represent an actual incident during a scheduled plant start-up. However, this scenario could just as easily be simulated in the virtual environment. The control room operator would be sitting in front of the HMI screen that is connected to the OTS. A field operator could be sitting in the room next door with a walkie-talkie and wearing 3-D goggles connected to the ITS. The field operator would move his avatar to the location of the on-site storage drum and locate the remote function valve. The field operator using his avatar would then note the setting of the valve and after receiving instructions from the control room operator would open the valve. At this point, the ITS would communicate to the OTS that a valve had been opened, and this would then allow the flow of product to continue to the drum; that is, the dynamic model of the process would respond to the valve being opened and model the flow to the drum. The control room operator, monitoring the HMI, would see the result of the flow of product as an increase in the drum level.

Clearly, any number of scenarios involving control room operators and field operators could be implemented. Moreover, maintenance operations, safety training, and a whole host of other operator functions could be simulated—all in the virtual plant.

Augmented Reality. From the previous example it is clear that any feasible scenario that might occur in the actual plant can be simulated in the virtual environment. However, a series of cases can be simulated that would be almost impossible to simulate in the actual plant but are easily accomplished in virtual reality. For example, it might be helpful to show a young engineer how a particular piece of equipment works by showing him or her the details of the internals of that equipment. In the actual plant, this opportunity might not be available until a scheduled plant shutdown occurs, and that might not happen for one or two years. However, in the virtual environment, the operation of a given piece of equipment can be easily displayed. In fact, the avatar can move into the plant and simply "strip away" the outer wall of a piece of equipment and look inside to see what is happening. This additional feature is sometimes referred to as augmented reality (AR). As an example of AR, the operation of a reboiler and a distillation column is illustrated in Figures 1.18(a) and 1.18(b), respectively.

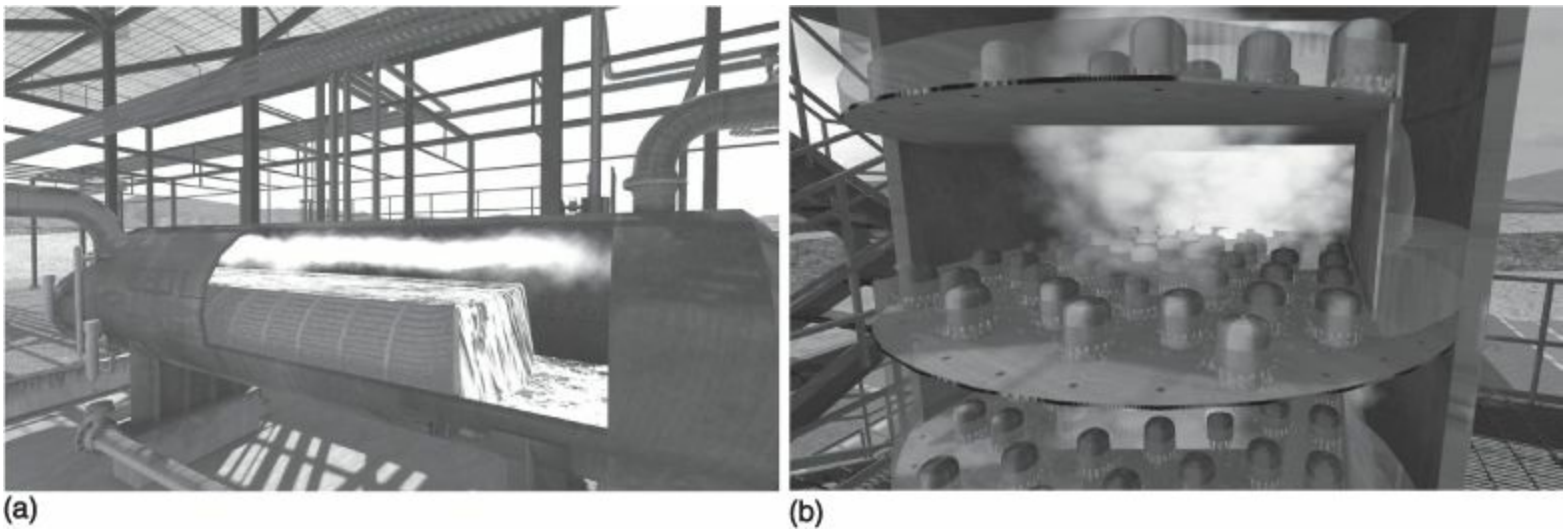


Figure 1.18. Augmented Reality in ITS: (a) Reboiler (b) Bubble-Cap Distillation Column (Reproduced by Permission of the DOE's National Energy Technical Laboratory and Invensys

Systems Inc., Property and Copyright of Invensys plc, UK)

Another example of AR is the display of process data in the virtual plant. For example, if an operator wanted to check on the trend of a certain process variable, say, the temperature in a reactor, or look at a schematic of a pump, the avatar can simply click on a piece of equipment and display that trend, as shown in Figure 1.19. Clearly, in the virtual environment, there are very few limitations on what information the operator (avatar) can access.

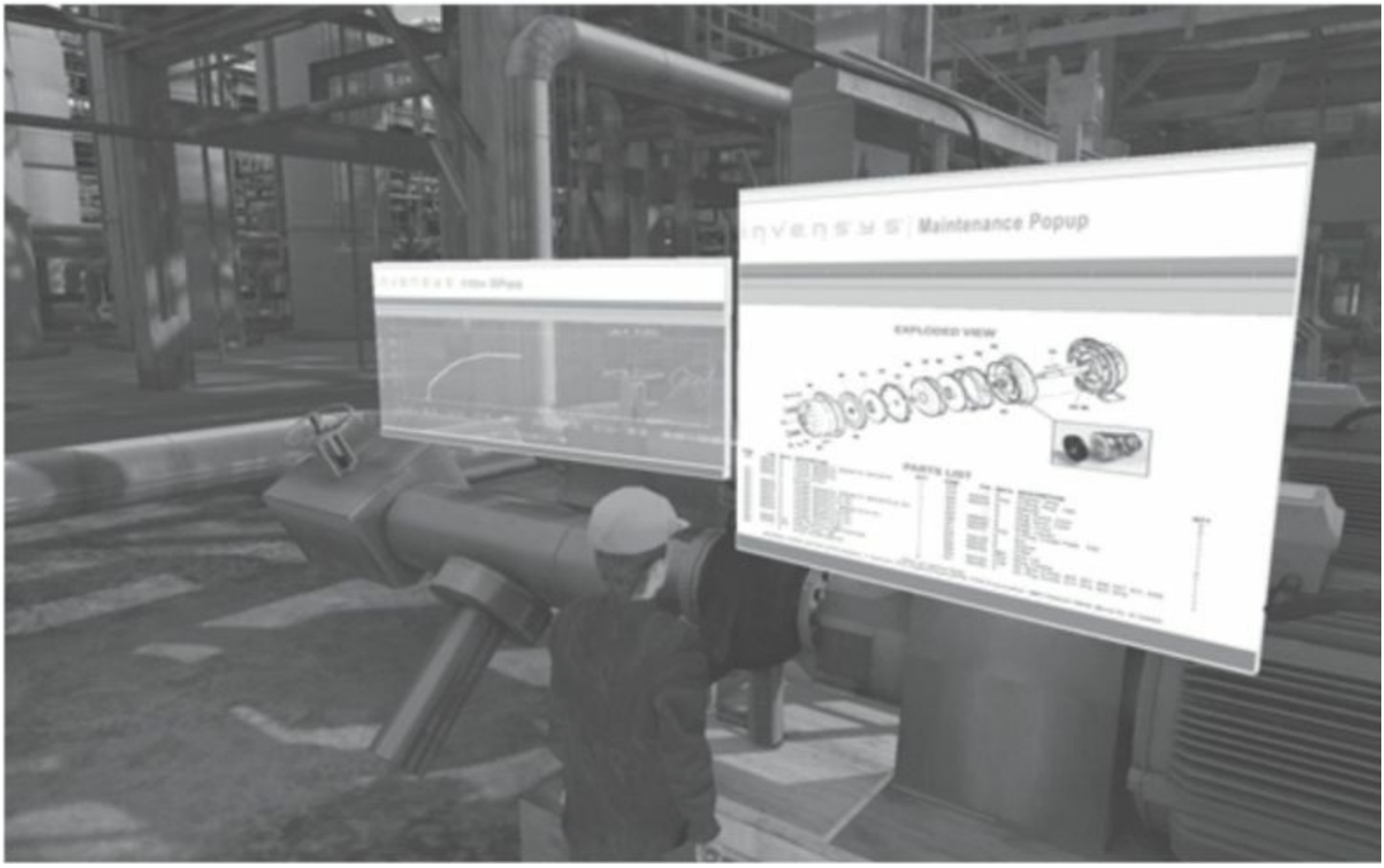


Figure 1.19. An Avatar Can Access Process Trends and Observe Equipment Schematics in AR (Reproduced by Permission of Invensys Systems Inc., Property and Copyright of Invensys plc, UK)

Training for Emergencies, Safety, and Maintenance. The possibilities for training operators and engineers in the virtual plant environment are unlimited. Of particular importance are the areas of safety, emergency response, and routine maintenance. For example, the response of an operator or team of operators to an emergency situation can be monitored, recorded, and played back in the virtual plant. Any mistakes made by the operator(s) can be analyzed, feedback given, and then the exercise can be repeated until the correct response is achieved. Although such training does not absolutely guarantee that when a real emergency arises in the plant the operators will respond correctly, it nevertheless provides crucial emergency training under realistic conditions without the fear of actual harm to personnel and equipment. Furthermore, the more often such scenarios are rehearsed, the more likely are operators to respond correctly when real emergencies occur in the plant.

Corresponding scenarios for safety and maintenance training can also be implemented. Often these activities must follow well-defined procedures, and again, the virtual environment offers a perfect

venue to record, analyze, and provide feedback to personnel as they perform these various tasks.

In summary, the use of the virtual plant environment (ITS linked to an OTS) provides unlimited opportunities to a new generation of engineers and operators to learn and to train as process plant personnel and to hone their respective skills in an environment that is both realistic and safe.

1.8. Summary

In this chapter, you have learned that the three principal types of diagrams used to describe the flow of chemical streams through a process are the block flow diagram (BFD), the process flow diagram (PFD), and the piping and instrumentation diagram (P&ID). These diagrams describe a process in increasing detail.

Each diagram serves a different purpose. The block flow diagram is useful in conceptualizing a process or a number of processes in a large complex. Little stream information is given, but a clear overview of the process is presented. The process flow diagram contains all the necessary information to complete material and energy balances on the process. In addition, important information such as stream pressures, equipment sizes, and major control loops is included. Finally, the piping and instrumentation diagram contains all the process information necessary for the construction of the plant. These data include pipe sizes and the location of all instrumentation for both the process and utility streams.

In addition to the three diagrams, there are a number of other diagrams used in the construction and engineering phase of a project. However, these diagrams contain little additional information about the process.

The logic for equipment placement and layout within the process was presented. The reasons for elevating equipment and providing access were discussed, and a 3-D representation of a DME plant was presented. The concept of operator training simulators is presented and the role of 3-D immersive training systems is also introduced.

The PFD is the single most important diagram for the chemical or process engineer and will form the basis of much of the discussion covered in this book.

What You Should Have Learned

- The difference between and uses of the block flow diagram, the process flow diagram, the piping and instrumentation diagram, plot plans, elevation diagrams, and piping isometrics
- A method for drawing consistent process flow diagrams
- How operator training systems and 3-D graphic process representations are used to train operators and engineers

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References

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Short Answer Questions

1. What are the three principal types of diagrams used by process engineers to describe the flow of chemicals in a process? On which of these diagrams would you expect to see the following items?
   a. The temperature and pressure of a process stream
   b. An overview of a multiple-unit process
   c. A major control loop
   d. A pressure indicator
   e. A pressure-relief valve
2. A problem has occurred in the measuring element of a level-indicating controller in a batch reactor. To what principal diagram should you refer in order to troubleshoot the problem?
3. Why is it important for a process engineer to be able to review a three-dimensional model (actual or virtual/electronic) of the plant prior to the construction phase of a project?
4. Name five things that would affect the locations of different pieces of equipment when determining the layout of equipment in a process unit.
5. Why are accurate plant models (made of plastic parts) no longer made as part of the design process? What function did these models play and how is this function now achieved?
6. In the context of process modeling tools, what do OTS and ITS stand for?
7. What is augmented reality? Give one example of it.

Problems

8. There are two common reasons for elevating the bottom of a tower by means of a "skirt." One reason is to provide enough $NPSH_A$ for bottoms product pumps to avoid cavitation. What is the other reason?
9. Which of the principal diagrams should be used to do the following:
   a. Determine the number of trays in a distillation column?
   b. Determine the top and bottom temperatures in a distillation column?
   c. Validate the overall material balance for a process?
   d. Check the instrumentation for a given piece of equipment in a "pre-start-up" review?
   e. Determine the overall material balance for a whole chemical plant?
10. What is the purpose(s) of a pipe rack in a chemical process?
11. When would a structure-mounted vertical plant layout arrangement be preferred over a grade-mounted, horizontal, in-line arrangement?

12. A process that is being considered for construction has been through several technical reviews; block flow, process flow, and piping and instrumentation diagrams are available for the process. Explain the changes that would have to be made to the three principal diagrams if during a final preconstruction review, the following changes were made:
    a. The efficiency of a fired heater had been specified incorrectly as 92% instead of 82%.
    b. A waste process stream flowrate (sent to a sludge pond) was calculated incorrectly and is now 30% greater than before.
    c. It has been decided to add a second (backup) drive for an existing compressor.
    d. The locations of several control valves have changed to allow for better operator access.
13. During a retrofit of an existing process, a vessel used to supply the feed pump to a batch reactor has been replaced because of excessive corrosion. The vessel is essentially identical to the original one, except it is now grounded differently to reduce the corrosion. If the function of the vessel (namely, to supply liquid to a pump) has not changed, answer the following questions:
    a. Should the new vessel have a new equipment number, or should the old vessel number be used again? Explain your answer.
    b. On which diagram or diagrams (BFD, PFD, or P&ID) should the change in the grounding setup be noted?
14. Draw a section of a P&ID diagram for a vessel receiving a process liquid through an insulated 4-in schedule-40 pipe. The purpose of the vessel is to store approximately 5 minutes of liquid volume and to provide "capacity" for a feed pump connected to the bottom of the pump using a 6-in schedule-40 pipe. The diagram should include the following features:
    a. The vessel is numbered V-1402 and the pump(s) are P-1407 A/B.
    b. The discharge side of the pump is made of 4-in schedule-40 carbon steel pipe and all pipe is insulated.
    c. A control valve is located in the discharge line of the pump, and a double block and bleed arrangement is used (see Problem 1.15 for more information).
    d. Both pumps and vessel have isolation (gate) valves.
    e. The pumps should be equipped with drain lines that discharge to a chemical sewer.
    f. The vessel is equipped with local pressure and temperature indicators.
    g. The vessel has a pressure-relief valve set to 50 psig that discharges to a flare system.
    h. The tank has a drain valve and a sampling valve, both of which are connected to the tank through separate 2-in schedule-40 CS lines.
    i. The tank level is used to control the flow of liquid out of the tank by adjusting the setting of the control valve on the discharge side of the pump. The instrumentation is similar to that shown for V-104 in Figure 1.7.
15. A standard method for instrumenting a control valve is termed the "double block and bleed," which is illustrated in Figure P1.15.

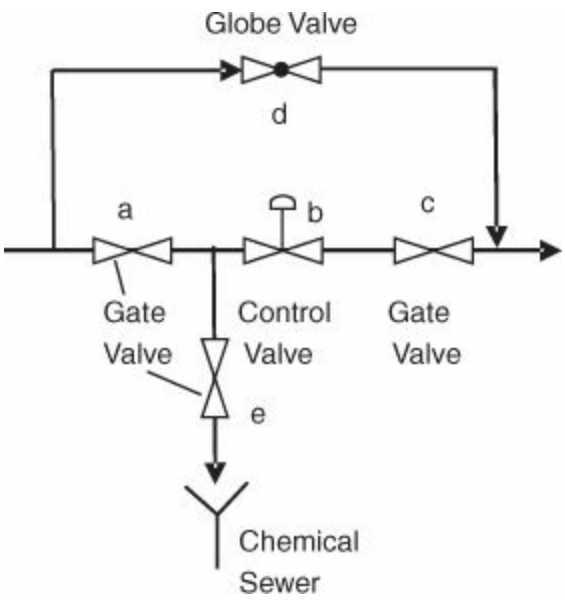


Figure P1.15. Double Block and Bleed Arrangement for Problem 1.15

Under normal conditions, valves a to c are open and valves d and e are closed. Answer the following:

a. Explain, carefully, the sequence of opening and closing valves required in order to change out the valve stem on the control valve (valve b).

b. What changes, if any, would you make to Figure P1.15 if the process stream did not contain a process chemical but contained process water?

c. It has been suggested that the bypass valve (valve d) be replaced with another gate valve to save money. Gate valves are cheap but essentially function as on-off valves. What do you recommend?

d. What would be the consequence of eliminating the bypass valve (valve d)?

16. Often, during the distillation of liquid mixtures, some noncondensable gases are dissolved in the feed to the tower. These noncondensables come out of solution when heated in the tower and may accumulate in the overhead reflux drum. In order for the column to operate satisfactorily, these vapors must be periodically vented to a flare or stack. One method to achieve this venting process is to implement a control scheme in which a process control valve is placed on the vent line from the reflux drum. A pressure signal from the drum is used to trigger the opening or closing of the vent line valve. Sketch the basic control loop needed for this venting process on a process flow diagram representing the top portion of the tower.

17. Repeat Problem 1.16, but create the sketch as a P&ID to show all the instrumentation needed for this control loop.

18. Explain how each of the following statements might affect the layout of process equipment:

a. A specific pump requires a large NPSH.

b. The flow of liquid from an overhead condenser to the reflux drum is gravity driven.

c. Pumps and control valves should be located for easy access and maintenance.

d. Shell-and-tube exchanges may require periodic cleaning and tube bundle replacement.

e. Pipes located at ground level present a tripping hazard.

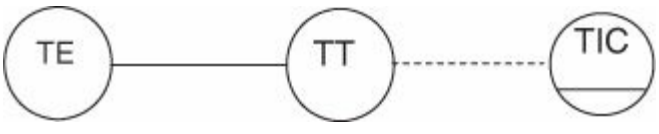
f. The prevailing wind is nearly always from the west.

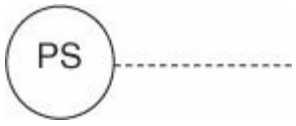
19. Estimate the footprint for a shell-and-tube heat exchanger from the following design data:

- Area = 145 m^2
- Hot side temperatures: in at 300°C, out at 195°C
- Cold side temperature: bfw at 105°C mps at 184°C
- Use 12 ft, 1-in OD tubes on a 1 1/4-in square pitch, use a single shell-and-tube pass because of change of phase on shell side
- Use a vapor space above boiling liquid = 3 times liquid volume

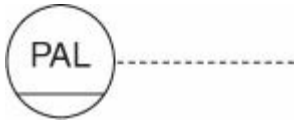
20. Make a sketch of a layout (plot plan only) of a process unit containing the following process equipment:
    - 3 reactors (vertical—diameter 1.3 m each)
    - 2 towers (1.3 and 2.1 m in diameter, respectively)
    - 4 pumps (each mounting pad is 1 m by 1.8 m)
    - 4 exchangers (footprints of 4 m by 1 m, 3.5 m by 1.2 m, 3 m by 0.5 m, and 3.5 m by 1.1 m)

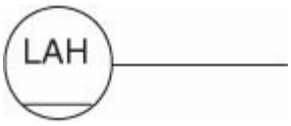
    The two columns and the three reactors should all be aligned with suitable spacing and all the exchangers should have clearance for tube bundle removal.
21. Using the data from Table 1.7, estimate the footprints of all the equipment in the toluene HDA process.
    - For the shell-and-tube exchangers, assume 12 ft, 1.25 in tubes on a 1.5 in square pitch, and assume 2 ft additional length at either end of the exchanger for tube return and feed header.
    - For double pipe exchangers, assume an 8-in schedule-20 OD and a 6-in schedule-40 ID pipe with a length of 12 ft including u-bend.
    - For the footprints of pumps, compressors, and fired heater, assume the following:
        - P-101 use 2 m by 1 m, P-102 use 2 m by 1 m
        - C-101 (+D-101) use 4 m by 2 m
        - H-101 use 5 m by 5 m
22. With the information from Problem 1.21 and the topology given in Figure 1.5, accurately sketch a plant layout (plot plan) of the toluene HDA process using a grade-mounted, horizontal, in-line arrangement similar to the one shown in Figure 1.9. You should assume that the area of land available for this process unit is surrounded on three sides by an access road and that a pipe rack runs along the fourth side. Use the information in Table 1.11 as a guide to placing equipment.
23. What do the following symbols (as seen on a P&ID) indicate?

(a) 

(b) 

(c) 

(d) 

(e) 

24. Determine all the errors in the section of a P&ID shown in Figure P1.24.

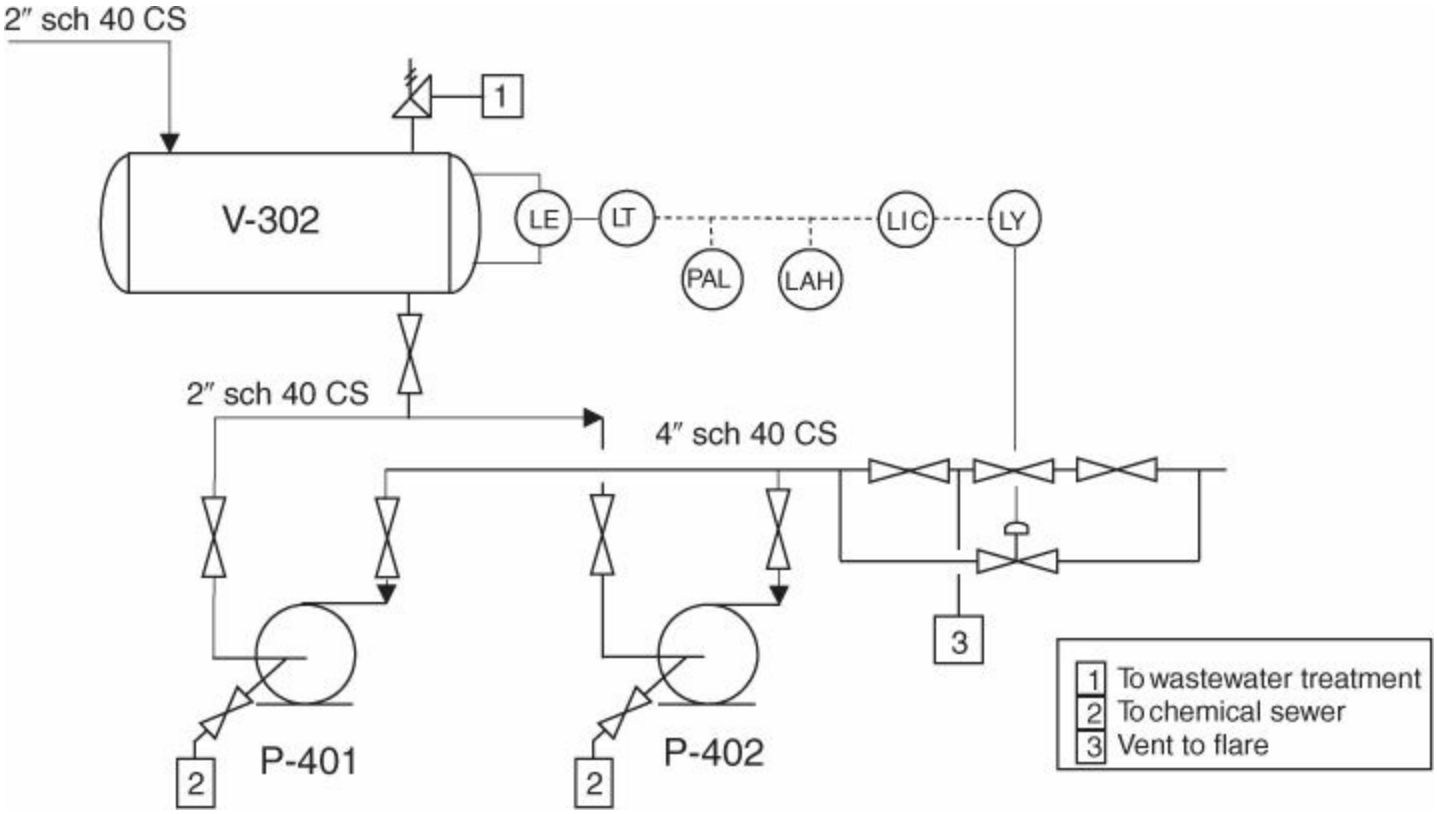


Figure P1.24. A Section of a P&ID to Be Used in Problem 1.24

Chapter 2. The Structure and Synthesis of Process Flow Diagrams

What You Will Learn

- The hierarchy of chemical process design
- The structure of continuous chemical processes
- The differences between batch and continuous processes

When looking at a process flow diagram (PFD) for the first time, it is easy to be confused or overwhelmed by the complexity of the diagram. The purpose of this chapter is to show that the evolution of every process follows a similar path. The resulting processes will often be quite different, but the series of steps that have been followed to produce the final processes are similar. Once the path or evolution of the structure of processes has been explained and is understood, the procedure for understanding existing PFDs is also made simpler. Another important benefit of this chapter is to provide a framework to generate alternative PFDs for a given process.

2.1. Hierarchy of Process Design

Before discussing the steps involved in the conceptual design of a process, it should be noted that often the most important decision in the evolution of a process is the choice of which chemical syntheses or routes should be investigated to produce a desired product. The identification of alternative process chemistries should be done at the very beginning of any conceptual design. The conceptual design and subsequent optimization of a process are "necessary conditions" for any successful new process. However, the greatest improvements (savings) associated with chemical processes are most often due to changes, sometimes radical changes, to the chemical pathway used to produce the product. Most often, there are at least two viable ways to produce a given chemical. These alternative routes may require different raw materials and may produce different byproducts. The cost of the raw materials, the value of the by-products, the complexity of the synthesis, and the environmental impact of any waste materials and pollutants produced must be taken into account when evaluating alternative synthesis routes.

Douglas [1, 2], among others, has proposed a hierarchical approach to conceptual process design. In this approach, the design process follows a series of decisions and steps. The order in which these decisions are made forms the hierarchy of the design process. These decisions are listed as follows:

1. Decide whether the process will be batch or continuous.
2. Identify the input/output structure of the process.
3. Identify and define the recycle structure of the process.
4. Identify and design the general structure of the separation system.
5. Identify and design the heat-exchanger network or process energy recovery system.

In designing a new process, Steps 1 through 5 are followed in that order. Alternatively, by looking at an existing process, and working backward from Step 5, it is possible to eliminate or greatly simplify the PFD. Hence, much about the structure of the underlying process can be determined.

This five-step design algorithm will now be applied to a chemical process. Each of the steps is

discussed in some detail, and the general philosophy about the decision-making process will be covered. However, because Steps 4 and 5 require extensive discussion, these will be covered in separate chapters (Chapter 12 for separations, and Chapter 15 for energy recovery).

2.2. Step 1—Batch Versus Continuous Process

It should be pointed out that there is a difference between a batch process and a batch (unit) operation. Indeed, there are very few, if any, processes that use only continuous operations. For example, most chemical processes described as continuous receive their raw material feeds and ship their products to and from the plant in rail cars, tanker trucks, or barges. The unloading and loading of these materials are done in a batch manner. Indeed, the demarcation between continuous and batch processes is further complicated by situations when plants operate continuously but feed or receive material from other process units within the plant that operate in a batch mode. Such processes are often referred to as semi-batch. A **batch process** is one in which a finite quantity (batch) of product is made during a period of a few hours or days. The batch process most often consists of metering feed(s) into a vessel followed by a series of unit operations (mixing, heating, reaction, distillation, etc.) taking place at discrete scheduled intervals. This is then followed by the removal and storage of the products, by-products, and waste streams. The equipment is then cleaned and made ready for the next process. Production of up to 100 different products from the same facility has been reported [3]. This type of operation is in contrast to **continuous processes,** in which feed is sent continuously to a series of equipment, with each piece usually performing a single unit operation. Products, by-products, and waste streams leave the process continuously and are sent to storage or for further processing.

There are a number of considerations to weigh when deciding between batch and continuous processes, and some of the more important of these are listed in Table 2.1. As this table indicates, there are many things to consider when making the decision regarding batch versus continuous operation. Probably the most important of these are size and flexibility. If it is desired to produce relatively small quantities, less than 500 tonne/y [1], of a variety of different products using a variety of different feed materials, then batch processing is probably the correct choice. For large quantities, greater than 5000 tonne/y of product [1], using a single or only a few raw materials, then a continuous process is probably the best choice. There are many trade-offs between the two types of processes. However, like most things, it boils down to cost. For a batch process compared to the equivalent continuous process, the capital investment is usually much lower because the same equipment can be used for multiple unit operations and can be reconfigured easily for a wide variety of feeds and products. On the other hand, operating labor costs and utility costs tend to be much higher. Recent developments in batch processing have led to the concept of the “pipeless batch process” [4]. In this type of operation, equipment is automatically moved to different workstations at which different processes are performed. For example, a reactor may be filled with raw materials and mixed at station 1, moved to station 2 for heating and reaction, to station 3 for product separation, and finally to station 4 for product removal. The workstations contain a variety of equipment to perform functions such as mixing, weighing, heating/cooling, filtration, and so on. This modular approach to the sequencing of batch operations greatly improves productivity and eases the scheduling of different events in the overall process.

Table 2.1. Some Factors to Consider When Deciding between Batch and Continuous Processes

Factor	Advantages/Disadvantages for Batch Processes	Advantages/Disadvantages for Continuous Processes
Size	Smaller throughput favors batch operations. As throughput increases, the required size of the process equipment increases, and the technical difficulties of moving large amounts of chemicals from equipment to equipment rapidly increase.	Economies of scale favor continuous processes for large throughput.
Batch Accountability/ Product Quality	When the product quality of each batch of material must be verified and certified, batch operations are preferred. This is especially true for pharmaceutical and food products. The manufacture of these products is strictly monitored by the Food and Drug Administration (FDA). If reworking (reprocessing) of off-specification product is usually not permitted, small batches are favored.	Continuous or periodic testing of product quality is carried out, but some potentially large quantities of off-specification product can be produced. If off-specification material may be blended or stored in dump/slop tanks and reworked through the process when the schedule permits, continuous processes are favored.
Operational Flexibility	Often the same equipment can be used for multiple operations—for example, a stirred tank can be used as a mixer, then a reactor, and then as a stage of a mixer-settler for liquid-liquid extraction.	Operational flexibility can be built in to continuous processes but often leads to inefficient use of capital. Equipment not required for one process but needed for another may sit idle for months. Often continuous processes are designed to produce a fixed suite of products from a well-defined feed material. If market forces change the feed/product availability or demand, then the plant will often be retrofitted to accommodate the change.
Standardized Equipment—Multiple Products	Often batch processes can be easily modified to produce several different products using essentially the same equipment. Examples of batch plants that can produce 100 different products are known [3]. For such processes the optimal control and sequencing of operations are critical to the success of such a plant.	The product suite or slate produced from continuous processes is usually fixed. Equipment tends to be designed and optimized for a single or small number of operating conditions.
Processing Efficiency	Operation of batch processes requires strict scheduling and control. Because different products are scheduled back-to-back, changes in schedules have a ripple effect and may cause serious problems with product availability for customers. If the same equipment is used to produce many different products, then this equipment will not be optimized for any one product. Energy integration is usually not possible, so utility usage tends to be higher than for continuous processes. Separation and reuse of raw materials are more difficult than for continuous processes.	Generally, as throughput increases, continuous processes become more efficient. For example, fugitive energy losses are reduced, and rotating equipment (pumps, compressors, etc.) operates with higher efficiency. Recycle of unused reactants and the integration of energy within the process or plant are standard practices and relatively easy to achieve.
Maintenance and Operating Labor	There are higher operating labor costs in standard batch plants due to equipment cleaning and preparation time. These costs have been shown to be reduced for the so-called pipeless batch plants [4].	For the same process, operating labor will be lower for continuous processes.
Feedstock Availability	Batch operations are favored when feedstock availability is limited, for example, seasonally. Canneries and wineries are examples of batch processing facilities that often operate for only part of the year.	Continuous plants tend to be large and need to operate throughout the year to be profitable. The only way that seasonal variations in feeds can be accommodated is through the use of massive storage facilities that are very expensive.
Product Demand	Seasonal demand for products such as fertilizers, gas-line antifreeze, deicing chips for roads and pavements, and so on, can be easily accommodated. Because batch plants are flexible, other products can be made during the off-season.	It is difficult to make other products during the off-season. However, similar but different products—for example, a family of solvents—can be produced using the same processes through a series of campaigns at different times during the year. Each campaign may last several months.
Rate of Reaction to Produce Products	Batch operations favor processes that have very slow reaction rates and subsequently require long residence times. Examples include fermentation, aerobic and anaerobic wastewater treatment, and many other biological reactions.	Very slow reactions require very large equipment. The flow through this equipment will be slow, and dispersion can be a problem if very high conversion is desired and plug flow is required.

Equipment Fouling	When there is significant equipment fouling, batch operations are favored because cleaning of equipment is always a standard operating procedure in a batch process and can be accommodated easily in the scheduling of the process.	Significant fouling in continuous operations is a serious problem and is difficult to handle. Operating identical units in parallel, one on-line and the other off-line for cleaning, can solve this problem. However, capital investment is higher, additional labor is required, and safety problems are more likely.
Safety	Generally, worker exposure to chemicals and operator error will be higher (per pound of product) than for continuous processes. Operator training in chemical exposure and equipment operation is critical.	Large chemical plants operating continuously have excellent safety records [6], and safety procedures are well established. Operator training is still of great importance, but many of the risks associated with operating equipment containing chemicals are eliminated.
Controllability	This problem arises because batch processes often use the same equipment for different unit operations and sometimes to produce different products. The efficient scheduling of equipment becomes very important. The control used for this scheduling is complicated [3].	Generally, continuous processes are easier to control. Also, more work and research have been done for these processes. For complicated and highly integrated (energy and/or raw materials) plants, the control becomes complex, and operational flexiblity is greatly reduced.

Finally, it is important to recognize the role of pilot plants in the development of processes. It has been long understood that what works well in the laboratory often does not work as well on the large scale. Of course, much of the important preliminary work associated with catalyst development and phase equilibrium is most efficiently and inexpensively completed in the laboratory. However, problems associated with trace quantities of unwanted side products, difficult material handling problems, and multiple reaction steps are not easily scaled up from laboratory-scale experiments. In such cases, specific unit operations or the entire process may be "piloted" to gain better insight into the proposed full-scale operation. Often, this pilot plant work is carried out in batch equipment in order to reduce the inventory of raw materials. Sometimes, the pilot plant serves the dual purpose of testing the process at an intermediate scale and producing enough material for customers and other interested parties to test. The role and importance of pilot plants are covered in detail by Lowenstein [5].

2.3. Step 2—The Input/Output Structure of the Process

Although all processes are different, there are common features of each. The purpose of this section is to investigate the input/output structure of the process. The inputs represent feed streams and the outputs are product streams, which may be desired or waste streams.

2.3.1. Process Concept Diagram

The first step in evaluating a process route is to construct a process concept diagram. Such a diagram uses the stoichiometry of the main reaction pathway to identify the feed and product chemicals. The first step to construct such a diagram is to identify the chemical reaction or reactions taking place within the process. The balanced chemical reaction(s) form the basis for the overall process concept diagram. Figure 2.1 shows this diagram for the toluene hydrodealkylation process discussed in Chapter 1. It should be noted that only chemicals taking place in the reaction are identified on this diagram. The steps used to create this diagram are as follows:

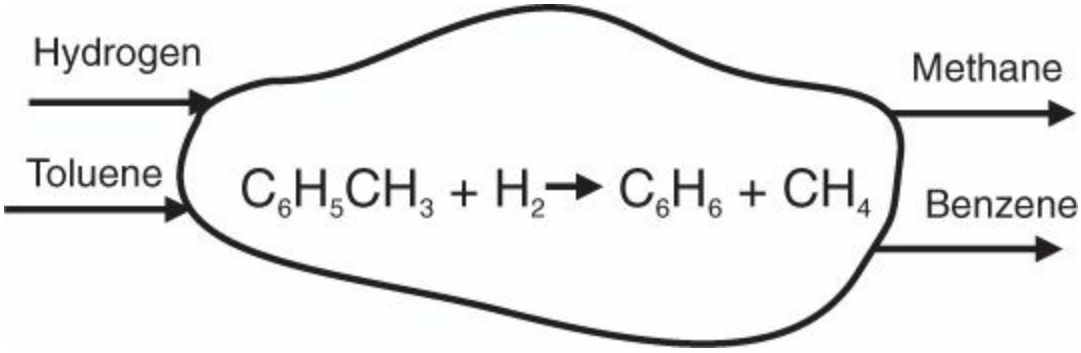


Figure 2.1. Input/Output Structure of the Process Concept Diagram for the Toluene Hydrodealkylation Process

1. A single "cloud" is drawn to represent the concept of the process. Within this cloud the stoichiometry for all reactions that take place in the process is written. The normal convention of the reactants on the left and products on the right is used.
2. The reactant chemicals are drawn as streams entering from the left. The number of streams corresponds to the number of reactants (two). Each stream is labeled with the name of the reactant (toluene and hydrogen).
3. Product chemicals are drawn as streams leaving to the right. The number of streams corresponds to the number of products (two). Each stream is labeled with the name of the product (benzene and methane).
4. Seldom does a single reaction occur, and unwanted side reactions must be considered. All reactions that take place and the reaction stoichiometry must be included. The unwanted products are treated as by-products and must leave along with the product streams shown on the right of the diagram.

2.3.2. The Input/Output Structure of the Process Flow Diagram

If the process concept diagram represents the most basic or rudimentary representation of a process, then the process flow diagram (PFD) represents the other extreme. However, the same input/output structure is seen in both diagrams. The PFD, by convention, shows the process feed stream(s) entering from the left and the process product stream(s) leaving to the right.

There are other auxiliary streams shown on the PFD, such as utility streams that are necessary for the process to operate but that are not part of the basic input/output structure. Ambiguities between process streams and utility streams may be eliminated by starting the process analysis with an overall input/output concept diagram.

Figure 2.2 shows the basic input/output structure for the PFD (see Figure 1.3). The input and output streams for the toluene HDA PFD are shown in bold. Both Figures 2.1 and 2.2 have the same overall input/output structure. The input streams labeled toluene and hydrogen shown on the left in Figure 2.1 appear in the streams on the left of the PFD in Figure 2.2. In Figure 2.2, these streams contain the reactant chemicals plus other chemicals that are present in the raw feed materials. These streams are identified as Streams 1 and 3, respectively. Likewise, the output streams, which contain benzene and methane, must appear on the right on the PFD. The benzene leaving the process, Stream 15, is clearly labeled, but there is no clear identification for the methane. However, by referring to Table 1.5 and looking at the entry for Stream 16, it can be seen that this stream contains a considerable amount of methane. From the stoichiometry of the reaction, the amount of methane and benzene produced in the process should be equal (on a mole basis). This is easily checked from the data for Streams 1, 3, 15,

and 16 (Table 1.5) as follows:

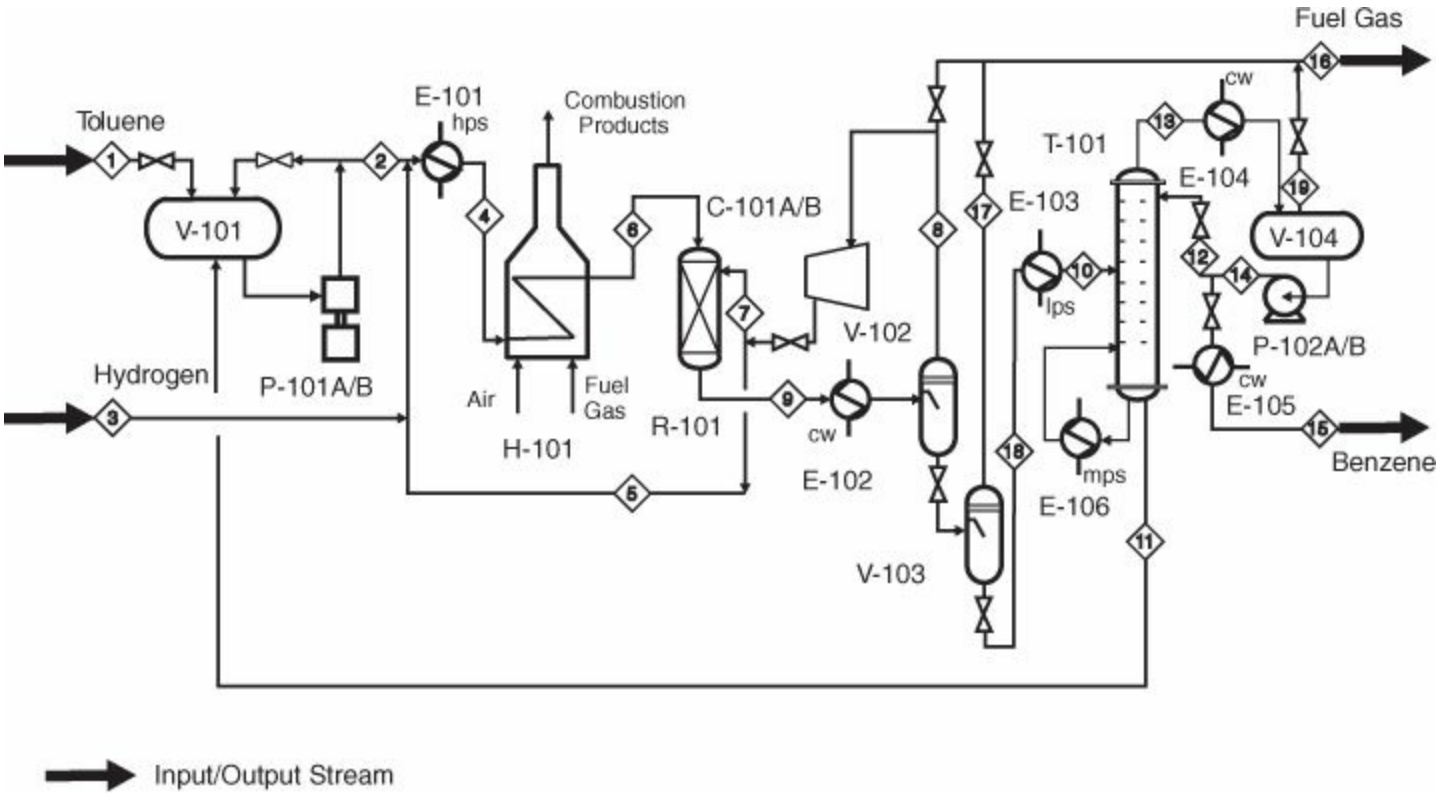


Figure 2.2. Input and Output Streams on Toluene Hydrodealkylation PFD

Benzene produced in process = Benzene leaving – Benzene entering
= 105.2 (Stream 15) + 2.85 (Stream 16) – 0
= 108.05 kmol/h

Amount of methane produced = Methane leaving – Methane entering
= 123.05 (Stream 16) – 15.0 (Stream 3)
= 108.05 kmol/h

At times, it will be necessary to use the process conditions or the flow table associated with the PFD to determine where a chemical is to be found.

There are several important factors to consider in analyzing the overall input/output structure of a PFD. Some of these factors are listed below.

1. Chemicals entering the PFD from the left that are not consumed in the chemical reactor are either required to operate a piece of equipment or are inert material that simply passes through the process. Examples of chemicals required but not consumed include catalyst makeup, solvent makeup, and inhibitors. In addition, feed materials that are not pure may contain inert chemicals. Alternatively, they may be added in order to control reaction rates, to keep the reactor feed outside of the explosive limits, or to act as a heat sink or heat source to control temperatures.
2. Any chemical leaving a process must either have entered in one of the feed streams or have been produced by a chemical reaction within the process.
3. Utility streams are treated differently from process streams. Utility streams, such as cooling water, steam, fuel, and electricity, rarely directly contact the process streams. They usually provide or remove thermal energy or work.

Figure 2.3 identifies, with bold lines, the utility streams in the benzene process. It can be seen that two streams—fuel gas and air—enter the fired heater. These are burned to provide heat to the process, but never come in direct contact (that is, mix) with the process streams. Other streams such

as cooling water and steam are also highlighted in Figure 2.3. All these streams are utility streams and are not extended to the left or right boundaries of the diagram, as were the process streams. Other utility streams are also provided but are not shown in the PFD. The most important of these is electrical power, which is most often used to run rotating equipment such as pumps and compressors. Other utilities, such as plant air, instrument air, nitrogen for blanketing of tanks, process water, and so on, are also consumed.

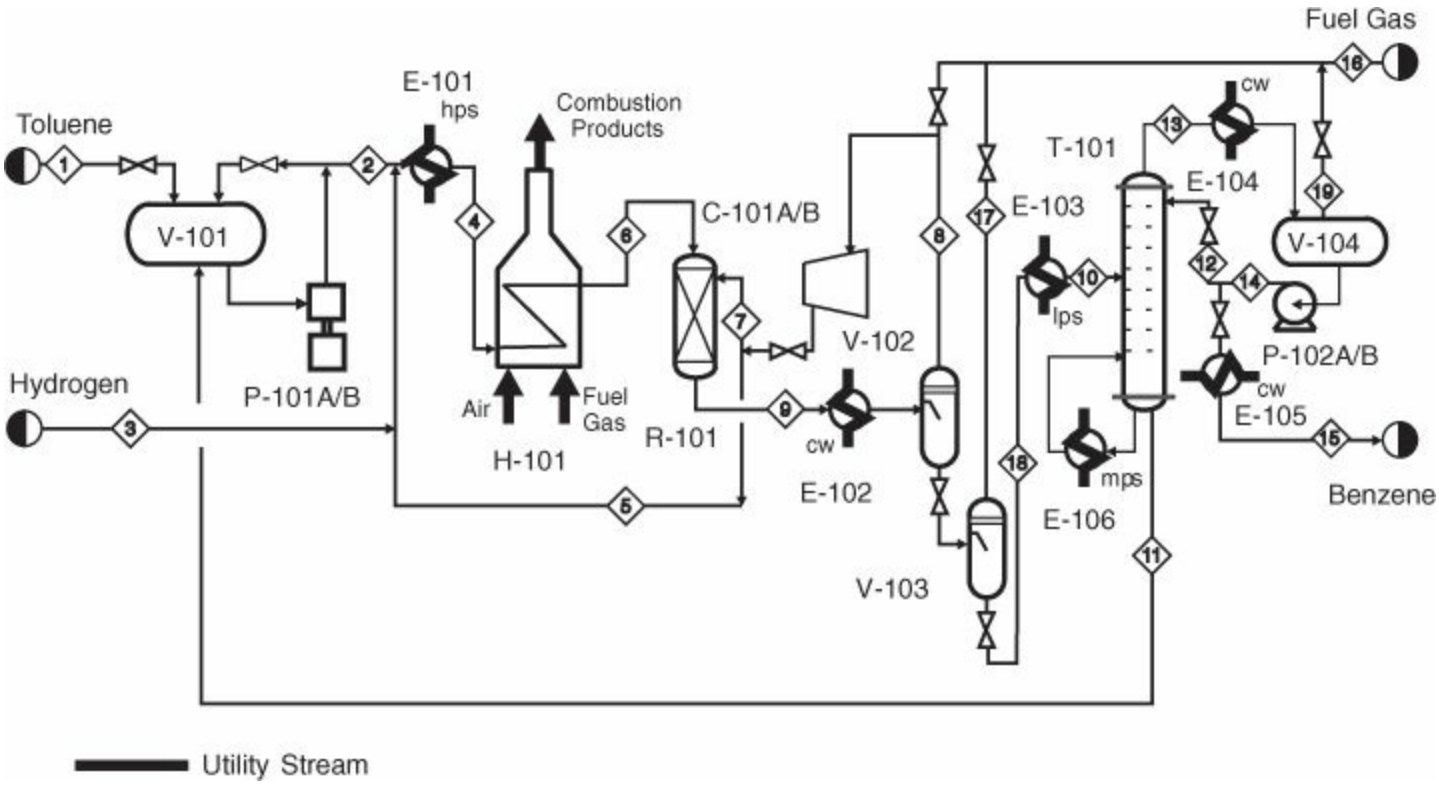


Figure 2.3. Identification of Utility Streams on the Toluene Hydrodealkylation PFD

2.3.3. The Input/Output Structure and Other Features of the Generic Block Flow Process Diagram

The **generic block flow diagram** is intermediate between the process concept diagram and the PFD. This diagram illustrates features, in addition to the basic input/output structure, that are common to all chemical processes. Moreover, in discussing the elements of new processes it is convenient to refer to this diagram because it contains the logical building blocks for all processes. Figure 2.4(a) provides a generic block flow process diagram that shows a chemical process broken down into six basic areas or blocks. Each block provides a function necessary for the operation of the process. These six blocks are as follows:

1. Reactor feed preparation
2. Reactor
3. Separator feed preparation
4. Separator

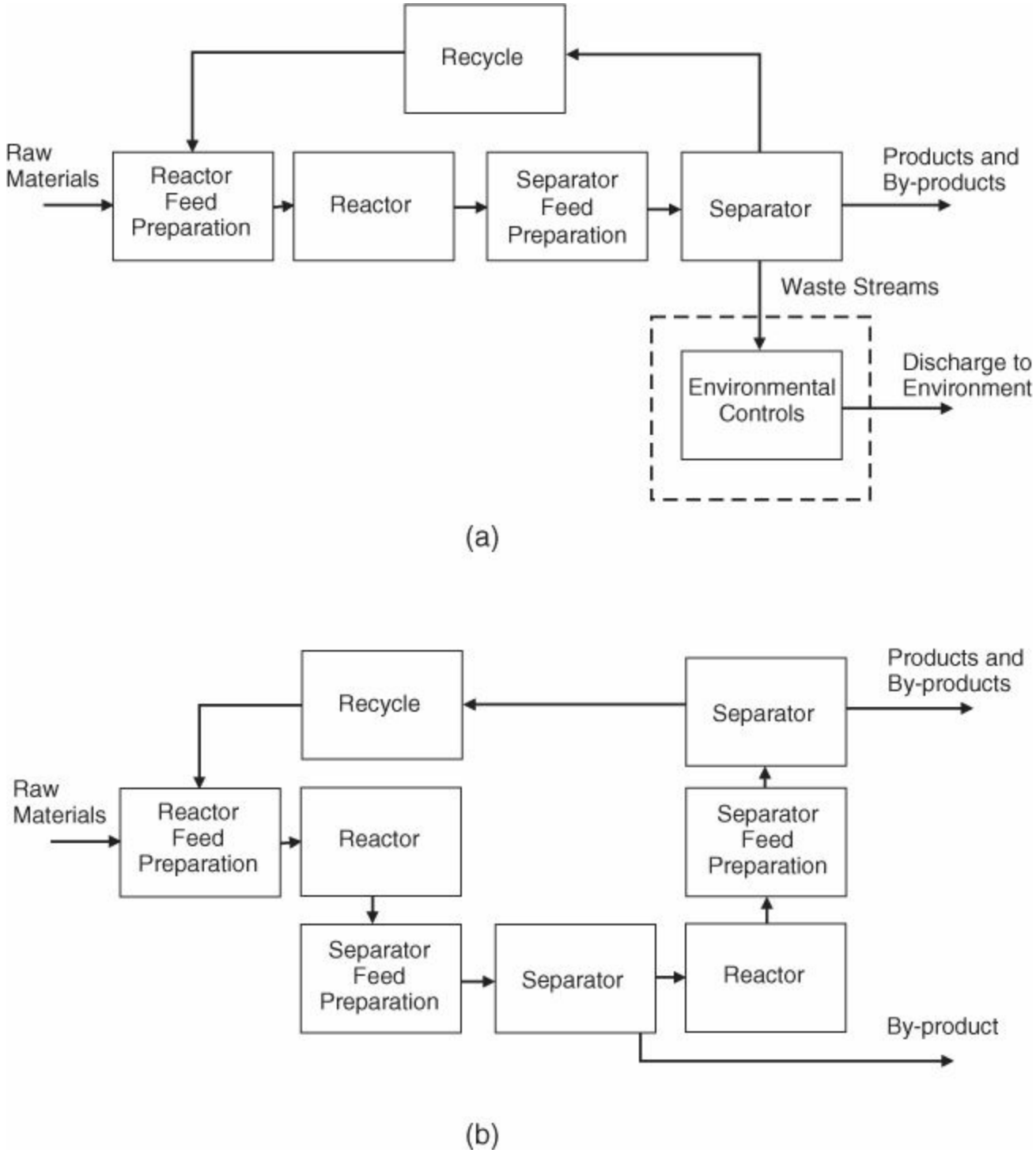


Figure 2.4. (a) The Six Elements of the Generic Block Flow Process Diagram; (b) A Process Requiring Multiple Process Blocks

5. Recycle
6. Environmental control

An explanation of the function of each block in Figure 2.4(a) is given below.

1. **Reactor Feed Preparation Block:** In most cases, the feed chemicals entering a process come from storage. These chemicals are most often not at a suitable concentration, temperature, and pressure for optimal performance in the reactor. The purpose of the reactor feed preparation section is to change the conditions of these process feed streams as required in the reactor.
2. **Reactor Block:** All chemical reactions take place in this block. The streams leaving this block contain the desired product(s), any unused reactants, and a variety of undesired by-products produced by competing reactions.

3. **Separator Feed Preparation Block:** The output stream from the reactor, in general, is not at a condition suitable for the effective separation of products, by-products, waste streams, and unused feed materials. The units contained in the separator feed preparation block alter the temperature and pressure of the reactor output stream to provide the conditions required for the effective separation of these chemicals.
4. **Separator Block:** The separation of products, by-products, waste streams, and unused feed materials is accomplished via a wide variety of physical processes. The most common of these techniques are typically taught in unit operations and/or separations classes—for example, distillation, absorption, and extraction.
5. **Recycle Block:** The recycle block represents the return of unreacted feed chemicals, separated from the reactor effluent, back to the reactor for further reaction. Because the feed chemicals are not free, it most often makes economic sense to separate the unreacted reactants and recycle them back to the reactor feed preparation block. Normally, the only equipment in this block is a pump or compressor and perhaps a heat exchanger.
6. **Environmental Control Block:** Virtually all chemical processes produce waste streams. These include gases, liquids, and solids that must be treated prior to being discharged into the atmosphere, sequestered in landfills, and so on. These waste streams may contain unreacted materials, chemicals produced by side reactions, fugitive emissions, and impurities coming in with the feed chemicals and the reaction products of these chemicals. Not all of the unwanted emissions come directly from the process streams. An example of an indirect source of pollution results when the energy needs of the plant are met by burning high sulfur oil. The products of this combustion include the pollutant sulfur dioxide, which must be removed before the gaseous combustion products can be vented to the atmosphere. The purpose of the environmental control block is to reduce significantly the waste emissions from a process and to render all nonproduct streams harmless to the environment.

It can be seen that a dashed line has been drawn around the block containing the environmental control operations. This identifies the unique role of environmental control operations in a chemical plant complex. A single environmental control unit may treat the waste from several processes. For example, the wastewater treatment facility for an oil refinery might treat the wastewater from as many as 20 separate processes. In addition, the refinery may contain a single stack and incinerator to deal with gaseous wastes from these processes. Often, this common environmental control equipment is not shown in the PFD for an individual process, but is shown on a separate PFD as part of the "off-site" section of the plant. Just because the environmental units do not appear on the PFD does not indicate that they do not exist or that they are unimportant.

Each of the process blocks may contain several unit operations. Moreover, several process blocks may be required in a given process. An example of multiple process blocks in a single process is shown in Figure 2.4(b). In this process, an intermediate product is produced in the first reactor and is subsequently separated and sent to storage. The remainder of the reaction mixture is sent to a second stage reactor in which product is formed. This product is subsequently separated and sent to storage, and unused reactant is also separated and recycled to the front end of the process. Based upon the reason for including the unit, each unit operation found on a PFD can be placed into one of these blocks. Although each process may not include all the blocks, all processes will have some of these blocks.

In Example 2.6, at the end of this chapter, different configurations will be investigated for a given process. It will be seen that these configurations are most conveniently represented using the building blocks of the generic block flow diagram.

2.3.4. Other Considerations for the Input/Output Structure of the Process Flowsheet

The effects of feed impurities and additional flows that are required to carry out specific unit operations may have a significant impact on the structure of the PFD. These issues are covered in the following section.

Feed Purity and Trace Components. In general, the feed streams entering a process do not contain pure chemicals. The option always exists to purify further the feed to the process. The question of whether this purification step should be performed can be answered only by a detailed economic analysis. However, some commonsense heuristics may be used to choose a good base case or starting point. The following heuristics are modified from Douglas [1]:

- If the impurities are not present in large quantities (say, <10%–20%) and these impurities do not react to form by-products, then *do not separate* them prior to feeding to the process. For example, the hydrogen fed to the toluene HDA process contains a small amount of methane (5 mol%—see Stream 3 in Table 1.5). Because the methane does not react (it is inert) and it is present as a small quantity, it is probably not worth considering separating it from the hydrogen.
- If the separation of the impurities is difficult (for example, an impurity forms an azeotrope with the feed or the feed is a gas at the feed conditions), then *do not separate* them prior to feeding to the process. For example, again consider the methane in Stream 3. The separation of methane and hydrogen is relatively expensive (see Example 2.3) because it involves low temperature and/or high pressure. This fact, coupled with the reasons given above, means that separation of the feed would not normally be attempted.
- If the impurities foul or poison the catalyst, then *purify the feed.* For example, one of the most common catalyst poisons is sulfur. This is especially true for catalysts containing Group VIII metals such as iron, cobalt, nickel, palladium, and platinum [7]. In the steam reformation of natural gas (methane) to produce hydrogen, the catalyst is rapidly poisoned by the small amounts of sulfur in the feed. A guard bed of activated carbon (or zinc oxide) is placed upstream of the reactor to reduce the sulfur level in the natural gas to the low ppm level.
- If the impurity reacts to form difficult-to-separate or hazardous products, then *purify the feed.* For example, in the manufacture of isocyanates for use in the production of polyurethanes, the most common synthesis path involves the reaction of phosgene with the appropriate amine [8]. Because phosgene is a highly toxic chemical, all phosgene is manufactured on-site via the reaction of chlorine and carbon monoxide.

$$CO + Cl_2 \rightarrow \underset{\text{phosgene}}{COCl_2}$$

If carbon monoxide is not readily available (by pipeline), then it must be manufactured via the steam reformation of natural gas. The following equation shows the overall main reaction (carbon dioxide may also be formed in the process, but it is not considered here):

$$CH_4 + H_2O \rightarrow CO + 3H_2$$

The question to ask is, At what purity must the carbon monoxide be fed to the phosgene unit? The

answer depends on what happens to the impurities in the CO. The main impurity is hydrogen. The hydrogen reacts with the chlorine to form hydrogen chloride, which is difficult to remove from the phosgene, is highly corrosive, and is detrimental to the isocyanate product. With this information, it makes more sense to remove the hydrogen to the desired level in the carbon monoxide stream rather than send it through with the CO and cause more separation problems in the phosgene unit and further downstream. Acceptable hydrogen levels in carbon monoxide feeds to phosgene units are less than 1%.

- If the impurity is present in large quantities, then *purify the feed.* This heuristic is fairly obvious because significant additional work and heating/cooling duties are required to process the large amount of impurity. Nevertheless, if the separation is difficult and the impurity acts as an inert, then separation may still not be warranted. An obvious example is the use of air, rather than pure oxygen, as a reactant. Because nitrogen often acts as an inert compound, the extra cost of purifying the air is not justified compared with the lesser expense of processing the nitrogen through the process. An added advantage of using air, as opposed to pure oxygen, is the heat-absorbing capacity of nitrogen, which helps moderate the temperature rise of many highly exothermic oxidation reactions.

Addition of Feeds Required to Stabilize Products or Enable Separations. Generally, product specifications are given as a series of characteristics that the product stream must meet or exceed. Clearly, the purity of the main chemical in the product is the major concern. However, other specifications such as color, density or specific gravity, turbidity, and so on, may also be specified. Often many of these specifications can be met in a single piece or train of separation equipment. However, if the product stream is, for example, reactive or unstable, then additional stabilizing chemicals may need to be added to the product before it goes to storage. These stabilizing chemicals are additional feed streams to the process. The same argument can be made for other chemicals such as solvent or catalyst that are effectively consumed in the process. If a solvent such as water or an organic chemical is required to make a separation take place—for example, absorption of a solvent-soluble chemical from a gas stream—then this solvent is an additional feed to the process (see Appendix B, Problem 5—the production of maleic anhydride via the partial oxidation of propylene). Accounting for these chemicals both in feed costs and in the overall material balance (in the product streams) is very important.

Inert Feed Material to Control Exothermic Reactions. In some cases, it may be necessary to add additional inert feed streams to the process in order to control the reactions taking place. Common examples of this are partial oxidation reactions of hydrocarbons. For example, consider the partial oxidation of propylene to give acrylic acid, an important chemical in the production of acrylic polymers. The feeds consist of nearly pure propylene, air, and steam. The basic reactions that take place are as follows:

$$C_3H_6 + \frac{3}{2}O_2 \rightarrow C_3H_4O_2 + H_2O \qquad \text{Reaction 1}$$

$$C_3H_6 + \frac{5}{2}O_2 \rightarrow C_2H_4O_2 + H_2O + CO_2 \qquad \text{Reaction 2}$$

$$C_3H_6 + \frac{9}{2}O_2 \rightarrow 3H_2O + 3CO_2 \qquad \text{Reaction 3}$$

All these reactions are highly exothermic, not limited by equilibrium, and potentially explosive. In order to eliminate or reduce the potential for explosion, steam is fed to the reactor to dilute the feed and provide thermal ballast to absorb the heat of reaction and make control easier. In some processes, enough steam (or other inert stream) is added to move the reaction mixture out of the flammability limits, thus eliminating the potential for explosion. The steam (or other inert stream) is considered a feed to the process, must be separated, and leaves as a product, by-product, or waste stream.

Addition of Inert Feed Material to Control Equilibrium Reactions. Sometimes it is necessary to add an inert material to shift the equilibrium of the desired reaction. Consider the production of styrene via the catalytic dehydrogenation of ethyl benzene:

$$\underset{\text{ethyl benzene}}{C_6H_5CH_2CH_3} \rightleftharpoons \underset{\text{styrene}}{C_6H_5CH=CH_2} + H_2$$

This reaction takes place at high temperature (600–750°C) and low pressure (<1 bar) and is limited by equilibrium. The ethyl benzene is co-fed to the reactor with superheated steam. The steam acts as an inert in the reaction and both provides the thermal energy required to preheat the ethyl benzene and dilutes the feed. As the steam-to-ethyl benzene ratio increases, the equilibrium shifts to the right (Le Chatelier's principle) and the single-pass conversion increases. The optimum steam-to-ethyl benzene feed ratio is based on the overall process economics.

2.3.5. What Information Can Be Determined Using the Input/Output Diagram for a Process?

The following basic information, obtained from the input/output diagram, is limited but nevertheless very important:

- Basic economic analysis on profit margin
- What chemical components must enter with the feed and leave as products
- All the reactions, both desired and undesired, that take place

The potential profitability of a proposed process can be evaluated and a decision whether to pursue the process can be made. As an example, consider the profit margin for the toluene HDA process given in Figure 2.1.

The profit margin will be formally introduced in Chapter 10, but it is defined as the difference between the value of the products and the cost of the raw materials. To keep things simple the stoichiometry of the reaction is used as the basis. If the profit margin is a negative number, then there is no potential to make money. The profit margin for the HDA process is given in Example 2.1.

Example 2.1.

Evaluate the profit margin for the HDA process.

From Tables 8.3 and 8.4, the following prices for raw materials and products are found:

Benzene = \$0.919/kg

Toluene = \$1.033/kg

Natural gas (methane and ethane, MW = 18) = \$11.10/GJ = \$11.89/1000 std. ft^3 = \$0.302/kg

Hydrogen = \$1.000/kg (based on the same equivalent energy cost as natural gas)

Using 1 kmol of toluene feed as a basis

Cost of Raw Materials

92 kg of Toluene = (92 kg)($1.033/kg) = $95.04

2 kg of Hydrogen = (2 kg)($1.000/kg) = $2.00

Value of Products

78 kg of Benzene = (78 kg)($0.919/kg) = $71.68

16 kg of Methane = (16 kg)($0.302/kg) = $4.83

Profit Margin

Profit Margin = (71.68 + 4.83) – (95.04 + 2.00) = –$20.53 or –$0.223/kg toluene

Based on this result, it is concluded that further investigation of this process is definitely not warranted.

Despite the results illustrated in Example 2.1, benzene has been produced for the last 50 years and is a viable starting material for a host of petrochemical products. Therefore, how is this possible? It must be concluded that benzene can be produced via at least one other route, which is less sensitive to changes in the price of toluene, benzene, and natural gas. One such commercial process is the disproportionation or transalkylation of toluene to produce benzene and a mixture of para-, ortho-, and meta-xylene by the following reaction:

$$\underset{\textit{toluene}}{2C_7H_8} \rightarrow \underset{\textit{benzene}}{C_6H_6} + \underset{\textit{xylene}}{C_8H_{10}}$$

The profit margin for this process is given in Example 2.2.

Example 2.2.

Evaluate the profit margin for the toluene disproportionation process.

From Table 8.4:

Mixed Xylenes = 0.820 $/kg

Using 2 kmols of toluene feed as a basis

Cost of Raw Materials

184 kg of Toluene = (184 kg)($1.033/kg) = $190.07

Value of Products

78 kg of Benzene = (78 kg)($0.919/kg) = $71.68

106 kg of Xylene = (106 kg)($0.820/kg) = $86.92

Margin

Profit Margin = 86.92 + 71.68 – 190.07 = –$31.47 or –$0.171/kg toluene feed

Based on the results of Example 2.2, the production of benzene via the disproportionation of toluene is better than the toluene HDA process but is still unprofitable. However, a closer look at the cost of purified xylenes (from Table 8.4) shows that these purified xylenes are considerably more valuable (ranging from $1.235 to $2.91/kg) than the mixed xylene stream ($0.820/kg). Therefore, the addition of a xylene purification section to the disproportionation process might well yield a potentially profitable process—namely, a process that is worth further, more-detailed analysis. Historically, the

prices of toluene and benzene fluctuate in phase with each other, but the toluene price ($1.033/kg) is currently elevated relative to that of benzene ($0.919/kg). In general, toluene disproportionation has been the preferred process for benzene production over the last two decades.

Examples 2.1 and 2.2 make it apparent that a better approach to evaluating the margin for a process would be to find cost data for the feed and product chemicals over a period of several years to get average values and then use these to evaluate the margin. Another important point to note is that there are often two or more different chemical paths to produce a given product. These paths may all be technically feasible; that is, catalysts for the reactions and separation processes to isolate and purify the products probably exist. However, it is the costs of the raw materials that usually play the major role when deciding which process to choose.

2.4. Step 3—The Recycle Structure of the Process

The remaining three steps in building the process flow diagram basically involve the recovery of materials and energy from the process. It may be instructive to break down the operating costs for a typical chemical process. This analysis for the toluene process is given in Chapter 8, Example 8.10. From the results of Example 8.10, it can be seen that raw material costs (toluene and hydrogen) account for (92.589)/(126.3) × 100 = 73% of the total manufacturing costs. This value is typical for chemical processes. Peters and Timmerhaus [9] suggest that raw materials make up between 10% and 50% of the total operating costs for processing plants; however, due to increasing conservation and waste minimization techniques this estimate may be low, and an upper limit of 75% is more realistic. Because these raw materials are so valuable, it is imperative that unused reactants are separated and recycled. Indeed, high efficiency for raw material usage is a requirement of the vast majority of chemical processes. This is why the generic block flow process diagram (Figure 2.4) has a recycle stream shown. However, the extent of recycling of unused reactants depends largely on the ease with which these unreacted raw materials can be separated (and purified) from the products that are formed within the reactor.

2.4.1. Efficiency of Raw Material Usage

It is important to understand the difference between single-pass conversion in the reactor, the overall conversion in the process, and the yield.

$$\text{Single-pass conversion} = \frac{\text{Reactant consumed in reaction}}{\text{Reactant fed to the reactor}} \tag{2.1}$$

$$\text{Overall conversion} = \frac{\text{Reactant consumed in process}}{\text{Reactant fed to the process}} \tag{2.2}$$

$$\text{Yield} = \frac{\text{Moles of reactant to produce desired product}}{\text{Moles of limiting reactant reacted}} \tag{2.3}$$

For the hydrodealkylation process introduced in Chapter 1, the following values are obtained for the most costly reactant (toluene) from Table 1.5:

$$\text{Single-pass conversion} = \frac{(144.0 - 36.0)}{144.0} = 0.75 \text{ or } 75\%$$

$$\text{Overall conversion} = \frac{(108.7 - 0.4 - 0.31)}{108.7} = 0.993 \text{ or } 99.3\%$$

$$\text{Yield} = \frac{(105.2 + 2.85)}{(108.7 - 0.4 - 0.31)} = 0.9995 \text{ or } 99.95\%$$

The single-pass conversion tells us how much of the toluene that enters the reactor is converted to benzene. The lower the single-pass conversion, the greater the recycle must be, assuming that the unreacted toluene can be separated and recycled. In terms of the overall economics of the process, the single-pass conversion will affect equipment size and utility flows, because both of these are directly affected by the amount of recycle. However, the raw material costs are not changed significantly, assuming that the unreacted toluene is separated and recycled.

The overall conversion tells us what fraction of the toluene in the feed to the process (Stream 1) is converted to products. For the hydrodealkylation process, it is seen that this fraction is high (99.3%). This high overall conversion is typical for chemical processes and shows that unreacted raw materials are not being lost from the process.

Finally the yield tells us what fraction of the reacted toluene ends up in our desired product: benzene. For this case, the yield is unity (within round-off error), and this is to be expected because no competing or side reactions were considered. In reality, there is at least one other significant reaction that can take place, and this may reduce the yield of toluene. This case is considered in Problem 2.1 at the end of the chapter. Nevertheless, yields for this process are generally very high. For example, Lummus [10] quotes yields from 98% to 99% for their DETOL, hydrodealkylation process.

By looking at the conversion of the other reactant, hydrogen, it can be seen from the figures in Table 1.5 that

$$\text{Single-pass conversion} = \frac{(735.4 - 652.6)}{735.4} = 0.113 \text{ or } 11.3\%$$

$$\text{Overall conversion} = \frac{(286.0 - 178.0)}{286.0} = 0.378 \text{ or } 37.8\%$$

Clearly these conversions are much lower than for toluene. The single-pass conversion is kept low because a high hydrogen-to-hydrocarbon ratio is desired everywhere in the reactor so as to avoid or reduce coking of the catalyst. However, the low overall conversion of hydrogen indicates poor raw material usage. Therefore, the questions to ask are, Why is the material usage for toluene so much better than that of hydrogen? and, How can the hydrogen usage be improved? These questions can be answered by looking at the ease of separation of hydrogen and toluene from their respective streams and leads us to investigate the *recycle structure* of the process.

2.4.2. Identification and Definition of the Recycle Structure of the Process

There are basically three ways that unreacted raw materials can be recycled in continuous processes.

1. Separate and purify unreacted feed material from products and then recycle.
2. Recycle feed and product together and use a purge stream.
3. Recycle feed and product together and do not use a purge stream.

Separate and Purify. Through the ingenuity of chemical engineers and chemists, technically feasible separation paths exist for mixtures of nearly all commercially desired chemicals. Therefore, the decision on whether to separate the unreacted raw materials must be made purely from economic considerations. In general, the ease with which a given separation can be made is dependent on two principles.

- First, for the separation process (unit operation) being considered, what conditions (temperature and pressure) are necessary to operate the process?
- Second, for the chemical species requiring separation, are the differences in physical or chemical properties for the species, on which the separation is based, large or small?

Examples that illustrate these principles are given below.

For the hydrodealkylation process, the reactor effluent, Stream 9, is cooled and separated in a two-stage flash operation. The liquid, Stream 18, contains essentially benzene and toluene. The combined vapor stream, Streams 8 and 17, contain essentially methane and hydrogen. In Example 2.3, methods to separate the hydrogen in these two streams are considered and are used to screen potential changes in the recycle structure of the HDA process.

Example 2.3.

For the separation of methane and hydrogen, first look at distillation:

Normal boiling point of methane = –161°C

Normal boiling point of hydrogen = –252°C

Separation should be easy using distillation due to the large difference in boiling points of the two components. However, in order to obtain a liquid phase, a combination of high pressure and low temperature must be used. This will be very costly and suggests that distillation is not the best operation for this separation.

Absorption

It might be possible to absorb or scrub the methane from Streams 8 and 17 into a hydrocarbon liquid. In order to determine which liquids, if any, are suitable for this process, the solubility parameters for both methane and hydrogen in the different liquids must be determined. This information is available in Walas [11]. Because of the low boiling point of methane, it would require a low temperature and high pressure for effective absorption.

Pressure-Swing Adsorption

The affinity of a molecule to adhere (either chemically or physically) to a solid material is the basis of adsorption. In pressure-swing adsorption, the preferential adsorption of one species from the gas phase occurs at a given pressure, and the desorption of the adsorbed species is facilitated by reducing the pressure and allowing the solid to "de-gas." Two (or more) beds operate in parallel, with one bed adsorbing and the other desorbing. The separation and purification of hydrogen contained in gaseous hydrocarbon streams could be carried out using pressure-swing adsorption. In this case, the methane would be preferentially adsorbed onto the surface of a sorbent, and the stream leaving the unit would contain a higher proportion of hydrogen than the feed. This separation could be applied to the HDA process.

Membrane Separation

Commercial membrane processes are available to purify hydrogen from hydrocarbon streams. This separation is facilitated because hydrogen passes more readily through certain membranes than does methane. This process occurs at moderate pressures, consistent with the operation of the HDA process. However, the hydrogen is recovered at a fairly low pressure and would have to be recompressed prior to recycling. This separation could be applied to the HDA process.

From Example 2.3, it can be seen that pressure-swing adsorption and membrane separation of the gas stream should be considered as viable process alternatives, but for the preliminary PFD for this process, no separation of hydrogen was attempted. In Example 2.4, the separation of toluene from a mixture of benzene and toluene is considered.

Example 2.4.

What process should be used in the separation of toluene and benzene?

Distillation

Normal boiling point of benzene = 79.8°C

Normal boiling point of toluene = 110°C

Separation should be easy using distillation, and neither excessive temperatures nor pressures will be needed. This is a viable operation for this separation of benzene and toluene in the HDA process.

Economic considerations often make distillation the separation method of choice. The separation of benzene and toluene is routinely practiced through distillation and is the preferred method in the preliminary PFD for this process.

Recycle Feed and Product Together with a Purge Stream. If separation of unreacted feed and products is not accomplished easily, then recycling both feed and product should be considered. In the HDA process, the methane product will act as an inert because it will not react with toluene. In addition, this process is not limited by equilibrium considerations; therefore, the reaction of methane and benzene to give toluene and hydrogen (the undesired path for this reaction), under the conditions used in this process, is not significant. It should be noted that for the case when a product is recycled with an unused reactant and the product does not react further, then a purge stream must be used to avoid the accumulation of product in the process. For the HDA process, the purge is the fuel gas containing the methane product and unused hydrogen, Stream 16, leaving the process. The recycle structure for the hydrogen and methane in the HDA process is illustrated in Figure 2.5.

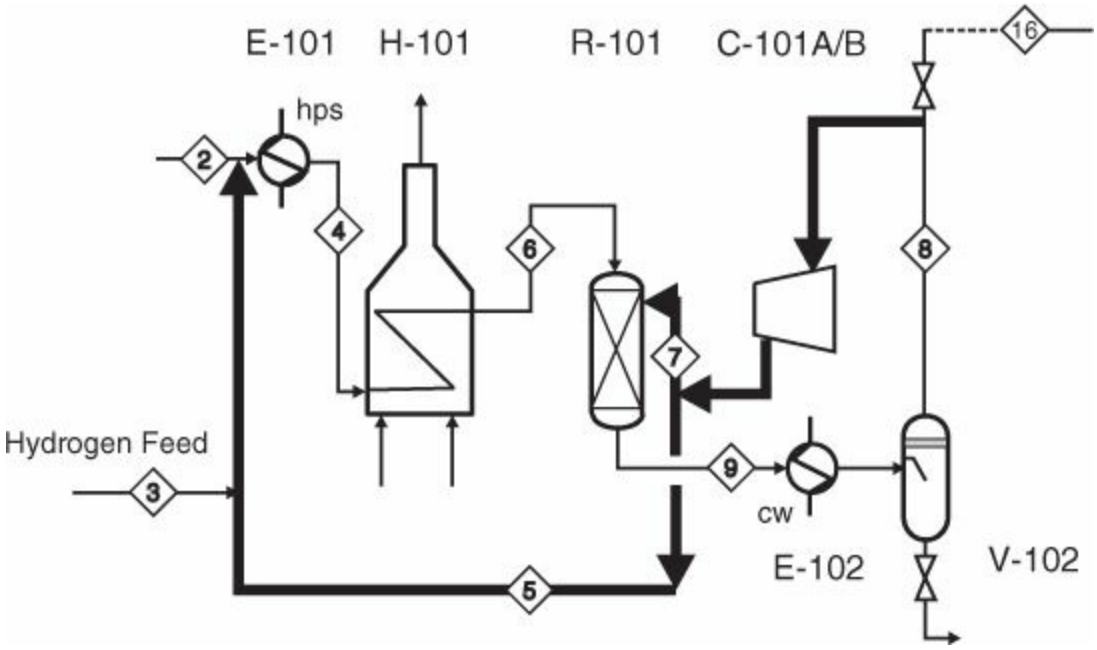


Figure 2.5. Recycle Structure of Hydrogen Stream in Toluene Hydrodealkylation Process. Methane Is Purged from the System via Stream 16.

Recycle Feed and Product Together without a Purge Stream. This recycle scheme is feasible only when the product can react further in the reactor and therefore there is no need to purge it from the process. If the product does not react and it does not leave the system with the other products, then it would accumulate in the process, and steady-state operations could not be achieved. In the previous case, with hydrogen and methane, it was seen that the methane did not react further and that it was necessary to purge some of the methane and hydrogen in Stream 16 in order to prevent accumulation of methane in the system.

An example where this strategy could be considered is again given in the toluene HDA process. Up to this point, only the main reaction between toluene and hydrogen has been considered:

$$\underset{\textit{toluene}}{C_7H_8} + H_2 \rightarrow \underset{\textit{benzene}}{C_6H_6} + CH_4$$

However, even when using a catalyst that is very specific to the production of benzene, some amount of side reaction will occur. For this process, the yield of toluene for commercial processes is on the order of 98% to 99%. Although this is high, it is still lower than the 100% that was originally assumed. A very small amount of toluene may react with the hydrogen to form small-molecule, saturated hydrocarbons, such as ethane, propane, and butane. More important, a proportion of the benzene reacts to give a two ring aromatic, diphenyl:

$$\underset{\textit{benzene}}{2C_6H_6} \rightleftharpoons \underset{\textit{diphenyl}}{C_{12}H_{10}} + H_2$$

The primary separation between the benzene and toluene in T-101 (see Figure 2.1) will remain essentially unchanged, because the light ends (hydrogen, methane, and trace amounts of $C_2 - C_4$ hydrocarbons) will leave in the flash separators (V-102 and V-103) or from the overhead reflux drum (V-104). However, the bottoms product from T-101 will now contain toluene and essentially all the diphenyl produced in the reactor, because it has a much higher boiling point than toluene. It is known that the benzene/diphenyl reaction is equilibrium limited at the conditions used in the reactor. Therefore, if the diphenyl is recycled with the toluene, it will simply build up in the recycle loop until it reaches its equilibrium value. At steady state, the amount of diphenyl entering the reactor in Stream

6 will equal the diphenyl in the reactor effluent, Stream 9. Because diphenyl reacts back to benzene, it can be recycled without purging it from the system. The changes to the structure of the process that would be required if diphenyl were produced are considered in Example 2.5.

Example 2.5.

Consider the following two process alternatives for the toluene HDA process when the side reaction of benzene to form diphenyl occurs.

Clearly for Alternative B, shown in Figure E2.5(b), an additional separator is required, shown here as a second distillation column T-102, along with the associated equipment (not shown) and extra utilities to carry out the separation. For Alternative A, shown in Figure E2.5(a), the cost of additional equipment is avoided, but the recycle stream (Stream 11) will be larger because it now contains toluene and diphenyl, and the utilities and equipment through which this stream passes (H-101, E-101, R-101, E-102, V-102, V-103, T-101, E-106) will all be greater. Which is the economically preferable alternative?

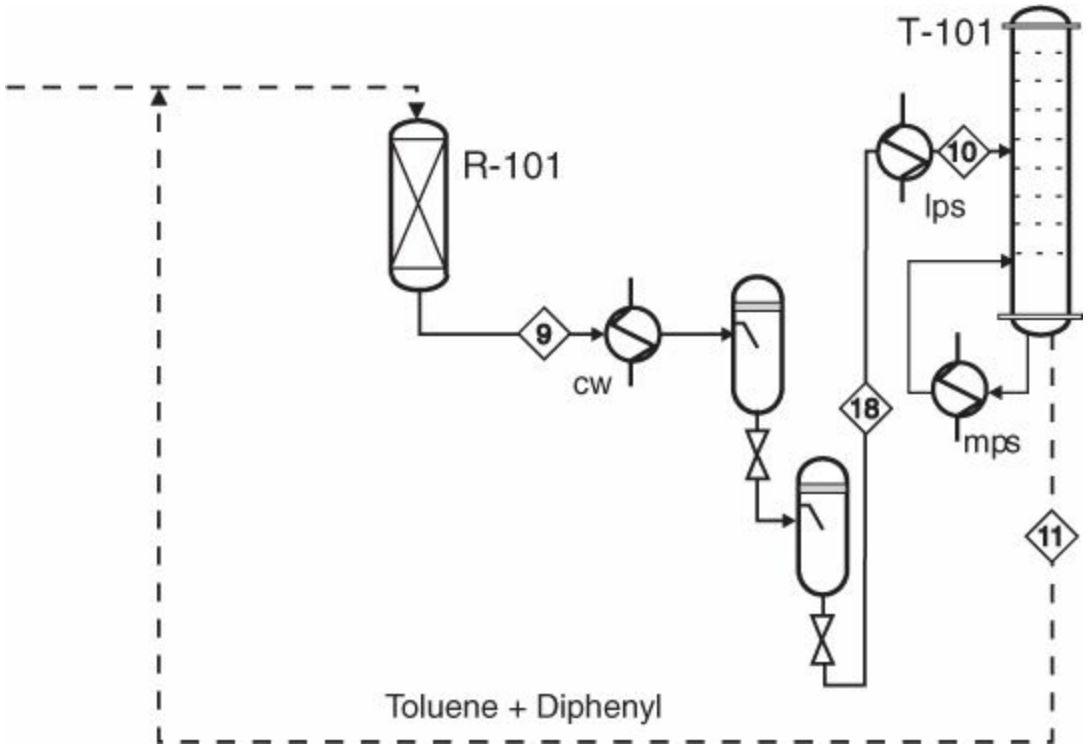


Figure E2.5(a). PFD for Alternative A in Example 2.5—Recycle of Diphenyl without Separation (E-101 and H-101 Not Shown)

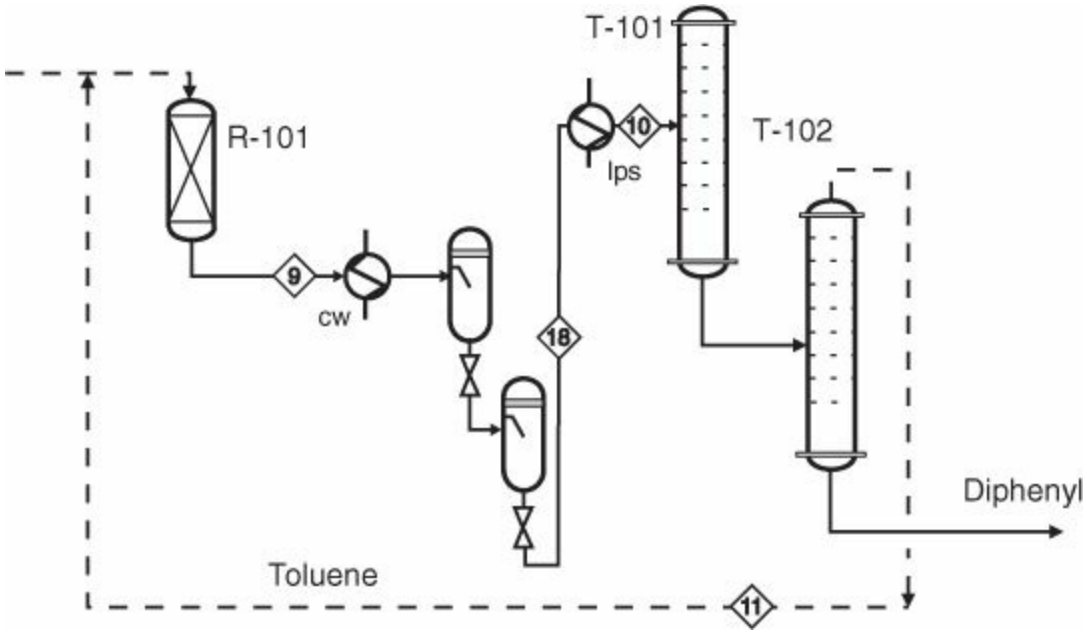


Figure E2.5(b). PFD for Alternative B in Example 2.5—Recycle of Diphenyl with Separation (E-101 and H-101 Not Shown)

The answer depends upon the value of the equilibrium constant for the benzene-diphenyl reaction. If the equilibrium conversion of benzene is high, then there will be a large amount of diphenyl in the recycle and the costs to recycle this material will be high, and vice versa. The equilibrium constant for this reaction is given as

$$\ln K_{eq} = 1.788 - \frac{4135.2}{T(K)}$$

The exit conditions of the reactor can be estimated by assuming that the benzene-diphenyl reaction has reached equilibrium, a conservative assumption. Using this assumption and data from Table 1.5 for Stream 9, if x kmol/h of diphenyl is present in the reactor effluent, then:

$$K_{eq} = \frac{[C_{10}H_{12}][H_2]}{[C_6H_6]^2} \Rightarrow \exp\left[1.788 - \frac{4135.2}{(654 + 273)}\right] = \frac{(x)(652.6 + x)}{(116 - 2x)^2}$$

Solving for the only unknown gives $x = 1.36$ kmol/h. Thus, the toluene recycle, Stream 11, will be increased from 35.7 to 37.06 kmol/h, an increase of 4%, while the increases in Streams 4 and 6 will be approximately 0.1%. Based on this result, Alternative A will probably be less expensive than Alternative B.

2.4.3. Other Issues Affecting the Recycle Structure That Lead to Process Alternatives

There are many other issues that affect the recycle structure of the PFD. The use of excess reactant, the recycling of inert materials, and the control of an equilibrium reaction are some examples that are addressed in this section.

How Many Potential Recycle Streams Are There? Consider first the reacting species that are of value. These are essentially all reactants except air and maybe water. Each reacting species that does not have a single-pass conversion > 99% should be considered as a potential recycle stream. The value of 99% is an arbitrarily high number, and it could be anywhere from 90% to > 99%, depending on the cost of raw materials, the cost to separate and recycle unused raw materials, and the cost of disposing of any waste streams containing these chemicals.

How Does Excess Reactant Affect the Recycle Structure? When designing the separation of recycled raw materials, it is important to remember which reactant, if any, should be in excess and how much this excess should be. For the toluene HDA process, the hydrogen is required to be in excess in order to suppress coking reactions that foul the catalyst. The result is that the hydrogen:toluene ratio at the inlet of the reactor (from Table 1.5) is 735.4:144, or slightly greater than 5:1. This means that the hydrogen recycle loop must be large, and a large recycle compressor is required. If it were not for the fact that this ratio needs to be high, the hydrogen recycle stream, and hence the recycle compressor, could be eliminated.

How Many Reactors Are Required? The reasons for multiple reactors are as follows:

- **Approach to Equilibrium:** The classic example is the synthesis of ammonia from hydrogen and nitrogen. As ammonia is produced in a packed-bed reactor, the heat of reaction heats the products and moves the reaction closer to equilibrium. By adding additional reactants between staged packed beds arranged in series, the concentration of the reactants is increased, and the temperature is decreased. Both these factors move the reaction away from equilibrium and allow the reaction to proceed further to produce the desired product, ammonia.
- **Temperature Control:** If the reaction is mildly exothermic or endothermic, then internal heat transfer may not be warranted, and temperature control for gas-phase reactions can be achieved by adding a "cold (or hot) shot" between staged adiabatic packed beds of catalyst. This is similar to the ammonia converter described earlier.
- **Concentration Control:** If one reactant tends to form by-products, then it may be advantageous to keep this reactant at a low concentration. Multiple side feeds to a series of staged beds or reactors may be considered. See Chapter 23 for more details.
- **Optimization of Conditions for Multiple Reactions:** When several series reactions (A→R→S→T) must take place to produce the desired product (T) and these reactions require different catalysts and/or different operating conditions, then operating a series of staged reactors at different conditions may be warranted.

Do Unreacted Raw Material Streams Need to Be Purified Prior to Recycling? The next issue is whether the components need to be separated prior to recycle. For example, if distillation is used to separate products from unused reactants, and if two of the reactants lie next to each other in a list of relative volatility, then no separation of these products is necessary. They can be simply recycled as a mixed stream.

Is Recycling of an Inert Warranted? The components in the feed streams that do not react, that is, are inert, are considered next. Depending on the process, it may be worth recycling these streams. For example, consider the water feed to the absorber, Stream 8, in the acetone production process (Appendix B, Figure B.10.1). This water stream is used to absorb trace amounts of isopropyl alcohol and acetone from the hydrogen vent, Stream 5. After purification, the water leaves the process as a wastewater stream, Stream 15. This water has been purified in column T-1103 and contains only trace amounts of organics. An alternative process configuration would be to recycle this water back to the absorber. This type of pollution prevention strategy is discussed further in Chapter 27.

Can Recycling an Unwanted Product or an Inert Shift the Reaction Equilibrium to Produce Less

of an Unwanted Product? Another example of recycling an inert or unwanted product is to use that material to change the conversion and selectivity of an equilibrium reaction. For example, consider the production of synthesis gas (H_2 and CO) via the partial oxidation (gasification) of coal:

$$C_mH_n + \left(\frac{m}{2} + \frac{n}{4}\right)O_2 \rightarrow mCO + \frac{n}{2}H_2O \quad \text{Partial oxidation}$$

$$C_mH_n + \left(m + \frac{n}{4}\right)O_2 \rightarrow mCO_2 + \frac{n}{2}H_2O \quad \text{Complete oxidation}$$

$$CO + H_2O \rightleftharpoons CO_2 + H_2 \quad \text{Water-gas shift}$$

Coal, shown here simply as a mixture of carbon and hydrogen, is reacted with a substoichiometric amount of pure oxygen in a gasifier, and steam is added to moderate the temperature. The resulting mixture of product gases forms the basis of the synthesis gas. The carbon dioxide is an unwanted by-product of the reaction and must be removed from the product stream, usually by a physical or chemiphysical absorption process. A viable process alternative is recycling a portion of the separated carbon dioxide stream back to the reactor. This has the effect of pushing the equilibrium of the water-gas shift reaction to the left, thus favoring the production of carbon monoxide.

Is Recycling of an Unwanted Product or an Inert Warranted for the Control of Reactor Operation? As mentioned previously, for highly exothermic reactions such as the partial oxidation of organic molecules, it is sometimes necessary to add an inert material to the reactor feed to moderate the temperature rise in the reactor and/or to move the reacting components outside of the explosive (flammability) limits. The most often used material for this purpose is steam, but any inert material that is available may be considered. For example, in the coal gasification example given earlier, steam is used to moderate the temperature rise in the reactor. For the case of recycling carbon dioxide to affect the water-gas shift reaction, there is another potential benefit. The recycling of carbon dioxide reduces the amount of steam needed in the feed to the reactor, because the carbon dioxide can absorb heat and reduce the temperature rise in the reactor.

What Phase Is the Recycle Stream? The phase of the stream to be recycled plays an important role in determining the separation and recycle structure of the process. For liquids, there are concerns about azeotropes that complicate the separations scheme. For gases, there are concerns about whether high pressures and/or low temperatures must be used to enable the desired separation to take place. In either case gas compression is required, and, generally, this is an expensive operation. For example, the use of membrane separators or pressure-swing adsorption requires that the gas be fed at an elevated pressure to these units. If separation of a gas (vapor) is to be achieved using distillation, then a portion of the gas must be condensed, which usually requires cooling the gas significantly below ambient temperatures. This cooling process generally requires the use of compressors in the refrigeration cycle; the lower the desired temperature, the more expensive the refrigeration. Some typical refrigerants and their range of temperature are given in Table 2.2. Because separations of gases require expensive, low-temperature refrigeration, they are avoided unless absolutely necessary.

Table 2.2. Common Refrigerants and Their Ranges of Cooling (Data from References [12] and [13])

Refrigerant	Typical Operating Temperature Range (°C)	Vapor Pressure at 45°C (bar)	Critical Pressure and Temperature (bar) and (°C)	
Methane	–129 to –184	749	46.0	–82.5
Ethane	–59 to –115	1453	48.8	32.3
Ethylene	–59 to –115	2164	50.3	9.3
Propane	4 to –46	15.3	42.5	96.7
Propylene	4 to –46	18.45	46.1	91.6
N-Butane	16 to –12	4.35	38.0	152.0
Ammonia	27 to –32	17.8	112.8	132.5
Carbon Dioxide	4 to –50	787	73.8	31.1
Methylene Chloride	4 to –12	1.21	60.8	236.9
Methyl Chloride	4 to –62	9.84	66.8	143.1
R-134a (1,1,1,2-tetrafluoro-ethane)	4 to –50	11.6	40.6	101.0
R-152a (1,1-difluoro-ethane)	4 to –50	10.4	45.0	113.5

Only refrigerants with critical temperatures above the typical cooling water condenser temperature of 45°C can be used in single-stage, noncascaded refrigeration systems. Therefore, such systems are usually limited to the range of –45 to –60°C (for example, propylene, propane, and methyl chloride). For lower temperatures, refrigeration systems with two different refrigerants are required, with the lower-temperature refrigerant rejecting heat to the higher-temperature refrigerant, which in turn rejects heat to the cooling water. Costs of refrigeration are given in Chapter 8, and these costs increase drastically as the temperature decreases. For this reason, separations of gases requiring very low temperatures are avoided unless absolutely necessary.

As a review of the concepts covered in this chapter, Example 2.6 is presented to illustrate the approach to formulating a preliminary process flow diagram.

Example 2.6.

Illustrative Example Showing the Input/Output and Recycle Structure Decisions Leading to the Generation of Flowsheet Alternatives for a Process

Consider the conversion of a mixed feed stream of methanol (88 mol%), ethanol (11 mol%), and water (1 mol%) via the following dehydration reactions:

$$2CH_3OH \rightleftharpoons (CH_3)_2O + H_2O \qquad \Delta H_{reac} = -11{,}770 \text{ kJ/kmol}$$

methanol *dimethyl ether (desired product)*

$$2C_2H_5OH \rightleftharpoons (C_2H_5)_2O + H_2O \qquad \Delta H_{reac} = -11{,}670 \text{ kJ/kmol}$$

ethanol *diethyl ether (valuable by-product)*

$$C_2H_5OH \rightarrow C_2H_4 + H_2O \qquad \Delta H_{reac} = -1570 \text{ kJ/kmol}$$

ethanol *ethylene (less valuable by-product)*

The reactions take place in the gas phase, over an alumina catalyst [14, 15], and are mildly exothermic but do not require additional diluents to control reaction temperature. The stream leaving the reactor (reactor effluent) contains the following components, listed in order of decreasing volatility (increasing boiling point):

1. Ethylene (C_2H_4)
2. Dimethyl Ether (DME)
3. Diethyl Ether (DEE)
4. Methanol (MeOH)
5. Ethanol (EtOH)
6. Water (H_2O)

Moreover, because these are all polar compounds, with varying degrees of hydrogen bonding, it is not surprising that these compounds are highly non-ideal and form a variety of azeotropes with each other. These azeotropes are as follows:

- DME – H_2O (but no azeotrope with significant presence of alcohol)
- DME – EtOH
- DEE – EtOH
- DEE – H_2O
- EtOH – H_2O

For this problem, it is assumed that the mixed alcohol stream is available at a relatively low price from a local source ($0.75/kg). However, pure methanol ($0.672/kg) and/or ethanol ($1.138/kg) streams may be purchased if necessary. The selling prices for DME, DEE, and ethylene are $0.841/kg, $1.75/kg, and $1.488/kg, respectively. Preliminary market surveys indicate that up to 15,000 tonne/y of DEE and up to 10,000 tonne/y of ethylene can be sold.

For a proposed process to produce 50,000 tonne/y of DME, determine the viable process alternatives.

Step 1: Batch versus Continuous

For a plant of this magnitude, a continuous process would probably be chosen. However, this issue will be reviewed after considering some process alternatives and it will be seen that a hybrid batch/continuous process should also be considered.

Step 2: Define the Input/Output Structure of the Process

The basic input/output diagram of the process is shown in the process concept diagram of Figure E2.6(a). First, consider a material balance for the process and estimate the profit margin:

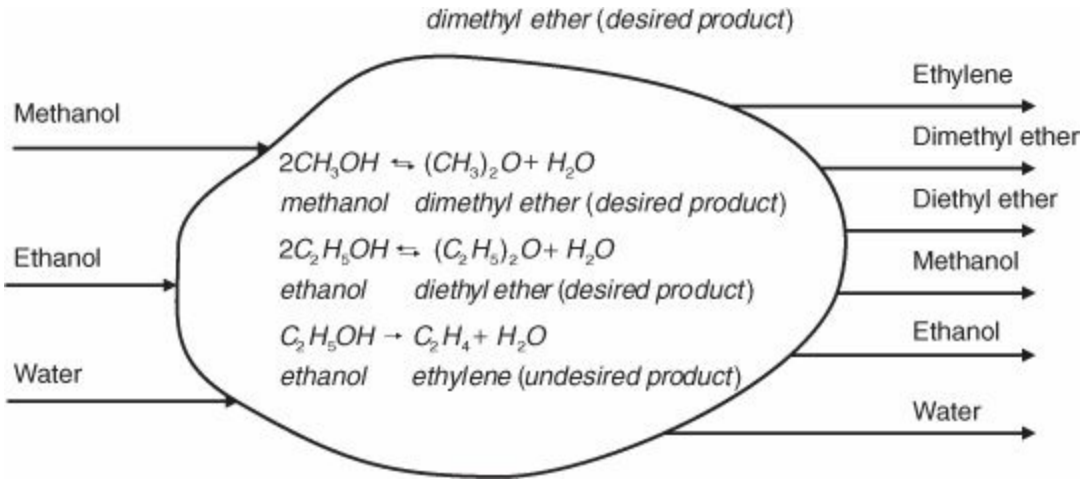


Figure E2.6(a). Process Concept Diagram for the Mixed Ethers Process of Example 2.6

$$\text{Desired DME production} = 50{,}000{,}000 \text{ kg/y} = \frac{50 \times 10^6}{46} = 1.087 \times 10^6 \text{ kmol/y}$$

$$\text{Required MeOH feed} = (2)(1.087 \times 10^6) = 2.174 \times 10^6 \text{ kmol/y}$$

$$\text{EtOH feed entering with methanol} = \frac{2.174 \times 10^6}{88}(11) = 0.2718 \times 10^6 \text{ kmol/y}$$

$$\text{Maximum DEE production} = \frac{0.2718 \times 10^6}{2} = 0.1309 \times 10^6 \text{ kmol/y or } 9.69 \times 10^3 \text{ tonne/y}$$

Maximum ethylene production = 0.2718×10^6 kmol/y or 7.61×10^3 tonne/y

$$\text{Cost of feed} = \left((2.174 \times 10^6)(30) + (0.2718 \times 10^6)(46) + \frac{(2.174 \times 10^6)}{88}(18)\right)(0.75) = \$58.62 \times 10^6$$

Value of DME = $(50 \times 10^6)(0.841) = \$42.05 \times 10^6$/y

Value of DEE (maximum production) = $(0.1309 \times 10^6)(74)(1.75) = \$16.95 \times 10^6$/y

Value of ethylene (maximum production) = $(0.2718 \times 10^6)(28)(1.488) = \$11.32 \times 10^6$/y

Margin will vary between (42.05 + 16.95 – 58.62) = \$0.38 million and (42.05 + 11.32 – 58.62) = –\$5.24 million per year.

Important Points

From this margin analysis, it is clear that the amount of DEE produced should be optimized, because making ethylene is far less profitable. In addition, the maximum amount of DEE that the market can support is not currently being produced. Therefore, supplementing the feed with ethanol should be considered.

Because the main feed stream contains both reactants and an impurity (water), separation or purification of the feed prior to processing should be considered.

In order to minimize the production of by-products (ethylene), the selectivity of the DEE reaction should be optimized.

Alternative 1

In this option, shown in Figure E2.6(b), the mixed alcohol feed is not separated, but feed is supplemented with ethanol. One reactor is used for both reactions. The disadvantages of this case are that the separations are complicated and the reactor for both DME and DEE production cannot be optimized easily.

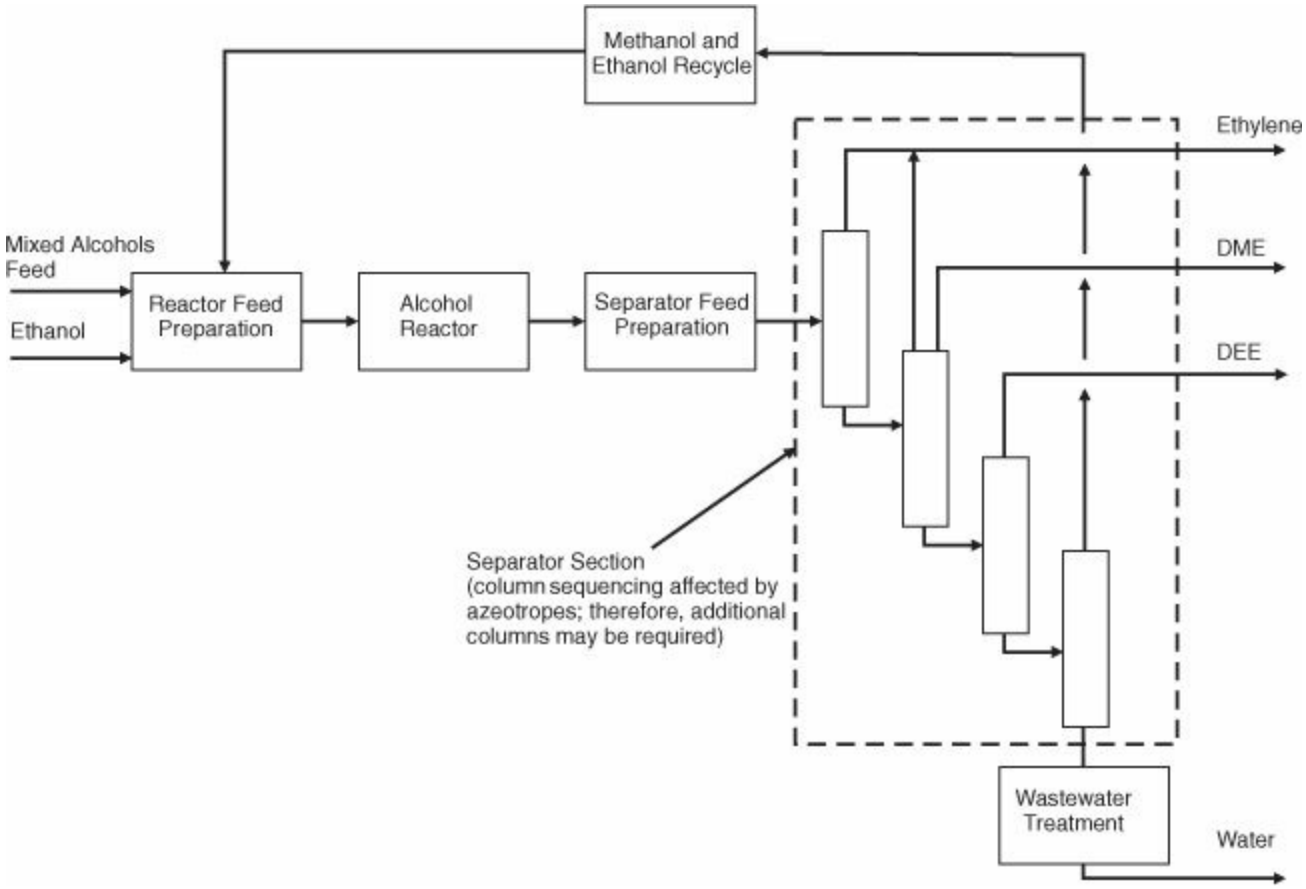


Figure E2.6(b). Structure of Process for Alternative 1 in Example 2.6

Alternative 2

In this option, shown in Figure E2.6(c), feed is supplemented with ethanol and is separated into separate methanol and ethanol streams. Two reaction trains are used: one for DME and the other for DEE production. This allows the production of DME and DEE to be optimized separately and eliminates problems associated with the DME-ethanol azeotrope. However, there are two reactors and at least one more separation (column).

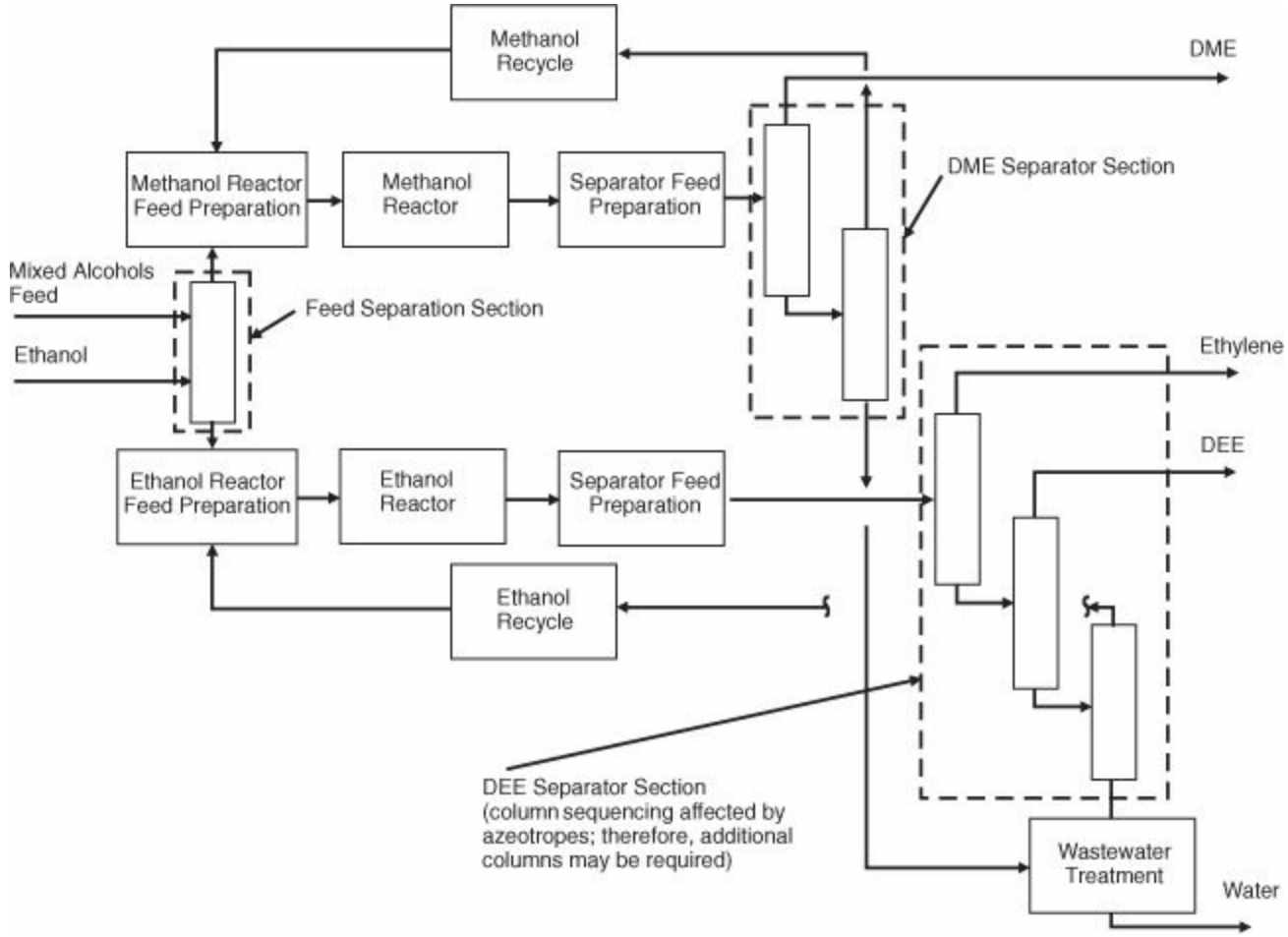


Figure E2.6(c). Structure of Process for Alternative 2 in Example 2.6

Alternative 3

This option is a hybrid between batch and continuous processes. The methanol is continuously separated from ethanol in the first column. However, the same equipment is used to produce both DME and DEE but at different times. The equipment is run in two "campaigns" per year. In the first campaign (Figure E2.6[d]), DME is produced and ethanol is stored for use in the second campaign.

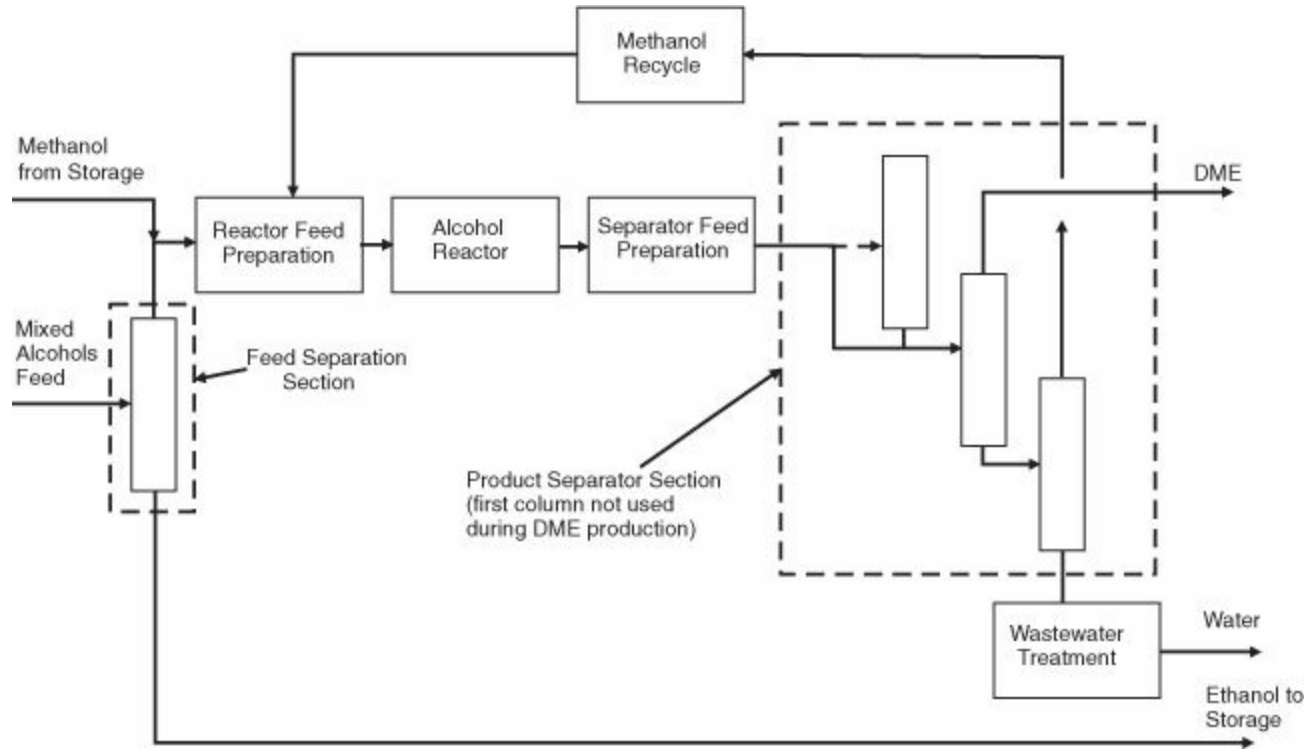


Figure E2.6(d). Structure of Process for Alternative 3—DME Campaign in Example 2.6

In the second campaign, shown in Figure E2.6(e), methanol is sent to storage, and ethanol is taken from storage to produce DEE and ethylene using the same equipment as was used to produce DME. For this part of the campaign, the first column is used to remove the ethylene.

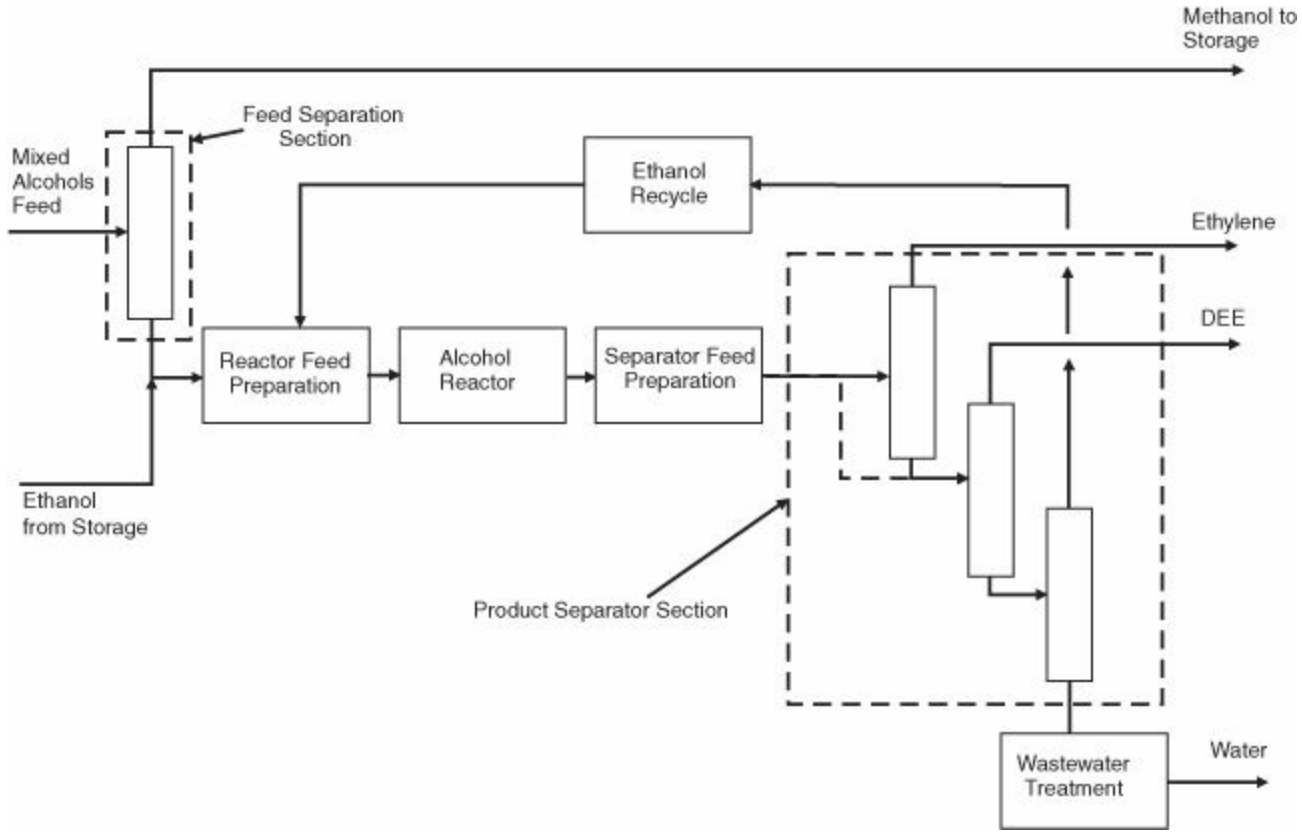


Figure E2.6(e). Structure of Process for Alternative 3—DEE Campaign in Example 2.6

For this option, there is significantly less equipment to buy. However, the design and optimization of the process are more complicated because the equipment must be designed to perform two separate and quite different functions.

2.5. Step 4—General Structure of the Separation System

As pointed out previously, the structure of the separation sequence is covered in detail in Chapter 12. In that chapter, considerable emphasis is placed on the sequencing of distillation columns, and some of the problems associated with azeotropic systems are covered.

2.6. Step 5—Heat-Exchanger Network or Process Energy Recovery System

The main objective of process energy recovery is to optimize the energy that a process exchanges with the utilities. At the expense of capital investment, the utility usage can be decreased by exchanging energy between process streams. The amount of energy integration is a function of the relative costs of the utilities. In addition, the process becomes more complex and more difficult to control. This loss in flexibility must be weighed against the savings in operating costs. These and other issues are covered in more detail in Chapter 15.

2.7. Information Required and Sources

In formulating a process flow diagram, one of the most important tasks is the collection and synthesis of data. These data are available in a wide variety of publications. As a guide, a summary of useful resources is presented in Table 2.3. The data in this table are partitioned into information pertaining

to new and existing processes and data on new and existing chemical pathways.

Table 2.3. Summary of Resources for Obtaining Information on Chemical Processes

Resource	Information Available
	Existing Processes
Shreve's Chemical Process Industries [16]	Gives a good review of basic processes to produce a wide variety of chemicals. Both organic and inorganic chemicals are covered.
Refinery Processes Handbook [17]	Published every other year in *Hydrocarbon Processing*. Gives basic block flow diagrams and operating cost and capital investment data for a wide range of refinery operations.
Gas Processes Handbook [18]	Published every other year in *Hydrocarbon Processing*. Gives basic block flow diagrams and operating cost and capital investment data for a wide range of gas processing operations.
Petrochemical Processes Handbook [19]	Published every other year in *Hydrocarbon Processing*. Gives basic block flow diagrams and operating cost and capital investment data for a wide range of gas petrochemical operations.
Kirk-Othmer Encyclopedia of Chemical Technology [20]	Comprehensive 25-volume encyclopedia has background information and PFDs for a wide variety of organic and inorganic chemical processes.
Encyclopedia of Chemical Processing and Design [21]	Comprehensive 20-volume encyclopedia contains background information on a variety of chemical processes. Many solutions to previous AIChE student contest problems are published as case studies.
	Reactions and Kinetics
Chemical Reactor Design for Process Plants [22]	Vol. 2 has several excellent case studies for processes, includingreaction kinetics and reactor designs.
Industrial and Engineering Chemistry Research	This journal is published monthly by the American Chemical Society and contains numerous research articles containing information about processes and reaction kinetics.
Journal of Catalysis—Academic Press *Applied Catalysis*—Elsevier *Catalysis Today*—Elsevier	These (and other) journals concentrate on research conducted into the field of heterogeneous catalysis. Kinetic expressions and activity data are given for many processes of industrial importance.
Patents	The patent literature contains a wealth of information about new processes. Typically, single-pass conversions and catalyst activities are given. However, reaction kinetics are generally not provided and may not be derived easily from patent data. An excellent on-line patent search engine is at http://www.delphion.com.
SRI Reports	Excellent source of background information on all aspects of processes. Unfortunately, this information is available only to industrial clients of this service.

2.8. Summary

In this chapter, the development of a process flow diagram has been investigated. The first step in synthesizing a PFD was to establish and examine all possible chemical routes that form the desired product(s). The next step was to establish whether the process should operate in a batch or continuous manner. Guidelines to make this decision were presented in Table 2.1. The next step was to establish the input/output structure of the process. The process concept diagram was introduced that only required the identification of the raw materials, products, and stoichiometry of all the reactions that take place. At the process level, it was shown that all processes possess the same basic structure given in the generic block flow diagram.

The recycle structure of the PFD was introduced, and the three basic methods of recycle were discussed. Reasons and examples were provided to illustrate why inert material or products are sometimes recycled with unreacted raw materials. Difficulties in separating streams of products and reactants were given, and these were shown to influence the recycle structure and type of separation used.

The separation of products and unreacted raw materials and the integration of energy were covered briefly and are covered in greater depth in Chapters 12 and 15, respectively. An example showing how process alternatives are generated using the methods outlined in this chapter was provided, and several process alternatives were illustrated for this example using generic block flow diagrams. Finally, a list of resources was presented to help guide the reader to obtain basic data on chemical reactions and processes.

What You Should Have Learned

- The first choice is whether to use batch or continuous operation.
- Continuous chemical processes have a general structure:
  - Input-output
  - Recycle
  - Separation
- The input-output structure of a continuous chemical process consists of
  - Reactor feed preparation
  - Reactor
  - Separation feed preparation
  - Separation
  - Recycle
  - Environmental control

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Short Answer Questions

1. What are the five elements of the hierarchy of process design?

2. What are the three types of recycle structures possible in a chemical process? Explain when each is used.
3. Give three criteria for choosing a batch process as opposed to a continuous process.
4. When would one purposely add an inert material to a feed stream? Illustrate this strategy with an example, and explain the advantages (and disadvantages) of doing this.
5. In general, when would one purify a material prior to feeding it to a process unit? Give at least one example for each case you state.

Problems

6. In modern integrated gasification combined cycle (IGCC) coal-fed power plants, oxygen is produced via cryogenic separation of air and is fed to the IGCC plant along with coal. The separation of oxygen from air is expensive; what reason(s) can you give for doing this?
7. The production of ethylbenzene is described in Appendix B, Project B.2. From the PFD (Figure B.2.1) and accompanying stream table (Table B.2.1), determine the following:
   a. The single-pass conversion of benzene
   b. The single-pass conversion of ethylene
   c. Overall conversion of benzene
   d. Overall conversion of ethylene

   Suggest two strategies to increase the overall conversion of ethylene and discuss their merits.
8. Consider the following statement: "If a reactant (G) in a process is a gas at the feed conditions, subsequent separation from the reactor effluent is difficult, hence unused G cannot be recycled." Do you agree with this statement? Give your reasoning why you agree or disagree.
9. Most pharmaceutical products are manufactured using batch processes. Give at least three reasons why this is so.
10. The formation of styrene via the dehydrogenation of ethylbenzene is a highly endothermic reaction. In addition, ethylbenzene may decompose to benzene and toluene and also may react with hydrogen to form toluene and methane:

$$\underset{\text{ethylbenzene}}{C_6H_5C_2H_5} \overset{1}{\rightleftharpoons} \underset{\text{styrene}}{C_6H_5C_2H_3} + \underset{\text{hydrogen}}{H_2} \qquad \text{(B.2.1)}$$

$$\underset{\text{ethylbenzene}}{C_6H_5C_2H_5} \overset{3}{\rightarrow} \underset{\text{benzene}}{C_6H_6} + \underset{\text{ethylene}}{C_2H_4} \qquad \text{(B.2.2)}$$

$$\underset{\text{ethylbenzene}}{C_6H_5C_2H_5} + \underset{\text{hydrogen}}{H_2} \overset{4}{\rightarrow} \underset{\text{toluene}}{C_6H_6CH_3} + \underset{\text{methane}}{CH_4} \qquad \text{(B.2.3)}$$

This process is presented in Appendix B as Project B.3. From the information given in Appendix B, determine the following:

a. The single-pass conversion of ethylbenzene
b. The overall conversion of ethylbenzene
c. The yield of styrene

Suggest one strategy to increase the yield of styrene, and sketch any changes to the PFD that this strategy would require.

11. There are two technically viable routes to the production of a hydrocarbon solvent, *S*, starting with feed material *A*. Route 1 uses a disproportionation reaction, in which feed material *A* is converted to the desired solvent *S* and another solvent *R*, both of which are marketable products. Route 2 starts with the same chemical *A* but uses a hydrodealkylation reaction to produce the desired solvent. The reaction schemes for each process are shown below.

Route 1 $2A \rightarrow S + R$

Route 2 $A + H_2 \rightarrow S + CH_4$

Assuming that pure *A* is fed to the process, the solvents *S* and *R* are separable by simple distillation, and both are much less volatile than either methane or hydrogen, sketch PFDs for Routes 1 and 2. Which process do you think will be more profitable? Explain your reasoning and assumptions.

12. When considering the evolution of a process flowsheet, it was noted that there are three forms of recycle structure for unused reactants, given as a–c below. For each case, carefully explain under what conditions you would consider or implement each strategy.
    a. Separate, purify, and recycle.
    b. Recycle without separation and use a purge.
    c. Recycle without separation and do not use a purge.

13. Acetaldehyde is a colorless liquid with a pungent, fruity odor. It is primarily used as a chemical intermediate, principally for the production of acetic acid, pyridine and pyridine bases, peracetic acid, pentaeythritol, butylene glycol, and chloral. Acetaldehyde is a volatile and flammable liquid that is miscible in water, alcohol, ether, benzene, gasoline, and other common organic solvents. In this problem, the synthesis of acetaldehyde via the dehydrogenation of ethanol is to be considered. The following reactions occur during the dehydrogenation of ethanol:

$$CH_3CH_2OH \rightarrow \underset{\textit{acetaldehyde}}{CH_3CHO} + H_2 \quad (1)$$

$$2CH_3CH_2OH \rightarrow \underset{\textit{ethyl acetate}}{CH_3COOC_2H_5} + 2H_2 \quad (2)$$

$$2CH_3CH_2OH \rightarrow \underset{\textit{butanol}}{CH_3(CH_2)_3OH} + H_2O \quad (3)$$

$$CH_3CH_2OH + H_2O \rightarrow \underset{\textit{acetic acid}}{CH_3COOH} + 2H_2 \quad (4)$$

The single-pass conversion of ethanol is typically 60%. The yields for each reaction are approximately:

(1) Acetaldehyde 92%

(2) Ethyl acetate 4%

(3) Butanol 2%

(4) Acetic acid 2%

a. For this process, generate a process concept diagram showing all the input and output chemicals.

b. Develop two alternative preliminary process flow diagrams for this process.

14. Consider the following process in which liquid feed material *A* (normal BP of 110°C) is reacted with gaseous feed material *G* to produce main product *C* and by-products *R* and *S* via the

following reactions:

$$A + G \rightarrow C + S$$

$$G + C \rightarrow R$$

Both feeds enter the process at ambient temperature and pressure. Both reactions occur in the gas phase at moderate temperature and pressure (250°C and 10 bar). The normal boiling points of *G*, *S*, and *C* are less than –120°C. By-product *R* has a normal boiling point of 75°C and is highly soluble in water. Product *C* is very soluble in water but *G* and *S* are insoluble. The single-pass conversion through the reactor is low for feed *A*, and the ratio of *G* to *A* in the feed to the reactor should be maintained in excess of 4 to minimize the chance of other unwanted side reactions. Using this information, and assuming that both *A* and *G* are expensive, do the following:

a. Draw a preliminary process flow diagram identifying the main unit operations (reactors, compressors, pumps, heat exchangers, and separators), and identify the recycle structure of the process.

b. Justify the methods used to recycle *A* and *G*.

c. What unit operations do you suggest for your separators? Justify your choices.

d. How would your PFD change if the price of feed material *G* were very low?

15. How is Scotch whisky made?

The following descriptions of malt and grain whisky manufacturing are given here courtesy of the University of Edinburgh at http://www.dcs.ed.ac.uk/home/jhb/whisky/swa/chap3.html. For each of the two processes, sketch a process flow diagram.

There are two kinds of Scotch whisky: malt whisky, which is made by the pot still process, and grain whisky, which is made by the patent still (or Coffey still) process. Malt whisky is made from malted barley only, whereas grain whisky is made from malted barley together with unmalted barley and other cereals.

Malt Whisky

The pot still process by which malt whisky is made may be divided into four main stages: malting, mashing, fermentation, and distillation.

(1) Malting

The barley is first screened to remove any foreign matter and then soaked for two or three days in tanks of water known as steeps. After this it is spread out on a concrete floor known as the malting floor and allowed to germinate. Germination may take from 8 to 12 days depending on the season of the year, the quality of the barley used, and other factors. During germination the barley secretes the enzyme diastase, which makes the starch in the barley soluble, thus preparing it for conversion into sugar. Throughout this period the barley must be turned at regular intervals to control the temperature and rate of germination.

At the appropriate moment germination is stopped by drying the malted barley or green malt in the malt kiln. More usually nowadays malting is carried out in Saladin boxes or in drum maltings, in both of which the process is controlled mechanically. Instead of germinating on the distillery floor, the grain is contained in large rectangular boxes (Saladin) or in large cylindrical drums. Temperature is controlled by blowing air at selected temperatures upward through the germinating grain, which is turned mechanically. A recent development caused by the rapid expansion of the Scotch whisky industry is for distilleries to obtain their malt from

centralized maltings that supply a number of distilleries, thereby enabling the malting process to be carried out more economically.

(2) Mashing

The dried malt is ground in a mill, and the grist, as it is now called, is mixed with hot water in a large circular vessel called a mash tun. The soluble starch is thus converted into a sugary liquid known as wort. This is drawn off from the mash tun, and the solids remaining are removed for use as cattle feed.

(3) Fermentation

After cooling, the wort is passed into large vessels holding anything from 9000 to 45,000 liters of liquid, where it is fermented by the addition of yeast. The living yeast attacks the sugar in the wort and converts it into crude alcohol. Fermentation takes about 48 hours and produces a liquid known as wash, containing alcohol of low strength, some unfermentable matter, and certain by-products of fermentation.

(4) Distillation

Malt whisky is distilled twice in large copper pot stills. The liquid wash is heated to a point at which the alcohol becomes vapor. This rises up the still and is passed into the cooling plant, where it is condensed into liquid state. The cooling plant may take the form of a coiled copper tube or worm that is kept in continuously running cold water, or it may be another type of condenser.

The first distillation separates the alcohol from the fermented liquid and eliminates the residue of the yeast and unfermentable matter. This distillate, known as low wines, is then passed into another still, where it is distilled a second time. The first runnings from this second distillation are not considered potable, and it is only when the spirit reaches an acceptable standard that it is collected in the spirit receiver. Again, toward the end of the distillation, the spirit begins to fall off in strength and quality. It is then no longer collected as spirit but drawn off and kept, together with the first running, for redistillation with the next low wines.

Pot-still distillation is a batch process.

Grain Whisky

The patent still process by which grain whisky is made is continuous in operation and differs from the pot still process in four other ways.

a. The mash consists of a proportion of malted barley together with unmalted cereals.

b. Any unmalted cereals used are cooked under steam pressure in converters for about 3½ hours. During this time the mixture of grain and water is agitated by stirrers inside the cooker.

c. The starch cells in the grain burst, and when this liquid is transferred to the mash tun, with the malted barley, the diastase in the latter converts the starch into sugar.

d. The wort is collected at a specific gravity lower than in the case of the pot still process.

e. Distillation is carried out in a patent or Coffey still, and the spirit collected at a much higher strength.

Storage and aging of the whisky are also an important part of the overall process but need not be considered for this problem. Storage occurs in oak barrels that previously stored either sherry or

bourbon (or both, in the case of double-aged whisky). The length of storage in the barrel determines the vintage of the whisky. Unlike wine, the time after bottling does not count, and so a 15-year-old scotch that was bought in 1960 is today still a 15-year-old scotch.

Chapter 3. Batch Processing

What You Will Learn

- Batch processing is very different from continuous processing.
- The design equations are different—unsteady state.
- Scheduling of equipment is important.
- There are different types of scheduling patterns.

Some key reasons for choosing to manufacture a product using a batch process were discussed in Chapter 2. These include small production volume, seasonal variations in product demand, a need to document the production history of each batch, and so on. When designing a batch plant, there are many other factors an engineer must consider. The types of design calculations are very different for batch compared with continuous processes. Batch calculations involve transient balances, which are different from the steady-state design calculations taught in much of the traditional chemical engineering curriculum. Batch **sequencing**—the order and timing of the processing steps—is probably the most important factor to be considered. Determining the optimal batch sequence depends on a variety of factors. For example, will there be more than one product made using the same equipment? What is the optimal size of the equipment? How long must the equipment run to make each different product? What is the trade-off between economics and operability of the plant? In this chapter, these questions will be addressed, and an introduction to other problems that arise when considering the design and operation of batch processes will be provided.

3.1. Design Calculations for Batch Processes

Design calculations for batch processes are different from the steady-state design calculations taught in most unit operations classes. The batch nature of the process makes all design calculations unsteady state. This is best demonstrated by example; Example 3.1 illustrates the types of design calculations required for batch processing.

Example 3.1.

In the production of an API (active pharmaceutical ingredient), the following batch recipe is used.

Step 1: 500 kg of reactant A (MW = 100 kg/kmol) is added to 5000 kg of a mixture of organic solvent (MW = 200 kg/kmol) containing 60% excess of a second reactant B (MW = 125 kg/kmol) in a jacketed reaction vessel (R-301), the reactor is sealed, and the mixture is stirred and heated (using steam in the jacket) until the temperature has risen to 95°C. The density of the reacting mixture is 875 kg/m^3 (time taken = 1.5 h).

Step 2: Once the reaction mixture has reached 95°C, a solid catalyst is added, and reaction takes place while the batch of reactants is stirred. The required conversion is 94% (time taken = 2.0 h).

Step 3: The reaction mixture is drained from the reactor and passed through a filter screen (Sc-301) that removes the catalyst and stops any further reaction (time taken = 0.5 h).

Step 4: The reaction mixture (containing API, solvent, and unused reactants) is transferred to a

distillation column, T-301, where it is distilled under vacuum. Virtually all of the unused reactants and approximately 50% of the solvent are removed as overhead product (time taken = 3.5 h). The end point for the distillation is when the solution remaining in the still contains less than 1 mol% of reactant B. This ensures that the crystallized API, produced in Step 5, meets specification.

Step 5: The material remaining in the still is pumped to a crystallizer, CR-301, where the mixture is cooled under vacuum and approximately 60% of the API from Step 2 crystallizes out (time taken = 2.0 h).

Step 6: The API is filtered from the crystallizer and placed in a tray dryer, TD-301, where any entrapped solvent is removed (time taken = 4 h).

Step 7: The dried API is sealed and packaged in a packing machine, PK-301, and sent to a warehouse for shipment to the customer (time taken = 1.0 h).

Perform a preliminary design on the required equipment items for this batch process.

Solution

The equipment items will be designed in sequence.

Step 1: Reaction Vessel—Preheat

The reaction vessel, which is used to preheat the reactants and subsequently run the reaction, is designed first. For the batch size specified, the volume of the liquid in the tank, V, and the volume required for the reaction vessel, V_{tank}, are given by Equations (E3.1a) and (E3.1b), in which it is assumed that the vessel is approximately 60% full during operation.

$$V = \frac{5500\ [\text{kg}]}{875\ [\text{kg/m}^3]} = 6.286\ \text{m}^3 \qquad \text{(E3.1a)}$$

$$V_{required} = \frac{5500\ [\text{kg}]}{875\ [\text{kg/m}^3]}\frac{1}{0.6} = 10.48\ \text{m}^3 = 2768\ \text{gal} \qquad \text{(E3.1b)}$$

Because reactors of this sort come in standard sizes, a 3000 gal (V_{tank}) reactor is selected.

The heat transfer characteristics of this vessel are then checked. For a jacketed vessel, the unsteady-state design equation is

$$\rho V C_p \frac{dT}{dt} = UA(T_s - T) \qquad \text{(E3.1c)}$$

where ρ is the liquid density, C_p is the liquid heat capacity, T is the temperature of the liquid in the tank (95°C is the desired value in 1.5 h), U is the overall heat transfer coefficient from the jacket to the liquid in the tank, A is the heat transfer area of the jacket (cylinder surface), and T_s is the temperature of the condensing steam. (Normally, there is also a jacketed bottom to such a vessel, but this added heat transfer area is ignored in this example for simplification.) Integration of this equation yields

$$\ln\frac{(T_s - T_{final})}{(T_s - T_o)} = -\frac{UA\Delta t}{\rho V C_p} \qquad \text{(E3.1d)}$$

where T_o is the initial temperature in the tank (assumed to be 25°C). The following "typical" values are assumed for this design:

C_p = 2000 J/kg°C

T_s = 120°C (200 kPa Saturated Steam)

U = 300 W/m^2°C

Tank Height to Diameter Ratio = 3/1 (so $H = 3D$)

Assuming the tank to be cylindrical and ignoring the volume of the bottom elliptical head, the tank volume is $V_{tank} = \pi D^2 H/4 = 3\pi D^3/4$. Thus, the tank diameter, D, is 1.689 m. The height of fill is $H_{fill} = 4V/(\pi D^2) = 2.806$ m. The area for heat transfer is $A = \pi D \boldsymbol{H}_{fill} = 14.89$ m^2, because it was assumed there was negligible heat transfer to the vapor space. When these values are used in Equation (E3.1d), it is found that the time required for preheating the reactor, Δt, is 3288 s (55 min). Thus, the step time requirement of 1.5 h for this step is met. The additional time is required for filling, sealing, and inspecting the vessel prior to heating. It should be noted that there may be process issues that require a slower temperature ramp, which can be accomplished by controlling the steam pressure. Note also that it is assumed that the time requirement for cleaning the vessels in this example is included in the step times given in the problem statement.

Step 2: Reaction Vessel—Reaction

It is assumed that the reaction of one mole each of A and B to form one mole of the product is second order (first order in each reactant) and that the rate constant is 7.09 × 10^{-4} m^3/kmol s. The relationship for a batch reactor is

$$\frac{dC_A}{dt} = -kC_AC_B \qquad \text{(E3.1e)}$$

where A and B are the two reactants, and A is the limiting reactant. The standard analysis for conversion in a reactor yields

$$C_A = C_{Ao}(1 - X) \qquad \text{(E3.1f)}$$

$$C_B = C_{Ao}(\Theta - X) \qquad \text{(E3.1g)}$$

$$\frac{dX}{dt} = kC_{Ao}(1 - X)(\Theta - X) \qquad \text{(E3.1h)}$$

where C_{Ao} = (500 kg/100 kg/kmol)(875 kg/m^3)/5500 kg = 0.796 kmol/m^3. Because reactant B is present in 60% excess, $\Theta = 1.6$. The desired conversion, X_{final}, is 0.94. Integration of Equation (E3.1h) with an initial condition of zero conversion at time zero yields

$$\frac{1}{\Theta - 1}\left[ln\frac{\Theta - X_{final}}{1 - X_{final}}\right] = kC_{Ao}\Delta t \qquad \text{(E3.1i)}$$

When all of the values are inserted into Equation (E3.1i), the time (Δt) is found to be 7082 s, or 118 min, which is just less than the desired 2 h allotted for the reaction. For simplicity, the additional reaction time that occurs after the mixture leaves the reactor until the catalyst is removed from the reacting mixture has been ignored.

Step 3: Draining Reaction Vessel and Catalyst Filtration

This step will be modeled as a draining tank, which may significantly underestimate the actual required time for draining and filtering. In reality, experimental data on the filter medium and inclusion of the exit pipe frictional resistance would have to be included to determine the actual time

for a specific tank. Generally, the filter is the bottleneck in such a step. Here, a 2-in schedule-40 exit pipe, with a cross-sectional area of 0.00216 m^2, is assumed.

For a draining tank, the model is

$$\frac{dm}{dt} = \frac{d(\rho A_t H)}{dt} = -m = -\rho A_p v_p \qquad \text{(E3.1j)}$$

where ρ is the density of the liquid in the tank, A_t is the cross-sectional area of the tank, H is the height of liquid in the tank, A_p is the cross-sectional area of the exit pipe, and v_p is the velocity of liquid in the exit pipe, which, from Bernoulli's equation (turbulent flow), is $(2gH)^{1/2}$, where g is the gravitational acceleration. Therefore, Equation (E3.1j) becomes

$$\frac{dH}{dt} = -\frac{(2g)^{1/2} A_p}{A_t} H^{1/2} \qquad \text{(E3.1k)}$$

Integrating from $H = 2.806$ m at $t = 0$ to find the time when $H = 0$ yields

$$-2H^{0.5}\Big|_{2.806\ m}^{0} = \frac{2^{0.5}(9.81\ [\text{m/s}^2])^{0.5}(0.00216\ [\text{m}^2])}{\frac{\pi(1.689\ [\text{m}])^2}{4}}\Delta t \qquad \text{(E3.1l)}$$

which gives $\Delta t = 785$ s = 13 min, which is rounded up to 30 minutes for this step. Note that this time can be further reduced by pressurizing the vessel with an inert gas.

Step 4: Distillation of Reaction Products

A material balance on the reactor at the end of Step 2 yields the following:

Component, i	kmoles	x_i	MW	mass (kg)
Reactant A	= (1 – 0.94)(5.0) = 0.3	0.0106	100	30.0
Reactant B	= (1.6)(5) – (5.0 – 0.3) = 3.3	0.1166	125	412.5
Solvent S	20.0	0.7067	200	4000.0
Product P	= (0.94)(5.0) = 4.7	0.1661	225	1057.5
Total	**28.3**	**1.0000**		**5500.0**

Initially, the reaction mixture is heated to its boiling point of 115°C at the operating pressure. This is done by condensing steam in a heat exchanger located in the still of the column. The time to heat the mixture from 95°C (the temperature leaving the reactor, assuming no heat loss in the filter) to 115°C is given by Equation (E3.1d) with the following variable values:

$T_s = 120$°C

ρ= 875 kg/m^3

$C_p = 2000$ J/kg°C

$U = 420$ W/m^2°C

$A = 10$ m^2

Solving for the unknown time gives $t = 4215$ s = 70.3 min.

The distillation is performed using a still with three theoretical stages ($N = 3$), a boil-up rate, $V = 30$ kmol/h, and a reflux ratio, $R = 4.5$. The volatilities of each component relative to the product are given as follows:

$\alpha_{AP} = 3.375$

$\alpha_{BP} = 2.700$

$\alpha_{SP} = 1.350$

$\alpha_{PP} = 1.000$

The solution methodology involves a numerical integration using the method of Sundaram and Evans [1]. The overall material and component balances are given by

$$-\frac{dW}{dt} = D = \frac{V}{1+R}$$

or in finite difference form,

$$W^{(k+1)} = W^{(k)} - \left(\frac{V}{1+R}\right)\Delta t \qquad \text{(E3.1m)}$$

$$\frac{d(Wx_{W_i})}{dt} = x_{D_i}\frac{dW}{dt}$$

or in finite difference form,

$$x_{W_i}^{(k+1)} = x_{W_i}^{(k)} + (x_{D_i}^{(k)} - x_{W_i}^{(k)})\frac{W^{(k+1)} - W^{(k)}}{W^{(k)}} \qquad \text{(E3.1n)}$$

where W is the total moles in the still; x_{Di} and x_{Wi} are the mole fractions of component i, at any time t, in the overhead product and in the still, respectively; k is the index for time in the finite difference representation; and Δt is the time step. These equations are solved in conjunction with the sum of the gas-phase mole fraction equaling unity and the Fenske-Underwood-Gilliland method for multicomponent distillation. This leads to the following additional equations:

$$x_{D_r} = \frac{x_{W_r}}{\sum_{i=1}^{C} x_{W_i}\alpha_{1,C}^{N_{min}}} \text{ and } x_{D_i} = x_{W_i}\left(\frac{x_{D_i}}{x_{w_i}}\right)\alpha_{i,r}^{N_{min}} \qquad \text{(E3.1o)}$$

$$R_{min} = \frac{\alpha_{1,C}^{N_{min}} - \alpha_{1,C}}{(\alpha_{1,C}-1)\sum_{i=1}^{C} x_{w_i}\alpha_{1,C}^{N_{min}}} \text{ and } \frac{N - N_{min}}{N+1} = 0.75\left[1 - \left(\frac{R - R_{min}}{R+1}\right)^{0.5668}\right] \qquad \text{(E3.1p)}$$

where R_{min} and N_{min} are the minimum values for the reflux ratio and the number of theoretical stages, respectively. The solution of these equations is explained in detail by Seader and Henley [2], and the results for this example are shown in Figures E3.1(a) and E.3.1(b).

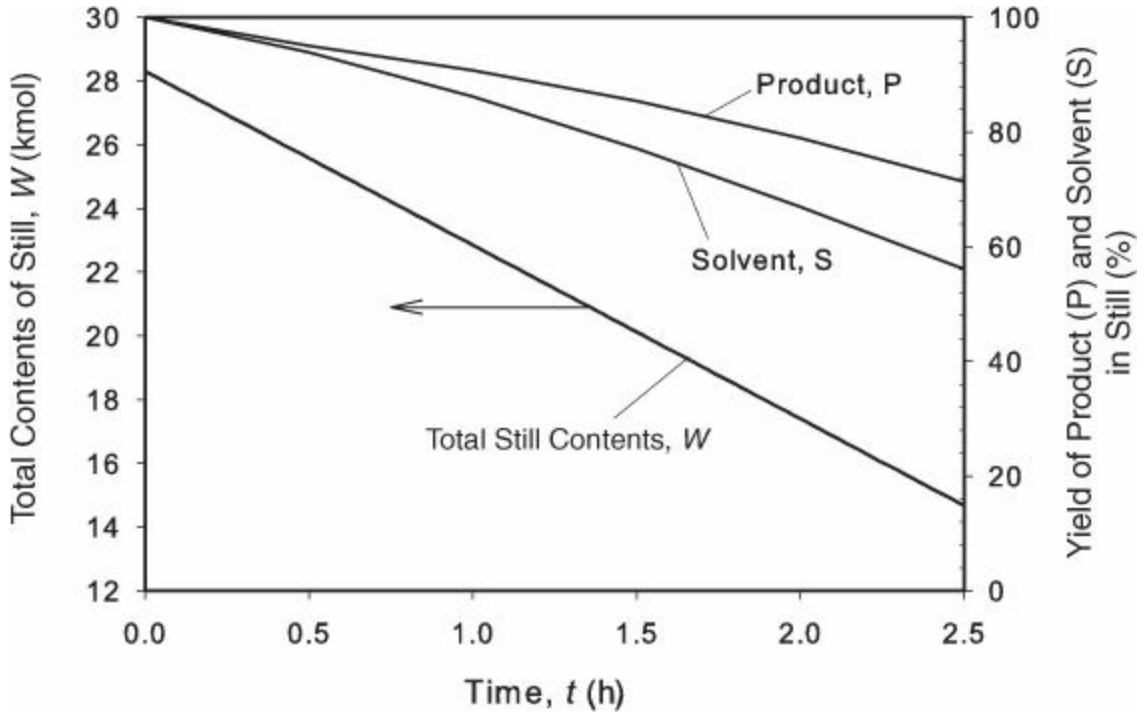


Figure E3.1(a). Change of Still Contents and Yields of P and S with Time

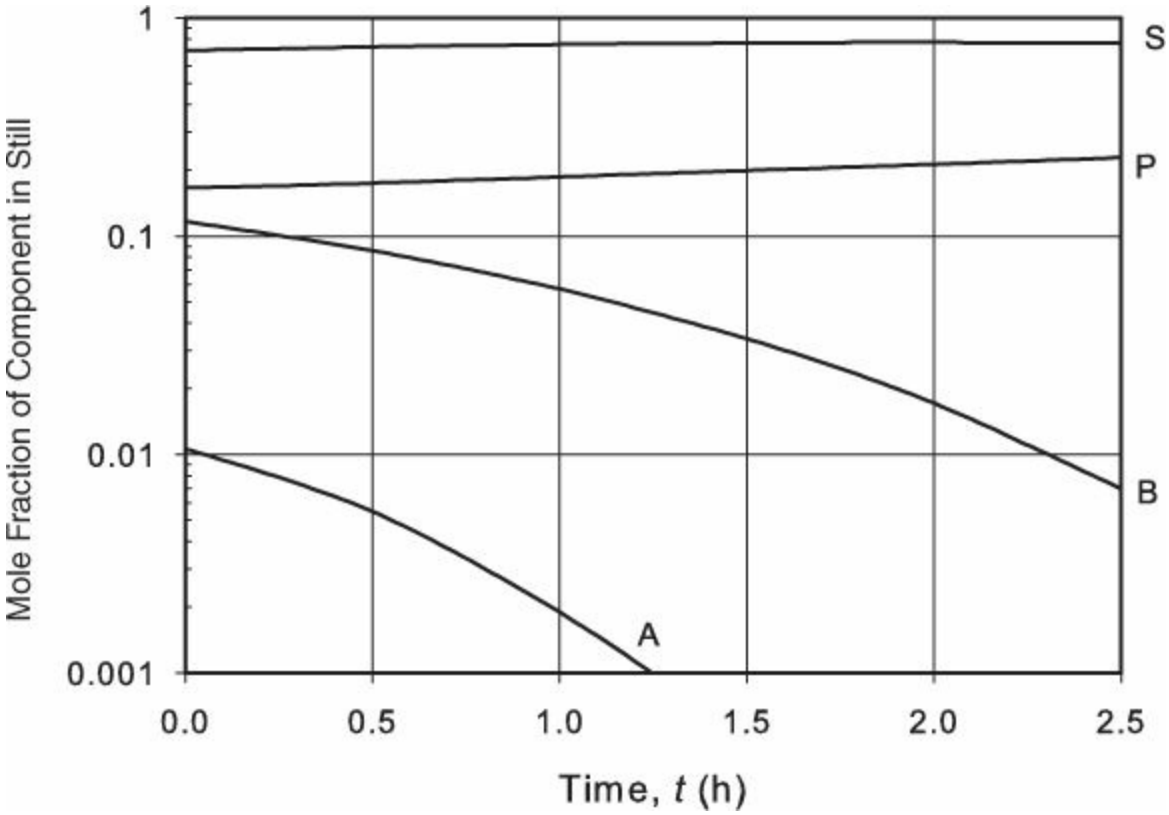


Figure E3.1(b). Change in Composition of Still Material with Time

From Figures E3.1(a) and (b), the mole fraction of reactant B is seen to drop to less than the specification of 0.01 (1 mol%) at a time of approximately 2.3 h. This time, coupled with the heating time of 70.2 min, gives a total of 3.5 h. However, note that only about 75% of the product remains in the still to be recovered in the next step.

Step 5: Cooling and Crystallization of Product

The analysis of the crystallization, filtration, drying, and packaging steps is beyond the scope of this analysis. Therefore, it is assumed that the times for each of these steps have been determined through laboratory-scale experiments, and those times are simply stated here. The amount of product

crystallized is 80% of the product recovered from the still, or 60% of the 1057.5 kg produced in the reactor (634.5 kg). The time required to cool and crystallize is 2 h.

Step 6: Filtration and Drying

The time required for filtration and drying is 4 h.

Step 7: Packaging

The time required for packaging is 1 h.

There are several unique features of batch operations observed in Example 3.1. First, the heating, reaction, and separations steps are unsteady state, which is different from the typical steady-state analysis with which most undergraduate chemical engineers are familiar. Secondly, it is observed that no provision was made to recycle the unreacted raw materials. In Chapter 2, recycle was shown to be a key element of a steady-state chemical process. Raw materials are almost always the largest item in the cost of manufacturing; therefore, recycling unreacted raw materials is essential to ensure profitability. So, how is this done in a batch process? In Example 3.1, the overhead product from the batch distillation contains unreacted raw material and product in the solvent. This could be sent to a holding tank and periodically mixed with a stream containing pure solvent and just enough reactants A and/or B to make up a single charge to the process in Step 1. However, the recycling of product to the reactor would have to be investigated carefully to determine whether unwanted side reactions take place at higher product concentrations. Even though an additional tank would need to be purchased, it is almost certain that the cost benefit of recycling the raw materials would far outweigh the cost of the additional tank. Third, it is observed that, overall, only 60% of the product made in the reactor is crystallized out in Step 5. This means that the **mother liquor** (solution containing product to be crystallized after some has crystallized out) contains significant amounts of valuable product. Additional crystallization steps could recover some, if not most, of the valuable product. The strategy for accomplishing this could be as simple as scheduling a second or third cooling or crystallization step, or it could involve storing the mother liquor from several batch processes until a sufficient volume is available for another cooling or crystallization step. These additional crystallization steps are tantamount to adding additional separation stages.

3.2. Gantt Charts and Scheduling

Gantt charts (see, for example, Dewar [3]) are tabular representations used to illustrate a series of tasks (rows) that occur over a period of time (columns). These charts graphically represent completion dates, milestone achievements, current progress, and so on [3] and are discussed further in Chapter 28 as a planning tool for completing large design projects. In this chapter, a simplified Gantt chart is used to represent the scheduling of equipment needed to produce a given batch product. Example 3.2 illustrates the use of Gantt charts to show the movement of material as it passes through several pieces of equipment during a batch operation.

Example 3.2.

Draw a Gantt chart that illustrates the sequence of events in the production of the API in Example 3.1.

Solution

Gantt charts for this process are shown in Figure E3.2. Note that in both charts, Steps 1 and 2 have

been consolidated into one operation because they occur sequentially in the same piece of equipment. The top chart shows the row names as tasks, and the bottom figure simply identifies each row with the equipment number. In general, the notation used in the bottom figure will be adopted.

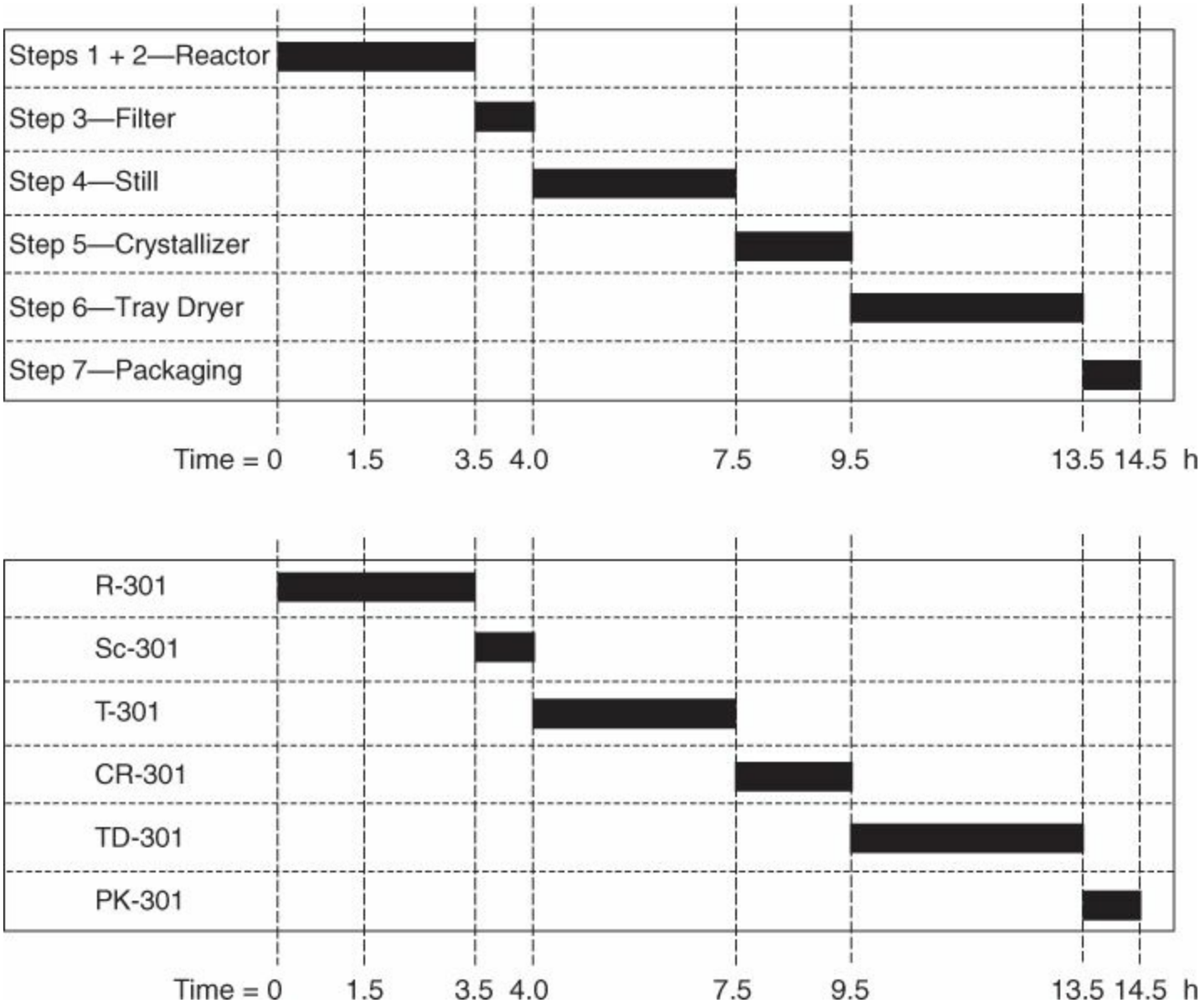


Figure E3.2. Gantt Chart Showing Sequence of Events for the Manufacture of API in Example 3.1

3.3. Nonoverlapping Operations, Overlapping Operations, and Cycle Times

In general, product is produced throughout an extended period of time by using a repeating sequence of operations. For example, the batch process described in Example 3.1 produces a certain amount of crystallized API, namely, 634.5 kg. If it is desired to produce 5000 kg, then the sequence of steps must be repeated 5000/634.5 ≅ 8 times. There are several ways to repeat the sequence of tasks needed to make one batch, in order to make the desired total amount of product (5000 kg). An example of one such **nonoverlapping** scheme is shown in Figure 3.1.

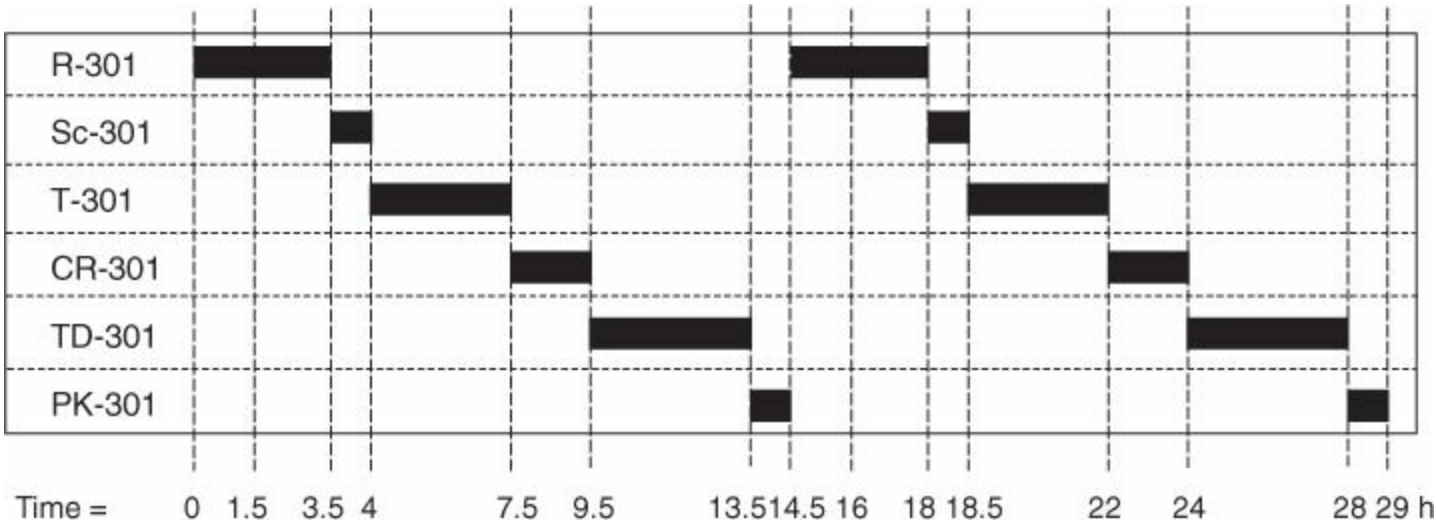


Figure 3.1. Example of a Nonoverlapping Sequence of Batch Operations

For the nonoverlapping (designated by the subscript *NO*) scheme, the total processing time is the number of batches multiplied by the time to process a single batch.

$$T_{NO} = n\sum_{i=1}^{m} t_i \qquad (3.1)$$

where T_{NO} is the total time to process n batches without overlapping, each batch having m steps of duration $t_1, t_2, \ldots, t_m$. For this example, the total time is equal to (8)(3.5 + 0.5 + 3.5 + 2 + 4.0 + 1.0) = (8)(14.5) = 116.0 h.

For the process described in Figure 3.1, using the nonoverlapping scheme, the equipment is used infrequently, and the total processing time is unduly long. However, such a scheme might be employed in plants that operate only a single shift per day. In such cases, the production of a single batch might be tailored to fit an 8 or 10 h shift (for this example, the shift would have to be 14.5 h), with the limitation that only one batch would be produced per day. Although such a scheme does not appear to be very efficient, it eliminates prolonged storage of intermediate product and certainly makes the scheduling problem easy.

The total time to process all the batches can be reduced by starting a batch before the preceding batch has finished. This is equivalent to shifting backward the time blocks representing the steps in the batch process, as shown in Figure 3.2.

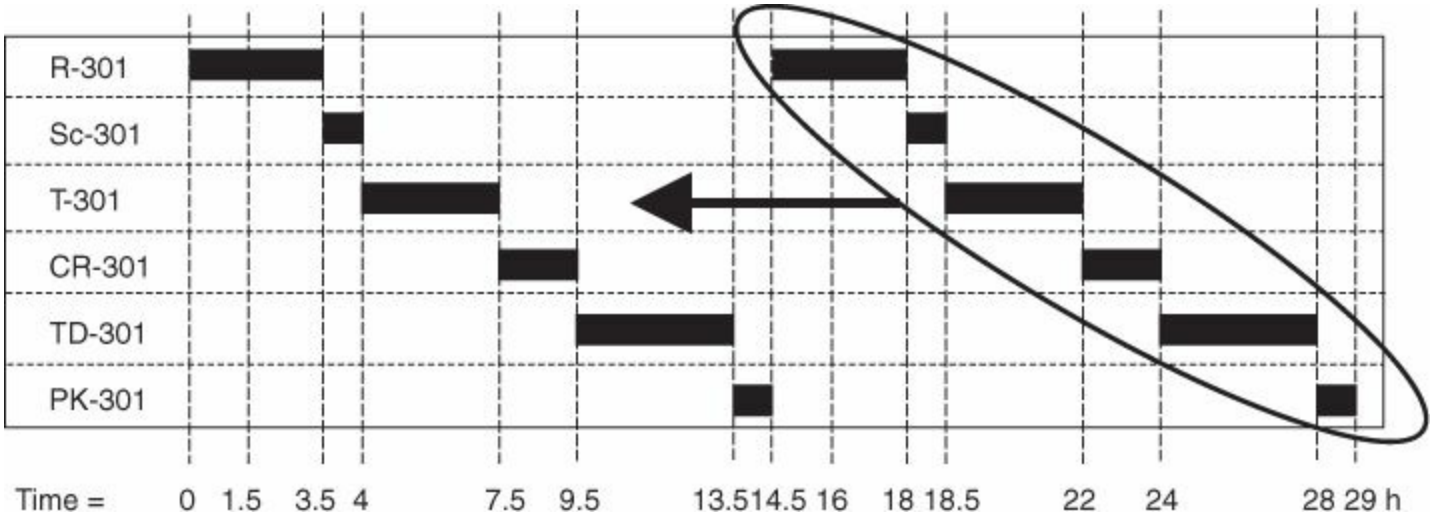


Figure 3.2. Backward Shifting of Batches, Giving Rise to Overlapping Sequencing

This shifting of batches backward in time leads to the concept of **overlapping** sequencing of batches.

The limit of this shifting or overlapping process occurs when two time blocks in consecutive batches just touch each other (assuming that cleaning, inspection, and charging times are included). This situation is shown in Figure 3.3.

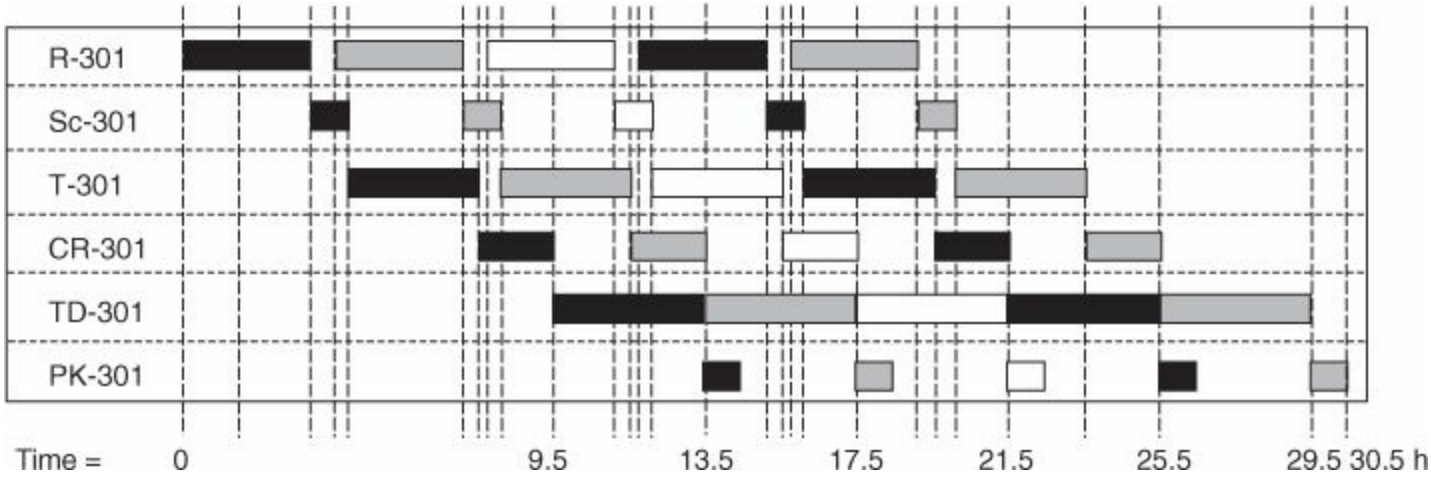


Figure 3.3. The Limiting Case for Overlapping Batch Sequencing

From Figure 3.3, it can be seen that the limiting case for overlapping occurs when the step taking the longest time (here, the tray drying step in TD-301, which takes 4 h to complete) repeats itself without a waiting time between batches. The time to complete n batches using this limiting overlapping scheme is given by

$$T_O = T = (n-1)\max_{i=1,\ldots,m}(t_i) + \sum_{i=1}^{m} t_i \qquad (3.2)$$

where T_O is the minimum total (overlapping) time, and [max (t_i)] is the maximum individual time step for the batch process. The subscript O denoting overlapping will be dropped, and T will be used as the total processing time from this point on. For the example, $T = (8–1)(4.0) + (14.5) = 42.5$ h.

Comparing Figures 3.1 and 3.3, the use of overlapping sequencing reduces the processing time significantly (from 116 to 42.5 h) and makes much better use of the equipment; specifically, the equipment is operated for a higher fraction of time in the overlapping scheme compared with the nonoverlapping scheme.

In batch operations, the concept of **cycle time** is used to refer to the average time required to cycle through all necessary steps to produce a batch. The formal definition is found by dividing the total time to produce a number of batches by the number of batches. Thus, from Equations (3.1) and (3.2),

$$t_{cycle,NO} = \frac{T_{NO}}{n} = \frac{n\sum_{i=1}^{m} t_i}{n} = \sum_{i=1}^{m} t_i \qquad (3.3)$$

$$t_{cycle,O} = t_{cycle} = \frac{T}{n} = \frac{(n-1)\max_{i=1,\ldots,m}(t_i) + \sum_{i=1}^{m} t_i}{n} \qquad (3.4)$$

For the overlapping scheme, when the number of batches (n) to be produced is large, the cycle time is approximated by

$$t_{cycle} \cong \max_{i=1,\ldots,m}\{t_i\} \qquad (3.5)$$

Therefore, for Example 3.1, the nonoverlapping and overlapping cycle times are 14.5 h and 4 h, respectively.

3.4. Flowshop and Jobshop Plants

Thus far, the discussion has focused on the production of only a single product. However, most batch plants produce multiple products. All these products may require the same processing steps, or more often will require only a subset of all possible steps. Moreover, the order in which a batch process uses different equipment might also differ from product to product.

3.4.1. Flowshop Plants

Consider a plant that must make three products: A, B, and C. Figure 3.4 shows an example of the sequence of equipment used to produce these three products. In Figure 3.4, all the products use the same equipment in the same order or sequence, but not necessarily for the same lengths of time. This type of plant is sometimes referred to as a **flowshop** plant [4]. The total time for operation of overlapping schedules depends on the number of runs of each product and how these runs are scheduled. One approach to scheduling multiple products is to run each product in a campaign during which only that product is made. Then the plant is set up to run the next product in a campaign, and so on. The case when multiple products, using the same equipment in the same order, are to be produced in separate campaigns is considered first. If the corresponding numbers of batches for products A, B, C in a campaign are n_A, n_B, and n_C, respectively, then the total processing time, or production cycle time, can be found by adding the operation times for each product. If the number of batches per campaign is large (for example, >10), then the production cycle time can be approximated by

$$T = \sum_{j=A}^{C} n_j \{t_{cycle}\}_j \cong \sum_{j=A}^{C} n_j \left\{ \max_{i=1,\ldots,m} \{t_i\} \right\}_j \qquad (3.6)$$

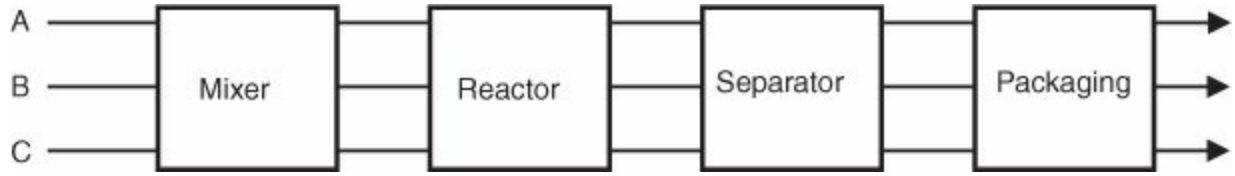


Figure 3.4. An Example of a Flowshop Plant for Three Products A, B, and C

An illustration of a multiple-product process is given in Example 3.3.

Example 3.3.

Consider three batch processes, producing products A, B, and C, as illustrated in Table E3.3. Each process uses the four pieces of equipment in the same sequencing order but for different times.

Table E3.3. Equipment Times (in Hours) Needed to Produce A, B, and C

Product	Time in Mixer	Time in Reactor	Time in Separator	Time in Packaging	Total Time
A	1.5	1.5	2.5	2.5	8.0
B	1.0	2.5	4.5	1.5	9.5
C	1.0	4.5	3.5	2.0	11.0

Market demand dictates that equal numbers of batches of the three products be produced over a prolonged period of time.

Determine the total number of batches that can be produced in a production cycle equal to one month of operation of the plant using separate campaigns for each product, assuming that a month of

operation is equivalent to 500 h (based on 1/12 of a 6000 h year for a three-shift plant operating five days per week).

Solution

The time to produce each product is given by Equation (3.2). Assume that each product is run x times during the month:

$$T = 500 = \sum_{j=A}^{C} \left\{ (n-1) \max_{i=1,\ldots,m} \{t_i\} + \sum_{i=1}^{m} t_i \right\}_j$$

$$500 = [(x-1)(2.5) + 8] + [(x-1)(4.5) + 9.5] + [(x-1)(4.5) + 11]$$

$$500 = (x-1)(11.5) + 28.5 \Rightarrow x = \frac{(500-28.5)}{11.5} + 1 = 42$$

Thus, 42 batches each of A, B, and C can be run as campaigns in a 500 h period. The cycle times are $t_{cycle,A} = [(41)(2.5) + 8/(42)] = 2.631$ h, $t_{cycle,B} = 4.619$ h, and $t_{cycle,C} = 4.655$ h.

Using Equation (3.6) with the approximations $t_{cycle,A} = 2.5$, $t_{cycle,B} = 4.5$, and $t_{cycle,C} = 4.5$,

$$T = 500 = x(2.5 + 4.5 + 4.5) \Rightarrow x = \frac{500}{11.5} = 43$$

Equation (3.6) slightly overestimates the number of batches that can be run in the 500 h period but is a very good approximation. In general, Equation (3.6) will be used to estimate cycle times and other calculations for single-product campaigns for multiproduct plants.

Running campaigns for the production of the same product is efficient and makes scheduling relatively easy. However, this strategy suffers from a drawback: The longer the production cycle, the greater the amount of product that must be stored. The concept of product storage is addressed in the following section. However, the bottom line is that storage requires additional equipment or warehouse floor space that must be purchased or rented. On the other hand, a strategy of single-product campaigns may decrease cleaning times and costs, which generally are greater when switching from one process to another. Therefore, the implementation of a batch sequencing strategy that uses sequences of single-product campaigns involves additional costs that should be included in any design and optimization. The extreme case for single-product batch campaigning occurs for seasonal produce (a certain vegetable oil, for example), where the feed material is available only for a short period of time and must be processed quickly, but the demand for the product lasts the whole year.

An alternative to running single-product campaigns (AAA…, BBB…, CCC…) over the production cycle is to run multiproduct campaigns—for example, ABCABCABC, ACBACBACB, AACBAACBAACB, and so on. In this strategy, products are run in a set sequence and the sequence is repeated. This approach is illustrated in Example 3.4.

Example 3.4.

Consider the same processes given in Example 3.3. Determine the number of batches that can be produced in a month (500 h) using a multiproduct campaign strategy with the sequence ABCABCABC.. …

The Gantt chart for this sequence is shown in Figure E3.4.

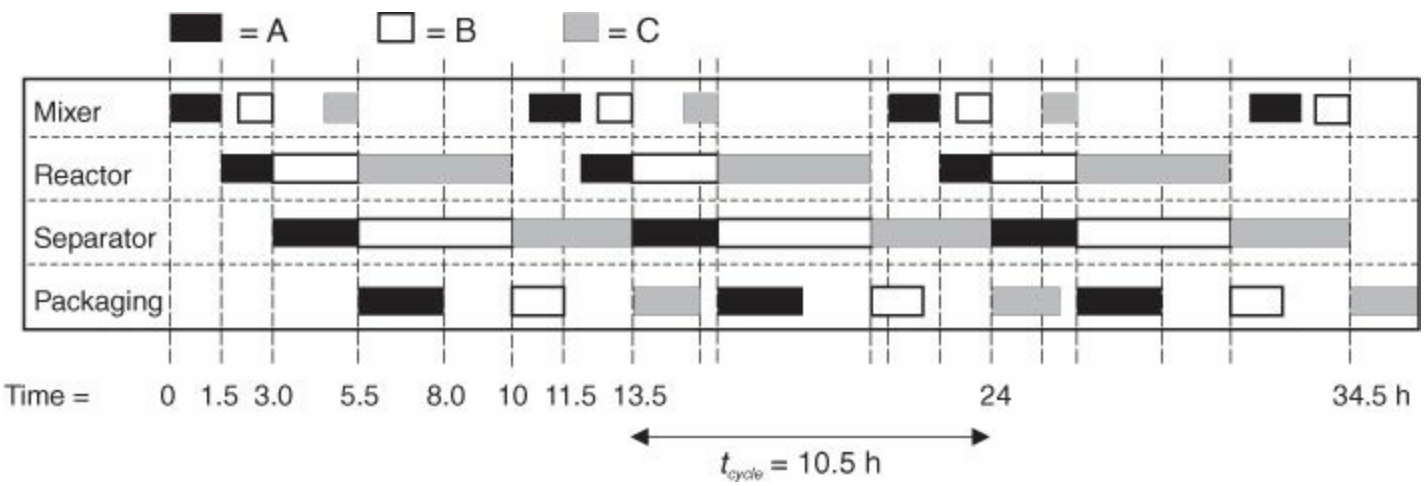


Figure E3.4. Gantt Chart Showing the Multiproduct Sequence ABCABCABC. …

From Figure E3.4, it can be seen that the limiting equipment for this sequence is the separator. This means that the separator is used without downtime for the duration of the 500 h. If x batches are produced during the 500 h period, then

$$T = 500 = (3 + x(2.5 + 4.5 + 3.5) + 2) \Rightarrow x = \frac{(500-5)}{10.5} = 47$$

Therefore, an additional five batches of each product can be produced using this sequence compared with the single-product campaign discussed in Example 3.3, assuming no additional cleaning time. It should be noted that other sequences, such as BACBACBAC, could be used, and these may give more or fewer batches than the sequence used here.

3.4.2. Jobshop Plants

The flowshop plant discussed previously is one example of a batch plant that processes multiple products. When not all products use the same equipment or the sequence of using the equipment is different for different products, then the plant is referred to as a **jobshop** plant [4]. Figure 3.5 gives two examples of such plants. In Figure 3.5(a), all the products move from the left to the right—that is, they move in the same direction through the plant, but not all of them use the same equipment. In Figure 3.5(b), products A and B move from left to right, but product C uses the equipment in a different order from the other two products. The sequencing of multiproduct campaigns for this type of plant is more complex and is illustrated in Example 3.5. The relative efficiencies of different processing schemes for the plant shown in Figure 3.5(b) are calculated in Example 3.6.

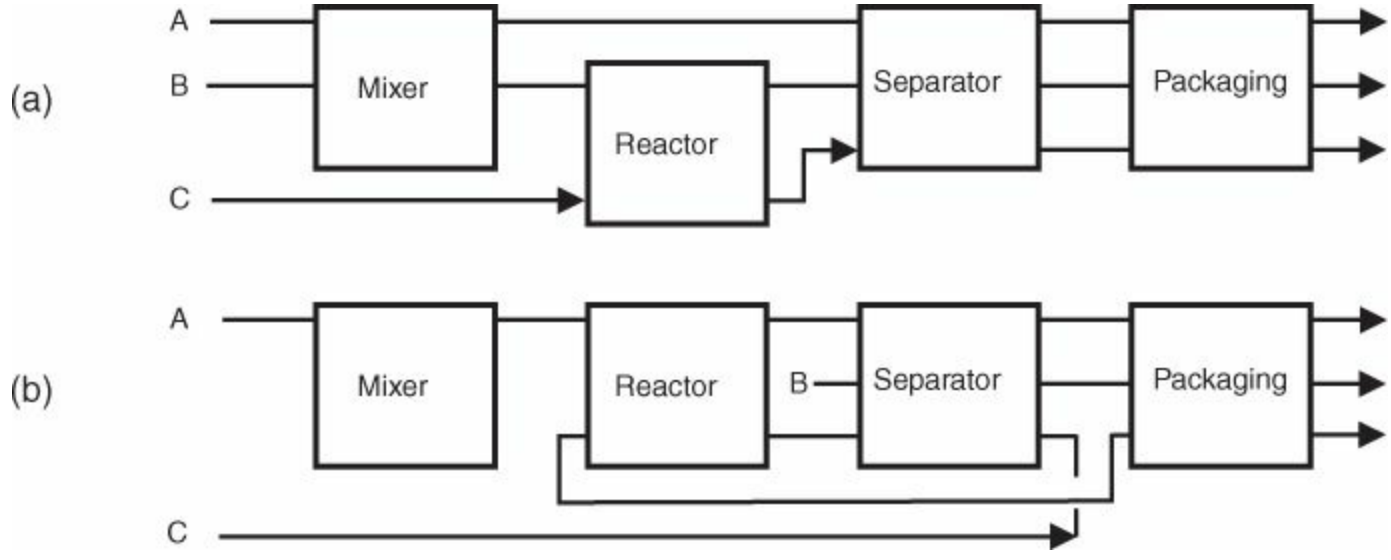


Figure 3.5. Two Examples of Jobshop Plants for Three Products A, B, and C

Example 3.5.

Consider the jobshop plant following the sequence shown in Figure 3.5(b) and described in Table E3.5. Construct the Gantt charts for overlapping single-product campaigns for products A, B, and C and for the multiproduct campaign with sequence ABCABCABC. …

Table E3.5. Equipment Processing Times (in Hours) for Processes A, B, and C

Process	Mixer	Reactor	Separator	Packaging
A	1.0	5.0	4.0	1.5
B	—	—	4.5	1.0
C	—	3.0	5.0	1.5

Solution

The Gantt charts for the three processes are shown in Figure E3.5. The top chart shows the timing sequences for each batch, and the next three charts show overlapping campaigns for products A, B, and C, respectively. It can be seen that the rules and equations for overlapping campaigns given previously still apply. The bottom chart shows the overlapping multiproduct campaign using the sequence ABCABCABC… Note that there are many time gaps separating the use of the different pieces of equipment, and no one piece of equipment is used all the time. This situation is common in jobshop plants, and strategies to increase equipment usage become increasingly important and complicated as the number of products increases.

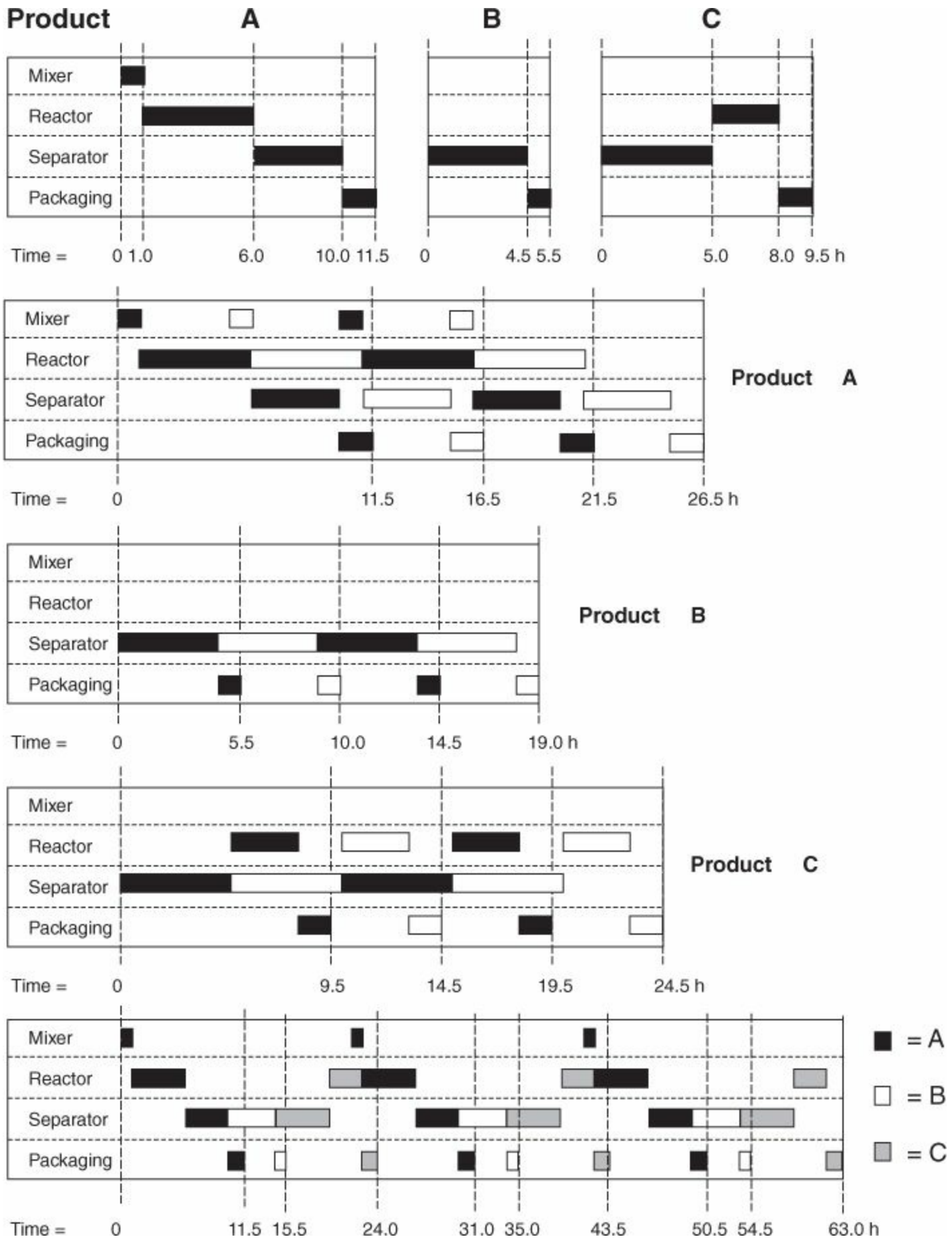


Figure E3.5. Gantt Charts for Single-Product and Multiproduct Campaigns

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Example 3.6.

It is desired to produce the same number of batches of A, B, and C. Using information from Example

3.5, determine the total number of batches of each product that can be produced in an operating period of 1 month = 500 h, using single-product campaigns and a multiproduct campaign following the sequence ABCABCABCABC. …

Solution

For the single-product campaigns, the number of batches of each product, x, can be estimated using Equation (3.6). Thus

$$500 = x(5 + 4.5 + 5) \Rightarrow x = \frac{500}{14.5} = 34$$

Therefore, 34 batches of each product can be made in a 500 h period using single-product campaigns.

For the multiproduct campaign, referring to Figure E3.5, the cycle time for the sequence ABC is 19.5 h. This is found by determining the time between successive completions of product C: 43.5 – 24 = 19.5 h, and 63 – 43.5 = 19.5 h. Therefore, the number of batches of A, B, and C that can be produced is given by

$$500 = x(19.5) \Rightarrow x = \frac{500}{19.5} = 25$$

This multiproduct sequence is clearly less efficient than the single-product campaign approach, but it does eliminate intermediate storage. It should be noted that different multiproduct sequences give rise to different results, and the ABCABC sequence may not be the most efficient sequence for the production of these products.

3.5. Product and Intermediate Storage and Parallel Process Units

In this section, the effect of intermediate and product storage on the scheduling of batch processes and the use of parallel process units or equipment are investigated. Both of these concepts will, in general, increase the productivity of batch plants.

3.5.1. Product Storage for Single-Product Campaigns

When using combinations of single-product campaigns in a multiproduct plant, it is necessary to store product during the campaign. For example, considering the products produced in Example 3.3, the plant will produce 43 batches each of products A, B, and C in a 500 h period. If the required production rates for these three products are 10,000, 15,000, and 12,000 kg/month, respectively, then what is the amount of storage required? In practice, it is the volume, and not the weight, of each product that determines the required storage capacity. For this example, it is assumed that the densities of each product are the same and equal to 1000 kg/m^3. Considering product A first and assuming that demand is steady, the demand rate (r_d) is equal to 10,000/500 = 20 kg/h = 0.020 m^3/h. Note that the demand rate is calculated on the basis of plant operating hours, and not on the basis of a 24-hour day. During the campaign, 10,000 kg of A must be made in 43 batch runs, with each run taking $t_{cycle,\ A}$ = 2.5 h. Thus, during production, the production rate (r_p) of A is equal to 10,000/(43)(2.5) = 93.0 kg/h = 0.0930 m^3/h. Results for all the products are given in Table 3.1.

Table 3.1. Production and Demand Rates for Products A, B, and C in Example 3.3

Rate	Product A	Product B	Product C
Volume (m^3) of product required per month	10.0	15.0	12.0
Cycle time (h)	2.5*	4.5*	4.5*
Production rate, r_p (m^3/h)	(10)/[(43)(2.5)] = 0.0930	0.07752	0.06202
Demand rate, r_d (m^3/h)	(10)/(500) = 0.020	0.030	0.024

*These are approximate cycle times based on Equation (3.5).

When a campaign for a product is running, the rate of production is greater than the demand rate. When the campaign has stopped, the demand rate is greater than the production rate of zero. Therefore, the accumulation and depletion of product over the monthly period are similar to those shown in Figure 3.6. The changing inventory of material is represented on this figure by the bottom diagram. The maximum inventory, V_s, is the minimum storage capacity that is required for the product using this single-product campaign strategy. The expression for calculating V_s is

$$V_s = (r_p - r_d)t_{camp} \quad (3.7)$$

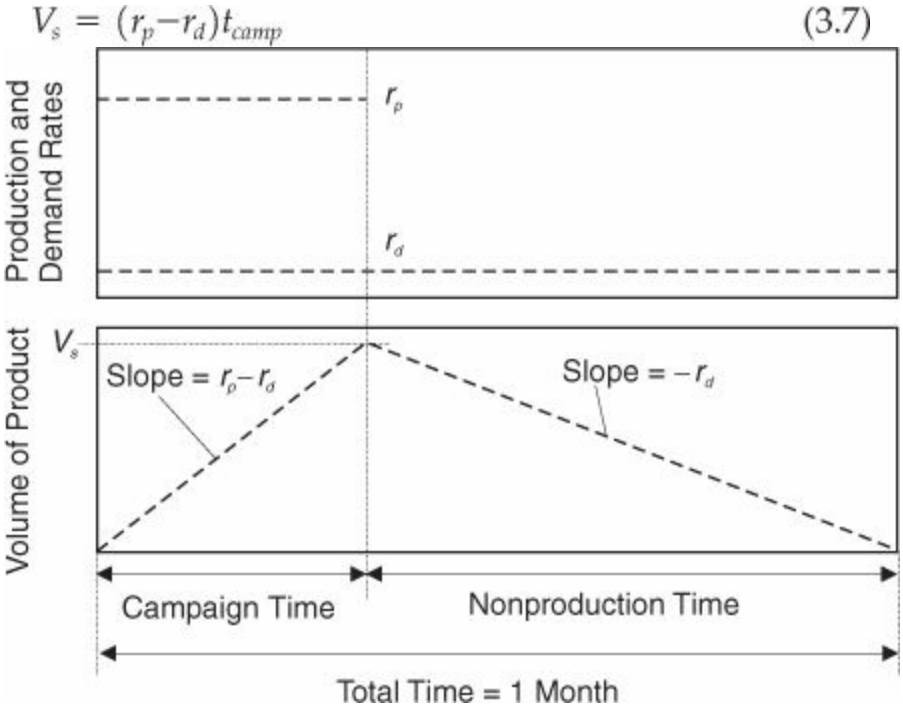


Figure 3.6. Changing Inventory of Product during Single-Product Campaign Run within a Multiproduct Process

where t_{camp} is the campaign time. This assumes that the shipping rate of product from the plant is constant during plant operating hours. Because shipping is usually itself a batch process, the actual minimum storage capacity could be more or less than that calculated in Equation (3.7). The strategies for matching shipping schedules to minimize cost (including storage costs and missed-delivery risks) are known as logistics and are not covered here.

Determination of the minimum storage capacities for all products in Example 3.3 is given in Example 3.7.

Example 3.7.

For the products A, B, and C in Example 3.3, determine the minimum storage capacities for the single-product campaign strategy outlined in Example 3.3.

Solution

Table E3.7 shows the results using data given in Example 3.3 and Table 3.1.

Table E3.7. Results for the Estimation of Minimum Storage Volume from Equation (3.7)

Product	Campaign Time, t_{camp} (h)	$r_p - r_d$ (m^3/h)	V_s (m^3)
A	(43)(2.5) = 107.5	0.09302 – 0.020 = 0.07302	(0.07302)(107.5) = 7.85
B	(43)(4.5) = 193.5	0.07752 – 0.030 = 0.04752	(0.04752)(193.5) = 9.20
C	(43)(4.5) = 193.5	0.06202 – 0.024 = 0.03802	(0.03802)(193.5) = 7.36

It should be noted that the production cycle time is equal to the sum of the campaign times, or (107.5 + 193.5 + 193.5) = 494.5 h, which is slightly less than 500 h. This discrepancy reflects the approximation of cycle times given by Equation (3.6). The actual cycle times for A, B, and C are found from Example 3.3 and are equal to 2.63, 4.62, and 4.65 h, respectively. The corresponding values of V_s are 7.79, 9.18, and 7.31 m^3. Clearly, these differences are small, and the approach using Equation (3.6) is acceptable when the number of production runs per campaign is 10 or more.

3.5.2. Intermediate Storage

Up to this point, it has been assumed that there is no intermediate product storage available. This type of process is also known as a **zero wait,** or a **zw process** [4]. Specifically, as soon as a unit operation is completed, the products are transferred to the next unit operation in the sequence, or they go to final product storage. The concept of storing the final product to match the supply with the demand was demonstrated in Example 3.7. However, it may also be beneficial to store the output from a given piece of equipment for a period of time to increase the overall efficiency of a process. It may be possible to store product in the equipment that has just been used. For example, if two feed streams are mixed in a vessel, the mixture could be stored until the next process unit in the production sequence becomes available. In this case, the storage time is limited based on the scheduling of equipment. This **holding-in-place** method may not work for some unit operations. For example, in a reactor, a side reaction may take place, and unless the reaction can be quenched, the product yield and selectivity will suffer. The upper limit of the intermediate storage concept occurs when there is **unlimited intermediate storage (uis)** available, and this is referred to as a **uis process** [4]. In general, cycle times can be shortened when intermediate product storage is available. This concept is illustrated in Figure 3.7, which is based on the information given in Table 3.2.

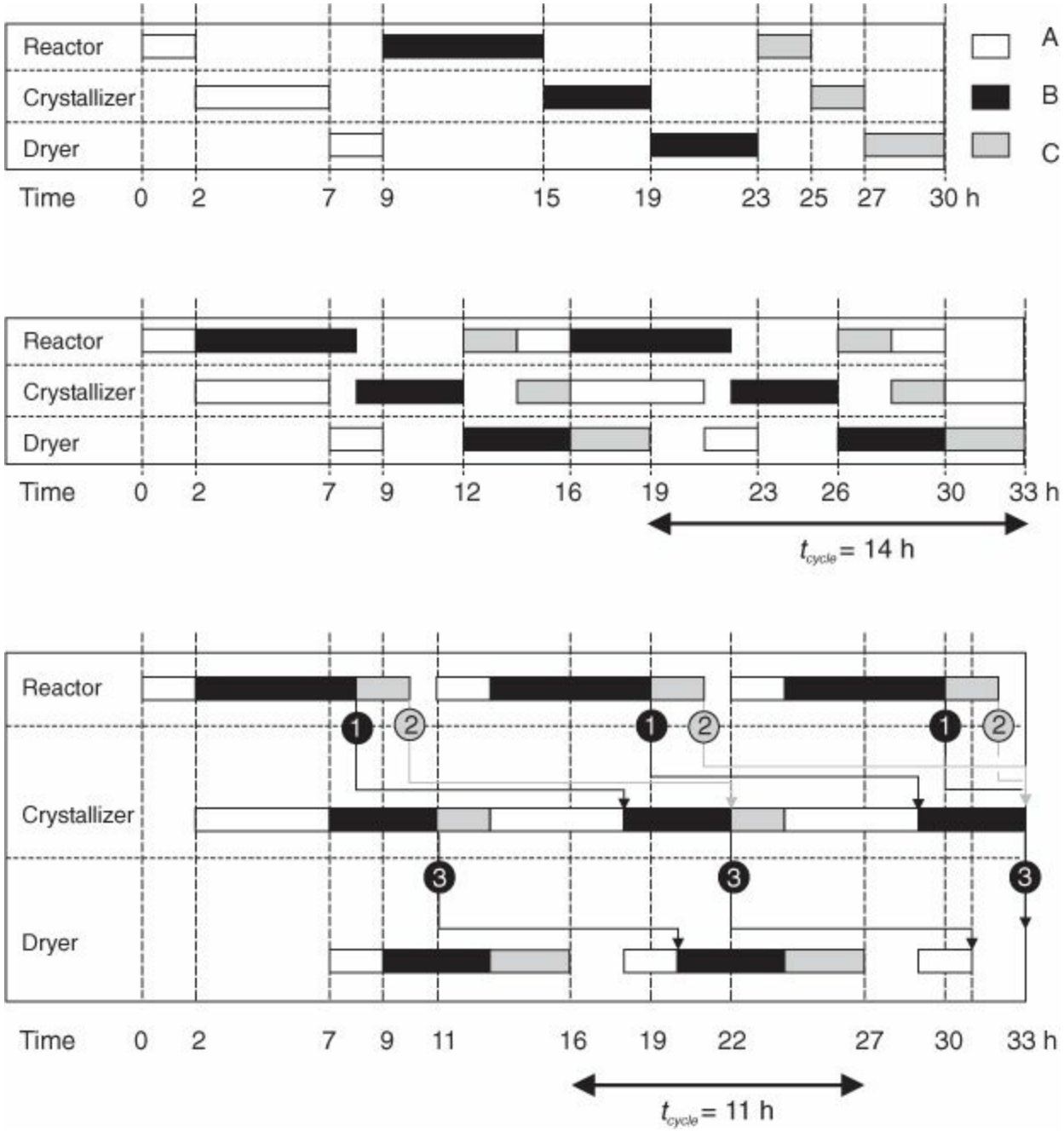


Figure 3.7. Multiproduct Sequence (ABC) for Products Given in Table 3.2 Showing Effect of Intermediate Storage (Storage Shown as Circles; Number Identifies Individual Tanks for Each Intermediate Product)

Table 3.2. Equipment Times (in Hours) Required for Products A, B, and C

Product	Reactor	Crystallizer	Dryer	Total
A	2.0	5.0	2.0	9.0
B	6.0	4.0	4.0	14.0
C	2.0	2.0	3.0	7.0
Total Time per Equipment	10.0	11.0	9.0	

Without intermediate product storage, the shortest multiproduct campaign, as given by Equation (3.6), is 14 h, as shown in Figure 3.7. However, if the materials leaving the reactor and crystallizer are placed in storage prior to transfer to the crystallizer and dryer, respectively, then this time is reduced to 11 h. The limiting cycle time for a uis process is given by

$$t_{cycle,uis} = \max_{j=1,m} \sum_{i=1}^{N} nc_i t_{i,j} \qquad (3.8)$$

where m is the number of unit operations, N is the number of products, and nc_i is the number of campaigns of product i produced in a single multiproduct sequence. For the case shown in Table 3.2 and Figure 3.7, $n = 1$ (because only one campaign for each product (A, B, and C) is used in the multiproduct sequence), and Equation (3.8) is the maximum value given in the last row of Table 3.2, or 11.0 h.

The total amount of storage required for this example is fairly small, because only three storage vessels are required, each dedicated to one intermediate product. The downside of this approach is that there are many more material transfers required, and the potential for product contamination and operator error increases significantly.

3.5.3. Parallel Process Units

Another strategy that can be employed to increase production is to use duplicate equipment. This strategy is most beneficial when there is a bottleneck involving a single piece of equipment that can be relieved by adding a second (or more) units in parallel. This strategy can be extended to a limiting case in which parallel trains of equipment are used for each product. This strategy eliminates the dependence of scheduling between the different products but is more expensive, because the number of pieces of equipment increases m-fold, where m is the number of products. An example of using parallel equipment is shown in Figure 3.8 based on the data in Table 3.3.

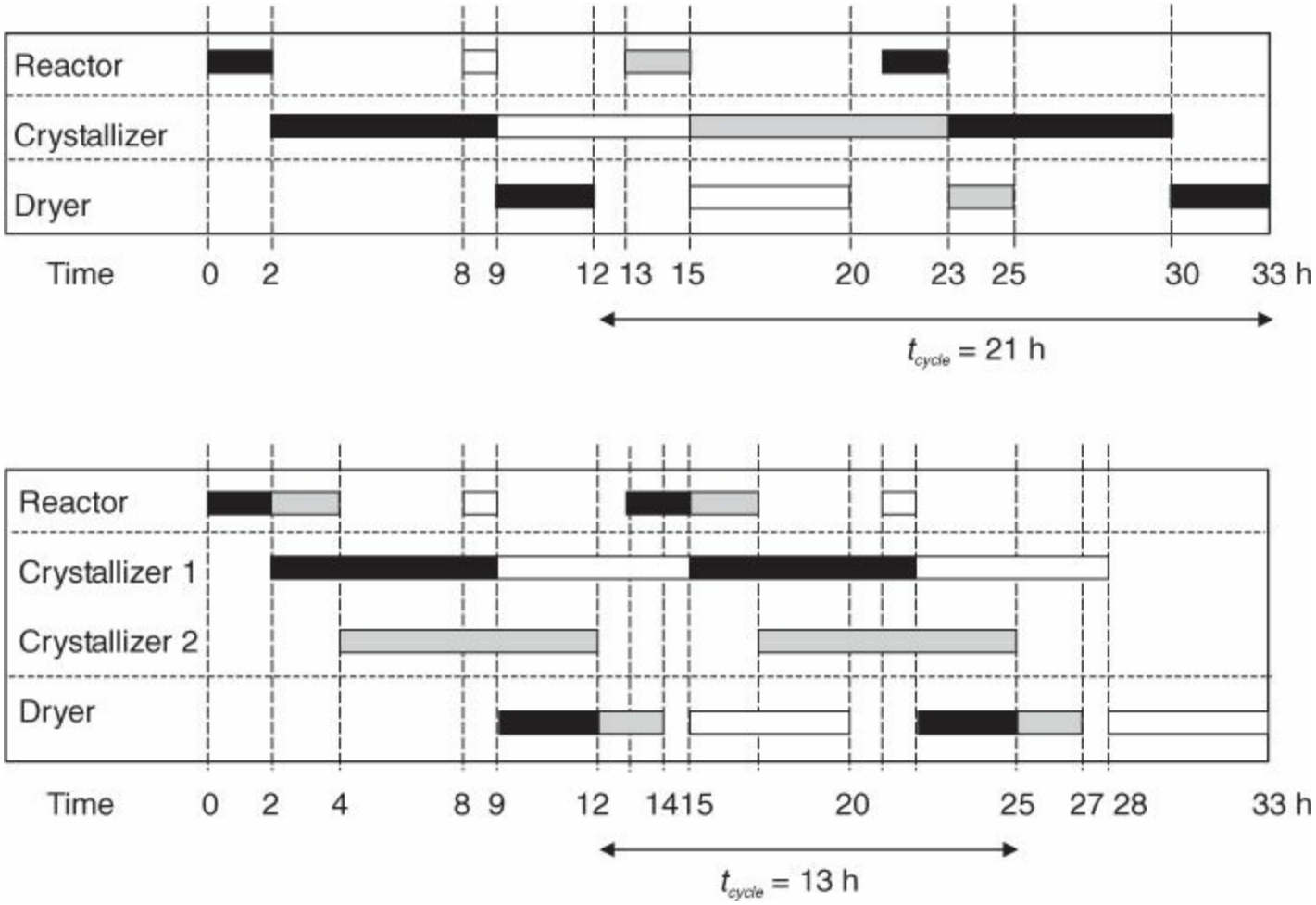


Figure 3.8. The Effect of Adding an Additional Crystallizer to the Process Given in Table 3.2

Table 3.3. Data (Times in Hours) for Multiproduct Batch Process Shown in Figure 3.8

Process	Reactor	Crystallizer	Dryer
A	2.0	7.0	3.0
B	1.0	6.0	5.0
C	2.0	8.0	2.0

From the top chart in Figure 3.8, the limiting piece of equipment is seen to be the crystallizer. The bottom chart shows the effect of adding a second crystallizer that processes product C. The effect is to reduce the cycle time from 21 h to 13 h, a considerable improvement in throughput. The determination of whether to make this change must be made using an appropriate economic criterion, such as net present value (NPV) or equivalent annual operating cost (EAOC), which are discussed in Chapter 10. The resulting tradeoff is between increased product revenues and the cost of purchasing a second crystallizer plus additional operators to run the extra equipment.

3.6. Design of Equipment for Multiproduct Batch Processes

The design of equipment sizes for multiproduct batch processes depends on the production cycle time, whether single- or multiproduct campaigns are used, the sequence of products for multiproduct campaigns, and the use of parallel equipment. As an example, the multiproduct process described in Table 3.4 will be analyzed. It is assumed that each product will be produced using a single-product campaign. The production cycle will be 500 h (equivalent to one month in a 6000 h year). The production cycle will be repeated 12 times in a year. The required amount of each product is given in Table 3.4 along with the processing times.

Table 3.4. Data for a Multiproduct Batch Process

Process	Reactor and Mixer	Filtration	Distillation	Yearly Production	Production in 500 h
A	7.0 h	1.0 h	2.0 h	120,000 kg	10,000 kg
B	9.0 h	1.0 h	1.5 h	180,000 kg	15,000 kg
C	10.0 h	1.0 h	3.0 h	420,000 kg	35,000 kg

By studying Table 3.4, it is apparent that the limiting piece of equipment is the mixing and reaction vessel, and the cycle times can be found from this piece of equipment. To estimate equipment volume, it is necessary to determine the volume of each piece of equipment per unit of product produced. To determine these quantities, descriptions of the method (recipe) for using each piece of equipment for each product must be known. The procedure to estimate the specific volume of the reactor for process A in Table 3.4 is given in Example 3.8.

Example 3.8.

The following is a description of the reaction in process A, based on a laboratory-scale experiment. First, 10 kg of liquid reactant (density = 980 kg/m^3) is added to 50 kg of a liquid mixture of organic solvent containing excess of a second reactant (density of mixture = 1050 kg/m^3) in a jacketed reaction vessel, the reactor is sealed, and the mixture is stirred and heated. Once the reaction mixture has reached 95°C, a solid catalyst (negligible volume) is added, and reaction takes place while the batch of reactants continues to be stirred. The required conversion is 94%, 17.5 kg of product is

produced, and the time taken is 7.0 h. The reactor is filled to 60% of maximum capacity to allow for expansion and to provide appropriate vapor space above the liquid surface. Determine the volume of reaction vessel required to produce 1 kg of product.

Solution

$$\text{volume of reactor} = \left(\frac{10\ [\text{kg}]}{980\ [\text{kg/m}^3]} + \frac{50\ [\text{kg}]}{1050\ [\text{kg/m}^3]}\right)\frac{100}{60} = 0.09637\ \text{m}^3$$

$$v_{react} = \frac{\text{volume of reactor}}{\text{mass of product}} = \frac{0.09637}{17.5} = 0.005507\ \text{m}^3\text{/kg-product}$$

Similar calculations can be made for the reactor/mixer for processes B and C in Table 3.4, and these results are given in Table 3.5 along with the cycle times for each process. It should be noted that even for a preliminary design and cost estimate, other attributes of the equipment should also be considered. For example, in order to specify fully the reactor and estimate its cost, the heating duty and the size of the motor for the mixer impeller must be calculated. To simplify the current example, only the volumes of the reactor are considered, but it should be understood that other relevant equipment properties must also be considered before a final design can be completed. This procedure should be applied to all the equipment in the process.

Table 3.5. Specific Reactor/Mixer Volumes for Processes A, B, and C

Process	A	B	C
v_{react} (m^3/kg-product)	0.005507	0.007860	0.006103
t_{cycle} (h)	7.0	9.0	10.0

Let the single-product campaign times for the three products be t_A, t_B, and t_C, respectively. Applying Equation (3.6), the following relationship is obtained:

$$t_A + t_B + t_C = 500 \tag{3.9}$$

The number of batches per campaign for each product is then given by $t_x/t_{cycle,x}$ and

$$\text{Batch size (kg/batch)} = \frac{\text{production of } x}{t_x/t_{cycle,x}} \tag{3.10}$$

Furthermore, the volume of a batch is found by multiplying Equation (3.10) by $v_{reac,x}$, and equating batch volumes for the different products yields

$$\text{Volume of batch} = \frac{(\text{production of } x)(v_{react,x})}{t_x/t_{cycle,x}} \tag{3.11}$$

$$\frac{(10{,}000)(0.005507)}{t_A/7.0} = \frac{(15{,}000)(0.007860)}{t_B/9.0} = \frac{(35{,}000)(0.006103)}{t_B/10.0} \tag{3.12}$$

Solving Equations (3.9) and (3.12) yields

$$t_A = 53.8\ \text{h}$$

$$t_B = 148.1\ \text{h}$$

$$t_C = 298.1\ \text{h}$$

$$v_{react,A} = v_{react,B} = v_{react,C} = 7.17 \text{ m}^3$$

Number of batches per campaign for product A = 7.7

Number of batches per campaign for product B = 16.5

Number of batches per campaign for product C = 29.8

Clearly the number of batches should be an integer value. Rounding these numbers yields

For product A

Number of batches = 8

$t_A = (8)(7) = 56$ h

$V_A = (10{,}000)(0.005507)(7)/(56) = 6.88 \text{ m}^3$

For product B

Number of batches = 16

$t_B = (16)(9) = 144$ h

$V_B = (15{,}000)(0.007860)(9)/(144) = 7.37 \text{ m}^3$

For product C

Number of batches = 30

$t_C = (30)(10) = 300$ h

$V_C = (35{,}000)(0.006103)(10)/(300) = 7.12 \text{ m}^3$

Total time for production cycle = 500 h

Volume of reactor = 7.37 m^3 (limiting condition for product B)

= (7.37)(264.2) =1947 gallons

The closest standard size, 2000 gallons, is chosen.

3.7. Summary

In this chapter, concepts important to the design of batch processes were introduced. Gantt charts were used to illustrate the timing and movement of product streams through batch processes. The concepts of nonoverlapping and overlapping sequences were discussed for single-product and multiproduct processes. The differences between flowshop and jobshop plants were introduced, and the strategies for developing single-product and multiproduct campaigns for each type of process were discussed. The role of intermediate and final product storage and the methods to estimate the minimum product storage for single-product campaigns were illustrated. The addition of parallel equipment was shown to reduce product cycle time. Finally, an example of estimating the size of vessels required in a multiproduct process was given.

What You Should Have Learned

- The difference between design considerations for batch versus continuous processes
- Batch scheduling patterns
  - Flowshop versus jobshop plants

- Impact of storage requirements
- Single- versus multiproduct plants

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3. Dewar, J. D., "If You Don't Know Where You're Going, How Will You Know When You Get There?" *CHEMTECH* 19, no. 4 (1989): 214–217.
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Short Answer Questions

1. What is a flowshop plant?
2. What is a jobshop plant?
3. What are the two main methods for sequencing multiproduct processes?
4. Give one advantage and one disadvantage of using single-product campaigns in a multiproduct plant.
5. What is the difference between a zero-wait and a uis process?

Problems

6. Consider the processes given in Example 3.3. Determine the number of batches that can be produced in a month (500 h) using a series of single-product campaigns when the required number of batches for product A is twice that of either product B or product C.
7. Consider the processes given in Examples 3.3 and 3.4. Determine the number of batches that can be produced in a month (500 h) using a multiproduct campaign strategy with the sequence ACBACBACB. Are there any other sequences for this problem other than the one used in Example 3.4 and the one used here?
8. Consider the multiproduct batch plant described in Table P3.8.

Table P3.8. Equipment Processing Times for Processes A, B, and C

Process	Mixer	Reactor	Separator
A	2.0 h	5.0 h	4.0 h
B	3.0 h	4.0 h	3.5 h
C	1.0 h	3.0 h	4.5 h

It is required to produce the same number of batches of each product. Determine the number of batches that can be produced in a 500 h operating period using the following strategies:

a. Single-product campaigns for each product

b. A multiproduct campaign using the sequence ABCABCABC. …

c. A multiproduct campaign using the sequence CBACBACBA. …

9. Consider the process given in Problem 3.8. Assuming that a single-product campaign strategy is used over a 500 h operating period and further assuming that the production rates (for a year = 6000 h) for products A, B, C are 18,000 kg/y, 24,000 kg/y, and 30,000 kg/y, respectively, determine the minimum volume of product storage required. Assume that the product densities of A, B, and C are 1100, 1200, and 1000 kg/m^3, respectively.

10. Using the data from Tables P3.10(a) and (b), and following the methodology given in Section 3.6, determine the number of batches and limiting reactor size for each product.

Table P3.10(a). Production Rates for A, B, and C

Product	Yearly Production	Production in 500 h
A	150,000 kg	12,500 kg
B	210,000 kg	17,500 kg
C	360,000 kg	30,000 kg

Table P3.10(b). Specific Reactor/Mixer Volumes for Processes A, B, and C

Process	A	B	C
v_{react} (m^3/kg-product)	0.0073	0.0095	0.0047
t_{cycle} (h)	6.0	9.5	18.5

11. Referring to the batch production of amino acids described in Project 8 in Appendix B, the batch reaction times and product filtration times are given in Table P3.11.

Table P3.11. Batch Step Times (in Hours) for Reactor and Bacteria Filter for Project 8 in Appendix B

Product	Reactor*	Precoating of Bacteria Filter	Filtration of Bacteria
L-aspartic acid	35	25	5
L-phenylalanine	65	25	5

*Includes 5 h for filling, cleaning, and heating.

The capacity of the reactors chosen for both products is 10,000 gallons each. The precoating of the filters may occur while the batch reactions are taking place, and hence the critical time for the filtration is 5 h. It should be noted that intermediate storage is not used between the reactor and filter, and hence the batch times for the reactors must be extended an additional 5 h while the contents are fed through the filter to storage tank V-901. It is desired to produce L-aspartic acid and L-phenylalanine in the ratio of 1 to 1.25 by mass. Using a campaign period of 1 year = 8000 h and assuming that there is a single reactor and filter available, determine the following:

a. The number of batches of each product that can be produced in a year, maintaining the desired ratio of the two products, if one single-product campaign is used for each amino acid per year.

b. The amount of final product storage for each product assuming a constant demand of each product over the year. Express this amount of storage as a volume of final solid crystal product (bulk density of each amino acid is 1200 kg/m^3). You may assume that the recovery of

each amino acid is 90% of that produced in the reactor.

c. By how much would the answer to Part (b) change if the single-product campaigns for each amino acid were repeated every month rather than every year?

12. Referring to Problem 3.11, by how much would yearly production change if the following applied?

a. The reaction times for L-aspartic acid and L-phenylalanine were reduced by 5 h each. Use the same scenario as described in Problem 3.11, Part (a).

b. The reaction times for L-aspartic acid and L-phenylalanine were increased by 5 h each. Use the same scenario as described in Problem 3.11, Part (a).

13. It is desired to produce three different products, A, B, and C, using the same equipment in a batch processing plant. Each production method uses the same equipment in the same order for the times given in Table P3.13.

Table P3.13. Equipment Processing Times for Problem 3.13

Equipment Process	Mixer\Reactor	Filter	Crystallizer	Dryer	Density
A	2.5 h	1.5 h	4.5 h	5.0 h	900 kg/m^3
B	3.5 h	3.5 h	5.5 h	4.0 h	1000 kg/m^3
C	2.0 h	3.5 h	5.0 h	4.0 h	850 kg/m^3

It has been determined that market forces dictate that the rate of production of product B should be twice that of A and for C should be three times that of A. For a one-month campaign, equivalent to 600 h, answer the following questions:

a. Assume that each product will be produced in separate campaigns; for example, first make all A, then B, then C. Determine the number of batches for each product.

b. If the yearly demand for product C is 180,000 kg/y (180 tonne/y), determine the storage capacity (volume) for this product assuming constant demand for C throughout the campaign period.

c. Determine the number of batches that could be produced during a 600 h period if the multibatch sequence ABBCCCABBCCC . . . is used.

14. A batch chemical plant is to be used to produce three chemical products (A, B, and C) using a flowshop plant. The times for each product in each piece of equipment (in hours) are shown in Table P3.14.

Table P3.14. Equipment Processing Times for Problem 3.14

Unit Op/ Product	Heating	Reaction/ Mixing	Filtration	Distillation	Crystallization
A	1.0	3.0	1.0	2.5	3.5
B	1.5	3.5	1.0	1.5	4.0
C	2.5	2.0	0.5	2.5	3.0

Market demands for these products require that the ratio of A to B to C be 1/2/2. Therefore, n_B =

$n_C = 2n_A$. For this batch plant, answer the following questions:

a. In an operating period of 600 h, how many batches of A, B, and C can be made using three single-product campaigns (AAA…, BBBBBB…, CCCCCC…)?

b. Using multiple batch campaigns in the order ABBCCABBCC …, how many batches of A, B, and C can be made?

c. How would the answer to Part (a) change if the number of batches of A were twice those of B and C (instead of half)?

d. For Part (a), if the required production over the 600 h of operation for product B was 20,000 kg or 17.5 m^3 of product, what volume of intermediate storage would be required to ensure that a constant supply of B could be maintained over the 600 h operation?

Chapter 4. Chemical Product Design

What You Will Learn

- There is a difference between process design and product design.
- There is a strategy for chemical product design.

The subject of most of this book is chemical process design, the traditional capstone experience in chemical engineering curricula. For most of the history of chemical engineering, graduates have gone to work in chemical plants that manufacture commodity chemicals. **Commodity chemicals** are those manufactured by many companies in large quantities, usually in continuous processes like those illustrated in this textbook. There is little or no difference in commodity chemicals produced by different companies. The price for which a commodity chemical can be sold is essentially the same for all producers, and, because most raw materials are also commodity chemicals, the price of raw materials is also the same for all producers. For the most part, innovations regarding manufacture of commodity chemicals have occurred a long time in the past. Therefore, the only real way to be more profitable than a competitor is to have lower ancillary costs, such as a favorable union contract, a better deal on the costs of different sources of energy, superior automation, a better catalyst, and so on.

Before a chemical became a commodity, it was probably a specialty. A **specialty chemical** is one made in smaller quantities, often in batch processes, usually by the company that invented the chemical. Perhaps the best examples of specialty chemicals evolving into commodity chemicals are polymers. Polymers such as nylon, Teflon, and polyethylene were specialties when they were invented in the first half of the twentieth century, and they were seen only in selected applications. Now, they are ubiquitous commodities.

The chemical industry has also become more global. At one time, chemicals and products from chemicals for the entire world were manufactured in the centers of the chemical industry: the United States and Western Europe. This meant that a large, rapidly growing chemical industry in the United States and Western Europe was needed to serve the needs of developing countries. Now chemicals are manufactured all over the world, closer to where they are used, as are the raw materials for these chemicals. Therefore, the traditional commodity chemical industry is not in a growth phase in places such as the United States and Western Europe. Existing chemical processes continue to operate, and chemical engineers trained to understand and work with continuous, commodity chemical processes are still needed.

It has been suggested that the future of chemical engineering—that is, the place where chemical engineers can innovate—is in chemical product design [1, 2]. This is also the place where more and more chemical engineers are being employed [2]. It could be argued that the future is identical to the past. Since the 1970s, most large, commodity chemical companies have trimmed their long-range research, focusing instead on support for the global growth of commodity chemical production. They believed this to be a necessary shift of emphasis as chemicals that were once specialties evolved into commodities.

What is a chemical product? One possibility is a new specialty chemical. A new drug is a chemical product. A new catalyst or solvent for use in the commodity chemical industry is a chemical product.

Post-it Notes are a chemical product. A fuel cell is a chemical product. A device for indoor air purification is a chemical product. Technologies employing chemical engineering principles could be considered to be chemical products. Even the ChemE Cars that many students build as part of the AIChE competition could be considered chemical products.

In this chapter, an introduction to procedures used for chemical product design is provided. It will be seen that there are similarities to chemical process design; however, the focus of this chapter is on the differences between process and product design.

4.1. Strategies for Chemical Product Design

A strategy for chemical product design has been suggested by Cussler and Moggridge [1]. It has four steps:

1. Needs
2. Ideas
3. Selection
4. Manufacture

Needs means that a need for a product must be identified. This involves dealing with industrial customers and/or the public. If the business end of a commodity chemical industry determines there is a market for additional benzene, a process is constructed to make the same benzene product that all other benzene producers make, probably using the same process technology. If there is a market for the additional benzene, there will be customers. In contrast, in chemical product design, once the need is established, then the search for the best product begins.

Ideas means that the search for the best product has begun. This is similar to the brainstorming stage of the problem-solving strategy to be discussed in Chapter 24. Different ideas are identified as to the best possible product to serve the need.

Selection involves screening the ideas for those believed to be the best. There are quantitative methods for this step, and they are discussed later.

Manufacture involves determining how to manufacture the product in sufficient quantities. Unlike commodity chemicals, this usually involves batch rather than continuous processes.

The four-step process is a simplification that is most applicable to the design of chemical products that are actually chemicals. For the design of devices, there are additional steps needed. Two such product design strategies, suggested by Dym and Little [3] and Ulrich and Eppinger [4] are illustrated in Table 4.1 and compared with the strategy of Cussler and Moggridge [1]. The most significant difference is the inclusion of different stages of device design not apparent for design of a chemical, although it could be considered that these steps are all part of the selection and/or manufacture step.

Table 4.1. Comparison of Product Design Strategies

Strategy	Cussler and Moggridge [1]	Dym and Little [3]	Ulrich and Eppinger [4]
Steps	Needs	Need	Identify customer needs
	Ideas	Problem definition	Establish target specifications
	Selection	Conceptual design	Generate product concepts
	Manufacture	Preliminary design	Select product concepts
		Detailed design	Test product concepts
		Design communication	Set final specifications
		Final design	Plan downstream development

There are clear parallels among these three product design strategies. It is observed that the first step in each strategy is the identification of customer needs. The ideas and selection steps of Cussler and Moggridge [1] are identical to the generate product concepts and select product concepts steps of Ulrich and Eppinger [4], respectively. The strategies of Dym and Little [3] and Ulrich and Eppinger [4] all include several design and product-testing steps. Although these are not explicitly included in the strategy of Cussler and Moggridge [1], they will have to be part of any product design strategy. For example, no one would begin to manufacture a product without first making a small amount in the lab and testing it.

It is instructive to observe the parallel between the strategy of Dym and Little [3] and the increasing levels of capital cost estimates in process design illustrated in Table 7.1. Moving from a feasibility estimate through a detailed estimate parallels moving from a conceptual design to a detailed design. Similarly, the evolution of a detailed P&ID from a PFD also parallels the evolution from a conceptual design to a detailed design.

In the following sections, the strategy of Cussler and Moggridge [1] is illustrated using several examples.

4.2. Needs

A new chemical product is sought in response to a need. The needs might be those of individual customers, those of groups, or those of society. Consider the case of Freon refrigerants. In the 1980s, Freons were identified as having high ozone-depleting potential because of their chlorine content. Therefore, a need for an environmentally friendly chemical with the appropriate properties of a refrigerant was established. This led to the development of fluorocarbon refrigerants (e.g., R-134a) and methods for their synthesis. However, this did not solve the problem entirely. It was then determined that the new refrigerants were incompatible with typical compressor lubricants. This created the need for a new lubricant that was compatible with the new refrigerant. Subsequently, this new lubricant was developed, and the new refrigerant began to be phased in as Freons were phased out.

Chemical companies devoted to product design (e.g., food products, personal care) deal with customers all the time. Customers are interviewed, often in focus groups, and the results of these interviews must be interpreted and made into product specifications. This is an inexact "science." Care must be taken to define the correct need.

As an example, consider the needs of vessels used for space travel (e.g., the space shuttle) as they reenter Earth's atmosphere [5]. The customer, NASA, initially sought the development of a material

that would withstand the temperatures of reentry. Such a material was never developed. Once the problem was redefined, a more appropriate need was defined. The real need was not to have a material capable of withstanding the temperatures of reentry; the real need was to protect those inside the space vessel from the high temperatures generated by friction with the edge of Earth's atmosphere. This led to the development of the sacrificial tiles used in the space shuttle. The energy generated by friction is dissipated by vaporizing these sacrificial tiles, thereby protecting those inside the vessel from the heat. Only after the correct need was identified was the problem solved.

Examples 4.1 through 4.4 [6–8] illustrate definition of needs.

Example 4.1.

Zebra mussels are mollusks that have been known to infest the water intake pipes of water treatment and electric power plants. Entire towns have been shut down because the infestation of zebra mussels has halted the supply of water to purification plants. The initial solution to this problem was to remove the infested zebra mussels manually. Identify the need(s) to alleviate the infestation problem.

The need is for a method to prevent the infestation, because it is undesirable to shut down water treatment facilities for manual cleaning. If this method is to involve a chemical, it is important to specify the desired features of this chemical. For example, it should be inexpensive, it must prevent infestation, it should not harm other wildlife, and it should be removable in the water treatment facility.

Example 4.2.

Maintaining a swimming pool, either at home or in a public facility, is both expensive and time consuming. The water must be tested often, particularly for chlorine. The chlorine additive to a swimming pool emits a characteristic odor, irritates the eyes, and can fade colors on swimsuits due to its bleaching effect. Identify a product need.

There might be a need for a method to disinfect the pool water other than adding a chlorine-containing compound. Suppose a continuous-flow device could be developed that disinfected the pool water as it passed through the filter system. Is there a need for such a product? (This is one possible alternative to chlorine. There are others.) Such a device would undoubtedly increase the capital cost of installing a pool, even though it would save time and the cost of constantly adding chlorine. The unanswered question is whether pool purchasers would be willing to pay the incremental capital cost. Even though a net present value or an equivalent annual operating cost calculation, such as that illustrated in Chapter 10, might prove that the incremental cost of such a device is justified by the savings, it is still unclear whether people would purchase such a device. Most buyers will not sit down and do an incremental economic analysis. It is difficult to put a dollar value on the savings in time created by such a device. Clearly, it would be necessary to get feedback from potential customers before proceeding with development of such a device.

Example 4.3.

Research is under way to develop a magnetic refrigerator [9]. This refrigerator operates by using magnetocaloric materials, which are materials that heat up when in a magnetic field. A magnetic refrigerator operates without a compressor and therefore does not need a refrigerant like Freon,

which vaporizes and condenses in the vapor-compression cycle. Is there a need for such a refrigerator?

What are the advantages of such a refrigerator? There are two obvious ones. One is that a refrigerant like Freon is not needed. This may have spurred the initial research effort; however, the development of new refrigerants with more favorable environmental properties may have diminished this advantage. The other is the lack of a compressor, probably the most costly component of a vapor-compression refrigerator, both in capital cost and in operating cost. There are energy costs associated with the magnetic refrigerator, including a pump to circulate the cooling fluid and a motor to cycle the magnetocaloric material into and out of the magnetic field. Therefore, the savings created by compressor removal may be small. Based on these two factors, it is unclear whether there is a need for a magnetic refrigerator.

Example 4.4.

With the advent of portable electric devices such as laptop computers, cellular phones, personal digital assistants, MP3 players, and so on, the length of time they can run before recharging and/or replacement of their power source is becoming an issue. Is there a product need here?

Anyone who has ever used a laptop computer where there is no source of power has probably, at one time or another, been frustrated by a battery that has run out before the desired work was completed. However, does this mean there is a need for a longer-lasting power source? Or will this be a high-end, niche market? Consider the situations when one uses a laptop computer for long periods of time away from a power source. One of the most common situations is on an airplane. However, newer aircraft now have fitted power connections at every seat. Some older aircraft have already been retrofitted with such power connections. As older aircraft are replaced or as they are modernized, will all aircraft used for longer flights have power available? If so, this could diminish the need for a longer-lasting power source, especially one that might require new technology and be costly.

4.3. Ideas

The generation of ideas is tantamount to brainstorming. Just as in brainstorming, when ideas are being generated, there are no bad ideas. They will be screened in the next step, selection. Ideas can be sought from a variety of sources, including, but not limited to, members of the product development team, potential customers, and published literature. If there is a time for "pie in the sky," it is at this step.

It is important to remember not to "get married" to an idea at this stage. The chances of the first idea generated being the best one are slim or none. As many ideas as can be imagined should be generated before moving on to the selection step.

Examples 4.5 through 4.7 illustrate generation of ideas.

Example 4.5.

Suggest some ideas for the zebra mussel problem in Example 4.1.

One possible idea is to invent a chemical or determine whether there is a chemical that can kill existing infestations. It would be nice if this were combined with a chemical that can prevent the infestations. If either of these methods were to be used, some type of delivery system would be

needed. Another possibility is to place some type of filter at the water intake to keep the zebra mussels out of the water intake. Because zebra mussels are attracted to the warmer water near power plants and water treatment facilities, another possibility is to find a way to cool this water. There are undoubtedly other possibilities. Can you think of any?

Example 4.6.

Suggest some ideas for the chlorine problem in Example 4.2.

An alternative disinfectant to chlorine would be one possibility. A chemical would need to be developed that has similar disinfectant properties to chlorine, but without the smell and irritation. This would address those problems but not the problem of the time and effort needed to add disinfectant. Another possibility is some type of automatic dispenser for chlorine or a replacement disinfectant, so that a disinfectant reservoir would only have to be changed periodically and would not require daily attention. Another possibility is a device that makes chlorine from a less toxic chemical, in situ, somewhere in the filtration system. This would keep chlorine out of the pool, confining it to the region where water is circulated through the filter. There are undoubtedly other possibilities. Can you think of any?

Example 4.7.

Suggest some ideas for a power source for laptop computers, as discussed in Example 4.4.

One possibility is to develop better batteries. This is currently being done. Early laptop computers used NiCd batteries. The next generation was Ni-metal-hydride batteries, and the current generation is Li-ion batteries. There will probably be another generation forthcoming. Another possibility is to develop fuel cells that can be used to power a laptop computer. There may be other possibilities. Can you think of any?

4.4. Selection

Once a sufficient number of ideas has been generated, it is necessary to screen the ideas and select a few for more detailed investigation. Scientific principles can be applied. If it is thermodynamically impossible to manufacture an alternative, that idea can be eliminated. If it is determined that the kinetics of a desired reaction are unfavorable, that idea might be eliminated or downgraded, although this might stimulate development of a new catalyst to improve selectivity. If it is possible to determine at this stage that an alternative will be far too expensive relative to another idea, that idea might be eliminated or downgraded. However, when in doubt, it is probably best not to reject any idea too soon.

There are more quantitative methods for screening alternatives. One set of methods known as concept screening and concept scoring [4] will be briefly summarized here. More details can be found in Ulrich and Eppinger [4]. These methods are useful in that they allow subjective assessments to be quantified systematically for comparison purposes.

In **concept screening,** a selection matrix is prepared by listing a set of criteria to be used to evaluate the alternatives. Then one alternative is chosen as a reference alternative. This should be an alternative with which the team doing the evaluation is most familiar, perhaps an industry standard.

All criteria for the reference standard are assigned a value of zero, meaning "same as." The criteria for all other alternatives are assigned values of +, meaning "better than"; zero; or –, meaning "worse than." Then the number of "worse thans" is subtracted from the number of "better thans." The net score for each alternative provides a relative ranking. Some type of reflection is needed at this stage to determine whether the results make sense and whether each criterion was assigned a reasonable value. The number of alternatives is now reduced, though it is up to those involved to determine how many alternatives survive to the next step. An example of concept screening is shown in Table 4.2. Here, alternative 5 is chosen as the reference alternative. It is observed that alternatives with equal scores are assigned the same rank. To proceed to the next step, it will be assumed that only four alternatives—those with positive scores—remain in the selection process.

Table 4.2. Example of Concept Screening

	Alternative								
Criterion	1	2	3	4	5	6	7	8	9
1	+	–	0	+	0	+	0	–	0
2	0	+	+	0	0	0	+	0	+
3	+	0	0	0	0	+	+	–	0
4	0	0	–	0	0	–	+	0	0
5	0	–	+	–	0	0	–	+	–
Total Score	2	−1	1	0	0	1	2	−1	0
Rank	1	8	3	5	5	3	1	8	5

In **concept scoring,** the same matrix is used, but only on those alternatives that have survived the concept screening process. The results are now more quantitative. Each criterion is now assigned a relative weight, which reflects the team's judgment as to its relative importance. A reference alternative is chosen. Then, for each alternative, each criterion is assigned a value from 1 to 5, where 1 = much worse than reference, 2 = worse than reference, 3 = same as reference, 4 = better than reference, and 5 = much better than reference. The score is calculated for each alternative by weighting the evaluations using the relative weights. Once again, some degree of reflection on the result is needed because this is a subjective process, particularly the assigning of relative weights. The best alternative is the one with the highest score. Because there is a large degree of subjectivity here, care should be exercised when differentiating between alternatives with close scores. Table 4.3 illustrates concept scoring for the four alternatives chosen during concept screening. Based on this method, alternative 1 is chosen for further study, although alternative 7 is close. Once again, small differences in total score may not be significant. Also, information obtained during product development may change the relative weights and/or individual scores sufficiently so that the total score changes enough and alternative 7 is actually the best choice.

Table 4.3. Example of Concept Scoring

Criterion	Weight	Alternative			
		1	3	6	7
1	25%	5	3	4	3
2	5%	3	4	3	4
3	15%	5	3	5	5
4	35%	3	1	2	5
5	20%	3	4	3	1
Total Score		**3.80**	**2.55**	**3.20**	**3.65**
Rank		**1**	**3**	**4**	**2**

Caution should be exercised before using this method. There are subtleties associated with it, which are explained in more detail elsewhere [4].

4.5. Manufacture

This final step in the chemical product design structure is the most detailed. It includes determining whether the product can be manufactured, developing detailed product specifications, determining how the product is to be manufactured, and estimating the cost of manufacturing. It also includes sample or prototype testing, which may result in changes in the selection process and undoubtedly will result in modifications in every step of the manufacturing process until the optimal product and manufacturing process is obtained.

These feedback loops in the manufacturing process exist for the manufacture of any product, even a commodity chemical. Before a multimillion-dollar plant is constructed, a pilot plant is usually constructed. Before a new chemical product is manufactured, small quantities are made in the laboratory to determine whether the product satisfies the need for which it was designed. Similarly, before a device is manufactured, a prototype is built and tested.

One lesson is that device manufacture is likely to be a very interdisciplinary effort. In the magnetic refrigerator example, Example 4.3, mechanical engineers would be needed for the pulley system, and electrical engineers might be needed for the control systems. Industrial engineers may be needed to determine the most efficient manufacturing procedure and to help determine the unit cost in mass production, because the cost of a prototype always exceeds the unit cost in mass production. When interdisciplinary efforts are needed, it is recommended that the interdisciplinary team be involved from the beginning, if possible. Example 4.8 illustrates the type of product that might be manufactured.

Example 4.8.

Suppose the following scenario has evolved for the zebra mussel problem discussed in Examples 4.1 and 4.5. It is not possible to use a filter to prevent zebra mussel infestation because in the veliger (infancy) stage, zebra mussels are microscopic. They attach to the wall of the intake pipe, where they grow into maturity. Once the walls are saturated, they stack on each other, eventually occluding the pipe. Therefore, some type of chemical treatment is desirable. It has been determined from experimentation that alkylbenzyldimethylammonium chloride (alkyl chains between 12 and 16 carbons) will kill existing infestations, and dead mussels detach from the wall [10]. Also, assume that it has also been determined that 0.3 wt% hydrogen peroxide will inhibit veliger attachment. Describe

the manufacturing stage.

A delivery system is needed, both for the initial kill and for the hydrogen peroxide to prevent infestation. One possible solution is to design and market a technology for delivery of these chemicals. For example, suppose that a grating for the intake pipe containing flow channels with holes discharging into the intake pipe were designed. A pumping system would be needed to deliver the chemicals through the holes in the grating. If the fluid mechanics of the discharge into the intake pipe were studied to optimize hole placement, the hole placement could be optimized to ensure that the chemicals covered the entire cross section of the pipe at the desired concentration. This technology could then be marketed to water treatment facilities and power plants to prevent zebra mussel infestation.

4.6. Batch Processing

In the manufacture of a chemical product that is actually a chemical, batch operations are often employed. This is because specialty chemical products are usually produced in small batches. In the Douglas hierarchy discussed in Chapter 2, the first decision to be made in designing a chemical process is batch versus continuous. For production of a commodity chemical in the quantities reflected in the examples on the CD-ROM accompanying this book, the choice will always be a continuous process. Similarly, for production of a specialty chemical, the choice will almost always be a batch process.

The issues involved in batch processing were discussed in Chapter 3.

4.7. Economic Considerations

When a new process is constructed for a commodity chemical, the sale price for the chemical is largely determined by the price competitors charge for the same chemical. However, the law of supply and demand does affect the price. If new capacity exists without additional demand, the value of the chemical may drop; if new capacity is created in response to a demand, the value of the chemical can probably be estimated from its value before the demand increased. Either way, the value of the chemical can probably be bracketed reasonably easily.

However, when a new product enters the market, the initial price usually reflects the value of its uniqueness. This behavior is seen every day. When new electronic devices enter the market (CD players, DVD players, projection TVs, HDTV), they usually carry a high price tag. In part, this is because they are not being produced in large quantities, and in part it is because there are customers who will pay a huge premium to be the first to have one. Eventually, prices decrease to attract new customers and then decrease significantly if the product becomes a commodity. Pharmaceuticals, an example of a chemical product, also carry a high price tag when they are new. Pharmaceutical companies must recover the extremely high costs of product research and development and the regulatory process before their patents expire and low-cost, generic alternatives become available, or before a competitor invents a superior alternative.

Therefore, although the profitability criteria that will be discussed in Chapter 10 can be used to evaluate the economics of chemical products, the details of the analysis may change. Years of research and development costs are included as capital costs. However, remember that there may be 10 to 15 years of such costs, and the time value of money requires that the price charged for the product must be high to obtain a favorable rate of return. Furthermore, there is risk with developing

new products. One way to include risk in the profitability calculations that will be discussed in Chapter 10 is to increase the desired rate of return, which also increases the price of the product. (This is similar to the practice of lending institutions charging more for a loan to consumers with weaker credit histories, because they are poorer credit risks.)

4.8. Summary

The challenges of chemical product design are different from those of chemical process design. These challenges include dealing with customer needs, screening alternatives, batch processing and scheduling, and the need for interdisciplinary teams more than in chemical process design. This chapter has been only a brief introduction to chemical product design. The major issues have been introduced, and examples have been presented to illustrate these principles. The readers interested in a more detailed treatment of product design should consult references [1], [3], and [4].

What You Should Have Learned

- Chemical process design usually involves production of a chemical that eventually is used to make a product.
- Chemical product design involves the manufacture of a specific product such as a new chemical or a device that employs chemical engineering principles.
- The structure of solving a chemical product design problem is as follows:
  - Needs—what is needed
  - Ideas—list of alternatives to satisfy the need
  - Selection—select the final idea
  - Manufacture—how to produce the desired product

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Chapter 5. Tracing Chemicals through the Process Flow Diagram

What You Will Learn

- In a continuous chemical process, there are reactants, products, and inerts.
- These components enter, leave, are formed, or are consumed in the process.
- Each component can be followed through the process.

In Chapter 2, the unit operations from a PFD were classified into one of the six blocks of a generic block flow process diagram. In this chapter, you gain a deeper understanding of a chemical process by learning how to trace the paths taken by chemical species through a chemical process.

5.1. Guidelines and Tactics for Tracing Chemicals

In this chapter, guidelines and some useful tactics are provided to help you trace chemicals through a process. Two important operations for tracing chemical pathways in PFDs are the adiabatic mixer and adiabatic splitter.

Mixer: Two or more input streams are combined to form a single stream. This single output stream has a well-defined composition, phase(s), pressure, and temperature.

Splitter: A single input stream is split into two or more output streams with the same temperature, pressure, and composition as the input stream. All streams involved differ only in flowrate.

These operations are found where streams meet or a stream divides on a PFD. They are little more than tees in pipelines in the plant. These operations involve little design and minimal cost. Hence, they are not important in estimating the capital cost of a plant and would not appear on a list of major equipment. However, you will find in Chapter 13 that these units are included in the design of flowsheets for implementing and using chemical process simulators.

The mixers and splitters are highlighted as shaded boxes on the flow diagrams presented in this chapter. They carry an “m” and “s” designation, respectively.

5.2. Tracing Primary Paths Taken by Chemicals in a Chemical Process

Chemical species identified in the overall block flow process diagram (those associated with chemical reactions) are termed **primary chemicals.** The paths followed by primary chemicals between the reactor and the boundaries of the process are termed **primary flow paths.** Two general guidelines should be followed when tracing these primary chemicals:

1. **Reactants:** Start with the feed (left-hand side of the PFD) and trace chemicals forward toward the reactor.
2. **Products:** Start with the product (right-hand side of the PFD) and trace chemicals backward toward the reactor.

The following tactics for tracing chemicals apply to all unit operations *except for* chemical reactors:

Tactic 1: Any unit operation, or group of operations, that has a single or multiple input streams and a single output stream is traced in a forward direction. If chemical A is present in

any input stream, it must appear in the single output stream (see Figure 5.1[a]).

Tactic 2: Any unit operation, or group of operations, that has a single input stream and single or multiple output streams is traced in a backward direction. If chemical A is present in any output stream, it must appear in the single input stream (see Figure 5.1[b]).

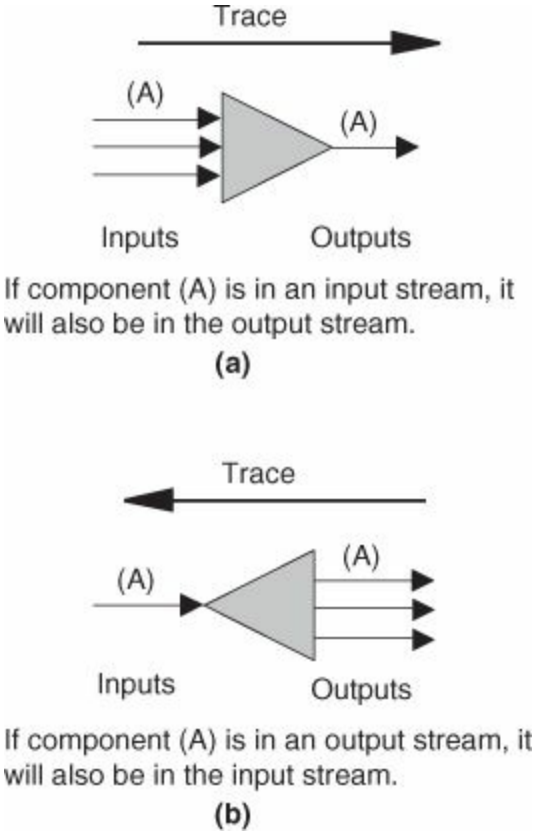


Figure 5.1. Tactics for Tracing Chemical Species

Tactic 3: Systems such as distillation columns are composed of multiple unit operations with a single input or output stream. It is sometimes necessary to consider such equipment combinations as blocks before implementing Tactics 1 and 2.

When tracing chemicals through a PFD, it is important to remember the following:

Only in reactors are feed chemicals transformed into product chemicals.

You may occasionally encounter situations where both reactions and physical separations take place in a single piece of equipment. In most cases, this is undesirable but unavoidable. In such situations, it will be necessary to divide the unit into two imaginary, or phantom, units. The chemical reactions take place in one phantom unit, and the separation in the second phantom unit. These phantom units are never shown on the PFD, but such units are useful when building a flowsheet for a chemical process simulator (see Chapter 13).

These guidelines are demonstrated in Example 5.1, by determining the paths of the primary chemicals in the toluene hydrodealkylation process. The only information used is that provided in the skeleton process flow diagram given in Figure 1.3.

Example 5.1.

For the toluene hydrodealkylation process, establish the primary flow pathway for

a. Toluene between the feed (Stream 1) and the reactor

b. Benzene between the reactor and the product (Stream 15)

Hint: Consider only one unit of the system at a time. Refer to Figure E5.1.

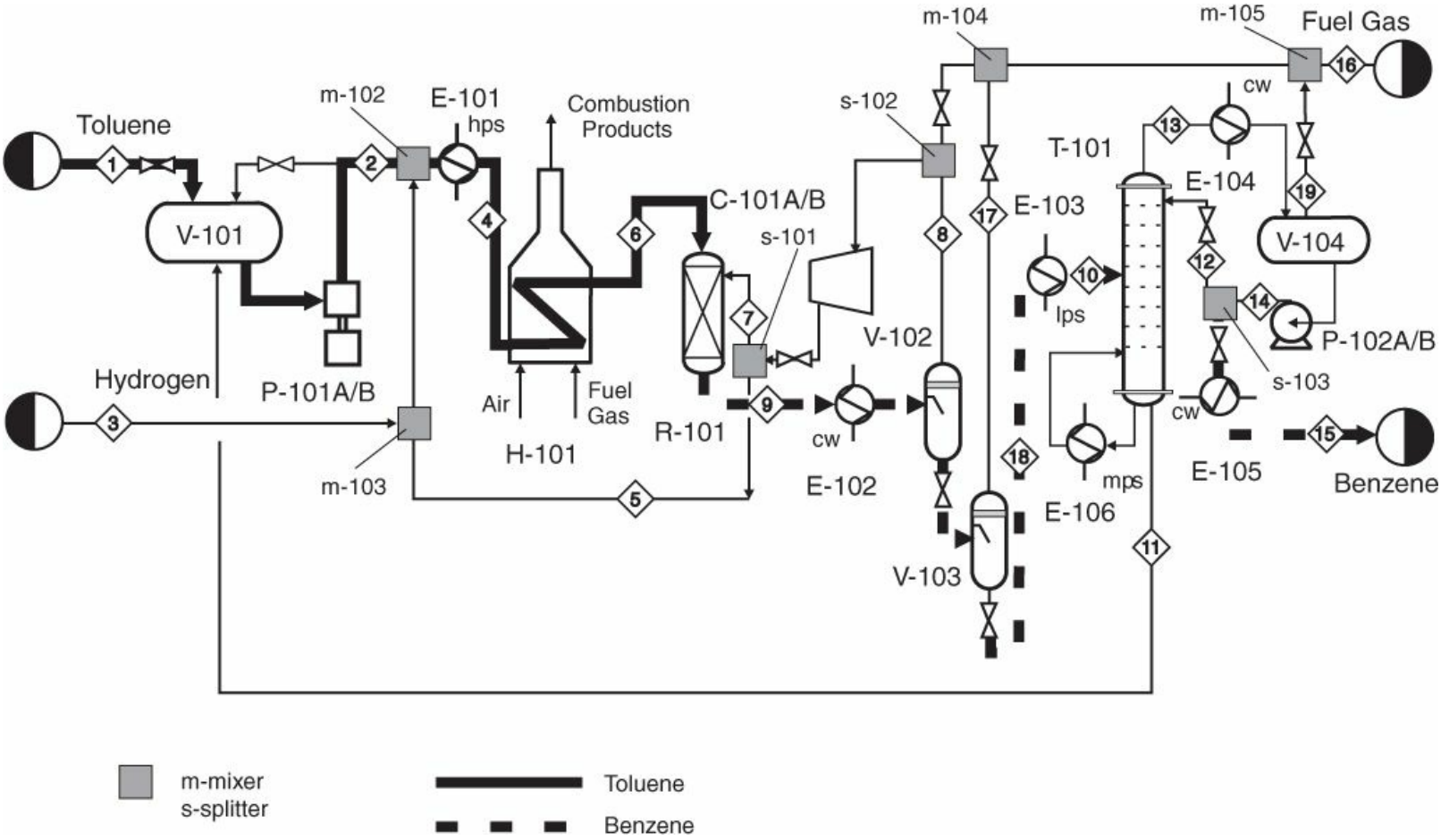


Figure E5.1. Primary Chemical Pathways for Benzene and Toluene in the Toluene Hydrodealkylation Process (Figure 1.3)

Toluene Feed: Tactic 1 is applied to each unit operation in succession.

a. Toluene feed Stream 1 mixes with Stream 11 in V-101. A single unidentified stream leaves tank V-101 and goes to pump P-101. All the toluene feed is in this stream.

b. Stream 2 leaves pump P-101 and goes to mixer m-102. All the feed toluene is in this stream.

c. A single unidentified stream leaves mixer m-102 and goes to exchanger E-101. All the feed toluene is in this stream.

d. Stream 4 leaves exchanger E-101 and goes to heater H-101. All the feed toluene is in this stream.

e. Stream 6 leaves heater H-101 and goes to reactor R-101. All the feed toluene is in this stream.

Benzene Product: Tactic 2 is applied to each unit operation in succession.

a. Product Stream 15 leaves exchanger E-105.

b. Entering exchanger E-105 is an undesignated stream from s-103 of the distillation system. It contains all of the benzene product.

c. Apply Tactic 3 and treat the tower T-101, pump P-102, exchangers E-104 and E-106, vessel V-104, and splitter s-103 as a system.

d. Entering this distillation unit system is Stream 10 from exchanger E-103. It contains all the benzene product.

e. Entering exchanger E-103 is Stream 18 from vessel V-103. It contains all the benzene product.

f. Entering vessel V-103 is an undesignated stream from vessel V-102. It contains all the benzene product.

g. Entering vessel V-102 is an undesignated stream from exchanger E-102. It contains all the benzene product.

h. Entering exchanger E-102 is Stream 9 from reactor R-101. It contains all the benzene product.

The path for toluene was identified as an enhanced solid line in Example 5.1. For this case, it was not necessary to apply any additional information about the unit operations to establish this path. The two streams that joined the toluene path did not change the fact that all the feed toluene remained as part of the stream. All the toluene fed to the process in Stream 1 entered the reactor, and this path represents the primary path for toluene.

The path for benzene was identified as an enhanced dotted line in Example 5.1. The equipment that makes up the distillation system was considered as an operating system and treated as a single unit operation. The fact that, within this group of process units, some streams were split with some of the flow returning upstream did not change the fact that the product benzene always remained in the part of the stream that continued to flow toward the product discharge. All the benzene product followed this path, and it represents the primary path for the benzene. The flow path taken for the benzene through the distillation column section is shown in more detail in Figure 5.2. The concept of drawing envelopes around groups of equipment in order to carry out material and energy balances is introduced early into the chemical engineering curriculum. This concept is essentially the same as the one used here to trace the path of benzene through the distillation column. The only information needed about unit operations used in this analysis was the identification of the multiple units that made up the distillation system. This procedure can be used to trace chemicals throughout the PFD and forms an alternative tracing method that is illustrated in Example 5.2.

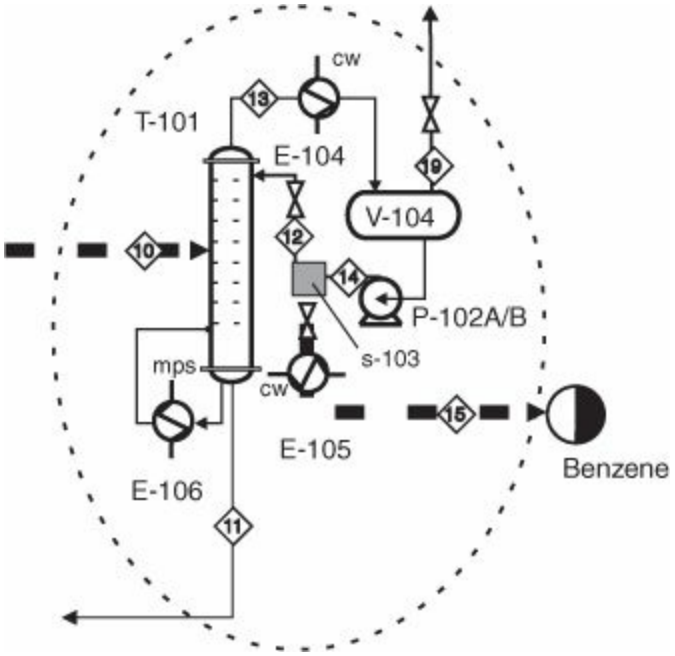


Figure 5.2. Envelope around Tower T-101 Showing Alternative Method for Tracing Benzene Stream

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Example 5.2.

Establish the primary flow pathway for

a. Hydrogen between its introduction as a feed and the reactor

b. Methane between its generation in the reactor and the discharge from the process as a product

In order to determine the primary flow paths, systems are developed (by drawing envelopes around equipment) that progressively include additional unit operations. Reference should be made to Figure E5.2(a) for viewing and identifying systems for tracing hydrogen.

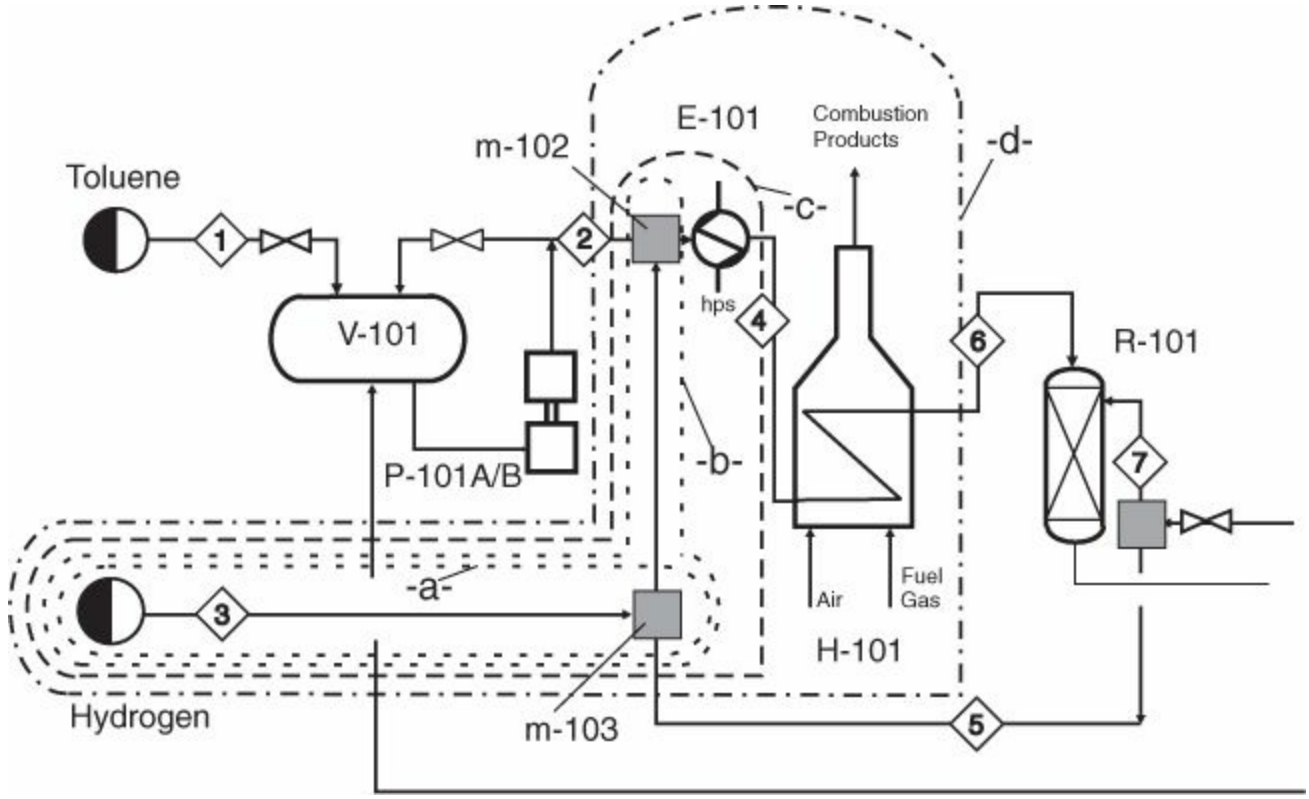


Figure E5.2(a). Tracing Primary Chemical Pathways Using the Envelope Method

Hydrogen Feed: Tactic 1 is applied to each system in a forward progression. Each system includes the hydrogen feed Stream 3, and the next piece of equipment to the right.

System -a-: This system illustrates the first step in our analysis. The system includes the first unit into which the hydrogen feed stream flows. The unidentified stream leaving mixer m-103 contains the feed hydrogen.

System -b-: Includes mixers m-103 and m-102. The exit stream for this system includes the feed hydrogen.

System -c-: Includes mixers m-103, m-102, and exchanger E-101. The exit stream for this system, Stream 4, includes the feed hydrogen.

System -d-: Includes mixers m-103, m-102, exchanger E-101, and heater H-101. The exit stream for this system, Stream 6, includes the feed hydrogen. Stream 6 goes to the reactor.

The four steps described above are illustrated in Figure E5.2(a). A similar analysis is possible for tracing methane, and the steps necessary to do this are illustrated in Figure E5.2(b). These steps are discussed briefly below.

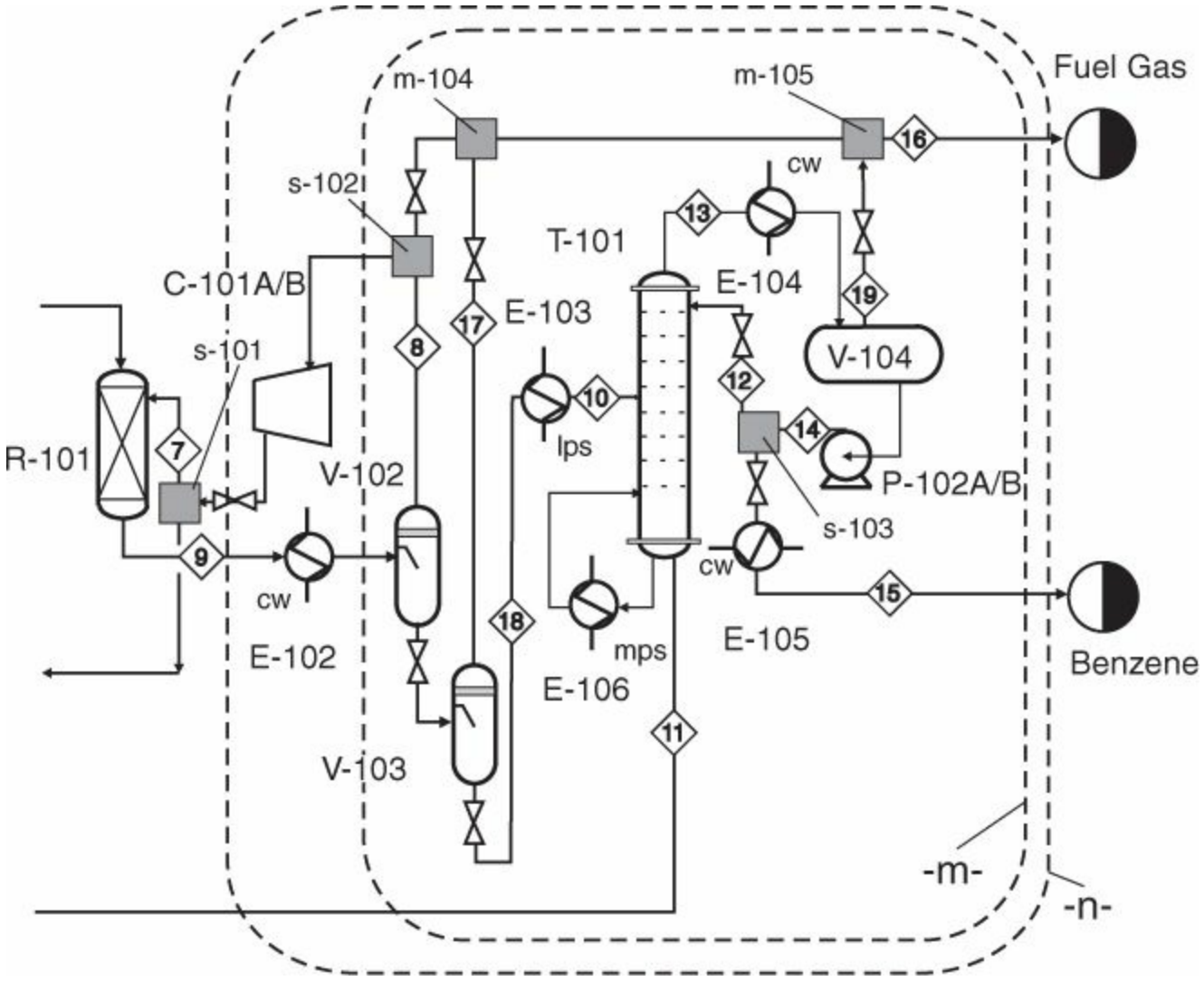


Figure E5.2(b). Tracing the Primary Flow Path for Methane in Toluene Hydrodealkylation PFD

Methane Product: The methane produced in the process leaves in the fuel gas, Stream 16. Tactic 2 is applied to each system containing the fuel gas product, in backward progression.

System -m-: Consists of m-105, m-104, E-105, T-101, V-104, P-102, s-103, E-104, E-106, E-103, V-102, V-103, and s-102. This is the smallest system that can be found that contains the fuel gas product stream and has a single input.

System -n-: Includes the system identified above plus exchanger E-102 and compressor C-101. The inlet to E-102 contains all the methane in the fuel stream. This is Stream 9, which leaves the reactor.

In the first step of tracing methane, including only m-105 was attempted. This unit had two input streams, and it was not possible to determine which of these streams carried the methane that made up the product stream. Thus, Tactic 2 could not be used. In order to move ahead, additional units were added to m-105 to create a system that had a single input stream. The resulting system, System -m-, has a single input, with the unidentified stream coming from exchanger E-102. An identical problem would arise if the procedure used in Example 5.1 were implemented. Figure 5.3 shows the primary paths for the hydrogen and methane.

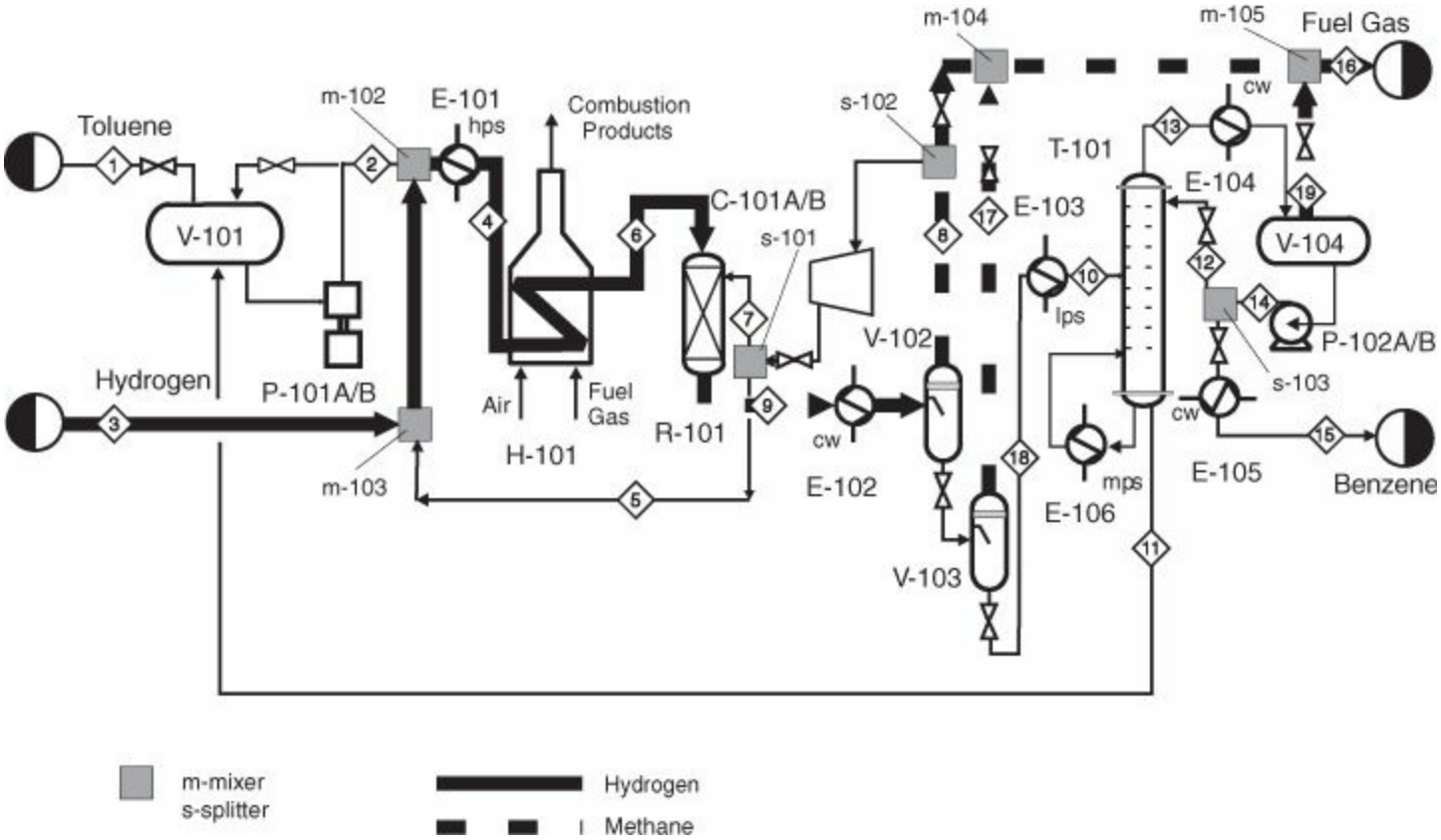


Figure 5.3. Primary Chemical Pathways for Methane and Hydrogen in the Toluene Hydrodealkylation PFD

5.3. Recycle and Bypass Streams

It is important to be able to recognize recycle and bypass streams in chemical processes. When identifying recycle and bypass streams, flow loops in the PFD are identified. Any time a flow loop is identified, either a recycle or a bypass stream exists. The direction of the streams, as indicated by the direction of the arrowheads, determines whether the loop contains a recycle or a bypass. The following tactics are applied to flow loops:

Tactic 4: If the streams in a loop flow so that the flow path forms a complete circuit back to the point of origin, then it is a **recycle loop.**

Tactic 5: If the streams in a loop flow so that the flow path does not form a complete circuit back to the place of origin, then it is a **bypass stream.**

It is worth noting that certain pieces of equipment normally contain recycle streams. In particular, distillation columns very often have top and bottoms product reflux streams, which are essentially recycle loops. When identifying recycle loops, which loops contain reflux streams and which do not can be determined easily. Example 5.3 illustrates the procedure for identifying recycle and bypass streams in the toluene hydrodealkylation PFD.

Example 5.3.

For the toluene hydrodealkylation PFD given in Figure E5.1, identify all recycle and bypass streams.

The recycle loops are identified in Figures E5.3(a) and E5.3(b). The main toluene recycle loop is highlighted in Figure E5.3(a), and the hydrogen recycle loops are shown in Figures E5.3(b)(a) and E5.3(b)(b). There are two reflux loops associated with T-101, and these are shown in Figures E5.3(b)(c) and E5.3(b)(d). Finally, there is a second toluene recycle loop identified in Figure

E5.3(b)(e).

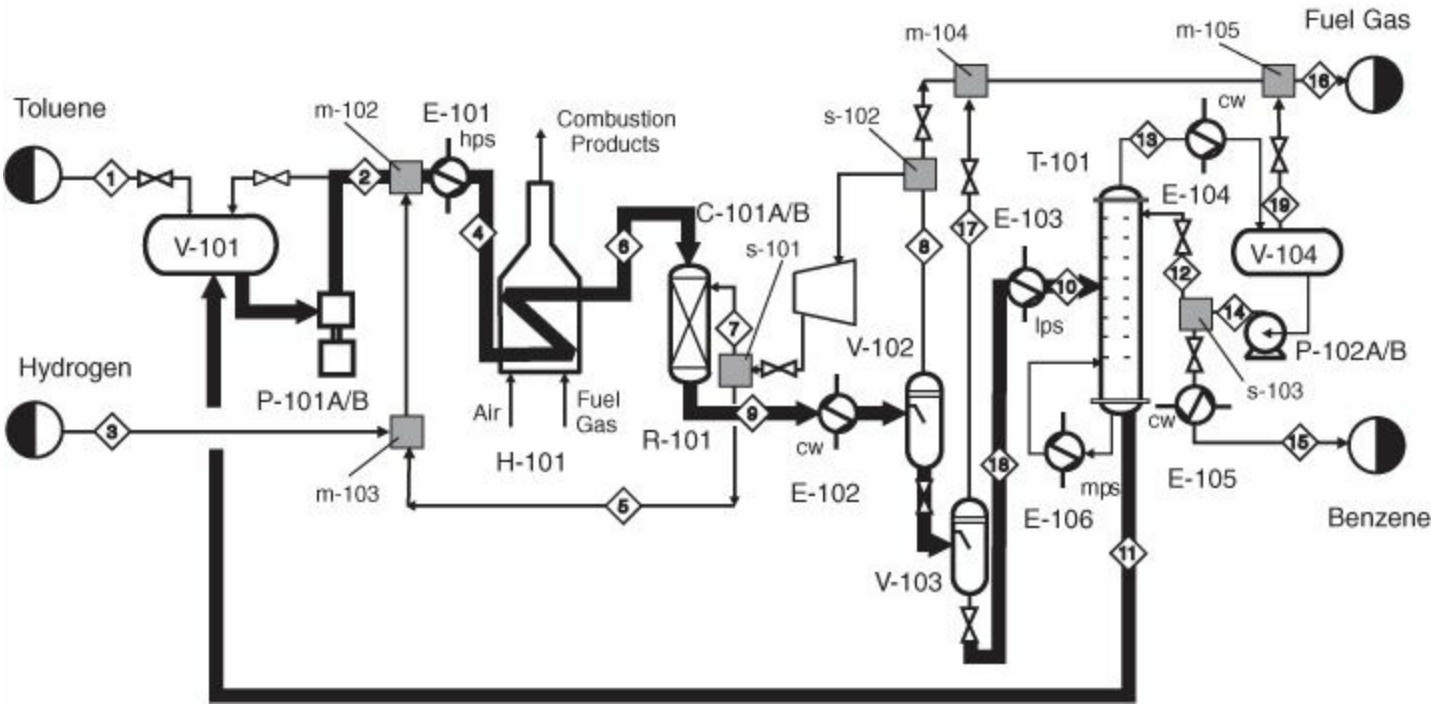


Figure E5.3(a). Identification of Toluene Recycle Loop in Toluene Hydrodealkylation PFD

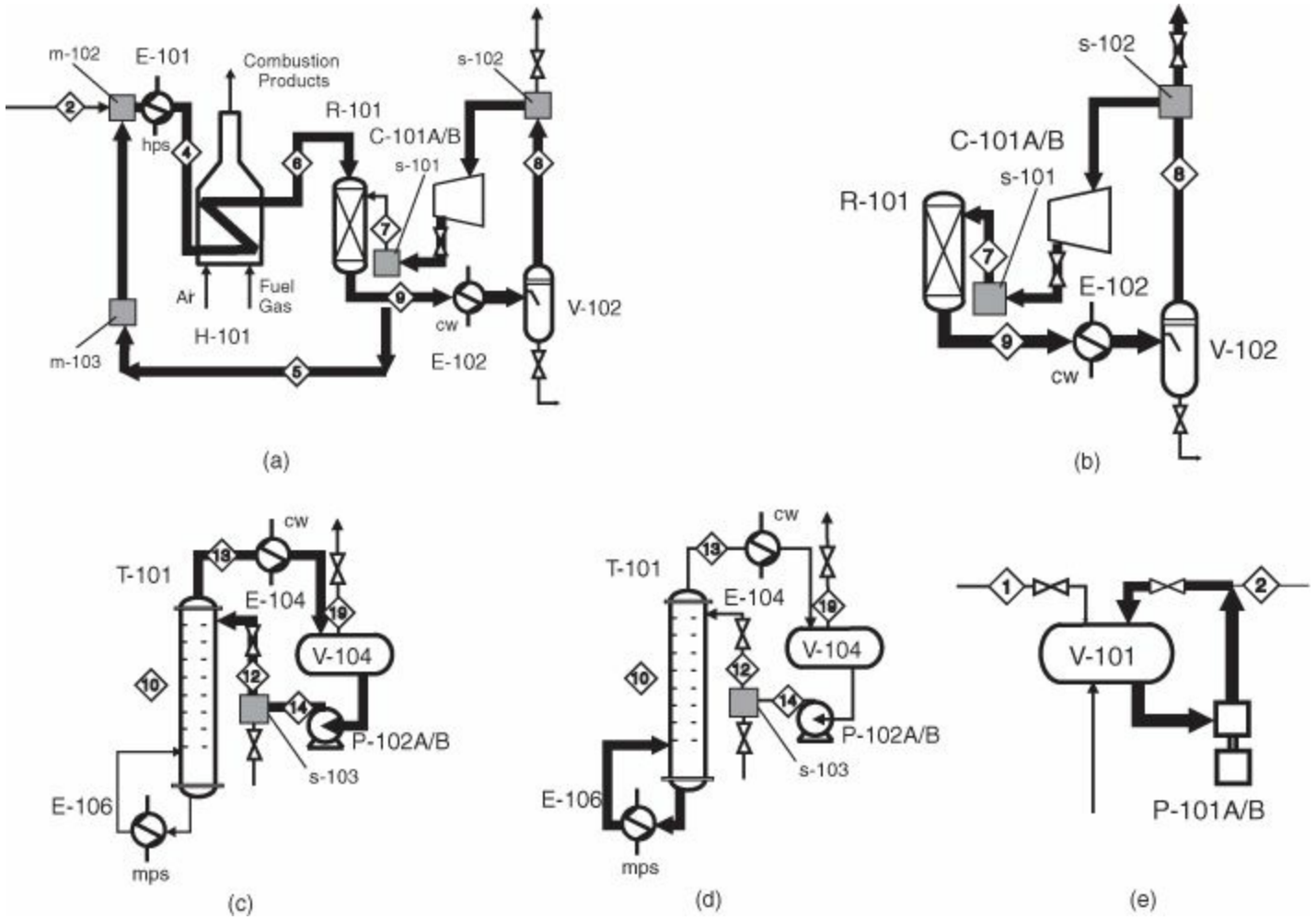


Figure E5.3(b). Identification of Other Recycle Loops in Toluene Hydrodealkylation PFD

This recycle loop is used for control purposes (see Chapter 18) and is not discussed further here. The logic used to deduce what chemical is being recycled in each loop is discussed in the next example.

The bypass streams are identified in Figure E5.3(c). These bypass streams contain mostly hydrogen

and methane and are combined to form the fuel gas stream, Stream 16.

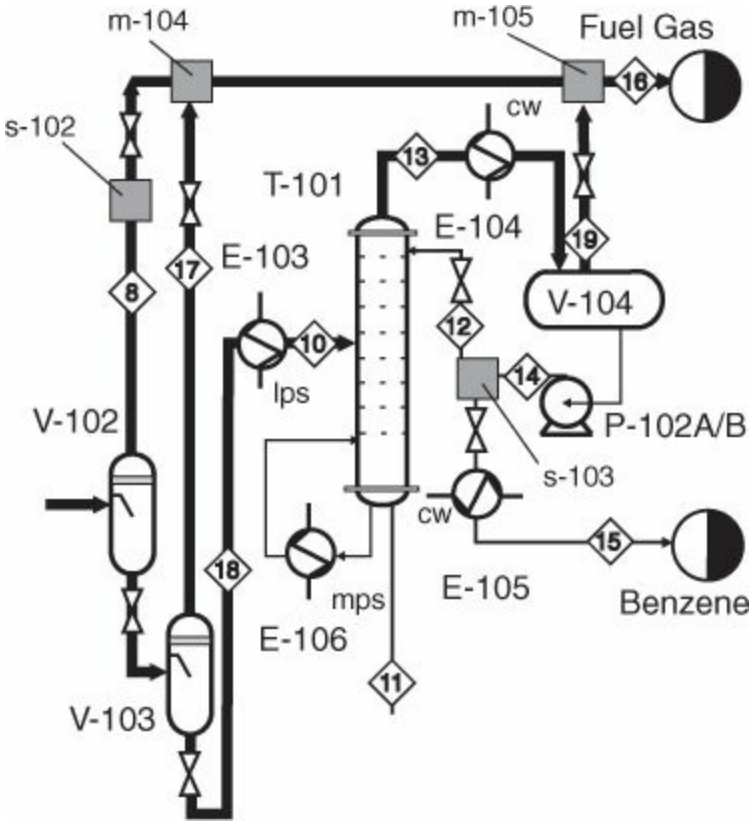


Figure E5.3(c). Identification of Bypass Streams in Toluene Hydrodealkylation PFD

It is important to remember that flow diagrams represent the most meaningful and useful documents to describe and understand a process. Although PFDs contain a lot of process information, it is sometimes necessary to apply additional knowledge about a unit operation to determine which chemicals are contained in a recycle stream. This idea is demonstrated in Example 5.4.

Example 5.4.

Provide preliminary identification of the important chemical species in each of the three recycle streams identified in Example 5.3. See Figures E5.3(a), E5.3(b)(a), and E5.3(b)(b).

Figure E5.3(a)

Stream 11: This is the bottoms product stream out of the distillation tower that provides the product benzene as distillate. The bottoms product stream must have a lower volatility than benzene. The only possible candidate is toluene. Stream 11 is essentially all toluene.

Figures E5.3(b)(a) and E5.3(b)(b)

Two undesignated streams leave splitter s-102: One stream leaves as part of a product stream and joins with other streams to form Stream 16. The other stream passes through C-101 to splitter s-101. The input and the two streams leaving s-101 have the same composition. If any of the stream compositions are known, then they are all known. In addition, methane is a reaction product and must leave the process. There are only two streams that leave the process, namely, Streams 15 and 16. Because the methane is unlikely to be part of the benzene stream, it must therefore be in the stream identified as fuel gas, Stream 16. The assumption is made that the product stream leaving is gaseous and not pure methane. If it were pure, it would be labeled methane.

The only other gas that could be present is hydrogen. Therefore, the fuel gas stream is a mixture of methane and hydrogen, and all three streams associated with s-101 have the same composition of methane and hydrogen.

The stream that leaves splitter s-102 and goes through compressor C-101 to splitter s-101 is split further into Streams 5 and 7. All streams have the same composition.

Stream 5 then mixes with additional hydrogen from Stream 3 in mixer m-103. The stream leaving m-103 contains both hydrogen and methane, but with a composition of hydrogen greater than that in the other gas streams discussed.

Finally, Stream 7, which also leaves splitter s-101, flows back to the reactor and forms the third recycle stream.

Before the analysis in Example 5.4 can be accepted, it is necessary to check out the assumption used to develop the analysis. Up to this point, the skeleton flow diagram was used, but it did not provide the important temperatures, pressures, and flowrates that are seen in the completed PFD (Figure 1.5). Figure 1.5 gives the following information for the flowrates of reactants:

Hydrogen (Stream 3): 572 kg/h (286.0 kmol/h)
Toluene (Stream 1): 10,000 kg/h (108.7 kmol/h)

Based on the information given in Table 1.5, only 108 kmol/h of hydrogen reacts to form benzene, and 178 kmol/h is excess reactant that leaves in the fuel gas. The fuel gas content is about 40 mol% methane and 60 mol% hydrogen. This confirms the assumption made in Example 5.4.

5.4. Tracing Nonreacting Chemicals

Chemical processes often contain nonreacting, or inert, compounds. These chemicals must appear in both the input and output streams and are neither created nor destroyed in the process. Unlike the reactants, it makes no difference in what direction these nonreacting chemicals are traced. They can be traced in the forward direction, the backward direction, or, starting in the middle, they can be traced in both directions. Other than this additional flexibility, the tactics provided above can be applied to all nonreacting chemicals.

5.5. Limitations

When the tracing procedure resorts to combining several unit operations into a single system that provides a single stream, the path is incomplete. This can be seen in the paths of both product streams, methane and benzene, in Figure E5.1.

> **Benzene:** The benzene flows into and out of the distillation system as the figure shows. There is no indication how it moves through the internal units consisting of V-104, s-103, E-104, E-106, and T-101.
>
> **Methane:** The methane flows into and out of a system composed of V-102, V-103, s-102, and m-104. Again, there is no indication of the methane path.

In order to determine the performance and the flows through these compound systems, you need more information than provided in the skeleton PFD, and you must know the function of each of the units.

The development given in the previous sections used only the information provided on the skeleton PFD, without the description of the unit operation, and did not include the important flows,

temperatures, and pressures that were given in the full PFD (Figure 1.5) and the flow table (Table 1.5). With this additional information and knowledge of the unit operations, you will be able to fill in some of the paths that are yet unknown.

Each step in tracing the flow paths increases our understanding of the process for the production of benzene represented in the PFD. As a last resort, reference should be made to the flow table to determine the composition of the streams, but this fails to develop analytical skills that are essential to understand the process.

5.6. Written Process Description

A process description, like a flow table, is often included with a PFD. When a description is not included, it is necessary to provide a description based upon the PFD. Based on the techniques developed in this and Chapter 1, you should be able to write a detailed description of the toluene hydrodealkylation process. Table 5.1 provides such a description. You should read this description carefully and make sure you understand it fully. It would be useful, if not essential, to refer to the PFD in Figure 1.5 during your review. It is a good idea to have the PFD in front of you while you follow the process description.

Table 5.1. Process Description of the Toluene Hydrodealkylation Process (Refer to Figures 5.3 and 1.5)

Fresh toluene, Stream 1, is combined with recycled toluene, Stream 11, in the storage tank, V-101. Toluene from the storage tank is pumped, via P-101, up to a pressure of 25.8 bar and combined with the recycled and fresh hydrogen streams, Streams 3 and 5. This two-phase mixture is then fed through the feed preheater exchanger, E-101, where its temperature is raised to 225°C, and the toluene is completely vaporized. Further heating is accomplished in the heater, H-101, where the temperature of the stream is raised to 600°C. The stream leaving the heater, Stream 6, enters the reactor, R-101, at 600°C and 25.0 bar. The reactor consists of a vertical packed bed of catalyst, down through which the hot gas stream flows. The hydrogen and toluene react catalytically to produce benzene and methane according to the following exothermic reaction:

$$\underset{\text{toluene}}{C_7H_8} + H_2 \rightarrow \underset{\text{benzene}}{C_6H_6} + CH_4$$

The reactor effluent, Stream 9, consisting of benzene and methane produced from the reaction, along with the unreacted toluene and hydrogen, is quenched in exchanger E-102, where the temperature is reduced to 38°C using cooling water. Most of the benzene and toluene condenses in E-102, and the two-phase mixture leaving this exchanger is then fed to the high-pressure phase separator, V-102, where the liquid and vapor streams are allowed to disengage.

The liquid stream leaving V-102 is flashed to a pressure of 2.8 bar and is then fed to the low-pressure phase separator, V-103. The liquid leaving V-103, Stream 18, contains toluene and benzene with only trace amounts of dissolved methane and hydrogen. This stream is heated in exchanger E-103 to a temperature of 90°C prior to being fed to the benzene purification column, T-101. The benzene column, T-101, contains 42 sieve trays and operates at approximately 2.5 bar. The overhead vapor, Stream 13, from the column is condensed using cooling water in E-104, and the condensate is collected in the reflux drum, V-104. Any methane and hydrogen in the column feed accumulates in V-104, and these noncon-densables, Stream 19, are sent to fuel gas. The condensed overhead vapor stream is fed from V-104 to the reflux pump P-102. The liquid stream leaving P-102, Stream 14, is split into two, one portion of which, Stream 12, is returned to the column to

provide reflux. The other portion of the condensed liquid is cooled to 38°C in E-105, prior to being sent to storage as benzene product, Stream 15. The bottoms product from T-101, Stream 11, contains virtually all of the toluene fed to the column and is recycled back to V-101 for further processing.

The vapor stream leaving V-102 contains most of the methane and hydrogen in the reactor effluent stream plus small quantities of benzene and toluene. This stream is split into two, with one portion being fed to the recycle gas compressor, C-101. The stream leaving C-101 is again split into two. The major portion is contained in Stream 5, which is recycled back to the front end of the process, where it is combined with fresh hydrogen feed, Stream 3, prior to being mixed with the toluene feed upstream of E-101. The remaining gas leaving C-101, Stream 7, is used for temperature control in the reactor, R-101. The second portion of the vapor leaving V-102 constitutes the major portion of the fuel gas stream. This stream is first reduced in pressure and then combined with the flashed vapor from V-103, Stream 17, and with the noncondensables from the overhead reflux drum, Stream 19. The combination of these three streams is the total fuel gas product from the process, Stream 16.

The process description should capture all the knowledge that you have developed in the last two chapters and represents a culmination of our understanding of the process up to this point.

5.7. Summary

This chapter showed how to trace many of the chemical species through a PFD, based solely upon the information shown on the skeleton PFD. It introduced operations involving splitting and mixing, not explicitly shown on the PFD, which were helpful in tracing these streams.

For situations where there was no single input or output stream, systems containing multiple unit operations were created. The tracing techniques for these compound systems did not provide the information needed to determine the internal flows for these systems. In order to determine reflux ratios for columns, for example, the process flow table must be consulted.

With the information provided, an authoritative description of the process can be prepared.

What You Should Have Learned

- Each component within a continuous chemical process can be traced.
- The tracing of chemical components is achieved using simple rules.

Problems

Identify the main reactant and product process streams for the following:

1. The ethylbenzene process shown in Figure B.2.1, Appendix B
2. The styrene production facility shown in Figure B.3.1, Appendix B
3. The drying oil production facility shown in Figure B.4.1, Appendix B
4. The maleic anhydride production process shown in Figure B.5.1, Appendix B
5. The ethylene oxide anhydride production process shown in Figure B.6.1, Appendix B
6. The formalin production process shown in Figure B.7.1, Appendix B

Identify the main recycle and bypass streams for the following:

7. The styrene production facility shown in Figure B.3.1, Appendix B
8. The drying oil production facility shown in Figure B.4.1, Appendix B
9. The maleic anhydride production process shown in Figure B.5.1, Appendix B

Write a process description for the following:

10. The ethylbenzene process shown in Figure B.2.1, Appendix B
11. The drying oil production facility shown in Figure B.4.1, Appendix B
12. The ethylene oxide production facility shown in Figure B.6.1, Appendix B

Chapter 6. Understanding Process Conditions

What You Will Learn

- There are typical ranges for process temperatures and pressures.
- There should be a reason for operating outside these ranges.

In previous chapters, process flow diagrams (PFDs) were accepted without evaluating the technical features of the process. The process topology and process operating conditions were provided but were not examined. Economic evaluations were carried out, but without confirming that the process would operate as indicated by the flow diagram.

It is not uncommon to investigate process economics based upon assumed process performance. For example, in order to justify spending the capital to develop a new catalyst, the economics of a process using a hypothetical catalyst with assumed characteristics, such as no unwanted side reactions, might be calculated.

> **The ability to make an economic analysis of a chemical process based on a PFD is not proof that the process will actually work.**

In this chapter, you will learn how to analyze the reasons why the specific temperatures, pressures, and compositions selected for important streams and unit operations have been chosen. Stream specifications and process conditions are influenced by physical processes as well as economic considerations and are not chosen arbitrarily. The conditions used in a process most often represent an economic compromise between process performance and the capital and operating costs of the process equipment. Final selection of operating conditions should not be made prior to the analysis of the process economics. In this chapter, the focus is on analyzing process conditions that require special consideration. As an example, the question of why a reactor is run at 600°C instead of 580°C is not addressed, but rather the reasons are addressed why the reactor is not run at a much lower temperature, for example, 200°C. This type of analysis leads to the question of how process conditions are chosen and what the consequences are of changing these conditions.

6.1. Conditions of Special Concern for the Operation of Separation and Reactor Systems

Process streams are rarely available at conditions most suitable for reactor and separation units. Temperatures, pressures, and stream compositions must be adjusted to provide conditions that allow effective process performance. This is discussed in Chapter 2, where the generic BFD was introduced (see Figure 2.4[a]). This figure showed two feed preparation blocks: one associated with the reactor and the second with the separation section.

Two generalizations are provided to assist in analyzing and understanding the selection of process conditions.

- It is usually easier to adjust the temperature and/or pressure of a stream than it is to change its composition. In fact, often the concentration of a compound in a stream (for a gas) is a dependent

variable and is controlled by the temperature and pressure of the stream.

- In general, pressures between 1 and 10 bar and temperatures between 40°C and 260°C do not cause severe processing difficulties.

The rationale for the conditions given in the second generalization are explained below.

6.1.1. Pressure

There are economic advantages associated with operating equipment at greater than ambient pressure when gases are present. These result from the increase in gas density and a decrease in gas volume with increasing pressure. All other things being equal, in order to maintain the same gas residence time in a piece of equipment, the size of the equipment through which the gas stream flows need not be as large when the pressure is increased.

Most chemical processing equipment can withstand pressures up to 10 bar without much additional capital investment (see the cost curves in Appendix A). At pressures greater than 10 bar, thicker-walled, more expensive equipment is necessary. Likewise, operating at less than ambient pressure (vacuum conditions) tends to make equipment large and may require special construction techniques, thus increasing the cost of equipment.

A decision to operate outside the pressure range of 1 to 10 bar must be justified.

6.1.2. Temperature

There are several critical temperature limits that apply to chemical processes. At elevated temperatures, common construction materials (primarily carbon steel) suffer a significant drop in physical strength and must be replaced by more costly materials. This drop in strength with temperature is illustrated in Example 6.1.

Example 6.1.

The maximum allowable tensile strengths for typical carbon steel and stainless steel at ambient temperature, 400°C, and 550°C are provided below (Walas [1]).

	Tensile Strength of Material at Temperature Indicated (bar)		
Temperature	**Ambient**	**400°C**	**550°C**
Carbon Steel (grade 70)	1190	970	170
Stainless Steel (Type 302)	1290	1290	430

Determine the fractional decrease in the maximum allowable tensile strength (relative to the strength at ambient conditions) for the temperature intervals (a) ambient to 400°C and (b) 400°C to 550°C.

a. Interval: ambient to 400°C:

Carbon Steel: (1190–970)/1190 = 0.18

Stainless Steel: (1290–1290)/1290 = 0.0

b. Interval: 400°C to 550°C:

Carbon Steel: (970–170)/1190 = 0.67

Stainless Steel: (1290–430)/1290 = 0.67

Example 6.1 has shown that carbon steel suffers a loss of 18%, and stainless steel suffers no loss in tensile strength, when heated to 400°C. With an additional temperature increase of 150°C to 550°C, stainless steel suffers a 67% loss while carbon steel suffers an additional 67% loss in strength. At operating temperatures of 550°C, carbon steel has a maximum allowable tensile strength of about 15% of its value at ambient conditions. For stainless steel, the maximum allowable strength at 550°C is about 33% of its ambient value. For this example, it is clear that carbon steel is unacceptable for service temperatures greater than 400°C, and that the use of stainless steel is severely limited. For higher service temperatures, more exotic (and expensive) alloys are required and/or equipment may have to be refractory lined.

A decision to operate at greater than 400°C must be justified.

Thus, if higher temperatures are specified, a justification must be found for the economic penalty associated with more complicated processing equipment, such as refractory-lined vessels or expensive materials of construction. In addition to the critical temperature of 400°C, there are temperature limits associated with the availability of common utilities for heating and cooling a process stream.

Steam: High-pressure steam between 40 and 50 bar is commonly available and provides heat at 250 to 265°C. Above this temperature additional costs are involved.

Water: Water from a cooling tower is commonly available at about 30°C (and is returned to the cooling tower at around 40°C). For utilities below this temperature, costs increase due to refrigeration. As the temperature decreases, the costs increase dramatically (see Table 8.3).

If cryogenic conditions are necessary, there may be an additional need for expensive materials of construction.

A decision to operate outside the range of 40°C to 260°C, thus requiring special heating/cooling media, must be justified.

6.2. Reasons for Operating at Conditions of Special Concern

When you review the PFD for different processes, you are likely to encounter conditions in reactors and separators that lie outside the temperature and pressure ranges presented in Section 6.1. This does not mean to say that these are “bad” processes, but rather that these conditions had to be used, despite the additional costs involved, to have the process operate effectively. These conditions, outside the favored temperature and pressure ranges, are identified as **conditions of special concern.**

When you encounter these conditions, you should seek a rational explanation for their selection. If no explanation can be identified, the condition used may be unnecessary. In this situation, the condition may be changed to a less severe one that provides an economic advantage.

A list of possible justifications for using temperature and pressure conditions outside the ranges given above are identified in Tables 6.1 through 6.3. The material provided in Tables 6.1 to 6.3 is based upon elementary concepts presented in undergraduate texts covering thermodynamics and reactor design.

Table 6.1. Possible Reasons for Operating Reactors and Separators Outside the Temperature Ranges of Special Concern

Stream Condition	Process Justification for Operating at This Condition	Penalty for Operating at This Condition
High Temperature [$T > 250°C$]	**Reactors** • Favorable equilibrium conversion for endothermic reactions • Increase reaction rates • Maintain a gas phase • Improve selectivity • • **Separators** • Obtain a gas phase required for vapor-liquid equilibrium • •	• Use of special process heaters • $T > 400°C$ requires special materials of construction • • •
Low Temperature [$T < 40°C$]	**Reactors** • Favorable equilibrium conversion for exothermic reactions • Temperature-sensitive materials • Improve selectivity • Maintain a liquid phase • • **Separators** • Obtain a liquid phase required for vapor-liquid or liquid-liquid equilibrium • Obtain a solid phase for crystallization • Temperature-sensitive materials • •	• Uses expensive refrigerant • May require special materials of construction for very low temperatures • • •

Table 6.2. Possible Reasons for Operating Reactors and Separators Outside the Pressure Range of Special Concern

Stream Condition	Process Justification for Operating at This Condition	Penalty for Operating at This Condition
High Pressure ($P > 10$ bar)	**Reactors** • Favorable equilibrium conversion • Increase reaction rates for gas-phase reactions (due to higher concentration) • Maintain a liquid phase • • **Separators** • Obtain a liquid phase for vapor-liquid or liquid-liquid equilibrium • •	• Requires thicker-walled equipment • Requires expensive compressors if gas streams must be compressed • • •
Low Pressure ($P < 1$ bar)	**Reactors** • Favorable equilibrium conversion • Maintain a gas phase • • **Separators** • Obtain a gas phase for vapor-liquid equilibrium • Temperature-sensitive materials • •	• Requires large equipment • Special design for vacuum operation • Air leaks into equipment that may be dangerous and expensive to prevent • • •

Table 6.3. Possible Reasons for Non-stoichiometric Reactor Feed Compositions of Special Concern

Stream Condition	Process Justification for Operating at This Condition	Penalty for Operating at This Condition
Inert Material in Feed to Reactor	• Acts as a diluent to control the rate of reaction and/or to ensure that the reaction mixture is outside the explosive limits (exothermic reactions) • Inhibits unwanted side reactions • •	• Causes reactor and downstream equipment to be larger since inert takes up space • Requires separation equipment to remove inert material • May cause side reactions (material is no longer inert) • Decreases equilibrium conversion • •
Excess Reactant	• Increases the equilibrium conversion of the limiting reactant • Inhibits unwanted side reactions • •	• Requires separation equipment to remove excess reactant • Requires recycle • Added feed material costs (due to losses in separation and/or no recycle) • •
Product Present in Feed to Reactor	• Product cannot easily be separated from recycled feed material. • Recycled product retards the formation of unwanted by-products formed from side reactions. • Product acts as a diluent to control the rate of reaction and/or to ensure that the reaction mixture is outside the explosive limits, for exothermic reactions. • •	• Causes reactor and downstream equipment to be larger • Requires larger recycle loop • Decreases equilibrium conversion • •

The rationale used to justify operating at temperatures that are of special concern and that are presented in Table 6.1 is given in the following list. The justification for entries in Tables 6.2 and 6.3 has a similar rationale.

For chemical reactors, possible justifications for operating at conditions of special concern are as follows.

1. **Favorable Equilibrium Conversion:** If the reaction is endothermic and approaches equilibrium, it benefits from operating at high temperatures. Le Chatelier's principle states that "for a reacting system at equilibrium, the extent of the reaction will change so as to oppose any changes in temperature or pressure." For an endothermic reaction, an increase in temperature tends to push the reaction equilibrium to the right (toward products). Conversely, low temperatures decrease the equilibrium conversion.
2. **Increase Reaction Rates:** All chemical reaction rates are strongly dependent upon

temperature through an Arrhenius type equation:

$$k_{reaction} = k_0 e^{-\frac{E_{act}}{RT}} \qquad (6.1)$$

As temperature increases, so does the reaction rate constant, $k_{reaction}$, for both catalytic and noncatalytic reactions. Therefore, temperatures greater than 250°C may be required to obtain a high enough reaction rate in order to keep the size of the reaction vessel reasonable.

3. **Maintain a Gas Phase:** Many catalytic chemical reactions used in processes today require both reactants and products to be in the gas phase. For high-boiling-point materials or operations where high pressure is used, a temperature in excess of 400°C may be required in the reactor in order to maintain all the species in the vapor phase.
4. **Improve Selectivity:** If competing reactions (series, parallel, or a combination of both) occur and the different reactions have different activation energies, then the production of the desired product may be favored by using a high temperature. Schemes for competing reactions are covered in greater detail in many of the well known texts on chemical reaction engineering, as well as in Chapter 23.

For separators, the following item of justification is presented:

1. **Obtain a Vapor Phase for Vapor-Liquid Equilibrium:** This situation arises quite frequently when high-boiling-point materials need to be distilled. An example is the distillation of crude oil in which the bottom of the atmospheric column is typically operated in the region of 310°C to 340°C (590°F to 645°F).

You would benefit by spending time to acquaint yourself with the information presented in Tables 6.1 to 6.3 and to convince yourself that you understand the justifications given in these tables. These tables should not be considered an exhaustive list of possible reasons for operating in the ranges of special concern. Instead, they represent a starting point in analyzing process conditions. As you discover other explanations for reasons to operate equipment in the ranges of special concern you may wish to add them to Tables 6.1–6.3. Additional blank entries are provided for this purpose.

6.3. Conditions of Special Concern for the Operation of Other Equipment

Additional equipment (such as pumps, compressors, heaters, exchangers, and valves) produces the temperature and pressure required by the feed streams entering the reactor and separation sections. When initially choosing the stream conditions for the reactor and separator sections, it is worthwhile using certain guidelines or heuristics. These technical heuristics are useful guidelines for doing design. Comprehensive lists of heuristics are described and applied in Chapter 11. In this chapter, some of the more general guidelines that apply to streams passing through process equipment are presented. These are presented in Table 6.4. Some of these guidelines are explored in Example 6.2.

Table 6.4. Changes in Process Conditions That Are of Special Concern for a Stream Passing through a Single Piece of Equipment

Type of Equipment	Change in Stream Condition Causing Concern	Justification or Remedy	Penalty for Operating Equipment in This Manner
1. Compressors	$P_{out}/P_{in} > 3$	**Remedy:** Use multiple stages and intercoolers.	High theoretical work requirement due to large temperature rise of gas stream.
	High-temperature inlet gas	**Remedy:** Cool the gas before compression.	High theoretical work requirement and special construction materials required.
2. Heat Exchangers	$\Delta T_{lm} > 100°C$	**Remedy:** Integrate heat better within process (see Chapter 15).	Large temperature driving force means that valuable high-temperature energy is wasted.
		Justification: Heat integration not possible or not profitable.	
3. Process Heaters	$T_{out} < T_{steam\ available}$	**Remedy:** Use high-pressure steam to heat process stream.	Process heaters are expensive and unnecessary if heating can be accomplished by using an available utility.
		Justification: Heater may be needed during start-up.	
4. Valves	Large ΔP across valve	**Remedy:** For gas streams install a turbine to recover lost work.	Wasteful expenditure of energy due to throttling.
		Justification: (a) Valve used for control purposes. (b) Installation of turbine not profitable. (c) Liquid is being throttled.	
5. Mixers (Streams Mixing)	Streams of greatly differing temperatures mix	**Remedy:** Bring temperatures of streams closer together using heat integration.	Wasteful expenditure of high-temperature energy.
	Streams of greatly differing composition mix	**Justification:** (a) Quenching of reaction products. (b) Provides driving force for mass transfer.	Causes extra separation equipment and cost.

Example 6.2.

It is necessary to provide a nitrogen stream at 80°C and a pressure of 6 bar. The source of the nitrogen is at 200°C and 1.2 bar. Determine the work and cooling duty required for three alternatives.

a. Compress in a single compression stage and cool the compressed gas.

b. Cool the feed gas to 80°C and then repeat Part (a).

c. Repeat Part (b), except use two stages of compression with an intercooler.

d. Identify any conditions of special concern that occur.

Nitrogen can be treated as an ideal diatomic gas for this comparison. Use as a basis 1 kmol of nitrogen and assume that the efficiency, ε, of each stage of compression is 70%.

For ideal diatomic gas: $C_p = 3.5R$, $C_v = 2.5R$, $\gamma = C_p/C_v = 1.4$, $R = 8.314$ kJ/kmol K, and assuming an efficiency, $\varepsilon = 0.70$

$$\text{Equations used: } q = C_p\Delta T,\ w = RT_{in}\gamma/(\gamma-1)[(P_{out}/P_{in})^{(\gamma-1)/\gamma}-1]/\varepsilon,$$

$$T_{out} = T_{in}\left(1+\frac{1}{\varepsilon}[(P_{out}/P_{in})^{(\gamma-1)/\gamma}-1]\right)$$

Figure E6.2 gives the process flow diagrams for the three alternatives and identifies stream numbers and utilities.

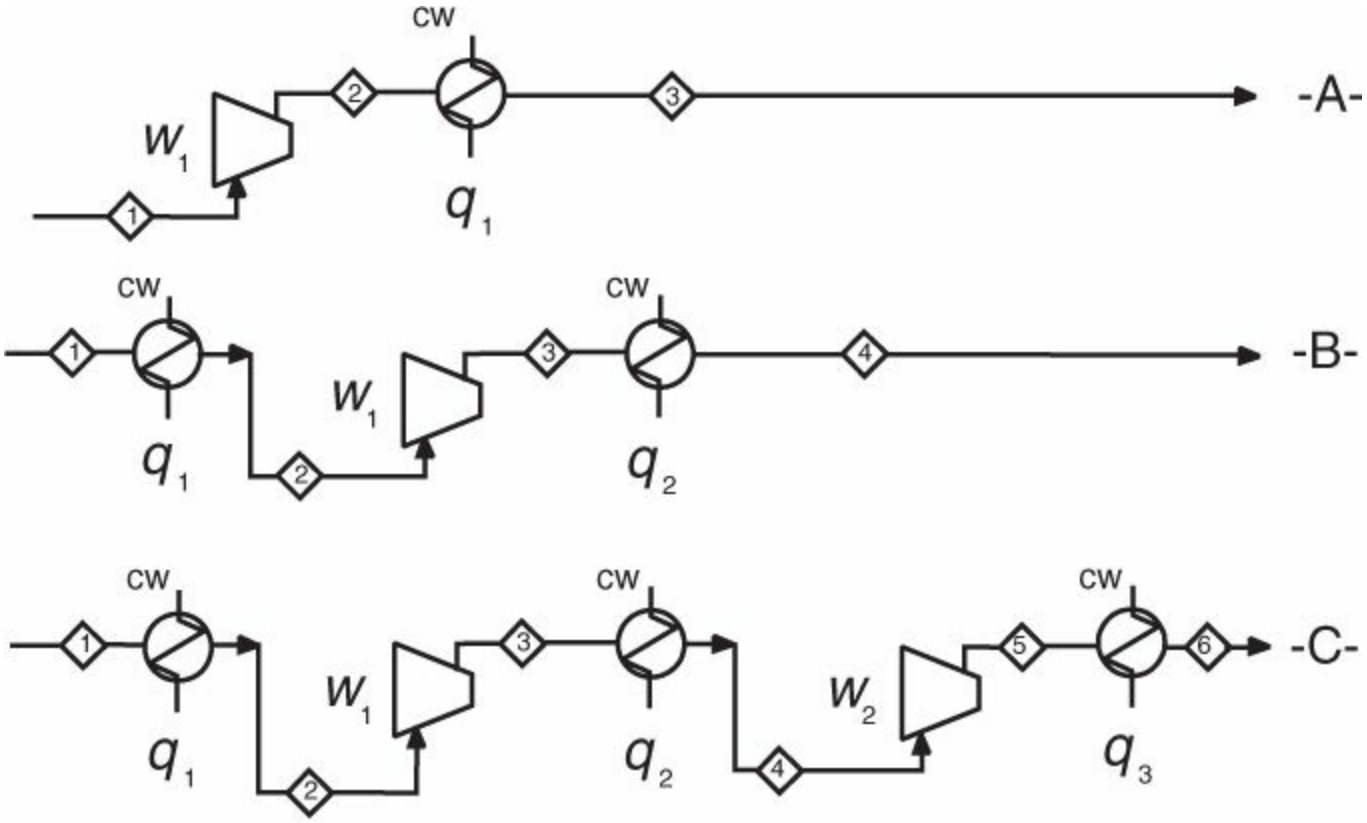


Figure E6.2. Alternative Process Schemes for Compression of Nitrogen

The results of the calculations for Parts (a), (b), and (c) are provided in Table E6.2, which shows stream conditions and utility requirements. To keep the calculations simple, the pressure drops across and between equipment have been ignored.

Table E6.2. Flow Summary Table for Example 6.2 and Figure E6.2

Stream Number in Figure E6.2	System -A-		System -B-		System -C-	
	T(°C)	P(bar)	T(°C)	P(bar)	T(°C)	P(bar)
1	200	1.2	200	1.2	200	1.2
2	595	6.0	80	1.2	80	1.2
3	80	6.0	374	6.0	210	2.68
4	—	—	80	6.0	80	2.68
5	—	—	—	—	210	6.0
6	—	—	—	—	80	6.0
Work: kJ/kmol						
w_1	11,470		8560		3780	
w_2	—		—		3780	
w_{total}	11,470		8560		7560	
Heat: kJ/kmol						
q_1	14,970		3490		3490	
q_2	—		8550		3780	
q_3	—		—		3780	
q_{total}	14,970		12,040		11,050	

Part (d): Alternative -A- requires a compressor exit temperature of 595°C, which is a condition of special concern. Note also that although the intermediate temperature of the gas (stream) in Alternative -B- was 374°C, because this stream is to be cooled there are no concerns about utility requirements.

Example 6.2 showed three alternatives of differing complexity for achieving the same final conditions. The amount of work (w) and cooling utilities (q) required for each alternative were calculated. Based solely upon process complexity, Alternative -A- is the most desirable. However, this alternative has several disincentives that should be considered before final selection:

1. The highest electric utility demand and cost (assuming that the compressor is electrically driven)
2. The highest cooling utility demand and cost
3. A condition of special concern, that is, T > 400°C (see Table 6.1)

   Note: Compressors are high-speed rotating devices where the loss of material strength and thermal expansion is critical. It would be expected that the purchase cost of the compressor would undergo a quantum jump for high-temperature operations.
4. Exceeds the 3/1 pressure ratio provided as a guideline (see Table 6.4)

Alternative -B- is more complex than Alternative -A- because it requires an additional heat exchanger, but it avoids the condition of special concern in item 3. The result of using this extra exchanger is a significant decrease in utilities over Alternative -A-. As a result, it is likely that

Alternative -B- would be preferred to Alternative -A-.

Alternative -C- requires an extra stage of compression and an additional cooler before the second compressor, something that is not required by Alternative -B-. However, Alternative -C- results in an additional savings in utilities over Alternative -B-.

The qualitative analysis given above suggests that both Alternatives -B- and -C- are superior to Alternative -A-. This conclusion is consistent with the two heuristics for compressors in Table 6.4: It is better to cool a hot gas prior to compressing it, and it is usually desirable to keep the compression ratio less than 3:1. Before a final selection is made, an economic analysis, which must include both the capital investment and the operating costs, should be carried out on each of the competing schemes. The equivalent annual operating cost (EAOC), described in Chapter 10, would be a suitable criterion to make such a comparison.

You should review the information given in Table 6.4 and convince yourself that you understand the rules, along with the penalties, remedies, and justifications, for operating equipment under these conditions. You may also be able to provide additional reasons why operating the equipment in this way would be justified. You should add these reasons to the list provided along with additional heuristics that are uncovered as you work problems and gain experience.

6.4. Analysis of Important Process Conditions

In this section, the focus is to analyze and to justify the conditions of special concern found in a process flow diagram. To help with this analysis, it is beneficial to prepare a process conditions matrix (PCM). In the PCM, all the equipment is listed vertically and the conditions of special concern are listed horizontally. Each unit is reviewed for conditions of special concern, and a check mark is used to identify which pieces of equipment have been identified. The PCM for the toluene hydrodealkylation process is shown in Table 6.5. The information for this PCM was obtained from Chapter 1, and you should verify that none of the areas of special concern have been missed.

Table 6.5. Process Conditions Matrix for the PFD of the Toluene Hydrodealkylation Process Shown in Figure 1.5

Equipment	Reactors and Separators Tables 6.1–6.3					Other Equipment Table 6.4				
	High Temp	*Low Temp*	*High Pres.*	*Low Pres.*	*Non-Stoich. Feed*	*Comp*	*Exch.*	*Htr.*	*Valve*	*Mix*
R-101	X		X		X					
V-101										
V-102			X							
V-103										
V-104										
T-101										
H-101										
E-101							X			
E-102							X			
E-103										
E-104										
E-105										
E-106										
C-101										
P-101										
P-102										
PCV on Stream 8									X	
PCV on Stream from V-101 to V-103									X	

The special conditions identified in Table 6.5 are now considered and justified.

6.4.1. Evaluation of Reactor R-101

Three conditions of concern have been identified for the reactor. They are high temperature, high pressure, and non-stoichiometric feed conditions.

In order to understand why these conditions are needed, additional information about the toluene hydrodealkylation reaction is required. Table 6.6 provides additional but limited information. This information is divided into two groups.

Table 6.6. Equilibrium and Reaction Kinetics Data for the Toluene Hydrodealkylation Process

Reaction Stoichiometry

$$\underset{\textit{toluene}}{C_6H_5CH_3} + H_2 = \underset{\textit{benzene}}{C_6H_6} + CH_4$$

Equilibrium Constant (T is in units of K)

$$\ln(K_p) = 13.51 + \frac{5037}{T} - 2.073\ln(T) + 3.499 \times 10^{-4}T + 4.173 \times 10^{-8}T^2 + \frac{3017}{T^2}$$

Heat of Reaction

$$\Delta H_{reaction} = -37{,}190 - 17.24T + 29.09 \times 10^{-4}T^2 + 0.6939 \times 10^{-6}T^3 + \frac{50{,}160}{T} \quad \frac{\text{kJ}}{\text{kmol}}$$

At the Reaction Conditions of 600°C (873 K)

Equilibrium Constant, $K_p = 265$

Heat of Reaction, $\Delta H_{reaction} = -49{,}500 \quad \frac{\text{kJ}}{\text{kmol}}$

Information on Reaction Kinetics

No side reactions

Reaction is kinetically controlled

Thermodynamic Information: This is information found in most chemical engineering thermodynamic textbooks:

a. Information required to perform energy balances, including heats of reaction and phase change, heat capacities, and so on

b. Information required to determine equilibrium conversion, including heats of formation, free energy of formation, and so on

Figure 6.1 is a plot of the heat of reaction and the equilibrium constant as a function of temperature, evaluated from the information provided in Table 6.6. From these plots it is evident that the chemical reaction is slightly exothermic, causing the equilibrium constant to decrease with temperature.

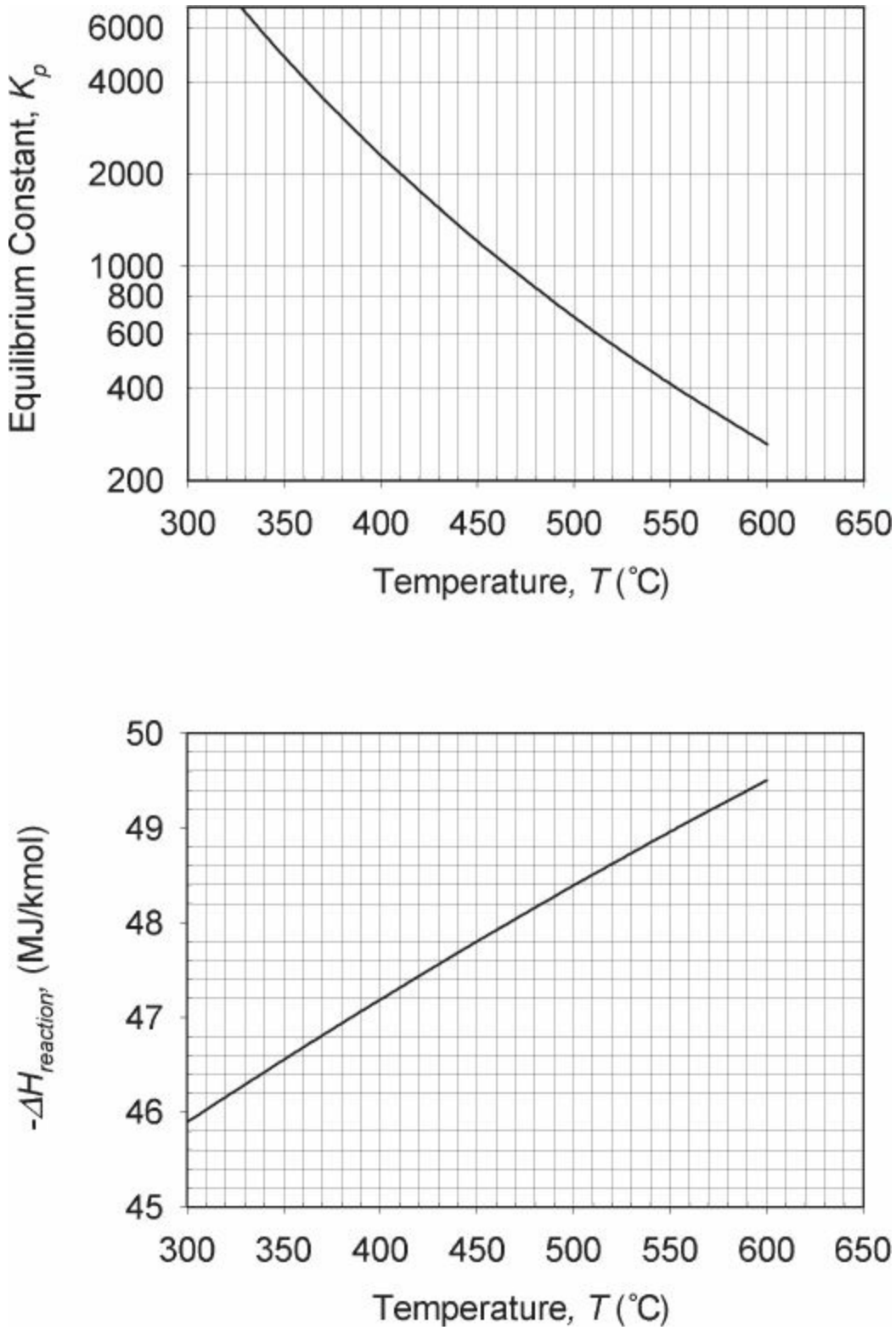


Figure 6.1. Equilibrium Constant and Heat of Reaction as a Function of Temperature for the Toluene Hydrodealkylation Reaction

Reaction Kinetics Information: This information is reaction specific and must be obtained experimentally. The overall kinetics may involve homogeneous and heterogeneous reactions both catalytic and noncatalytic. The expressions are often complex.

Before a process is commercialized, reaction kinetics information, such as space velocity and residence times, must be obtained for different temperatures and pressures from pilot plant studies. Such data are necessary to design the reactor. At this point, the specific details of the reactor design are not of interest, and hence specific kinetics expressions have not been included in Table 6.6 and are not necessary for the following analysis.

The analysis of the reactor takes place in two parts.

a. Evaluation of the special conditions from the thermodynamic point of view. This assumes that chemical equilibrium is reached and provides a limiting case.

b. Evaluation of the special conditions from the kinetics point of view. This accounts for the limitations imposed by reaction kinetics, mass transfer, and heat transfer.

If a process is unattractive under equilibrium (thermodynamic) conditions, analysis of the kinetics is not necessary. For processes in which the equilibrium conditions give favorable results, further study is necessary. The reason for this is that conditions that favor high equilibrium conversion may be unfavorable from the standpoint of reaction kinetics.

Thermodynamic Considerations. The use of high-temperature, high-pressure, and non-stoichiometric feed conditions are considered separately.

High-Temperature Concern (see Table 6.1). Figure 6.1 provided the important information that the reaction is exothermic. Table 6.1 notes that for an exothermic reaction, the result of increasing temperature is a reduction in equilibrium conversion. This is confirmed by the plot of the equilibrium constant versus temperature given in Figure 6.1. The decrease in the equilibrium conversion is undesirable. The actual conversion for the HDA process is compared with the equilibrium conversion in Example 6.3.

Example 6.3.

For the PFD presented in Figure 1.5,

a. Calculate the actual conversion.

b. Evaluate the equilibrium conversion at 600°C.

Assuming ideal gas behavior: $K_p = (N_{benzene}\, N_{methane})/(N_{toluene}\, N_{hydrogen})$

where N represents the moles of each species at equilibrium.

Information on the feed stream to the reactor from Table 1.5 (Stream 6 on Figure 1.5):

Hydrogen	735.4 kmol/h
Methane	317.3
Benzene	7.6
Toluene	144.0
Total	1204.3

c. Actual Conversion: Toluene in exit stream (Stream 9) = 36 kmol/h

Conversion = (144 – 36)/144 = 0.75 (75%)

d. Equilibrium Conversion at 600°C. From Table 6.6 at 600°C $K_p = 265$

Let N = kmol/h of benzene formed

$265 = [(N + 7.6)(N + 317.3)]/[(735.4 - N)(144 - N)]$

$N = 143.6$

Equilibrium Conversion = 143.6/144 = 0.997 (99.7%)

The equilibrium conversion for the hydrodealkylation reaction remained high in spite of the high temperature. Although there is no real problem with using the elevated temperature in the reactor, it

cannot be justified from a thermodynamic point of view.

High-Pressure Concern (see Table 6.2). From the reaction stoichiometry, it can be seen that there are equal numbers of reactant and product moles in the hydrodealkylation reaction. For this case, there is no effect of pressure on equilibrium conversion. From a thermodynamic point of view there is no reason for the high pressure in the reactor.

Non-stoichiometric Feed (see Table 6.3). The component feed rates to the reactor (see Example 6.3) show that

1. Toluene is the limiting reactant.
2. Hydrogen is an excess reactant (more than 400% excess).
3. Methane, a reaction product, is present in significant amounts.

Reaction Products (Methane) in Feed. The presence of reaction product in the feed results in a reduction in the equilibrium conversion (see Table 6.3). However, Example 6.3 shows that at the conditions selected for the reactor, the equilibrium conversion remained high despite the presence of the methane in the feed.

Excess Reactant (Hydrogen) in Feed. The presence of excess reactants in the feed results in an increase in equilibrium conversion (see Table 6.3). Example 6.4 explores the effect of this excess hydrogen on conversion.

Example 6.4.

(Reference Example 6.3.) Reduce the amount of hydrogen in the feed to the reactor to the stoichiometric amount—that is, 144 kmol/h—and determine the effect on the equilibrium conversion at 600°C.

The calculations are not shown. They are similar to those in Example 6.3(b). The total moles of hydrogen in the feed were changed from 735.4 kmol/h to the stoichiometric value of 144 kmol/h.

The results obtained were $N = 128.8$ kmol/h, equilibrium conversion = 0.895 (89.5%).

Example 6.4 reveals that the presence of the large excess of hydrogen had a noticeable effect on the equilibrium conversion.

It is concluded that thermodynamic considerations do not explain the selection of the high temperature, the high pressure, and the presence of reaction products in the feed. The presence of a large excess of hydrogen is the only positive effect predicted by thermodynamics.

Consideration of Reaction Kinetics. The information on reaction kinetics is limited in this chapter. A more detailed description of the kinetics rate expression will be given in a case study in Chapter 23, and the predictions made in this chapter with this limited information will be investigated further. However, you will find that a great deal of understanding can be extracted from the limited information presented here.

From the information provided in Table 6.6 and Chapter 1 the following is known:

1. The reaction takes place in the gas phase.

2. The reaction is kinetically controlled.
3. There are no significant side reactions.

High-Temperature Concern (see Table 6.1). In a region where the reaction kinetics control, the reaction rate increases rapidly with temperature, as Example 6.5 illustrates.

Example 6.5.

The activation energy for the rate of reaction for the hydrodealkylation of toluene is equal to 148.1 kJ/mol (Tarhan [2]). What is the reaction rate at 600°C relative to that at 400°C?

$$\text{Ratio of Reaction Rates} = \exp[-E/R\{1/T_2 - 1/T_1\}]$$
$$= \exp[148100/8.314\{1/673 - 1/873\}] = 430$$

The size of a reactor would increase by nearly three orders of magnitude if the reaction were carried out at 400°C (the critical temperature for materials selection, Table 6.1) rather than 600°C. Clearly the effect of temperature is significant.

Most reactions are not kinetically controlled as is the case here. In most cases the rate is controlled by heat or mass transfer considerations. These are not as sensitive to temperature changes as chemical reaction rates. For more detail, see Chapter 23.

High-Pressure Concern (see Table 6.2). For gas-phase reactions, the concentration of reactants is proportional to the pressure. For a situation where the reaction rate is directly proportional to the concentration, operation at 25 bar rather than at 1 bar would increase the reaction rate by a factor of 25 (assuming ideal gas behavior). Although it is not known that the rate is directly proportional to the concentration, it can be predicted that the effect of pressure is likely to be substantial, and the reactor size will be substantially reduced.

Non-stoichiometric Feed (see Table 6.3). The reactor feed contains both excess hydrogen and the reaction product methane.

Methane in the Feed. The effect of methane is to reduce the reactant concentrations. This decreases the reaction rate and represents a negative impact. The methane could possibly reduce the formation of side products, but there is no information to suggest that this is the case.

Excess Hydrogen in the Feed. The large amount of excess hydrogen in the feed ensures that the concentration of hydrogen will remain large throughout the reactor. This increases the reaction rate. Although there is no information provided regarding the decision to maintain the high hydrogen levels, it may be linked to reducing the formation of side products.

With the exception of the presence of methane product in the feed, the high-temperature operation, the excess hydrogen, and the elevated pressure all support an increase in reaction rate and a reduction in reactor volume. This suggests that the catalyst is not "hot"—that is, the catalyst is still operating in the reaction-controlled regime and mass transfer effects have not started to intrude. For these conditions, the manipulation of temperatures and pressures is essential to limit the reactor size.

There is a significant economic penalty for using more than 400% excess hydrogen in the reactor feed. The raw material cost of hydrogen would be reduced significantly if excess hydrogen were not

used. The fact that this large excess is used in spite of the economic penalty involved suggests that the hydrogen plays an important role in the prevention of side products. The concept of selectivity is discussed further in Chapter 23.

The presence of methane in the feed has not yet been resolved. At best it behaves as an inert and occupies volume that must be handled downstream of the reactor, thus making all the equipment larger and more expensive. This question is considered in more detail in Example 6.6.

Example 6.6.

It has been proposed that the hydrogen/methane stream is handled in the same manner as was the toluene/benzene stream. Recall that the unreacted toluene was separated from the benzene product and then recycled. It is proposed that the methane be separated from the hydrogen. The methane would then become a process by-product and the hydrogen would be recycled. Discuss this proposal using the arguments provided in Tables 6.1 and 6.2.

To use distillation for the separation of methane from hydrogen, as was used with the toluene/benzene, requires a liquid phase. For methane/hydrogen systems, this requires extremely high pressures together with cryogenic temperatures.

If the hydrogen could be separated from the methane and recycled, then the reactor feed would not contain significant quantities of methane, and the large excess of hydrogen could be maintained without the steep cost of excess hydrogen feed. Note that the overall conversion of hydrogen in the process is only 37%, whereas for toluene it is 99%.

Alternative separation schemes that do not require a liquid phase (e.g., a membrane separator) should be considered. The use of alternative separation technologies is addressed further in Chapter 12.

6.4.2. Evaluation of High-Pressure Phase Separator V-102

This vessel separates toluene and benzene as a liquid from the noncondensable gases hydrogen and methane. The reactor product is cooled and forms a vapor and a liquid stream that are in equilibrium. The vapor-liquid equilibrium is that at the temperature and pressure of the stream entering V-102. From Tables 6.1 and 6.2, it can be concluded that the lower temperature (38°C) was provided to obtain a liquid phase for the vapor-liquid equilibrium. The pressure was maintained to support the formation of the liquid phase. Because the separation can be accomplished relatively easily at high pressure, it is worthwhile maintaining V-102 at this high pressure.

6.4.3. Evaluation of Large Temperature Driving Force in Exchanger E-101

There is a large temperature driving force in this exchanger, because the heating medium is at a temperature of approximately 250°C, and the inlet to the exchanger is only 30°C. This is greater than the 100°C suggested in Table 6.4. This is an example of poor heat integration, and a closer look at improving this will be taken in Chapter 15 (also see the case study presented in Chapter 30).

6.4.4. Evaluation of Exchanger E-102

Stream 9 is cooled from 654°C to 40°C using cooling water at approximately 35°C. Again this is greater than the 100°C suggested in Table 6.4, and the process stream has a lot of valuable energy that is being wasted. Again, a lot of money can be saved by using heat integration (see Chapter 15).

6.4.5. Pressure Control Valve on Stream 8

The purpose of this control valve is to reduce the pressure of the stream entering the fuel gas line from 23.9 bar to 2.5 bar. This reduction in pressure represents a potential loss of useful work due to the throttling action of the valve. Referring to Table 6.4, it can be seen that when a gas is throttled, work can be recovered by using a turbine, although this may not be economically attractive. The operation of this valve is justified because of its control function.

6.4.6. Pressure Control Valve on Stream from V-102 to V-103

The purpose of this valve is to reduce the pressure of the liquid leaving V-102. This reduction in pressure causes some additional flashing and recovery of dissolved methane and hydrogen from the toluene/benzene mixture. The flashed gas is separated in V-103 and sent to the fuel gas line. The purpose of this valve is to control the pressure of the material fed to the distillation column T-101. Because the stream passing through the valve is essentially all liquid, little useful work could be recovered from this stream.

This completes the review of the conditions of special concern for the toluene hydrodealkylation process.

6.5. Summary

In this chapter, you learned to identify process conditions that are of special interest or concern in the analysis of the PFD. A series of tables was presented in which justifications for using process conditions of special concern were given. The process conditions matrix (PCM) was introduced for the toluene hydrodealkylation process and all the equipment in which process conditions of special concern existed were identified. Finally, by comparing the process conditions from the PFD to those given in the tables, an analysis was made as to why these conditions were selected for the process and where improvements could be made.

What You Should Have Learned

- The preferred pressure range in a chemical process is 1–10 bar.
- The preferred temperature range in a chemical process is 40°C–260°C.
- Operating above 400°C requires justification.
- There are reasons for operating outside these ranges, and there are many examples in the chemical process industry.
- There are financial consequences of operating outside these ranges, such as the need for refrigeration, the inability to use steam for heating, and the need for more expensive materials of construction.

References

1. Walas, S. M., *Chemical Process Equipment: Selection and Design* (Stoneham, MA: Butterworth, 1988).
2. Tarhan, M. O., *Catalytic Reactor Design* (New York: McGraw-Hill, 1983).

Short Answer Questions

1. State two common criteria for setting the pressure of a distillation column.

2. Suggest two reasons each why distillation columns are run *above* or *below* ambient pressure. Be sure to state clearly which explanation is for above and which is for below ambient pressure.
3. Suggest two reasons why reactors are run at elevated pressures and/or temperatures. Be sure to state clearly which explanation is for elevated pressure and which is for elevated temperature.
4. Give two reasons why operation of a process at greater than 250°C is undesirable. Give one reason each why one would operate a distillation column and a reactor at a temperature greater than 250°C.
5. Define a "condition of special concern." Define two such conditions, and state one possible justification for each.
6. In the food and drug industries, many processes used to produce new active ingredients (drugs) or to separate and purify drugs and foods occur at vacuum conditions and often at low temperatures (less than room temperature). What is it about these types of products that requires that these conditions of special concern be used?

Problems

7. For the separation of a binary mixture in a distillation column, what will be the effect of an increase in column pressure on the following variables?
   a. Tendency to flood at a fixed reflux ratio
   b. Reflux ratio for a given top and bottom purity at a constant number of stages
   c. Number of stages required for a given top and bottom purity at constant reflux ratio
   d. Overhead condenser temperature
8. In a new chemical process, a reboiler for a tower requires a heating medium at 290°C. Two possible solutions have been suggested: (a) Use high-pressure steam superheated to 320°C, and (b) use saturated steam at 320°C. Suggest one disadvantage for each suggestion.
9. As the ambient temperature and humidity increase, the temperature at which cooling water (cw) can be supplied to any piece of equipment increases. For example, in the winter, cw may be available at 27°C whereas in midsummer it may rise to 34°C. How, if at all, does this affect the pressure at which a distillation column operates (assuming that the overhead condenser uses cooling water as the heat exchange utility)?
10. It is desired to produce a hot vapor stream of benzene to feed a reactor for a certain petrochemical process. The benzene is available from an off-site storage facility at 1 atm pressure and ambient temperature (assume 25°C), and the reactor requires the benzene to be at 250°C at 10 atm. Two possible process schemes are being considered to heat and pressurize the feed: (1) Pump the liquid benzene to pressure and then vaporize it in a heat exchanger, and (2) vaporize the benzene first and then compress it to the desired pressure. Answer the following:
    a. Discuss qualitatively which scheme (if either) is better.
    b. Confirm your answer to Part (a) by comparing the costs using both schemes to feed 1000 kg/h of benzene to the reactor. (Assume that the cost of heating is $15/GJ and that electricity costs $0.06/kWh.)
11. One way to produce very pure oxygen and nitrogen is to separate air using a distillation process. For such a separation determine the following:
    a. Find the normal boiling point (at 1 atm pressure) of nitrogen and oxygen.

b. For a distillation column operating at 1 atm pressure, what would be the top and bottom temperatures and top and bottom compositions of a distillation column that separates air into nitrogen and oxygen? (For this problem, you may assume that air contains only nitrogen and oxygen and that pure components leave at the top and bottom of the column.)

c. At what pressure can oxygen and nitrogen be liquefied at ambient temperature (say, 40°C)?

d. What does the answer to Part (c) tell you about the potential to distill air at ambient conditions?

12. The production of ammonia (a key ingredient for fertilizer) using the Haber process takes place at temperatures of around 500°C and pressures of 250 atm using a porous iron catalyst according the following highly exothermic synthesis reaction:

$$N_2(g) + 3H_2(g) \rightleftharpoons 2NH_3(g) \qquad \Delta H = -92.4 \text{ kJ/mol}$$

Give possible reasons for the high temperature and pressure used for this reaction.

13. Consider the ammonia process in Problem 6.12. For the given conditions, the maximum single-pass conversion obtained in the reactor is about 15–20%. Explain how the temperature and pressure should be adjusted to increase this conversion and the penalties for making these changes.

14. For the production of drying oil shown as Project B.4 in Appendix B, do the following:

a. Construct a process conditions matrix (PCM) for the process, and determine all conditions of special concern.

b. For each condition of special concern identified in Part (a), suggest at least one reason why such a condition was used.

c. For each condition of special concern identified in Part (a), suggest at least one process alternative to eliminate the condition.

15. For the styrene production process given in Project B.3 in Appendix B, do the following:

a. Construct a process conditions matrix (PCM) for the process, and determine all conditions of special concern.

b. Explain the reasons for using the conditions of special concern in the reactor.

c. Suggest any process alternatives for Part (b).

Section II: Engineering Economic Analysis of Chemical Processes

This section concentrates on the evaluation of the economics of a chemical process. In order for a chemical engineer or cost engineer to evaluate the economic impact of a new (or existing) chemical process, certain technical information must be available. Although this information is gleaned from a variety of sources, it is generally presented in the form of the technical diagrams discussed in Chapter 1.

In the chapters of this section, methods to evaluate the economics of a chemical process are covered. The term *economics* refers to the evaluation of capital costs and operating costs associated with the construction and operation of a chemical process. The methods by which the one-time costs associated with the construction of the plant and the continuing costs associated with the daily operation of the process are combined into meaningful economic criteria are provided.

This material is treated in the following chapters.

Chapter 7: Estimation of Capital Costs

The common types of estimates are presented along with the basic relationships for scaling costs with equipment size. The concept of cost inflation is presented, and some common cost indexes are presented. The concept of total fixed capital investment to construct a new process is discussed, and the cost module approach to estimating is given. Finally, the software program (CAPCOST) to evaluate fixed capital costs (and other financial calculations) is described.

Chapter 8: Estimation of Manufacturing Costs

The basic components of the manufacturing costs of a process are presented. A method to relate the total cost of manufacturing (COM) to five elements—fixed capital investment, cost of operating labor, cost of raw materials, cost of utilities, and cost of waste treatment—is given. Examples of how utility costs can be calculated from the basic costs of fuel, power, and water are discussed. The estimation of labor costs based on the size and complexity of the process are also given.

Chapter 9: Engineering Economic Analysis

The concept of the time value of money is discussed. The following topics are presented: simple and compound interest, effective and nominal interest rates, annuities, cash flow diagrams, and discount factors. In addition, the concepts of depreciation, inflation, and taxation are covered.

Chapter 10: Profitability Analysis

The ideas discussed in Chapter 9 are extended to evaluate the profitability of chemical processes. Profitability criteria using nondiscounted and discounted bases are presented and include net present value (NPV), discounted cash flow rate of return (DCFROR), and payback period (PBP). A discussion of evaluating equipment alternatives using equivalent annual operating costs (EAOC) and other methods is presented. Finally, the concept of evaluating risk is covered and an introduction to the Monte-Carlo method is presented.

Chapter 7. Estimation of Capital Costs

What You Will Learn

- It takes up-front capital to construct a chemical plant.
- There are different levels of capital-cost estimation, roughly corresponding to the different levels of process diagrams discussed in Chapter 1.
- There are methods for estimating the cost of equipment for a chemical plant.

In Chapter 1, the information provided on a process flow diagram, including a stream table and an equipment summary table, was presented. In the next four chapters, this information will be used as a basis for estimating

1. How much money (capital cost) it takes to build a new chemical plant
2. How much money (operating cost) it takes to operate a chemical plant
3. How to combine items 1 and 2 to provide several distinct types of composite values reflecting process profitability
4. How to select a "best process" from competing alternatives
5. How to estimate the economic value of making process changes and modifications to an existing process
6. How to quantify uncertainty when evaluating the economic potential of a process

In this chapter, the focus is on the estimation of capital costs. **Capital cost** pertains to the costs associated with construction of a new plant or modifications to an existing chemical manufacturing plant.

7.1. Classifications of Capital Cost Estimates

There are five generally accepted classifications of capital cost estimates that are most likely to be encountered in the process industries [1, 2, 3]:

1. Detailed estimate
2. Definitive estimate
3. Preliminary estimate
4. Study estimate
5. Order-of-magnitude estimate

The information required to perform each of these estimates is provided in Table 7.1.

Table 7.1. Summary of Capital Cost Estimating Classifications (References [1], [2], and [3])

Order-of-Magnitude (also known as Ratio or Feasibility) Estimate **Data:** This type of estimate typically relies on cost information for a complete process taken from previously built plants. This cost information is then adjusted using appropriate scaling factors, for capacity, and for inflation to provide the estimated capital cost. **Diagrams:** Normally requires only a block flow diagram.
Study (also known as Major Equipment or Factored) Estimate **Data:** This type of estimate utilizes a list of the major equipment found in the process. This includes all pumps, compressors and turbines, columns and vessels, fired heaters, and exchangers. Each piece of equipment is roughly sized and the approximate cost determined. The total cost of equipment is then factored to give the estimated capital cost. **Diagrams:** Based on PFD as described in Chapter 1. Costs from generalized charts. **Note:** Most individual student designs are in this category.
Preliminary Design (also known as Scope) Estimate **Data:** This type of estimate requires more accurate sizing of equipment than is used in the study estimate. In addition, approximate layout of equipment is made along with estimates of piping, instrumentation, and electrical requirements. Utilities are estimated. **Diagrams:** Based on PFD as described in Chapter 1. Includes vessel sketches for major equipment, preliminary plot plan, and elevation diagram. **Note:** Most large student group designs are in this category.
Definitive (also known as Project Control) Estimate **Data:** This type of estimate requires preliminary specifications for all the equipment, utilities, instrumentation, electrical, and off-sites. **Diagrams:** Final PFD, vessel sketches, plot plan, and elevation diagrams, utility balances, and a preliminary P&ID.
Detailed (also known as Firm or Contractor's) Estimate **Data:** This type of estimate requires complete engineering of the process and all related off-sites and utilities. Vendor quotes for all expensive items will have been obtained. At the end of a detailed estimate, the plant is ready to go to the construction stage. **Diagrams:** Final PFD and P&ID, vessel sketches, utility balances, plot plan and elevation diagrams, and piping isometrics. All diagrams are required to complete the construction of the plant if it is built.

The five classifications given in Table 7.1 roughly correspond to the five classes of estimate defined in the AACE Recommended Practice No. 17R-97 [4]. The accuracy range and the approximate cost for performing each class of estimate are given in Table 7.2.

Table 7.2. Classification of Cost Estimates

Class of Estimate	Level of Project Definition (as % of Complete Definition)	Typical Purpose of Estimate	Methodology (Estimating Method)	Expected Accuracy Range (+/- Range Relative to Best Index of 1)	Preparation Effort (Relative to Lowest Cost Index of 1)
Class 5	0% to 2%	Screening or Feasibility	Stochastic or Judgment	4 to 20	1
Class 4	1% to 15%	Concept Study or Feasibility	Primarily Stochastic	3 to 12	2 to 4
Class 3	10% to 40%	Budget, Authorization, or Control	Mixed but Primarily Stochastic	2 to 6	3 to 10
Class 2	30% to 70%	Control or Bid/Tender	Primarily Deterministic	1 to 3	5 to 20
Class 1	50% to 100%	Check Estimate or Bid/Tender	Deterministic	1	10 to 100

(From AACE Recommended Practice No. 17R-97 [4], reprinted with permission of AACE International, 209 Prairie Ave., Morgantown, WV; http://www.aacei.org)

In Table 7.2, the accuracy range associated with each class of estimate and the costs associated with carrying out the estimate are ranked relative to the most accurate class of estimate (Class 1). In order to use the information in Table 7.2, it is necessary to know the accuracy of a Class 1 estimate. For the cost estimation of a chemical plant, a Class 1 estimate (detailed estimate) is typically +6% to –4% accurate. This means that by doing such an estimate, the true cost of building the plant would likely be in the range of 6% higher than and 4% lower than the estimated price. Likewise, the effort to prepare a Class 5 estimate for a chemical process is typically in the range of 0.015% to 0.30% of the total installed cost of the plant [1, 2].

The use of the information in Table 7.2, to estimate the accuracy and costs of performing estimates, is illustrated in Examples 7.1 and 7.2.

Example 7.1.

The estimated capital cost for a chemical plant using the study estimate method (Class 4) was calculated to be $2 million. If the plant were to be built, over what range would you expect the actual capital estimate to vary?

For a Class 4 estimate, from Table 7.2, the expected accuracy range is between 3 and 12 times that of a Class 1 estimate. As noted in the text, a Class 1 estimate can be expected to vary from +6% to –4%. The narrowest and broadest expected capital cost ranges can be evaluated as follows:

Lowest Expected Cost Range

High value for actual plant cost $(\$2.0 \times 10^6)[1 + (0.06)(3)] = \$2.36 \times 10^6$

Low value for actual plant cost $(\$2.0 \times 10^6)[1 - (0.04)(3)] = \$1.76 \times 10^6$

Highest Expected Cost Range

High value for actual plant cost $(\$2.0 \times 10^6)[1 + (0.06)(12)] = \$3.44 \times 10^6$

Low value for actual plant cost ($2.0 \times 10^6)[1 - (0.04)(12)] = \$1.04 \times 10^6$

The actual expected range would depend on the level of project definition and effort. If the effort and definition are at the high end, then the expected cost range would be between $1.76 and $2.36 million. If the effort and definition are at the low end, then the expected cost range would be between $1.04 and $3.44 million.

The primary reason that capital costs are underestimated stems from the failure to include all of the equipment needed in the process. Typically, as a design progresses, the need for additional equipment is uncovered, and the estimate accuracy improves. The different ranges of cost estimates are illustrated in Example 7.2.

Example 7.2.

Compare the costs for performing an order-of-magnitude estimate and a detailed estimate for a plant that cost $\$5.0 \times 10^6$ to build.

For the order-of-magnitude estimate, the cost of the estimate is in the range of 0.015% to 0.3% of the final cost of the plant:

Highest Expected Value: $(\$5.0 \times 10^6)(0.003) = \$15{,}000$

Lowest Expected Value: $(\$5.0 \times 10^6)(0.00015) = \$750$

For the detailed estimate, the cost of the estimate is in the range of 10 to 100 times that of the order-of-magnitude estimate.

For the lowest expected cost range:

Highest Expected Value: $(\$5.0 \times 10^6)(0.03) = \$150{,}000$

Lowest Expected Value: $(\$5.0 \times 10^6)(0.0015) = \$7500$

For the highest expected cost range:

Highest Expected Value: $(\$5.0 \times 10^6)(0.3) = \$1{,}500{,}000$

Lowest Expected Value: $(\$5.0 \times 10^6)(0.015) = \$75{,}000$

Capital cost estimates are essentially paper-and-pencil studies. The cost of making an estimate indicates the personnel hours required in order to complete the estimate. From Table 7.2 and Examples 7.1 and 7.2, the trend between the accuracy of an estimate and the cost of the estimate is clear. If greater accuracy is required in the capital cost estimate, then more time and money must be expended in conducting the estimate. This is the direct result of the greater detail required for the more accurate estimating techniques.

What cost estimation technique is appropriate? At the beginning of Chapter 1, a short narrative was given that introduced the evolution of a chemical process leading to the final design and construction of a chemical plant. Cost estimates are performed at each stage of this evolution.

There are many tens to hundreds of process systems examined at the block diagram level for each process that makes it to the construction stage. Most of the processes initially considered are screened out before any detailed cost estimates are made. Two major areas dominate this screening process. To continue process development, the process must be both technically sound and

economically attractive.

A typical series of cost estimates that would be carried out in the narrative presented in Chapter 1 is as follows:

- Preliminary feasibility estimates (order-of-magnitude or study estimates) are made to compare many process alternatives.
- More accurate estimates (preliminary or definitive estimates) are made for the most profitable processes identified in the feasibility study.
- Detailed estimates are then made for the more promising alternatives that remain after the preliminary estimates.
- Based on the results from the detailed estimate, a final decision is made whether to go ahead with the construction of a plant.

This text focuses on the preliminary and study estimation classification based on a PFD as presented in Chapter 1. This approach will provide estimates accurate in the range of +40% to –25%.

In this chapter, it is assumed that all processes considered are technically sound and attention is focused on the economic estimation of capital costs. The technical aspects of processes will be considered in later chapters.

7.2. Estimation of Purchased Equipment Costs

To obtain an estimate of the capital cost of a chemical plant, the costs associated with major plant equipment must be known. For the presentation in this chapter, it is assumed that a PFD for the process is available. This PFD is similar to the one discussed in detail in Chapter 1, which included material and energy balances with each major piece of equipment identified, materials of construction selected, and the size/capacity roughly estimated from conditions on the PFD. Additional PFDs and equipment summary tables are given for several processes in Appendix B.

The most accurate estimate of the purchased cost of a piece of major equipment is provided by a current price quote from a suitable vendor (a seller of equipment). The next best alternative is to use cost data on previously purchased equipment of the same type. Another technique, sufficiently accurate for study and preliminary cost estimates, utilizes summary graphs available for various types of common equipment. This last technique is used for study estimates emphasized in this text and is discussed in detail in Section 7.3. Any cost data must be adjusted for any difference in unit capacity (see Section 7.2.1) and also for any elapsed time since the cost data were generated (see Section 7.2.2).

7.2.1. Effect of Capacity on Purchased Equipment Cost

The most common simple relationship between the purchased cost and an attribute of the equipment related to units of capacity is given by Equation (7.1).

$$\frac{C_a}{C_b} = \left(\frac{A_a}{A_b}\right)^n \tag{7.1}$$

where A = Equipment cost attribute

C = Purchased cost

n = Cost exponent

Subscripts: a refers to equipment with the required attribute

b refers to equipment with the base attribute

The **equipment cost attribute** is the equipment parameter that is used to correlate capital costs. The equipment cost attribute is most often related to the unit capacity, and the term *capacity* is commonly used to describe and identify this attribute. Some typical values of cost exponents and unit capacities are given in Table 7.3. From Table 7.3, it can be seen that the following information is given:

Table 7.3. Typical Values of Cost Exponents for a Selection of Process Equipment

Range of Equipment Type	Correlation	Units of Capacity	Cost Exponent *n*
Reciprocating compressor with motor drive	0.75 to 1490	kW	0.84
Heat exchanger shell-and-tube carbon steel	1.9 to 1860	m^2	0.59
Vertical tank carbon steel	0.4 to 76	m^3	0.30
Centrifugal blower	0.24 to 71	std m^3/s	0.60
Jacketed kettle glass lined	0.2 to 3.8	m^3	0.48

(All data from Table 9-50, *Chemical Engineers' Handbook*, Perry, R.H., Green, D.W., and Maloney, J.O. (eds.), 7th ed., 1997. Reproduced by permission of the McGraw-Hill Companies, Inc., New York, NY.)

1. A description of the type of equipment used
2. The units in which the capacity is measured
3. The range of capacity over which the correlation is valid
4. The cost exponent (values shown for *n* vary between 0.30 and 0.84)

Equation (7.1) can be rearranged to give

$$C_a = KA_a^n \qquad (7.2)$$

where $K = C_b/A_b^n$.

Equation (7.2) is a straight line with a slope of *n* when the log of C_a is plotted versus the log of A_a. To illustrate this relationship, the typical cost of a single-stage blower versus the capacity of the blower, given as the volumetric flowrate, is plotted in Figure 7.1. The value for the cost exponent, *n*, from this curve is 0.60.

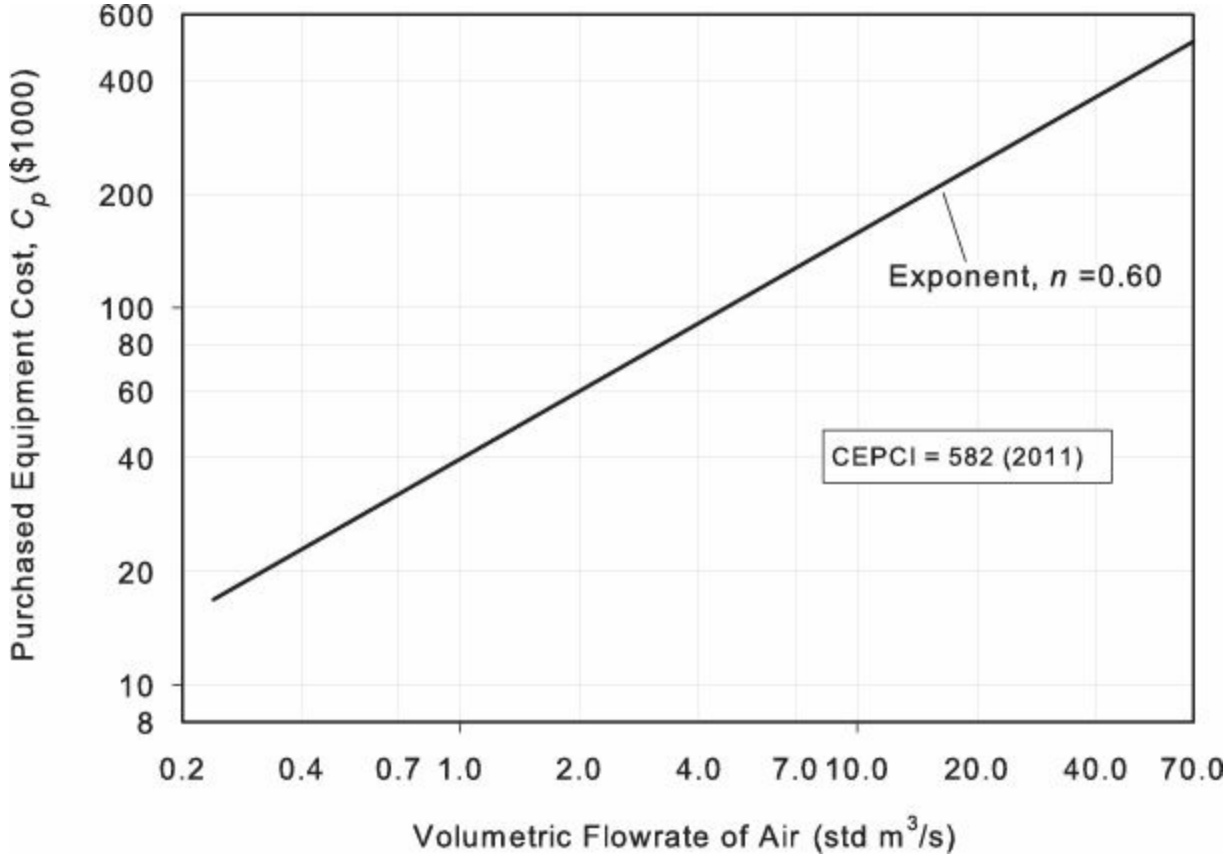


Figure 7.1. Purchased Cost of a Centrifugal Air Blower (Data adapted from Reference [3])

The value of the cost exponent, n, used in Equations (7.1) and (7.2), varies depending on the class of equipment being represented. See Table 7.3. The value of n for different items of equipment is often around 0.6. Replacing n in Equation (7.1) and/or 5.2 by 0.6 provides the relationship referred to as the **six-tenths rule.** A problem using the six-tenths rule is given in Example 7.3.

Example 7.3.

Use the six-tenths rule to estimate the percentage increase in purchased cost when the capacity of a piece of equipment is doubled.

Using Equation (7.1) with $n = 0.6$,

$$C_a/C_b = (2/1)^{0.6} = 1.52$$

$$\% \text{ increase} = ((1.52 - 1.00)/1.00)(100) = 52\%$$

This simple example illustrates a concept referred to as the **economy of scale**. Even though the equipment capacity was doubled, the purchased cost of the equipment increased by only 52%. This leads to the following generalization:

The larger the equipment, the lower the cost of equipment per unit of capacity.

Special care must be taken in using the six-tenths rule for a single piece of equipment. The cost exponent may vary considerably from 0.6, as illustrated in Example 7.4. The use of this rule for a total chemical process is more reliable and is discussed in Section 7.3.

Example 7.4.

Compare the error for the scale-up of a reciprocating compressor by a factor of 5 using the six-tenths rule in place of the cost exponent given in Table 7.3.

Using Equation (7.1),

Cost ratio using six-tenths rule (i.e., $n = 0.60$) = $5.0^{0.60} = 2.63$

Cost ratio using ($n = 0.84$) from Table 7.3 = $5.0^{0.84} = 3.86$

% Error = ((2.63 – 3.86)/3.86)(100) = –32 %

Another way to think of the economy of scale is to consider the purchased cost of equipment per unit capacity. Equation (7.2) can be rearranged to give the following relationship:

$$\frac{C}{A} = KA^{n-1} \qquad (7.3)$$

If Equation (7.3) is plotted on log-log coordinates, the resulting curve will have a negative slope, as shown in Figure 7.2. The meaning of the negative slope is that as the capacity of a piece of equipment increases, the cost per unit of capacity decreases. This, of course, is a consequence of $n < 1$ but also shows clearly how the economy of scale works. As cost curves for equipment are introduced in the text, they will be presented in terms of cost per unit capacity as a function of capacity to illustrate better the idea of economy of scale. For many equipment types, the simple relationship in Equation (7.1) is not very accurate, and an equation that is second order in the attribute is used.

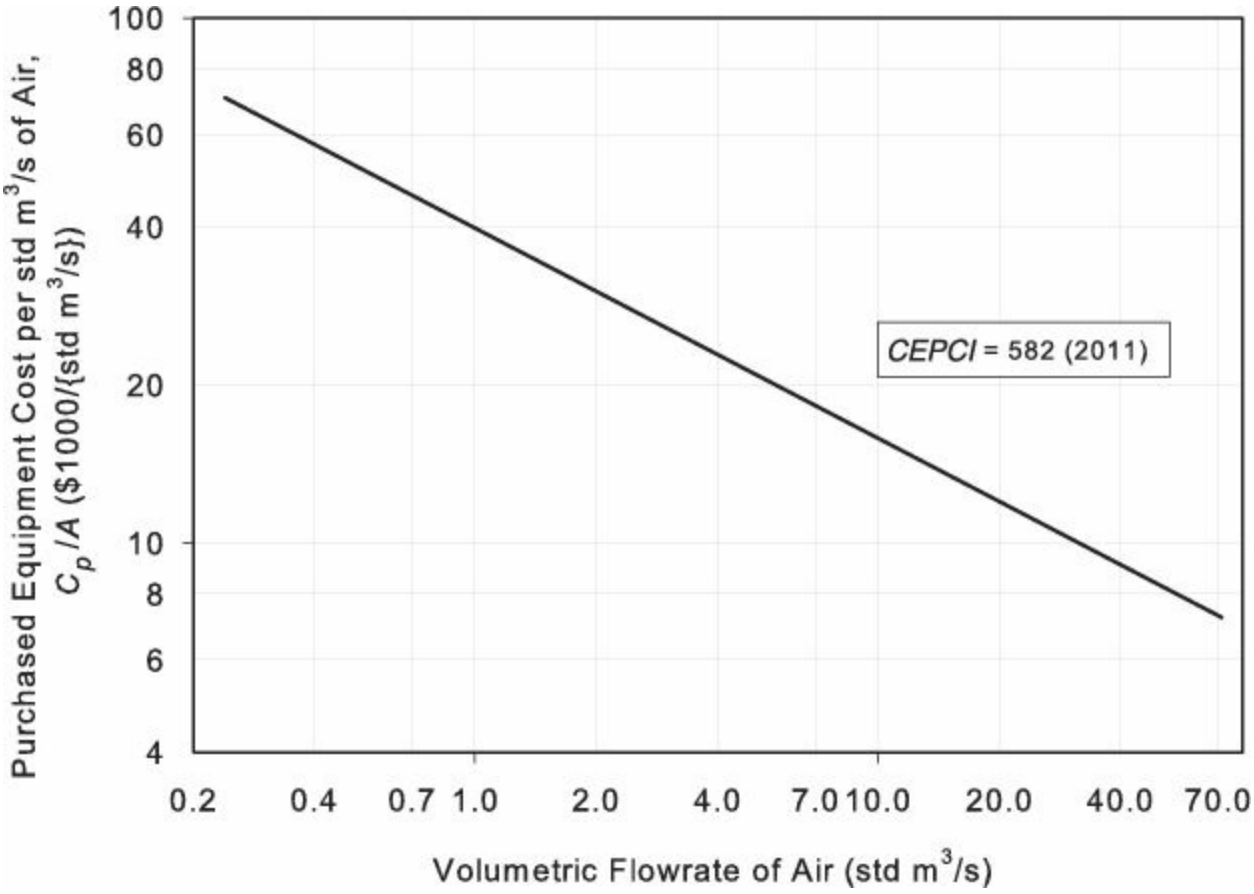


Figure 7.2. Purchased Cost per Unit of Flowrate of a Centrifugal Air Blower (Adapted from Reference [3])

In the last two examples, the relative costs of equipment of differing size were calculated. It is necessary to have cost information on the equipment at some "base case" in order to be able to determine the cost of other similar equipment. This base-case information must allow for the constant, K, in Equation (7.2), to be evaluated, as shown in Example 7.5. This base-case cost information may

be obtained from a current bid provided by a manufacturer for the needed equipment or from company records of prices paid for similar equipment.

Example 7.5.

The purchased cost of a recently acquired heat exchanger with an area of 100 m^2 was \$10,000.

Determine

a. The constant K in Equation (7.2)

b. The cost of a new heat exchanger with area equal to 180 m^2

From Table 7.3: $n = 0.59$: for Equation (7.2):

a. $K = C_b/(A_b)^n = 10{,}000/(100)^{0.59} = 661$ $\{\$/(m^2)^{0.59}\}$

b. $C_a = (661)(180)^{0.59} = \$14{,}100$

There are additional techniques that allow for the price of equipment to be estimated that do not require information from either of the sources given above. One of these techniques is discussed in Section 7.3.

7.2.2. Effect of Time on Purchased Equipment Cost

In Figures 7.1 and 7.2, the time at which the cost data were reported (2011) is given on each figure. This raises the question of how to convert this cost into one that is accurate for the present time. When one depends on past records or published correlations for price information, it is essential to be able to update these costs to take changing economic conditions (inflation) into account. This can be achieved by using the following expression:

$$C_2 = C_1\left(\frac{I_2}{I_1}\right) \qquad (7.4)$$

where C = Purchased cost

I = Cost index

Subscripts: 1 refers to base time when cost is known

2 refers to time when cost is desired

There are several cost indices used by the chemical industry to adjust for the effects of inflation. Several of these cost indices are plotted in Figure 7.3.

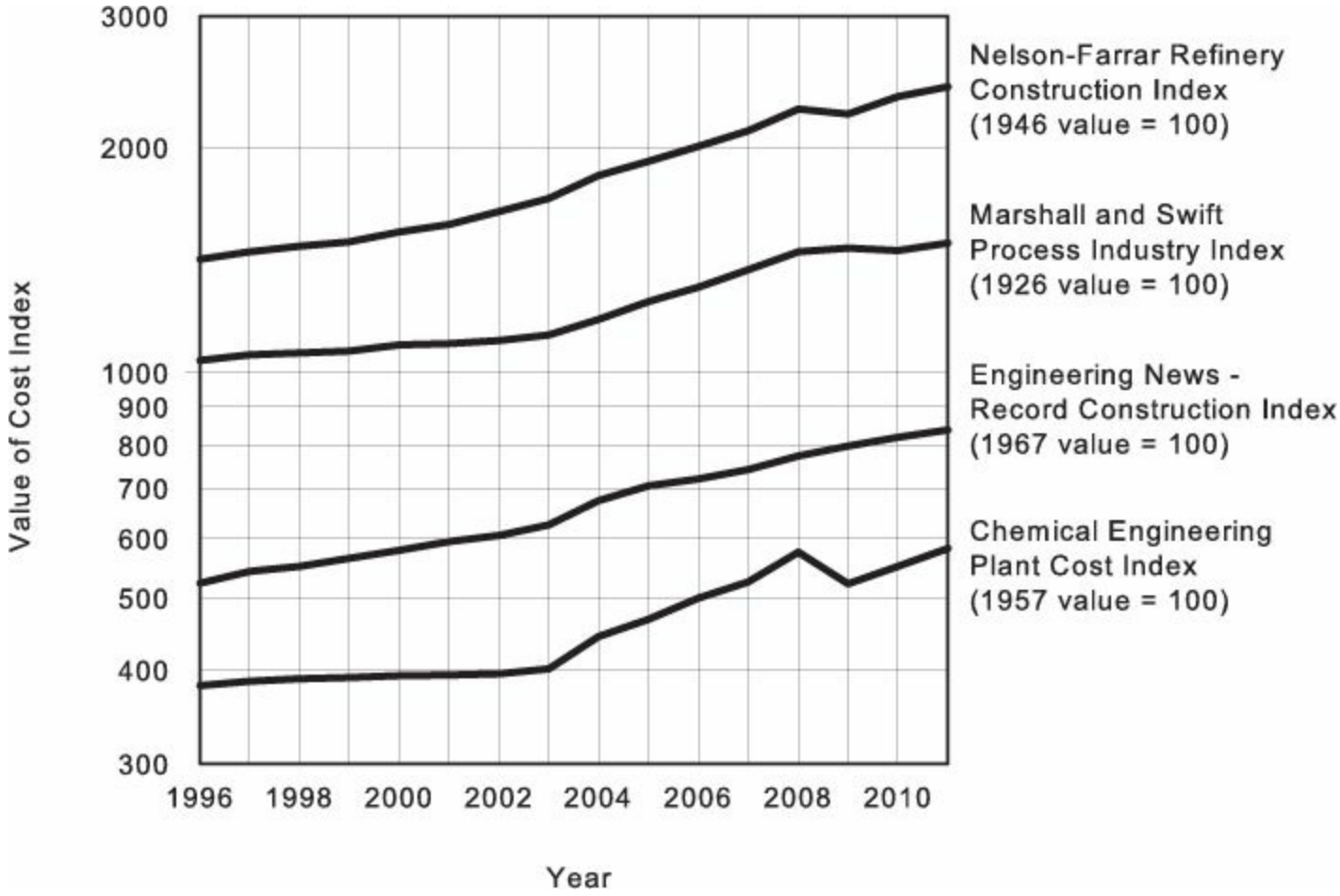


Figure 7.3. The Variations in Several Commonly Used Cost Indexes over the Past 15 Years (1996–2011)

All indices in Figure 7.3 show similar inflationary trends with time. The indices most generally accepted in the chemical industry and reported in the back page of every issue of *Chemical Engineering* are the Marshall and Swift Equipment Cost Index and the Chemical Engineering Plant Cost Index.

Table 7.4 provides values for both the Marshall and Swift Equipment Cost Index and the Chemical Engineering Plant Cost Index from 1996 to 2011.

Table 7.4. Values for the Chemical Engineering Plant Cost Index and the Marshall and Swift Equipment Cost Index from 1996 to 2011

Year	Marshall and Swift Equipment Cost Index	Chemical Engineering Plant Cost Index
1996	1039	382
1997	1057	387
1998	1062	390
1999	1068	391
2000	1089	394
2001	1094	394
2002	1104	396
2003	1124	402
2004	1179	444
2005	1245	468
2006	1302	500
2007	1373	525
2008	1449	575
2009	1469	521
2010	1457	551
2011 (estimated)	1490	582

Unless otherwise stated, the Chemical Engineering Plant Cost Index (CEPCI) will be used in this text to account for inflation. This is a composite index, and the items that are included in the index are listed in Table 7.5. A comparison between these two indices is given in Example 7.6.

Table 7.5. The Basis for the Chemical Engineering Plant Cost Index

Components of Index	Weighting of Component (%)	
Equipment, Machinery, and Supports		
(a) Fabricated equipment	37	
(b) Process machinery	14	
(c) Pipe, valves, and fittings	20	
(d) Process instruments and controls	7	
(e) Pumps and compressors	7	
(f) Electrical equipment and materials	5	
(g) Structural supports, insulation, and paint	10	
	100	61% of total
Erection and installation labor		22
Buildings, materials, and labor		7
Engineering and supervision		10
Total		100

Example 7.6.

The purchased cost of a heat exchanger of 500 m^2 area in 1996 was $25,000.

a. Estimate the cost of the same heat exchanger in 2011 using the two indices introduced above.

b. Compare the results.

From Table 7.4	1996	2011
Marshall and Swift Index	1039	1490
Chemical Engineering Plant Cost Index	382	582

a. Marshall and Swift: Cost = ($25,000)(1490/1039) = $39,852

Chemical Engineering: Cost = ($25,000)(582/382) = $38,089

b. Average Difference: (($35,852 – 38,089)/(($35,852 + 38,089)/2)(100) = –7.4%

7.3. Estimating the Total Capital Cost of a Plant

The capital cost for a chemical plant must take into consideration many costs other than the purchased cost of the equipment. As an analogy, consider the costs associated with building a new home.

> *The purchased cost of all the materials that are needed to build a home does not represent the cost of the home. The final cost reflects the cost of property, the cost for delivering materials, the cost of construction, the cost of a driveway, the cost for hooking up utilities, and so on.*

Table 7.6 presents a summary of the costs that must be considered in the evaluation of the total capital cost of a chemical plant.

The estimating procedures to obtain the full capital cost of the plant are described in this section. If an estimate of the capital cost for a process plant is needed and access to a previous estimate for a similar plant with a different capacity is available, then the principles already introduced for the scaling of purchased costs of equipment can be used.

1. The six-tenths rule (Equation [7.1] with n set to 0.6) can be used to scale up or down to a new capacity.
2. The Chemical Engineering Plant Cost Index should be used to update the capital costs (Equation [7.4]).

Table 7.6. Factors Affecting the Costs Associated with Evaluation of Capital Cost of Chemical Plants (from References [2] and [5])

Factor Associated with the Installation of Equipment	Symbol	Comments
1. **Direct Project Expenses**		
a. Equipment f.o.b. cost (f.o.b. = free on board)	C_P	Purchased cost of equipment at manufacturer's site.
b. Materials required for installation	C_M	Includes all piping, insulation and fireproofing, foundations and structural supports, instrumentation and electrical, and painting associated with the equipment.
c. Labor to install equipment and material	C_L	Includes all labor associated with installing the equipment and materials mentioned in (a) and (b).
2. **Indirect Project Expenses**		
a. Freight, insurance, and taxes	C_{FIT}	Includes all transportation costs for shipping equipment and materials to the plant site, all insurance on the items shipped, and any purchase taxes that may be applicable.
b. Construction overhead	C_O	Includes all fringe benefits such as vacation, sick leave, retirement benefits, etc.; labor burden such as social security and unemployment insurance, etc.; and salaries and overhead for supervisory personnel.
c. Contractor engineering expenses	C_E	Includes salaries and overhead for the engineering, drafting, and project management personnel on the project.

3. Contingency and Fee		
a. Contingency	C_{Cont}	A factor to cover unforeseen circumstances. These may include loss of time due to storms and strikes, small changes in the design, and unpredicted price increases.
b. Contractor fee	C_{Fee}	This fee varies depending on the type of plant and a variety of other factors.
4. Auxiliary Facilities		
a. Site development	C_{Site}	Includes the purchase of land; grading and excavation of the site; installation and hookup of electrical, water, and sewer systems; and construction of all internal roads, walkways, and parking lots.
b. Auxiliary buildings	C_{Aux}	Includes administration offices, maintenance shop and control rooms, warehouses, and service buildings (e.g., cafeteria, dressing rooms, and medical facility).
c. Off-sites and utilities	C_{Off}	Includes raw material and final product storage; raw material and final product loading and unloading facilities; all equipment necessary to supply required process utilities (e.g., cooling water, steam generation, fuel distribution systems, etc.); central environmental control facilities (e.g., wastewater treatment, incinerators, flares, etc.); and fire protection systems.

The six-tenths rule is more accurate in this application than it is for estimating the cost of a single piece of equipment. The increased accuracy results from the fact that multiple units are required in a processing plant. Some of the process units will have cost coefficients, n, less than 0.6. For this equipment, the six-tenths rule overestimates the costs of these units. In a similar way, costs for process units having coefficients greater than 0.6 are underestimated. When the sum of the costs is determined, these differences tend to cancel each other out.

The Chemical Engineering Plant Cost Index (CEPCI) can be used to account for changes that result from inflation. The CEPCI values provided in Table 7.4 are composite values that reflect the inflation of a mix of goods and services associated with the chemical process industries (CPI).

> *You may be familiar with the more common consumer price index issued by the government. This represents a composite cost index that reflects the effect of inflation on the cost of living. This index considers the changing cost of a "basket" of goods composed of items used by the "average" person. For example, the price of housing, cost of basic foods, cost of clothes and transportation, and so on, are included and weighted appropriately to give a single number reflecting the average cost of these goods. By comparing this number over time, it is possible to get an indication of the rate of inflation as it affects the average person.*

In a similar manner, the CEPCI represents a "basket" of items directly related to the costs associated with the construction of chemical plants. A breakdown of the items included in this index was given in Table 7.5. The index is directly related to the effect of inflation on the cost of an "average" chemical plant, as shown in Example 7.7.

Example 7.7.

The capital cost of a 30,000 metric ton/y isopropanol plant in 1996 was estimated to be $23 million. Estimate the capital cost of a new plant with a production rate of 50,000 metric tons/year in 2011.

Cost in 2011 = (Cost in 1996)(Capacity Correction)(Inflation Correction)

$= (\$23{,}000{,}000)(50{,}000/30{,}000)^{0.6}(582/382)$

$= (\$23{,}000{,}000)(1.359)(1.626) = \$47{,}610{,}000$

In most situations, cost information will not be available for the same process configuration; therefore, other estimating techniques must be used.

7.3.1. Lang Factor Technique

A simple technique to estimate the capital cost of a chemical plant is the Lang Factor method, due to Lang [6, 7, 8]. The cost determined from the Lang Factor represents the cost to build a major expansion to an existing chemical plant. The total cost is determined by multiplying the total purchased cost for all the major items of equipment by a constant. The major items of equipment are those shown in the process flow diagram. The constant multiplier is called the Lang Factor. Values for Lang Factors, F_{Lang}, are given in Table 7.7.

Table 7.7. Lang Factors for the Estimation of Capital Cost for Chemical Plant (from References [6, 7, 8])

Capital Cost = (Lang Factor)(Sum of Purchased Costs of All Major Equipment)	
Type of Chemical Plant	**Lang Factor = F_{Lang}**
Fluid processing plant	4.74
Solid-fluid processing plant	3.63
Solid processing plant	3.10

The capital cost calculation is determined using Equation (7.5).

$$C_{TM} = F_{Lang}\sum_{i=1}^{n} C_{p,i} \qquad (7.5)$$

where C_{TM} is the capital cost (total module) of the plant

$C_{p,i}$ is the purchased cost for the major equipment units

n is the total number of individual units

F_{Lang} is the Lang Factor (from Table 7.7)

Plants processing only fluids have the largest Lang Factor, 4.74, and plants processing only solids have a factor of 3.10. Combination fluid-solid systems fall between these two values. The greater the Lang Factor, the less the purchased costs contribute to the plant costs. For all cases, the purchased cost of the equipment is less than one-third of the capital cost of the plant. The use of the Lang Factor is illustrated in Example 7.8.

Example 7.8.

Determine the capital cost for a major expansion to a fluid processing plant that has a total purchased equipment cost of $6,800,000.

Capital Costs = ($6,800,000)(4.74) = $32,232,000

This estimating technique is insensitive to changes in process configuration, especially between processes in the same broad categories shown in Table 7.7. It cannot accurately account for the common problems of special materials of construction and high operating pressures. A number of alternative techniques are available. All require more detailed calculations using specific price information for the individual units/equipment.

7.3.2. Module Costing Technique

The equipment module costing technique is a common technique to estimate the cost of a new chemical plant. It is generally accepted as the best for making preliminary cost estimates and is used extensively in this text. This approach, introduced by Guthrie [9, 10] in the late 1960s and early 1970s, forms the basis of many of the equipment module techniques in use today. This costing technique relates all costs back to the purchased cost of equipment evaluated for some base conditions. Deviations from these base conditions are handled by using multiplying factors that depend on the following:

1. The specific equipment type
2. The specific system pressure
3. The specific materials of construction

The material provided in the next section is based upon information in Guthrie [9, 10], Ulrich [5], and Navarrete [11]. The reader is encouraged to review these references for further information.

Equation (7.6) is used to calculate the bare module cost for each piece of equipment. The bare module cost is the sum of the direct and indirect costs shown in Table 7.6.

$$C_{BM} = C_p^o F_{BM} \qquad (7.6)$$

where C_{BM} = bare module equipment cost: direct and indirect costs for each unit

F_{BM} = bare module cost factor: multiplication factor to account for the items in Table 7.6 plus the specific materials of construction and operating pressure

C_p^o = purchased cost for base conditions: equipment made of the most common material, usually carbon steel, and operating at near-ambient pressures

Because of the importance of this cost estimating technique, it is described below in detail.

7.3.3. Bare Module Cost for Equipment at Base Conditions

The bare module equipment cost represents the sum of direct and indirect costs shown in Table 7.6. The conditions specified for the base case are

1. Unit fabricated from most common material, usually carbon steel (CS)
2. Unit operated at near-ambient pressure

Equation (7.6) is used to obtain the bare module cost for the base conditions. For these base conditions, a superscript zero (0) is added to the bare module cost factor and the bare module equipment cost. Thus C_{BM}^o and F_{BM}^o refer to the base conditions.

Table 7.8 supplements Table 7.6 and provides the relationships and equations for the direct, indirect, contingency, and fee costs based on the purchased cost of the equipment. These equations are used to evaluate the bare module factor. The entries in Table 7.8 are described here:

Table 7.8. Equations for Evaluating Direct, Indirect, Contingency, and Fee Costs

Factor	Basic Equation	Multiplying Factor to Be Used with Purchased Cost, C_p^o
1. Direct		
a. Equipment	$C_p^o = C_p^o$	1.0
b. Materials	$C_M = \alpha_M C_p^o$	α_M
c. Labor	$C_L = \alpha_L(C_p^o + C_M)$	$(1.0 + \alpha_M)\alpha_L$
Total Direct	$\mathbf{C_{DE} = C_p^o + C_M + C_L}$	$\mathbf{(1.0 + \alpha_M)(1.0 + \alpha_L)}$
2. Indirect		
a. Freight, etc.	$C_{FIT} = \alpha_{FIT}(C_p^o + C_M)$	$(1.0 + \alpha_M)\alpha_{FIT}$
b. Overhead	$C_O = \alpha_O C_L$	$(1.0 + \alpha_M)\alpha_L\alpha_O$
c. Engineering	$C_E = \alpha_E(C_p^o + C_M)$	$(1.0 + \alpha_M)\alpha_E$
Total Indirect	$C_{IDE} = C_{FIT} + C_O + C_E$	$(1.0 + \alpha_M)(\alpha_{FIT} + \alpha_L\alpha_O + \alpha_E)$
Bare Module	$\mathbf{C_{BM}^o = C_{IDE} + C_{DE}}$	$\mathbf{(1.0 + \alpha_M)(1.0 + \alpha_L + \alpha_{FIT} + \alpha_L\alpha_O + \alpha_E)}$
3. Contingency and Fee		
a. Contingency	$C_{Cont} = \alpha_{Cont} C_{BM}^o$	$(1.0 + \alpha_M)(1.0 + \alpha_L + \alpha_{FIT} + \alpha_L\alpha_O + \alpha_E)\alpha_{Cont}$
b. Fee	$C_{Fee} = \alpha_{Fee} C_{BM}^o$	$(1.0 + \alpha_M)(1.0 + \alpha_L + \alpha_{FIT} + \alpha_L\alpha_O + \alpha_E)\alpha_{Fee}$
Total Module	$\mathbf{C_{TM} = C_{BM}^o + C_{Cont} + C_{Fee}}$	$\mathbf{(1.0 + \alpha_M)(1.0 + \alpha_L + \alpha_{FIT} + \alpha_L\alpha_O + \alpha_E)(1.0 + \alpha_{Cont} + \alpha_{Fee})}$

Column 1: Lists the factors given in Table 7.6.

Column 2: Lists equations used to evaluate each of the costs. These equations introduce multiplication cost factors, α_i. Each cost item, other than the purchased equipment cost, introduces a separate factor.

Column 3: For each factor, the cost is related to the purchased cost C_p^o by an equation of the form.

$$C_{XX} = C_p^o f(\alpha_{i,j,k...}) \qquad (7.7)$$

The function $f(\alpha_{i,\,j,\,k.\,...})$ is given in column 3 of Table 5.8.

From Table 7.8 and Equations (7.6) and (7.7), it can be seen that the bare module factor is given by

$$F_{BM}^o = [1 + \alpha_L + \alpha_{FIT} + \alpha_L\alpha_o + \alpha_E][1 + \alpha_M] \qquad (7.8)$$

The values for the bare module cost multiplying factors vary between equipment modules. The calculations for the bare module factor and bare module cost for a carbon steel heat exchanger are given in Example 7.9.

Example 7.9.

The purchased cost for a carbon steel heat exchanger operating at ambient pressure is $10,000. For a heat-exchanger module, Guthrie [9, 10] provides the following cost information:

Item	% of Purchased Equipment Cost
Equipment	100.0
Materials	71.4
Labor	63.0
Freight	8.0
Overhead	63.4
Engineering	23.3

Using the information given above, determine the equivalent cost multipliers given in Table 7.8 and the following:

a. Bare module cost factor, F_{BM}^{o}

b. Bare module cost, C_{BM}^{o}

Item	% of Purchased Equipment Cost	Cost Multiplier (Table 7.8)	Value of Multiplier
Equipment	100.0	1.0	
Materials	71.4	α_M	0.714
Labor	63.0	α_L	$0.63/(1 + 0.714) = 0.368$
Freight	8.0	α_{FIT}	$0.08/(1 + 0.714) = 0.047$
Overhead	63.4	α_O	$0.634/0.368/(1 + 0.714) = 1.005$
Engineering	23.3	α_E	$0.233/(1 + 0.714) = 0.136$
Bare Module	**329.1**		

a. Using Equation (7.8),

$$F_{BM}^{o} = (1 + 0.368 + 0.047 + (1.005)(0.368) + 0.136)(1 + 0.714) = 3.291$$

b. From Equation (7.6),

$$C_{BM}^{o} = (3.291)(\$10{,}000) = \$32{,}910$$

Fortunately, the procedure illustrated in Example 7.9 does not have to be repeated in order to estimate F_{BM}^{o} for every piece of equipment. This has already been done for a large number of equipment modules, and the results are given in Appendix A.

In order to estimate bare module costs for equipment, purchased costs for the equipment at base case conditions (ambient pressure using carbon steel) must be available along with the corresponding bare module factor and factors to account for different operating pressures and materials of construction. These data are made available for a variety of common gas/liquid processing equipment in Appendix A. These data were compiled during the summer of 2001 from information obtained from manufacturers and also from the R-Books software marketed by Richardson Engineering Services [12]. The method by which material and pressure factors are accounted for depends on the equipment type, and these are covered in the next section. The estimation of the bare module cost for a floating-head, shell-and-tube heat exchanger is illustrated in Example 7.10 and in subsequent examples in this chapter.

Example 7.10.

Find the bare module cost of a floating-head, shell-and-tube heat exchanger with a heat transfer area of 100 m^2 at the end of 2011. The operating pressure of the equipment is 1.0 bar, with both shell-and-tube sides constructed of carbon steel. The cost curve for this heat exchanger is given in Appendix A, Figure A.5, and is repeated as Figure 7.4. It should be noted that unlike the examples shown in

Figures 7.1 and 7.2, the log-log plot of cost per unit area versus area is nonlinear. In general this will be the case, and a second-order polynomial is normally used to describe this relationship.

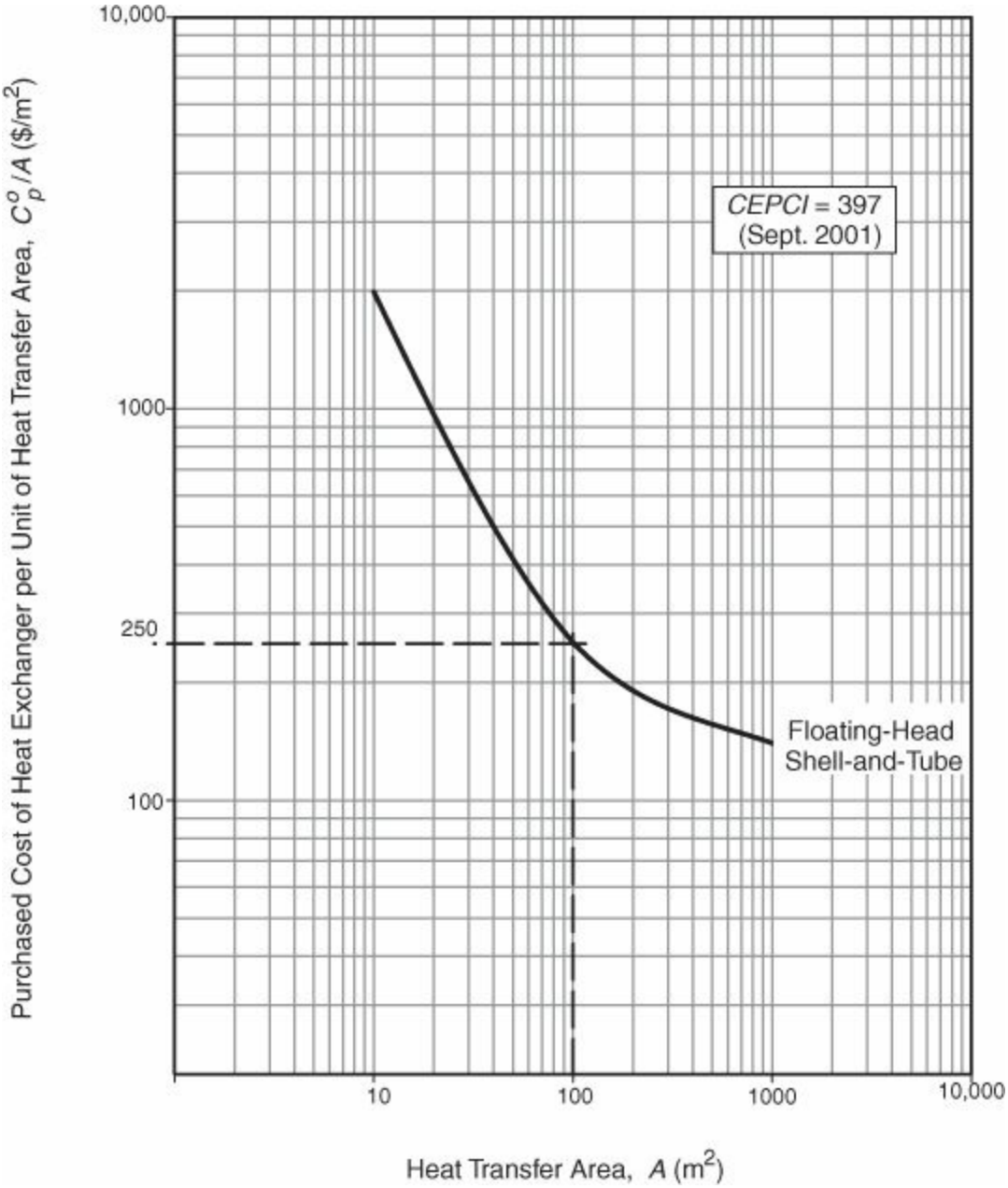


Figure 7.4. Purchased Costs for Floating-Head Shell-and-Tube Heat Exchangers

From Figure 7.4, C_p^o (2001) = ($250)(100) = $25,000 (the evaluation path is shown on Figure 7.4).

The bare module cost for shell-and-tube heat exchangers is given by Equation (A.4).

$$C_{BM} = C_p^o [B_1 + B_2 F_p F_M] \qquad \text{(A.4)}$$

The values of B_1 and B_2 for floating-head heat exchangers from Table A.4 are 1.63 and 1.66, respectively.

The pressure factor is obtained from Equation (A.3).

$$\log_{10} F_p = C_1 + C_2 \log_{10} P + C_3 (\log_{10} P)^2 \qquad \text{(A.3)}$$

From Table A.2, for pressures < 5 barg, $C_1 = C_2 = C_3 = 0$, and from Equation (A.3), $F_p = 1$.

Using data in Table A.3 for shell-and-tube heat exchangers with both shell and tubes made of carbon steel (Identification Number = 1) and Figure A.8, $F_M = 1$. Substituting this data into Equation (A.4) gives

$$C_{BM}^{o}(2001) = C_{p}^{o}(2001)[1.63 + 1.66(F_p = 1)(F_M = 1)] = 3.29C_{p}^{o} = (3.29)(\$25{,}000) = \$82{,}300$$
$$C_{BM}^{o}(2011) = C_{BM}^{o}(2001)\,(582/394) = \$82{,}300\,(582/397) = \$120{,}650$$

A comparison of the value of bare module cost factor for Example 7.10 shows that it is the same as the value of 3.29 evaluated using the individual values for α_i, given in Example 7.9.

7.3.4. Bare Module Cost for Non-Base-Case Conditions

For equipment made from other materials of construction and/or operating at nonambient pressure, the values for F_M and F_P are greater than 1.0. In the equipment module technique, these additional costs are incorporated into the bare module cost factor, F_{BM}. The bare module factor used for the base case, F_{BM}^{o}, is replaced with an actual bare module cost factor, F_{BM}, in Equation (7.6). The information needed to determine this actual bare module factor is provided in Appendix A. The effect of pressure on the cost of equipment is considered first.

Pressure Factors. As the pressure at which a piece of equipment operates increases, the thickness of the walls of the equipment will also increase. For example, consider the design of a process vessel. Such vessels, when subjected to internal pressure (or external pressure when operating at vacuum), are subject to rigorous mechanical design procedures. For the simple case of a cylindrical vessel operating at greater than ambient pressure, the relationship between design pressure and wall thickness required to withstand the radial stress in the cylindrical portion of the vessel, as recommended by the ASME [13], is given as

$$t = \frac{PD}{2SE - 1.2P} + CA \qquad (7.9)$$

where t is the wall thickness in meters, P is the design pressure (bar), D is the diameter of the vessel (m), S is the maximum allowable working pressure (maximum allowable stress) of material (bar), E is a weld efficiency, and CA is the corrosion allowance (m). The weld efficiency is dependent on the type of weld and the degree of examination of the weld. Typical values are from 1.0 to 0.6. The corrosion allowance depends on the service, and typical values are from 3.15 to 6.3 mm (0.125 to 0.25 inches). However, for very aggressive environments, inert linings such as glass and graphite are often used to protect the structural metal. Finally, the maximum working pressure of the material of construction, S, is dependent not only on the material but also on the operating temperature. Some typical values of S are given for common materials of construction in Figure 7.5. From this figure, it is clear that for typical carbon steel the maximum allowable stress drops off rapidly after 350°C. However, for stainless steels (ASME SA-240) the decrease in maximum allowable stress with temperature is less steep, and operation up to 600–650°C is possible for some grades. For even higher temperatures and very corrosive environments, when the lining of vessels is not practical, more exotic alloys such as titanium and titanium-based alloys and nickel-based alloys may be used. For example, Hastelloy B has excellent resistance to alkali environments up to 850°C. Inconel 600, whose main constituents are Ni 72%, Cr 15%, and Fe 8%, has excellent corrosion resistance to oxidizing environments such as acids and can be used from cryogenic temperatures up to 1100°C. The maximum allowable working pressure for Incoloy 800HT, which also has excellent corrosion resistance in acidic environments, is shown as a function of temperature in Figure 7.5.

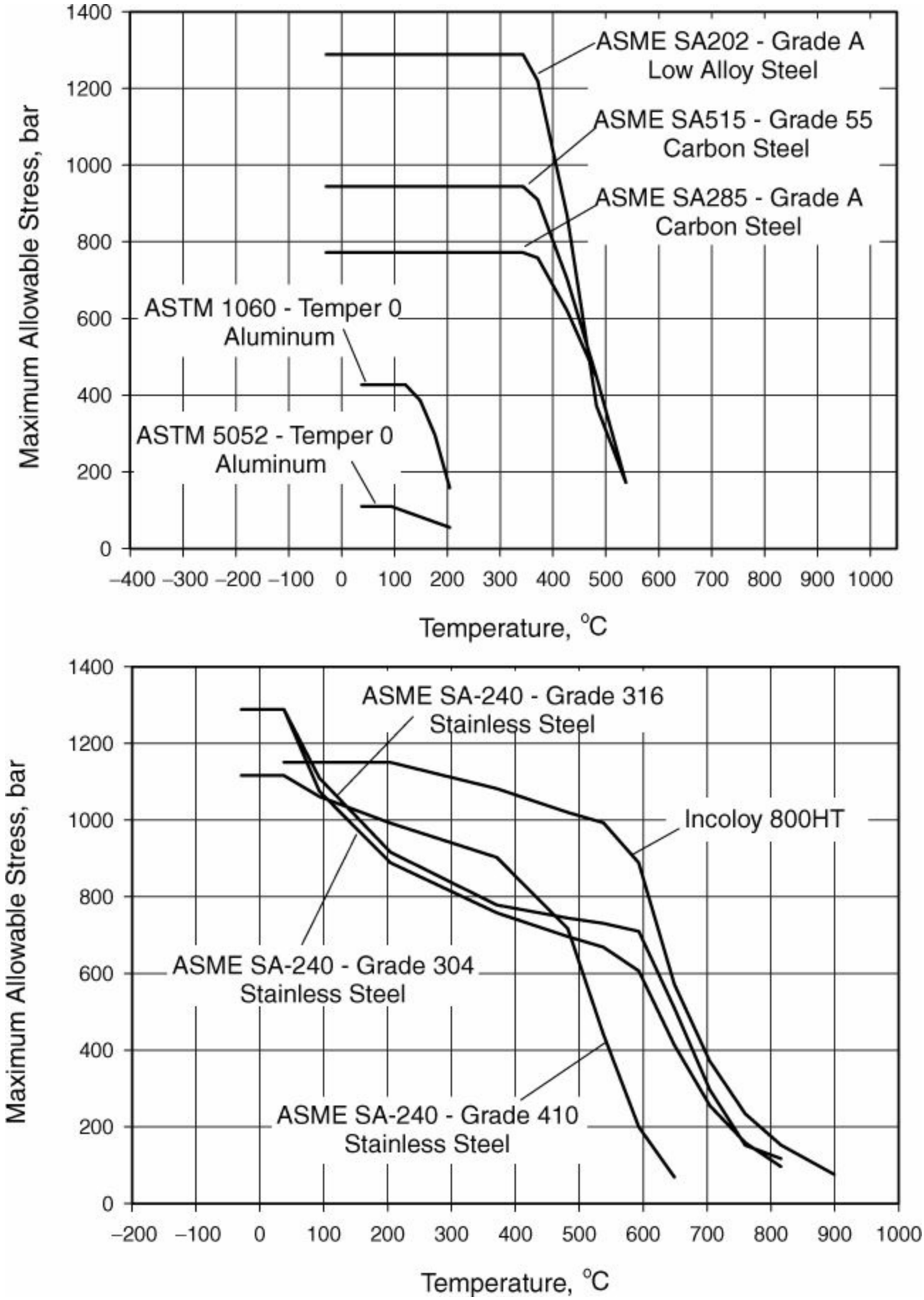


Figure 7.5. Maximum Allowable Stresses for Materials of Construction as a Function of Operating Temperature (Data from Perry et al. [3], Chapter 10, and Reference [15])

The relationship between cost of a vessel and its operating pressure is a complex one. However, with all other things being constant, the cost of the vessel is approximately proportional to the weight of the vessel, which in turn is proportional to the vessel thickness. From Equation (7.9), it is clear that

as the operating pressure approaches 1.67*SE*, the required wall thickness, and hence cost, becomes infinite. Moreover, the thickness of the vessel for a given pressure will increase as the vessel diameter increases. The effect of pressure on the weight (and ultimately cost) of carbon steel vessel shells as a function of vessel diameter is shown in Figure 7.6. The *y*-axis of the figure shows the ratio of the vessel thickness at the design pressure to that at ambient pressure, and the *x*-axis is the design pressure. A corrosion allowance of 3.15 mm (1/8 inch) and a value of $S = 944$ bar (13,700 psi) are assumed. It is also assumed that the vessel is designed with a minimum wall thickness of 6.3 mm (1/4 inch). A minimum wall thickness is often required to ensure that the vessel does not buckle under its own weight or when being transported. In addition to these factors, the costs for the vessel supports, manholes, nozzles, instrument wells, the vessel head, and so on, all add to the overall weight and cost of the vessel. For the sake of simplification, it is assumed that the pressure factor (F_P) for vertical and horizontal process vessels is equal to the value given on the *y*-axis of Figure 7.6. This, clearly, is a simplification but should be valid for the expected accuracy of this technique. Hence, the equation for F_P for process vessels is given by Equation (7.10).

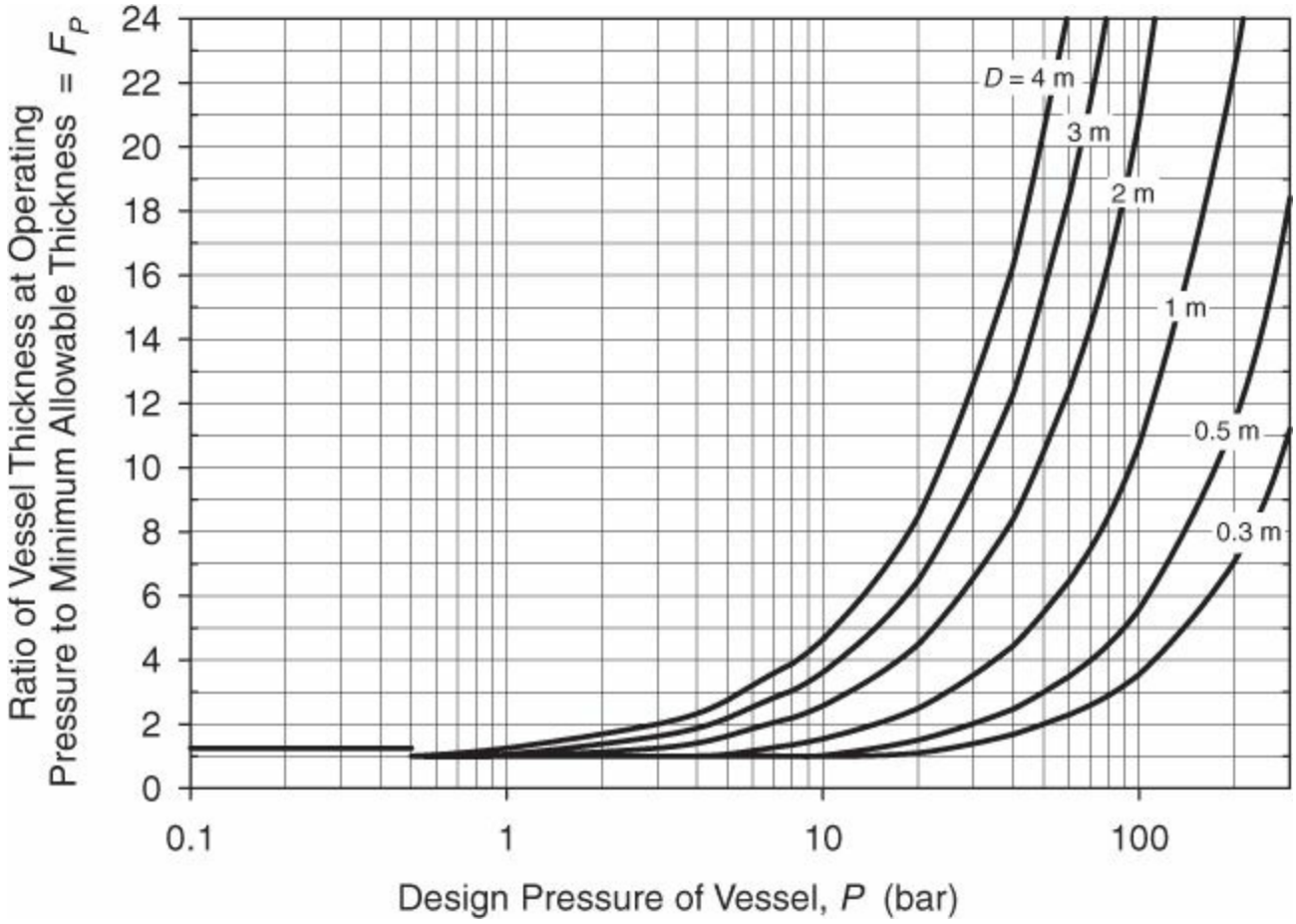


Figure 7.6. Pressure Factors for Carbon Steel Vessels

$$F_{P,vessel} \begin{cases} = 1 & \text{for } t < t_{min} \text{ and } P > -0.5 \text{ barg} \\ = \dfrac{(P+1)D}{\dfrac{(2)(944)(0.9) - 1.2(P+1)}{t_{min}}} + CA & \text{for } t > t_{min} \text{ and } P > -0.5 \text{ barg} \\ = 1.25 & \text{for } P < -0.5 \text{ barg} \end{cases} \qquad (7.10)$$

where D is the vessel diameter in m, P is the operating pressure in barg, CA is the corrosion

allowance (assumed to be 0.00315 m), and t_{min} is the minimum allowable vessel thickness (assumed to be 0.0063 m). A value of $S = 944$ bar has been assumed for carbon steel. As the operating temperature increases, the value of S decreases (see Figure 7.5) and the accuracy of F_p drops. For operating pressures less than –0.5 barg, the vessel must be designed to withstand full vacuum, that is, 1 bar of external pressure. For such operations, strengthening rings must be installed into the vessels to stop the vessel walls from buckling. A pressure factor of 1.25 should be used for such conditions, and this is shown in Figure 7.6.

Pressure factors for different equipment are given in Appendix A, Equation (A.3), and Table A.2. These pressure factors are presented in the general form given by Equation (A.3):

$$\log_{10} F_p = C_1 + C_2 \log_{10} P + C_3 (\log_{10} P)^2 \qquad \text{(A.3)}$$

This equation is clearly different from Equation (7.10) for process vessels. Moreover, the value predicted by this equation (using the appropriate constants) gives values of F_P much smaller than those for vessels at the same pressure. This difference arises from the fact that for other equipment, the internals of the equipment make up the major portion of the cost. Therefore, the cost of a thicker outer shell is a much smaller fraction of the equipment cost than for a process vessel, which is strongly dependent on the weight of the metal. Example 7.11 considers the effect of pressure on a shell-and-tube heat exchanger.

Example 7.11.

a. Repeat Example 7.10 except consider the case when the operating pressures in both the shell and the tube side are 100 barg.

b. Explain why the pressure factor for the heat exchanger is much smaller than for any of the process vessels shown in Figure 7.6.

Solution

a. From Example 7.10, $C_p^o(2001) = \$25{,}000$, $F_P = 1$

From Table A.2, for $5 < P < 140$ barg, $C_1 = 0.03881$, $C_2 = -0.11272$, $C_3 = 0.08183$

Using Equation (A.3) and substituting for $P = 100$ barg and the above constants,

$$\log_{10} F_p = 0.03881 - 0.11272\log_{10}(100) + 0.08183[\log_{10}(100)]^2 = 0.1407$$

$$F_P = 10^{0.1407} = 1.383$$

From Equation (A.4):

$$C_{BM}(2001) = C_p^o(2001)[B_1 + B_2 F_P F_M] = \$25{,}000[1.63 + 1.66(1.383)(1.0)] = \$98{,}100$$
$$C_{BM}(2011) = \$98{,}100\,(582/397) = \$143{,}810$$

b. Compared with Figure 7.6, this pressure factor (1.383) is much less than any of the vessels at $P = 100$ barg. Why?

The answer lies in the fact that much of the cost of a shell-and-tube heat exchanger is associated with the cost of the tubes that constitute the heat exchange surface area. Tubing is sold in standard sizes based on the BWG (Birmingham wire gauge) standard. Tubes for heat exchangers are typically between 19.1 and 31.8 mm (3/4 and 1-1/4 inch) in diameter and between 2.1 and 0.9 mm (0.083 and 0.035 inch) thick, corresponding to BWGs of 14 to 20, respectively. Using Equation (7.9), the maximum operating pressure of a 25.4 mm (1 inch) carbon steel tube can be estimated (assume that

CA is zero), the results are as follows:

BWG	Thickness (t) (mm)	P (from Eq. [7.9]) (barg)
20	0.889	59.1
18	1.244	81.8
16	1.651	106.9
14	2.108	134.1

From the table, it is evident that even the thinnest tube normally used for heat exchangers is capable of withstanding pressures much greater than atmospheric. Therefore, the most costly portion of a shell-and-tube heat exchanger (the cost of the tubes) is relatively insensitive to pressure. Hence, it makes sense that the pressure factors for this type of equipment are much smaller than those for process vessels at the same pressure.

The purchased cost of the equipment for the heat exchanger in Example 7.11 would be C_P (2011) = ($25,000)(1.383) (582/394) = $51,070. If this equipment cost were multiplied by the bare module factor for the base case, the cost would become C_{BM} = ($51,070)(3.29) = $168,020. This is 17% greater than the $143,810 calculated in Example 7.11. The difference between these two costs results from assuming, in the latter case, that all costs increase in direct proportion to the increase in material cost. This is far from the truth. Some costs, such as insulation, show small changes with the cost of materials, whereas other costs, such as installation materials, freight, labor, and so on, are impacted to varying extents. The method of equipment module costing accounts for these variations in the bare module factor.

Finally, some equipment is unaffected by pressure. Examples are tower trays and packing. This "equipment" is not subjected to significant differential pressure because it is surrounded by process fluid. Therefore, in Equation (A.3), use $C_1 = C_2 = C_3 = 0$. Some other equipment also has zero for these constants. For example, compressor drives are not exposed to the process fluid and so are not significantly affected by operating pressure. Other equipment, such as compressors, do not have pressure corrections because such data were not available. Use of these cost correlations for equipment outside the pressure range shown in Table A.2 should be done with extreme caution.

Materials of Construction (MOCs). The choice of what MOC to use depends on the chemicals that will contact the walls of the equipment. As a guide, Table 7.9, excerpted from Sandler and Luckiewicz [14], may be used for preliminary MOC selection. However, the interaction between process streams and MOCs can be very complex, and the compatibility of the MOC with the process stream must be investigated fully before the final design is completed.

Table 7.9. Corrosion Characteristics for Some Materials of Construction

Chemical Component	Carbon Steel	304 Stainless Steel	316 Stainless Steel	Aluminum	Copper	Brass	Monel	Hastelloy C	Titanium	TFE	Graphite
Acetaldehyde	N		A			C		A	A	A	A
Acetic acid, glacial	N		A	A	A	C	B	A	A	A	A
Acetic acid, 20%	N	A	A	A	A	C	B	A	A	A	A
Acetic anhydride	N	A	B	A	A	C		A	A	A	A
Acetone	A	A	A	A	A	A	A	A	A	A	
Ammonia, 10%	C	A	A	C	N	N	N	A	A	A	A
Aniline	A	A	A	N	N	N	A	A	A	A	A
Aqua regia	N	N	N	N	N	N	N	C	A	A	
Benzaldehyde		A	A	A	A	A	A	A	A	A	A
Benzene	A	A	A	A	A	A	A	A	A	A	A
Benzoic acid		C	A					A	B	A	A
Furfural	A	C	C	A	A	A	A	A	A	A	A
Gasoline	C	A	A	A	A	A	A	A	N	A	A
Heptane	A	A	A	A	A	A	A	A	A	A	A
Hexane		A	A	A			A	A	A	A	A
HCl, 0–25%	N	N	N	N	C	N	C	C	C	A	A
HCl, 25–37%	N	N	N	N	C	N	C	C	C	A	A
HF, 30%	N	B	B	N	N	N	A	A	N	A	A
HF, 60%	N	B	B	N	N	N	A	A	N	A	A
H_2O_2, 30%	C	C	A	C	C	N	C	A	A	A	A
H_2O_2, 90%	C	C	A	C	C	N		A	A	A	A
H_2S, aqueous	C	C	A	A	N	N	N	A	A	A	A
Maleic acid		A	A			A		A	A	A	A
Methanol		A	A	A	A		A	A	A	A	A
Methyl chloride		A	A	N			A	A	A	A	A
Methyl ethyl ketone	A	A	A	A	A		A	A	A	A	A
Methylene chloride		A	A		N		N	A	A	A	A

Naphthalene		A	A	A			A	A	A	A	A
Nitric acid, 10%	N	A	A	B	N		N	A	A	A	A
Nitric acid, 50%	N	C	C	B	N		N	A	A	A	N
Oleic acid	C	A	A	A	C		A	A	A	A	A
Oxalic acid	C	C	B	C	C		A	A	A	A	A
Phenol	N	C	C	B	N		A	A	A	A	A
Phosphoric acid, 0–50%	C	C	C	N	C		C	A	B	A	A
Phosphoric acid, 51–100%	C	C	C	N	C		C	A	B	A	A
Propyl alcohol		A	A	A	A			A	A	A	
Sodium hydroxide, 20%	A	A	A	N	C	N	A	A	A	A	A
Sodium hydroxide, 50%	A	A	A	N	C	N	A	A	A	A	A
Stearic acid		A	A	A	A		B	A	A	A	A
Sulfuric acid, 0–10%	N	N	N	N	N		C	A	B	A	A
Sulfuric acid, 10–75%	N	N	N	N	N		C	A	C	A	A
Sulfuric acid, 75–100%	N	N	N	N	N		C	C	N	A	A
Tartaric acid		A	A	A	A		C	A	A	A	A
Toluene	A	A	A	A	A		A	A	A	A	
Urea		A	A	A				A	A	A	A
Xylene		A	A					A	A	A	A

A = acceptable; B = acceptable up to 30°C; C = caution, use under limited conditions; N = not recommended; no entry = information is not available. (Reproduced from Sandler and Luckiewicz, *Practical Process Engineering, a Working Approach to Plant Design*, with permission of XIMIX, Inc., Philadelphia, 1987.)

Many *polymeric* compounds are nonreactive in both acidic and alkaline environments. However, polymers generally lack the structural strength and resilience of metals. Nevertheless, for operations at less than about 120°C in corrosive environments the use of polymers as liners for steel equipment or incorporated into fiberglass structures (at moderate operating pressures) often gives the most economical solution. The most common MOCs are still *ferrous* alloys, in particular carbon steel. *Carbon steels* are distinguished from other ferrous alloys such as wrought and cast iron by the amount of carbon in them. Carbon steel has less than 1.5 wt% carbon, can be given varying amounts of hardness or ductility, is easy to weld, and is cheap. It is still the material of choice in the CPI when corrosion is not a concern.

- *Low-alloy steels* are produced in the same way as carbon steel except that amounts of chromium and molybdenum are added (chromium between 4 and 9 wt%). The molybdenum increases the strength of the steel at high temperatures, and the addition of chromium makes the steel resistant to mildly acidic and oxidizing atmospheres and to sulfur-containing streams.
- *Stainless steels* are so-called high-alloy steels containing greater than 12 wt% chromium and possessing a corrosion-resistant surface coating, also known as a passive coating. At these chromium levels, the corrosion of steel to rusting is reduced by more than a factor of 10. Chemical resistance is also increased dramatically.
- *Nonferrous alloys* are characterized by higher cost and difficulty in machining. Nevertheless, they possess improved corrosion resistance.

  Aluminum and its alloys have a high strength-to-weight ratio and are easy to machine and cast but in some cases are difficult to weld. The addition of small amounts of other metals—for example, magnesium, zinc, silicon, and copper—can improve the weldability of aluminum.

Generally, corrosion resistance is very good due to the formation of a passive oxide layer, and aluminum has been used extensively in cryogenic (low-temperature) operations.

Copper and its alloys are often used when high thermal conductivity is required. Resistance to seawater and nonoxidizing acids such as acetic acid is very good, but copper alloys should not be used for services that contact ammonium ions (NH_4^-) or oxidizing acids. Common alloys of copper include *brasses* (containing 5–45 wt% zinc) and *bronzes* (containing tin, aluminum, and/or silicon).

- *Nickel and its alloys* are alloys in which nickel is the major component.

  Nickel-copper alloys are known by the name Monel, a trademark of the International Nickel Corp. These alloys have excellent resistance to sulfuric and hydrochloric acids, saltwater, and some caustic environments.

  Nickel-chromium alloys are known by the name Inconel, a trademark of the International Nickel Corp. These alloys have excellent chemical resistance at high temperatures. They are also capable of withstanding attack from hot concentrated aqueous solutions containing chloride ions.

  Nickel-chromium-iron alloys are known by the name Incoloy, a trademark of the International Nickel Corp. These alloys have characteristics similar to Inconel but with slightly less resistance to oxidizing agents.

  Nickel-molybdenum alloys are known by the name Hastelloy, a trademark of the Cabot Corp. These alloys have very good resistance to concentrated oxidizing agents.

- *Titanium and its alloys* have good strength-to-weight ratios and very good corrosion resistance to oxidizing agents. However, it is attacked by reducing agents, it is relatively expensive, and it is difficult to weld.

As previously shown, the combination of operating temperature and operating pressure will also affect the choice of MOC. From Table 7.9, it is evident that the number of MOCs available is very large and that the correct choice of materials requires input from a trained metallurgist.

Moreover, information about the cost of materials presented in this text is limited to a few different MOCs. The approximate relative cost of some common metals is given in Table 7.10. As a very approximate rule, if the metal of interest does not appear in Appendix A, then Table 7.10 can be used to find a metal that has approximately the same cost. As the metallurgy becomes more “exotic,” the margin for error becomes larger, and the data provided in this text will lead to larger errors in estimating the plant cost than for a plant constructed of carbon steel or stainless steel.

Table 7.10. Relative Costs of Metals Using Carbon Steel as the Base Case

Material	Relative Cost
Carbon steel	Base case (lowest)
Low-alloy steel	Low to moderate
Stainless steel	Moderate
Aluminum and aluminum alloys	Moderate
Copper and copper alloys	Moderate
Titanium and titanium-based alloys	High
Nickel and nickel-based alloys	High

To account for the cost of different materials of construction, it is necessary to use the appropriate material factor, F_M, in the bare module factor. This material factor is *not* simply the relative cost of the material of interest to that of carbon steel. The reason is that the cost to produce a piece of equipment is not directly proportional to the cost of the raw materials. For example, consider the cost of a process vessel as discussed in the previous section. Just as the bare module cost was broken down into factors relating to the purchased cost of the equipment (Tables 7.6 and 7.8), the purchased cost (or at least the manufacturing cost) can be broken down into factors relating to the cost of manufacturing the equipment. Many of these costs will be related to the size of the vessel that is in turn related to the vessel's weight, W_{vessel}. An example of these costs is given in Table 7.11.

Table 7.11. Costs Associated with the Manufacture of a Process Vessel

Factors Associated with the Manufacturing Cost of a Vessel	Relationship Relating Cost to Vessel Weight, W_{vessel}
Direct Expenses	
Cost of raw materials	$\beta_{RM} W_{vessel}$
Machining costs	$\beta_{MC} W_{vessel}$
Labor costs	$\beta_L W_{vessel}$
Indirect Costs	
Overhead	$\beta_{OH} \beta_L W_{vessel}$
Engineering expenses	$\beta_E (\beta_{RM} + \beta_{MC}) W_{vessel}$
Contingencies	$\beta_{Cont} W_{vessel}$
Total manufacturing cost	$[\beta_{RM} + \beta_{MC} + \beta_L + \beta_{OH} \beta_{LI} + \beta_E (\beta_{RM} + \beta_{MC}) + \beta_{Cont}] W_{vessel}$

From Table 7.11, it is clear that the cost of the vessel is proportional to its weight. Therefore, the cost will be proportional to the vessel thickness, and thus the pressure factor derived in the previous section is valid (or at least is a reasonably good approximation). The effect of different MOCs is connected to the factor β_{RM}. Clearly, as the raw material costs increase, the total manufacturing costs will not increase proportionally to β_{RM}. In other words, if material *X* is 10 times as expensive as carbon steel, a vessel made from material *X* will be less than 10 times the cost of a similar vessel made from carbon steel. For example, over the last 15 years, the cost of stainless steel has varied between 4.7 and 7.0 times the cost of carbon steel [16]. However, the cost of a stainless steel process vessel has varied in the approximate range of 2.3 to 3.5 times the cost of a carbon steel vessel for similar service.

Materials factors for the process equipment considered in this text are given in Appendix A, Tables A.3–A.6, and Figures A.18 and A.19. These figures are constructed using averaged data from the following sources: Peters and Timmerhaus [2], Guthrie [9, 10], Ulrich [5], Navarrete [11], and Perry et al. [3]. Example 7.12 illustrates the use of these figures and tables.

Example 7.12.

Find the bare module cost of a floating-head shell-and-tube heat exchanger with a heat transfer area of 100 m^2 for the following cases:

a. The operating pressure of the equipment is 1 barg on both shell and tube sides, and the MOC of the shell and tubes is stainless steel.

b. The operating pressure of the equipment is 100 barg on both shell and tube sides, and the MOC of the shell and tubes is stainless steel.

From Example 7.10, C_p^o (2001) = \$25,000 and C_p^o (2011) = \$25,000 (582/397) = \$36,650.

a. From Example 7.10, at 1 barg, $F_P = 1$

From Table A.3 for a shell-and-tube heat exchanger made of SS, Identification No. = 5 and using Figure A.8, $F_M = 2.73$

From Equation (A.4),

$$C_{BM}\ (2011) = C_p^o[B_1 + B_2F_PF_M] = \$36{,}650[1.63 + 1.66(1.0)(2.73)] = \$225{,}800$$

b. From Example 7.11 for P = 100 barg, $F_P = 1.383$

From (a) above, $F_M = 2.73$

Substituting these values in to Equation (A.4),

$$C_{BM}\ (2011) = C_p^o[B_1 + B_2F_PF_M] = \$36{,}650[1.63 + 1.66(1.383)(2.73)] = \$289{,}300$$

The last three examples all considered the same size heat exchanger made with different materials of construction and operating pressure. The results are summarized below.

Example	Pressure	Materials	F_{BM}	Cost
7.10	ambient	CS tubes/shell	3.29	\$120,650
7.11	100 barg	CS tubes/shell	3.93	\$143,810
7.12a	ambient	SS tubes/shell	6.16	\$225,800
7.12b	100 barg	SS tubes/shell	7.90	\$289,300

These results reemphasize the point that the cost of the equipment is strongly dependent on the materials of construction and the pressure of operation.

7.3.5. Combination of Pressure and MOC Information to Give the Bare Module Factor, F_{BM}, and Bare Module Cost, C_{BM}

In Examples 7.10–7.12, the bare module factors and costs were calculated using Equation (A.4). The form of this equation is not obvious, and its derivation is based on the approach used by Ulrich [5]:

$$\text{Cost of Equipment} = C_p^o F_P F_M \qquad (7.11)$$

This is the equipment cost at operating conditions:

$$\text{Cost for Equipment Installation (for base conditions)} = C_p^o(F_{BM}^o - 1) \qquad (7.12)$$

This cost is calculated by taking the bare module cost, at base conditions, and subtracting the cost of the equipment at the base conditions.

The incremental cost of equipment installation due to non-base-case conditions is

$$C_p^o(F_P F_M - 1)f_{P\&I} \qquad (7.13)$$

This cost is based on the incremental cost of equipment due to non-base conditions multiplied by a factor, ($f_{P\&I}$), that accounts for the fraction of the installation cost that is associated with piping and instrumentation. The values of $f_{P\&I}$ are modified from Guthrie [9, 10] to account for an increase in the level and cost of instrumentation that modern chemical plants enjoy compared with that at the time of Guthrie's work.

Equations (7.11) through (7.13) can be combined to give the following relationship:

$$\text{Bare module cost, } C_{BM} = C_p^o F_P F_M + C_p^o(F_{BM}^o - 1) + C_p^o(F_P F_M - 1)f_{P\&I}$$

$$= C_p^o[F_P F_M(1 + f_{P\&I}) + F_{BM}^o - 1 - f_{P\&I}] = C_p^o[B_1 + B_2 F_P F_M] \qquad (7.14)$$

Equation (7.13) is the same as Equation (A.4), with $B_1 = F_{BM}^o - 1 - f_{P\&I}$ and $B_2 = 1 + f_{P\&I}$.

7.3.6. Algorithm for Calculating Bare Module Costs

The following six-step algorithm is used to estimate actual bare module costs for equipment from the figures in Appendix A:

1. Using the correct figure in Appendix A (Figures A.1–A.17), or the data in Table A.1, obtain C_p^o for the desired piece of equipment. This is the purchased equipment cost for the base case (carbon steel construction and near-ambient pressure).
2. Find the correct relationship for the bare module factor. For exchangers, pumps, and vessels, use Equation (A.4) and the data in Table A.4. For other equipment, the form of the equation is given in Table A.5.
3. For exchangers, pumps, and vessels, find the pressure factor, F_P, Table A.2 and Equation (A.2) or (A.3), and the material of construction factor, F_M, Equation (A.4), Table A.3, and Figure A.18. Use Equation (A.4) to calculate the bare module factor, F_{BM}.
4. For other equipment find the bare module factor, F_{BM}, using Table A.6 and Figure A.19.
5. Calculate the bare module cost of equipment, C_{BM}, from Equation (7.6).
6. Update the cost from 2001 ($CEPCI$ – 397) to the present by using Equation (7.4).

Example 7.13 illustrates the six-step algorithm for the case of a distillation column with associated trays.

Example 7.13.

Find the bare module cost (in 2011) of a stainless steel tower 3 m in diameter and 30 m tall. The tower has 40 stainless steel sieve trays and operates at 20 barg.

The costs of the tower and trays are calculated separately and then added together to obtain the total cost.

For the tower,

a. Volume = $\pi D^2 L/4 = (3.14159)(3)^2(30)/4 = 212.1\ m^3$

From Equation (A.1),

$$\log_{10} C_p^o\,(2001) = 3.4974 + 0.4485\log_{10}(212.1) + 0.1074\{\log_{10}(212.1)\}^2 = 5.1222$$

$$C_p^o\,(2001) = 10^{5.1222} = \$132{,}500$$

$$C_p^o\,(2011) = \$132{,}500(582/397) = \$194{,}240$$

b. From Equation (A.3) and Table A.4, $F_{BM} = 2.25 + 1.82\,F_M F_P$

c. From Equation (7.10) with $P = 20$ barg and $D = 3$ m,

$$F_{P,vessels} = \frac{\dfrac{(20+1)3}{(2)[(944)(0.9) - 0.6(20+1)]} + 0.00315}{0.0063} = 6.47$$

From Table A.3, identification number for stainless steel vertical vessel = 20; from Figure A.8, $F_M = 3.11$

$$F_{BM} = 2.25 + 1.82(6.47)(3.11) = 38.87$$

d. $C_{BM}\,(2011) = (194{,}240)(38.87) = \$7{,}550{,}300$

For the trays,

a. Tray (tower) area = $\pi D^2/4 = 7.0686$

From Equation (A.1),

$$\log_{10} C_p^o\,(2001) = 2.9949 + 0.4465\log_{10}(7.0686) + 0.3961\{\log_{10}(7.0686)\}^2 = 3.6599$$

$$C_p^o\,(2001) = 10^{3.6599} = \$4570$$

$$C_p^o\,(2011) = \$4{,}570(582/397) = \$6{,}700$$

From Table A.5,

$$C_{BM} = C_p N F_{BM} f_q$$

$N = 40$

$f_q = 1.0$ (since number of trays > 20, Table A.5)

From Table A.6, SS sieve trays identification number = 61; from Figure A.9, $F_{BM} = 1.83$

$$C_{BM,trays}\,(2011) = (\$6{,}700)(40)(1.83)(1.0) = \$490{,}400$$

For the tower plus trays,

$$C_{BM,tower+trays}\,(2011) = \$7{,}550{,}300 + \$490{,}410 = \$8{,}040{,}700$$

7.3.7. Grassroots and Total Module Costs

The term *grassroots* (or green field) refers to a completely new facility in which the construction is started on essentially undeveloped land, a grass field. The term *total module cost* refers to the cost of making small to moderate expansions or alterations to an existing facility.

To estimate these costs, it is necessary to account for other costs in addition to the direct and indirect costs. These additional costs were presented in Table 7.6 and can be divided into two groups.

Group 1: Contingency and Fee Costs: The contingency cost varies depending on the

reliability of the cost data and completeness of the process flowsheet available. This factor is included in the evaluation of the cost as a protection against oversights and faulty information. Unless otherwise stated, values of 15% and 3% of the bare module cost are assumed for contingency costs and fees, respectively. These are appropriate for systems that are well understood. Adding these costs to the bare module cost provides the *total module cost*.

Group 2: Auxiliary Facilities Costs: These include costs for site development, auxiliary buildings, and off-sites and utilities. These terms are generally unaffected by the materials of construction or the operating pressure of the process. A review of costs for these auxiliary facilities by Miller [17] gives a range of approximately 20% to more than 100% of the bare module cost. Unless otherwise stated, these costs are assumed to be equal to 50% of the bare module costs for the base case conditions. Adding these costs to the total module cost provides the *grassroots cost*.

The total module cost can be evaluated from

$$C_{TM} = \sum_{i=1}^{n} C_{TM,i} = 1.18 \sum_{i=1}^{n} C_{Bm,i} \qquad (7.15)$$

and the grassroots cost can be evaluated from

$$C_{GR} = C_{TM} + 0.50 \sum_{i=1}^{n} C^{o}_{BM,i} \qquad (7.16)$$

where n represents the total number of pieces of equipment. The use of these equations is shown in Example 7.14.

Example 7.14.

A small expansion to an existing chemical facility is being investigated, and a preliminary PFD of the process is shown in Figure E7.14.

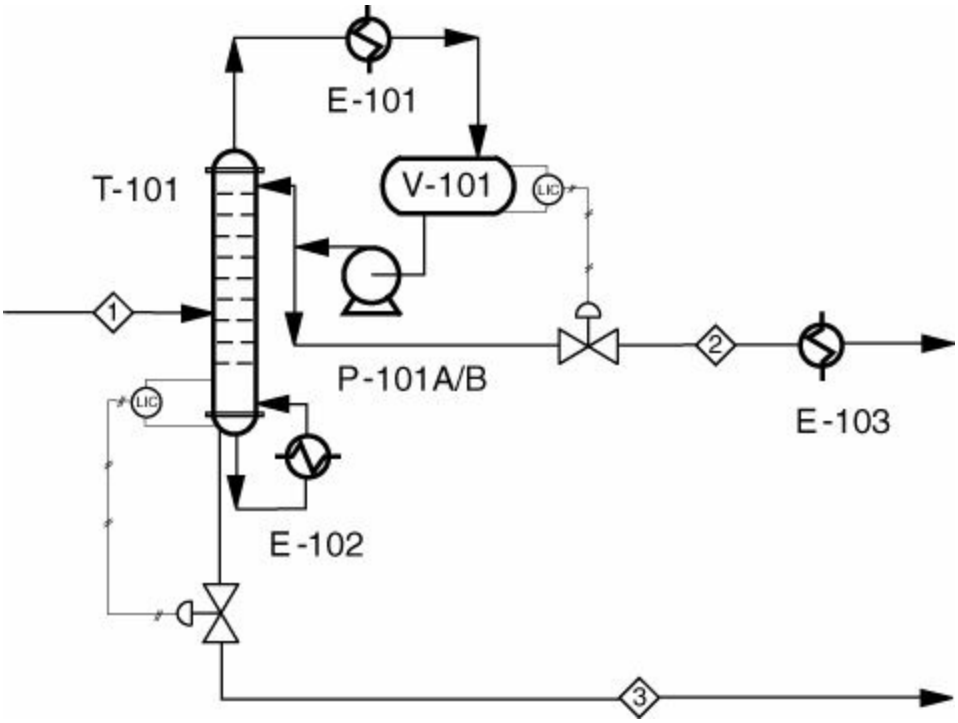


Figure E7.14. PFD for Example 7.14

The expansion involves the installation of a new distillation column with a reboiler, condenser, pumps, and other associated equipment. A list of the equipment, sizes, materials of construction, and

operating pressures is given in Table E7.14(a). Using the information in Appendix A, calculate the total module cost for this expansion in 2011.

Table E7.14(a). Information on Equipment Required for the Plant Expansion Described in Example 7.14

Equipment No.	Capacity / Size	Material of Construction*	Operating Pressure (barg†)
E-101 Overhead condenser	Area = 170 m^2 Shell and tube (floating head)	Tube—CS Shell—CS	Tube = 5.0 Shell = 5.0
E-102 Reboiler	Area = 205 m^2 Shell and tube (floating head)	Tube—SS Shell—CS	Tube = 18.0 Shell = 6.0
E-103 Product cooler	Area = 10 m^2 (double pipe)	All CS construction	Inner = 5.0 Outer = 5.0
P-101A/B Reflux pumps	$Power_{shaft}$ = 5 kW Centrifugal	CS	Discharge = 5.0
T-101 Aromatics column	Diameter = 2.1 m Height = 23 m	Vessel—CS	Column = 5.0
	32 sieve trays	Trays—SS	
V-101 Reflux drum	Diameter = 1.8 m Length = 6 m Horizontal	Vessel—CS	Vessel = 5.0

*CS = Carbon steel; SS = Stainless steel
†barg = bar gauge, thus 0.0 barg = 1.0 bar

The same algorithm presented above is used to estimate bare module costs for all equipment. This information is listed in Table E7.14(b), along with purchased equipment cost, pressure factors, material factors, and bare module factors.

Table E7.14(b). Results of Capital Cost Estimate for Example 7.14

Equipment	F_P	F_M	F_{BM}	C_p^o (2001) ($)	C_{BM} (2001) ($)	C_{BM}^o (2001) ($)
E-101	1.0	1.0	3.29	33,000	108,500	108,500
E-102	1.023	1.81	4.70	36,900	177,900	121,300
E-103	1.0	1.0	3.29	3700	12,300	12,300
P-101A/B	1.0	1.55	3.98	(2)(3200)	(2)(12,600)	(2)(10,300)
T-101	1.681	1.0	5.31	54,700	290,700	222,800
32 trays		1.83	1.83	(32)(2200)	131,200	71,700
V-101	1.513	1.0	3.79	13,500	51,200	40,600
Totals				219,900	797,000	597,800

CEPCI = 397

C_{BM} (2011) = (582/397)(797,000) = $1,168,400

The substitutions from Table E7.14(b) are made into Equations (7.15) and (7.16) to determine the total module cost and the grassroots cost.

$$\text{Total module cost } (C_{TM}) = 1.18\sum_{i=1}^{n} C_{BM,i} = 1.18(\$797{,}000)(582/397) = \$1{,}378{,}700$$

$$\text{Grassroots cost } (C_{GR}) = C_{TM} + 0.50\sum_{i=1}^{n} C^{o}_{BM,i} = \$1{,}378{,}700 + 0.50(\$597{,}800)(582/397)$$
$$= \$1{,}816{,}900$$

Although the grassroots cost is not appropriate here (because this involves only a small expansion to an existing facility), it is shown for completeness.

7.3.8. A Computer Program (CAPCOST) for Capital Cost Estimation Using the Equipment Module Approach

For processes involving only a few pieces of equipment, estimating the capital cost of the plant by hand is relatively easy. For complex processes with many pieces of equipment, these calculations become tedious. To make this process easier, a computer program has been developed that allows the user to enter data interactively and obtain cost estimates in a fraction of the time required for hand calculations with less chance for error. The program (CAPCOST_2011.xls) is programmed in Microsoft Excel, and a template copy of the program is supplied on the CD that accompanies this book.

The program is written in the Microsoft Windows programming environment. The program requires the user to input information about the equipment—for example, the capacity, operating pressure, and materials of construction. The cost data can be adjusted for inflation by entering the current value of the CEPCI. Other information such as output file names and the number of the unit (100, 200, etc.) is also required.

The equipment options available to the user are given below.

- Blenders
- Centrifuges
- Compressors and blowers without drives
- Conveyors
- Crystallizers
- Drives for compressors, blowers, and pumps
- Dryers
- Dust collectors
- Evaporators and vaporizers
- Fans with electric drives
- Filters
- Fired heaters, thermal fluid heaters, and packaged steam boilers
- Furnaces
- Heat exchangers
- Mixers

- Process vessels with/without internals
- Power recovery equipment
- Pumps with electric drives
- Reactors
- Screens
- Storage vessels (fixed roof and floating roof)
- Towers
- User-added modules

The type of equipment required can be entered by using the mouse-activated buttons provided on the first worksheet. The user will then be asked a series of questions that appear on the screen. The user will be required to identify or enter the same information as would be needed to do the calculations by hand—that is, operating pressure, materials of construction, and the size of the equipment. The same information as contained in the cost charts and tables in Appendix A is embedded in the program, and the program should give the same results as hand calculations using these charts.

When the data for equipment are entered, a list of the costs on the first worksheet is updated. The use of the spreadsheet is explained in the CAPCOST.avi help files contained on the CD, and the reader is encouraged to view the file prior to using the software. The results for Example E7.14 from CAPCOST2011 are shown in Table 7.12. As can be seen, the results are essentially identical to those found by hand calculation.

Table 7.12. Results from CAPCOST2011 for Example 7.14

Add Equipment | Unit Number 100

Edit Equipment | CEPCI 582

Remove All Equipment

User Added Equipment

Exchangers	Exchanger Type	Shell Pressure (barg)	Tube Pressure (barg)	MOC	Area (square meters)	Purchased Equipment Cost	Bare Module Cost
E-101	Floating Head	5	5	Carbon Steel/ Carbon Steel	170	$48,300	$159,000
E-102	Floating Head	6	18	Stainless Steel/ Carbon Steel	205	$54,100	$261,000
E-103	Double Pipe		5	Carbon Steel/ Carbon Steel	10	$5,470	$18,000

Pumps (with drives)	Pump Type	Power (kilowatts)	# Spares	MOC	Discharge Pressure (barg)	Purchased Equipment Cost	Bare Module Cost
P-101	Centrifugal	5	1	Carbon Steel	5	$9,310	$37,100

Towers	Tower Description	Height (meters)	Diameter (meters)	Tower MOC	Demister MOC	Pressure (barg)	Purchased Equipment Cost	Bare Module Cost
T-101	2 Stainless Steel Sieve Tray	23	2.1	Carbon Steel		5	$185,000	$619,000

Vessels	Orientation	Length/ Height (meters)	Diameter (meters)	MOC	Demister MOC	Pressure (barg)	Purchased Equipment Cost	Bare Module Cost
V-101	Horizontal	6	1.8	Carbon Steel	5	5	$19,800	$75,000
							Total Bare Module Cost	$1,169,100

Total Module Cost = $1,380,000
Total Grassroots Cost = $1,820,000

7.4. Summary

In this chapter, the different types of capital cost estimating techniques that are available were reviewed. The accuracy of the different estimates was shown to increase significantly with the time involved in completion and the amount of data required. The information required to make an equipment module estimate based on data from the major process equipment was also covered. The effects of operating pressure and materials of construction on the bare module cost of equipment were reviewed. Several examples were given to show how the installed cost of equipment is significantly greater than the purchased cost and how the installed cost increases with increased pressure and materials of construction. The use of cost indices to adjust for the effects of inflation on equipment costs was considered, and the Chemical Engineering Plant Cost Index (CEPCI) was adopted for all inflation adjustments. The concepts of grassroots and total module costs were introduced in order to make estimates of the total capital required to build a brand-new plant or make an expansion to an existing facility. To ease the calculation of the various costs, a computer program for cost estimation was introduced. This chapter contains the basic approach to estimating capital costs for new chemical plants and expansions to existing plants, and mastery of this material is assumed in the remaining chapters.

What You Should Have Learned

- Equipment costs can be estimated from correlations developed based on vendor quotes or based on historical purchase data.

- These correlations can be adjusted for changes in cost over time (inflation).
- The equipment cost is also a function of operating pressure and materials of construction.
- The capital cost of a chemical plant can be obtained by adding the individual equipment costs and including other factors such as site development and auxiliary facilities.

References

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Short Answer Questions

1. What are the three main factors that determine the capital cost of a piece of equipment such as a

heat exchanger at a given time?

2. What is the Chemical Engineering Plant Cost Index (CEPCI) used for, and what does it measure?
3. What is the difference between the total module cost and the grassroots cost of a chemical process?
4. When would you use a cost exponent of 0.6?
5. What is meant by the economy of scale?
6. What is a Lang Factor?
7. The pressure factor F_p for a shell-and-tube heat exchanger is significantly smaller than for a vessel over the same pressure range. Why is this so?

Problems

8. The cost* of a recent plant in Alberta, Canada, to produce 1.27 million tonne/y of polyethylene was $540 million. Estimate what the range of cost estimates would likely have been for a Class 5, a Class 3, and a Class 1 estimate.

   *http://www.chemicals-technology.com/projects/joffre/

9. In Appendix A, Figures A.1–A.17, the purchased costs for various types of equipment are given. The *y*-axis is given as the cost of the equipment per unit of capacity, and the *x*-axis is given as the capacity. The capacity is simply the relevant sizing parameter for the equipment. Identify all equipment that does not conform to the principle of the economy of scale.
10. A process vessel was purchased in the United Kingdom for our plant in the United States in 1993. A similar vessel, but of different capacity, was purchased in 1998. From the data given below, estimate the cost in U.S.$ of a vessel of 120 m^3 capacity purchased today (assume the current *CEPCI* = 582).

Date	Vessel Capacity (m^3)	Purchased Cost (Pounds Sterling = £)	Exchange Rate
1993	75	£7,800	$1.40/£
1998	155	£13,800	$1.65/£
2007	120		$2.00/£

11. You have been hired as a consultant to a legal firm. Part of your assignment is to determine the size of a storage tank purchased in 1978 (*CEPCI* = 219), before computerization of records. Many records from this era were destroyed in a fire (not in the plant, but in a distant office building). The tank was replaced every 10 years, and the sizes have changed due to plant capacity changes. You have the information in the table below. Estimate the original capacity of this vessel.

Date	Tank Capacity (1000 gal)	Purchased Cost
1978	?	$35,400
1988	105	$45,300
1998	85	$45,500

12. In your role as a consultant to a legal firm, you have been requested to determine whether

calculations submitted in a legal action are valid. The problem is to determine what year a compressor was placed into service. The information in the table is available. It is claimed that the compressor was placed into service in 1976. History suggests that during the period from 1976 to 1985 there was significant inflation. Do you believe the information submitted is correct? If not, what year do you believe the compressor to be placed into service? Use *CEPCI* = 500 for 2006.

Date	Compressor Power (kW)	Total Module Cost (in $10^3$$)
???	1000	645.93
2000	500	500.00
2006	775	811.68

Note: CEPCI (1986) = 318, *CEPCI* (1981) = 297, *CEPCI* (1976) = 192.

13. When designing equipment for high-temperature and high-pressure service, the maximum allowable stress as a function of temperature of the material of construction is of great importance. Consider a cylindrical vessel shell that is to be designed for pressure of 150 bar (design pressure). The diameter of the vessel is 3.2 m, it is 15 m long, and a corrosion allowance of 6.35 mm (1/4") is to be used. Construct a table that shows the thickness of the vessel walls in the temperature range of 300 to 500°C (in 20°C increments) if the materials of construction are (a) ASME SA515-grade carbon steel and (b) ASME SA-240-grade 316 stainless steel.
14. Using the results of Problem 7.13, determine the relative costs of the vessel using the two materials of construction (CS and 316 SS) over the temperature range. You may assume that the cost of the vessel is directly proportional to the weight of the vessel and that the 316 SS costs 3.0 times as much as CS. Based on these results, which material of construction is favored over the temperature range 300–500°C for this vessel?
15. A certain vendor estimates the cost of vertical drums made from stainless steel as a function of the volume (V) of the cylindrical portion of the drum and the diameter (d) of the end pieces. The cost function is

$$Cost(\$) = aV^{0.8} + bd^{0.3}$$

where V is in ft^3 and d is in ft. Your company has purchased two such drums in the past, and the information is given in Table P7.15. Estimate the cost when *CEPCI* = 550 of a 5 ft diameter and 12 ft tall drum.

Table P7.15. Size and Cost Data for Problem 7.15

Year Purchased	Height (ft)	Diameter (ft)	Purchased Cost ($)
1986	15	6	24,224
1998	10	3	7202

The following problems may be solved either by using hand calculations or by using CAPCOST (use a value of* CEPCI = *582).

16. Determine the bare module cost of a 1-shell-pass, 2-tube-pass (1-2) heat exchanger designed for the following operating conditions:

Maximum operating pressure (tube side) = 30 barg

Maximum operating pressure (shell side) = 5 barg

Process fluid in tubes requires stainless steel MOC

Shell-side utility (cooling water) requires carbon steel MOC

Heat exchange area = 160 m^2

17. Repeat Problem 7.16, except reverse the shell-side and tube-side fluids. Are your results consistent with the heuristics for heat exchangers given in Chapter 11? Which heuristic is relevant?
18. In Chapter 15, the concepts of heat-exchanger networks and pinch technology are discussed. When designing these networks to recover process heat, it is often necessary to have a close temperature approach between process streams, which leads to large heat exchangers with multiple shells. Multiple-shell heat exchangers are often constructed from sets of 1-2 shell-and-tube exchangers stacked together. For costing considerations, the cost of the multiple-shell heat exchanger is best estimated as a number of smaller 1-2 exchangers. Consider a heat exchanger constructed of carbon steel and designed to withstand a pressure of 20 barg in both the shell and tube sides. This equipment has a heat exchange area of 400 m^2. Do the following:
    a. Determine the bare module cost of this 4-shell and 8-tube pass heat exchanger as four, 1-2 exchangers, each with a heat-exchange area of 100 m^2.
    b. Determine the bare module cost of the same exchanger as if it had a single shell.
    c. What is the name of the principle given in this chapter that explains the difference between the two answers in (a) and (b)?
19. A distillation column is initially designed to separate a mixture of toluene and xylene at around ambient temperature (say, 100°C) and pressure (say, 1 barg). The column has 20 stainless steel valve trays and is 2 m in diameter and 14 m tall. Determine the purchased cost and the bare module cost using a *CEPCI* = 582.
20. A column with similar dimensions, number of trays, and operating at the same conditions as given in Problem 7.19 is to be used to separate a mixture containing the following chemicals. For each case determine the bare module cost using a *CEPCI* = 582.
    a. 10% nitric acid solution
    b. 50% sodium hydroxide solution
    c. 10% sulfuric acid solution
    d. 98% sulfuric acid solution

    Hint: You may need to look for the relevant MOC for Part (d) on the Internet or another resource.

It is recommended that the following problems be solved using CAPCOST (use a value of CEPCI ***= 582).***

Determine the bare module, total module, and grassroots cost of the following:

21. Toluene hydrodealkylation plant described in Chapter 1 (see Figures 1.3 and 1.5 and Tables 1.5 and 1.7)
22. Ethylbenzene plant described in Appendix B, Project B.2

23. Styrene plant described in Appendix B, Project B.3
24. Drying oil plant described in Appendix B, Project B.4
25. Maleic anhydride plant described in Appendix B, Project B.5
26. Ethylene oxide plant described in Appendix B, Project B.6
27. Formalin plant described in Appendix B, Project B.7

Chapter 8. Estimation of Manufacturing Costs

What You Will Learn

- It is necessary to quantify the cost of manufacture of a chemical process.
- The primary components of the cost of manufacture are raw materials, utilities, and waste treatment.

The costs associated with the day-to-day operation of a chemical plant must be estimated before the economic feasibility of a proposed process can be assessed. This chapter introduces the important factors affecting the manufacturing cost and provides methods to estimate each factor. In order to estimate the manufacturing cost, process information provided on the PFD, an estimate of the fixed capital investment, and an estimate of the number of operators required to operate the plant are all needed. The fixed capital investment is the same as either the total module cost or the grassroots cost defined in Chapter 7. Manufacturing costs are expressed in units of dollars per unit time, in contrast to the capital costs, which are expressed in dollars. How these two costs are treated, expressed in different units, to judge the economic merit of a process is covered in Chapters 9 and 10.

8.1. Factors Affecting the Cost of Manufacturing a Chemical Product

There are many elements that influence the cost of manufacturing chemicals. A list of the important costs involved, including a brief explanation of each cost, is given in Table 8.1.

Table 8.1. Factors Affecting the Cost of Manufacturing (*COM*) for a Chemical Product (from References [1, 2, and 3])

Factor	Description of Factor
1. Direct Costs	**Factors that vary with the rate of production**
a. Raw materials	Costs of chemical feedstocks required by the process. Flowrates obtained from the PFD.
b. Waste treatment	Costs of waste treatment to protect environment.
c. Utilities	Costs of utility streams required by process. Includes but not limited to a. Fuel gas, oil, and/or coal b. Electric power c. Steam (all pressures) d. Cooling water e. Process water f. Boiler feed water g. Instrument air h. Inert gas (nitrogen, etc.) i. Refrigeration Flowrates for utilities found on the PFD/P&IDs.
d. Operating labor	Costs of personnel required for plant operations.
e. Direct supervisory and clerical labor	Cost of administrative, engineering, and support personnel.
f. Maintenance and repairs	Costs of labor and materials associated with maintenance.
g. Operating supplies	Costs of miscellaneous supplies that support daily operation not considered to be raw materials. Examples include chart paper, lubricants, miscellaneous chemicals, filters, respirators and protective clothing for operators, etc.

h. Laboratory charges	Costs of routine and special laboratory tests required for product quality control and troubleshooting.
i. Patents and royalties	Cost of using patented or licensed technology.
2. Fixed Costs	**Factors not affected by the level of production**
a. Depreciation	Costs associated with the physical plant (buildings, equipment, etc.). Legal operating expense for tax purposes.
b. Local taxes and insurance	Costs associated with property taxes and liability insurance. Based on plant location and severity of the process.
c. Plant overhead costs (sometimes referred to as factory expenses)	Catch-all costs associated with operations of auxiliary facilities supporting the manufacturing process. Costs involve payroll and accounting services, fire protection and safety services, medical services, cafeteria and any recreation facilities, payroll overhead and employee benefits, general engineering, etc.
3. General Expenses	**Costs associated with management-level and administrative activities not directly related to the manufacturing process**
a. Administration costs	Costs for administration. Includes salaries, other administration, buildings, and other related activities.
b. Distribution and selling costs	Costs of sales and marketing required to sell chemical products. Includes salaries and other miscellaneous costs.
c. Research and development	Costs of research activities related to the process and product. Includes salaries and funds for research-related equipment and supplies, etc.

The cost information provided in Table 8.1 is divided into three categories:

1. **Direct Manufacturing Costs:** These costs represent operating expenses that vary with production rate. When product demand drops, production rate is reduced to less than the design capacity. At this lower rate, a reduction in the factors making up the direct manufacturing costs would be expected. These reductions may be directly proportional to the production rate, as for raw materials, or might be reduced slightly—for example, maintenance costs or operating labor.
2. **Fixed Manufacturing Costs:** These costs are independent of changes in production rate. They include property taxes, insurance, and depreciation, which are charged at constant rates even when the plant is not in operation.
3. **General Expenses:** These costs represent an overhead burden that is necessary to carry out business functions. They include management, sales, financing, and research functions. General expenses seldom vary with production level. However, items such as research and development and distribution and selling costs may decrease if extended periods of low production levels occur.

The equation used to evaluate the cost of manufacture using these costs becomes:

$$\text{Cost of Manufacture } (COM) = \text{Direct Manufacturing Costs } (DMC) + \text{Fixed Manufacturing Costs } (FMC) + \text{General Expenses } (GE)$$

The approach provided in this chapter is similar to that presented in other chemical engineering design texts [1, 2, 3].

The cost of manufacturing, *COM*, can be determined when the following costs are known or can be estimated:

1. Fixed capital investment (*FCI*): (C_{TM} or C_{GR})
2. Cost of operating labor (C_{OL})
3. Cost of utilities (C_{UT})
4. Cost of waste treatment (C_{WT})
5. Cost of raw materials (C_{RM})

Table 8.2 gives data to estimate the individual cost items identified in Table 8.1 (both tables carry the same identification of individual cost terms). With the exception of the cost of raw materials, waste treatment, utilities, and operating labor (all parts of the direct manufacturing costs), Table 8.2 presents equations that can be used to estimate each individual item. With each equation, a typical range for the constants (multiplication factors) to estimate an individual cost item is presented. If no other information is available, the midpoint value for each of these ranges is used to estimate the costs involved. It should be noted that the best information that is available should always be used to establish these constants. The method presented here should be used only when no other information on these costs is available.

Table 8.2. Multiplication Factors for Estimating Manufacturing Cost* (See Also Table 8.1)

Cost Item from Table 8.1	Typical Range of Multiplying Factors	Value Used in Text
1. Direct Manufacturing Costs		
a. Raw materials	C_{RM}†	
b. Waste treatment		C_{WT}†
c. Utilities	C_{UT}†	
d. Operating labor		C_{OL} C_{OL}
e. Direct supervisory and clerical labor	$(0.1–0.25)C_{OL}$	$0.18C_{OL}$
f. Maintenance and repairs	$(0.02–0.1)FCI$	$0.06FCI$
g. Operating supplies	(0.1–0.2)(Line 1.F)	$0.009FCI$
h. Laboratory charges	$(0.1–0.2)C_{OL}$	$0.15C_{OL}$
i. Patents and royalties	$(0–0.06)COM$	$0.03COM$
Total Direct Manufacturing Costs	$C_{RM} + C_{WT} + C_{UT} + 1.33C_{OL} + 0.03COM + 0.069FCI$	

2. Fixed Manufacturing Costs		
a. Depreciation	$0.1FCI^{\ddagger}$	$0.1FCI^{\ddagger}$
b. Local taxes and insurance	$(0.014–0.05)FCI$	$0.032FCI$
c. Plant overhead costs	(0.50–0.7)(Line 1.D. + Line 1.E + Line 1.F)	$0.708C_{OL} + 0.036FCI$
Total Fixed Manufacturing Costs	$\mathbf{0.708C_{OL} + 0.068FCI}$ **+ depreciation**	
3. General Manufacturing Expenses		
a. Administration costs	0.15(Line 1.D. + Line 1.E.+ Line 1.F.)	$0.177C_{OL} + 0.009FCI$
b. Distribution and selling costs	$(0.02–0.2)COM$	$0.11COM$
c. Research and development	$0.05COM$	$0.05COM$
Total General Manufacturing Costs	$\mathbf{0.177C_{OL} + 0.009FCI + 0.16COM}$	
Total Costs	$\mathbf{C_{RM} + C_{WT} + C_{UT} + 2.215C_{OL} + 0.190COM + 0.146FCI}$ **+ depreciation**	

*Costs are given in dollars per unit time (usually per year).
†Costs are evaluated from information given on the PFD and the unit cost.
‡Depreciation costs are covered separately in Chapter 9. The use of 10% of *FCI* is a crude approximation at best.
From references [1], [2], and [3].

By using the midpoint values given in Table 8.2, column 2, the resulting equations for the individual items are calculated in column 3. The cost items for each of the three categories are added together to provide the total cost for each category. The equations for estimating the costs for each of the categories are as follows:

$$DMC = C_{RM} + C_{WT} + C_{UT} + 1.33C_{OL} + 0.069FCI + 0.03COM$$

$$FMC = 0.708C_{OL} + 0.068FCI + \text{depreciation}$$

$$GE = 0.177C_{OL} + 0.009FCI + 0.16COM$$

The total manufacturing cost can be obtained by adding these three cost categories together and solving for the total manufacturing cost, *COM*. The result is

$$COM = 0.280FCI + 2.73C_{OL} + 1.23(C_{UT} + C_{WT} + C_{RM}) \qquad (8.1)$$

In Equation (8.1), the depreciation allowance of $0.10FCI$ is added separately.

The cost of manufacture without depreciation, COM_d, is

$$COM_d = 0.180FCI + 2.73C_{OL} + 1.23(C_{UT} + C_{WT} + C_{RM}) \qquad (8.2)$$

The calculation of manufacturing costs and expenses is given in Example 8.1.

Example 8.1.

The following cost information was obtained from a design for a 92,000 tonne/y nitric acid plant:

Fixed Capital Investment	$11,000,000
Raw Materials Cost	$ 7,950,000/y
Waste Treatment Cost	$ 1,000,000/y
Utilities	$ 356,000/y
Direct Labor Cost	$ 300,000/y
Fixed Costs	$ 1,500,000/y

Determine

a. The manufacturing cost in $/y and $/tonne of nitric acid

b. The percentage of manufacturing costs resulting from each cost category given in Tables 8.1 and 8.2

Using Equation (8.2),

COM_d = (0.180)($11,000,000) + (2.73)($300,000) + (1.23)($356,000 + $1,000,000 + $7,950,000) = $14,245,000/y

($14,245,000/y)/(92,000 tonne/y) = $155/tonne

From the relationships given in Table 8.2,

Direct Manufacturing Costs = $7,950,000 + $1,000,000 + $356,000 + (1.33)($300,000) + (0.069)($11,000,000) + (0.03)($14,245,000) = $10,891,000

Percentage of manufacturing cost = (100)(10.891)/14.25 = 76%

Fixed Manufacturing Costs = (0.708)($300,000) + (0.068)($11,000,000) = $960,000

Percentage of manufacturing cost = (100)(0.960)/14.25 = 7%

General Expenses = (0.177)($300,000) + (0.009)($11,000,000) + (0.16)($14,245,000) = $2,431,000

Percentage of manufacturing cost = (100)(2.431)/14.25 = 17%

In Example 8.1, the direct costs were shown to dominate the manufacturing costs, accounting for about 76% of the manufacturing costs. Of these direct costs, the raw materials cost, the waste treatment cost, and the cost of utilities accounted for more than $9 million of the $10.9 million direct costs. These three cost contributions are not dependent on any of the estimating factors provided in Table 8.2. Therefore, the manufacturing cost is generally insensitive to the estimating factors provided in Table 8.2. The use of the midrange values is acceptable for this situation.

8.2. Cost of Operating Labor

The technique used to estimate operating labor requirements is based on data obtained from five chemical companies and correlated by Alkhayat and Gerrard [4]. According to this method, the operating labor requirement for chemical processing plants is given by Equation (8.3):

$$N_{OL} = (6.29 + 31.7P^2 + 0.23N_{np})^{0.5} \qquad (8.3)$$

where N_{OL} is the number of operators per shift, P is the number of processing steps involving the handling of particulate solids—for example, transportation and distribution, particulate size control, and particulate removal. N_{np} is the number of nonparticulate processing steps and includes compression, heating and cooling, mixing, and reaction. In general, for the processes considered in this text, the value of P is zero, and the value of N_{np} is given by

$$N_{np} = \sum_{\substack{compressors \\ towers \\ reactors \\ heaters \\ exchangers}} Equipment \qquad (8.4)$$

Equation (8.3) was derived for processes with, at most, two solid handling steps. For processes with a greater number of solid handling operations, this equation should not be used.

The value of NOL in Equation (8.3) is the number of operators required to run the process unit per shift. A single operator works on the average 49 weeks a year (3 weeks' time off for vacation and sick leave), five 8-hour shifts a week. This amounts to (49 weeks/year × 5 shifts/week) 245 shifts per operator per year. A chemical plant normally operates 24 hours/day. This requires (365 days/year × 3 shifts/day) 1095 operating shifts per year. The number of operators needed to provide this number of shifts is [(1095 shifts/y)/(245 shifts/operator/y)] or approximately 4.5 operators. Four and one-half operators are hired for each operator needed in the plant at any time. This provides the needed operating labor but does not include any support or supervisory staff.

To estimate the cost of operating labor, the average hourly wage of an operator is required. Chemical plant operators are relatively highly paid, and data from the Bureau of Labor Statistics [5] give the hourly rate for miscellaneous plant and system operators in the Gulf Coast region at $28.64 in May 2010. This corresponds to $59,580 for a 2080-hour year. The cost of labor depends considerably on the location of the plant, and significant variations from the above figure may be expected. Historically, wage levels for chemical plant operators have grown slightly faster than the other cost indexes for process plant equipment given in Chapter 7. *The Oil and Gas Journal* and *Engineering News Record* provide appropriate indices to correct labor costs for inflation, or reference [5] can be consulted. The estimation of operating costs is illustrated in Example 8.2.

Example 8.2.

Estimate the operating labor requirement and costs for the toluene hydrodealkylation facility shown in Figures 1.3 and 1.5.

From the PFD in Figure 1.5, the number and type of equipment are determined.

Using Equation (8.4), an estimate of the number of operators required per shift is made. This information is shown in Table E8.2.

$$N_{OL} = [6.29 + (0)^{0.1} + (0.23)(11)]^{0.5} = [8.82]^{0.5} = 2.97$$

Table E8.2. Results for the Estimation of Operating Labor Requirements for the Toluene Hydrodealkylation Process Using the Equipment Module Approach

Equipment Type	Number of Equipment	N_{np}
Compressors	1	1
Exchangers	7	7
Heaters/Furnaces	1	1
Pumps*	2	—
Reactors	1	1
Towers	1	1
Vessels*	4	—
	Total	11

*Pumps and vessels are not counted in evaluating N_{np} in Equation (8.4).

The number of operators required per shift = 2.97.

Operating Labor = (4.5)(2.97) = 13.4 (rounding up to the nearest integer yields 14 operators)

Labor Costs (2010) = 14 × $59,580 = $834,100/y

8.3. Utility Costs

The costs of utilities are directly influenced by the cost of fuel. Specific difficulties emerge when estimating the cost of fuel, which directly impact the price of utilities such as electricity, steam, and thermal fluids. Figure 8.1 shows the general trends for fossil fuel costs from 1996 to 2009. The costs presented represent average values and are not site specific. These costs do not reflect the wide variability of cost and availability of various fuels throughout the United States.

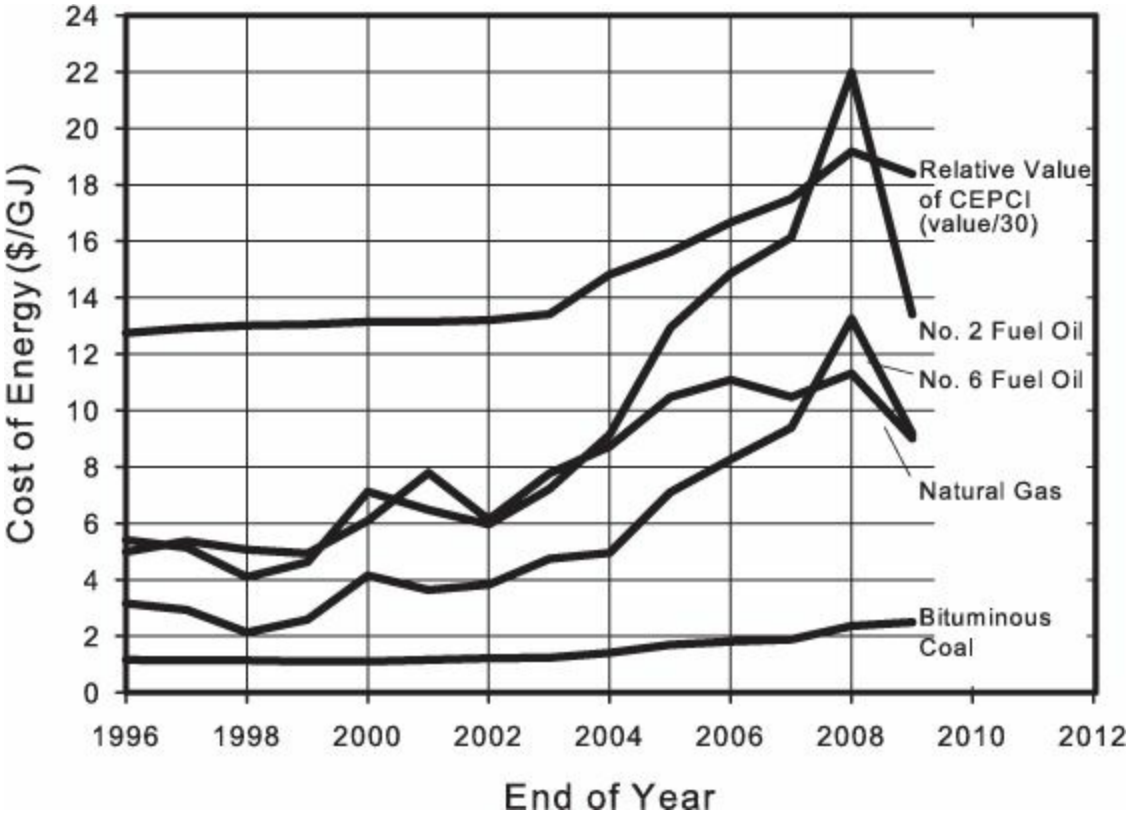


Figure 8.1. Changes in Fuel Prices from 1996 to 2009 (Information Taken from Energy Information Administration [6])

8.3.1. Background Information on Utilities

As seen from Figure 8.1, coal represents the lowest-cost fossil fuel on an energy basis. Most coal is consumed near the "mine mouth" in large power plants to produce electricity. The electricity is transported by power lines to the consumer. At locations remote from mines, both the availability and cost of transportation reduce and/or eliminate much of the cost advantage of coal. Coal suffers further from its negative environmental impact—for example, relatively high sulfur content and relatively high ratio of CO_2 produced per unit of energy.

From Figure 8.1, it is seen that no. 6 fuel oil (a heavy oil with a relatively high sulfur content) and natural gas are the next most expensive fuels. Natural gas fuel is the least damaging fossil fuel energy supply with respect to the environment. It is transported by pipelines throughout much of the country. The cost is less uniform than coal throughout different regions of the country. There remain, however, regions in the country that are not yet serviced by the natural gas distribution system. In these regions, the use of natural gas is not an option that can be considered. Although natural gas is a mixture of several light hydrocarbons, it consists predominantly of methane. For the calculations used in this text, it is assumed that methane and natural gas are equivalent.

No. 2 fuel oil is the final fossil fuel that is commonly used as an energy source in the chemical industry. Historically, it has been the highest-cost fossil fuel source. It is most readily available near coastal regions where oil enters the country and refining takes place. The United States has become increasingly dependent on imported oil, which may be subject to large upsets in cost and domestic availability. Uncertainties in the availability of supplies, high storage costs, and large fluctuations in cost make this source of energy the least attractive in many situations.

Figure 8.1 shows that fuel costs have increased somewhat more rapidly and in a much more chaotic fashion than the cost index (CEPCI) that has been used previously to correct costs for inflation. As a result of the regional variations in the availability and costs of fossil fuels, along with the inability of the cost index to represent energy costs, it is assumed that site-specific cost and availability information must be provided for a valid estimation of energy costs. It is assumed in this text that natural gas is the fuel of choice unless otherwise stated.

The PFD for the toluene hydrodealkylation process (Figure 1.5) represents the "battery-limits" plant. The equipment necessary to produce the various service or utility streams, which are used in the process and are necessary for the plant to operate, are not shown on the PFD. However, the utility streams such as cooling water and steam for heating are shown on the PFD. These streams, termed *utilities*, are necessary for the control of stream temperatures as required by the process. These utilities can be supplied in a number of ways:

1. **Purchasing from a Public or Private Utility:** In this situation no capital cost is involved, and the utility rates charged are based upon consumption. In addition the utility is delivered to the battery limits at known conditions.
2. **Supplied by the Company:** A comprehensive off-site facility provides the utility needs for many processes at a common location. In this case, the rates charged to a process unit reflect the fixed capital and the operating costs required to produce the utility.
3. **Self-Generated and Used by a Single Process Unit:** In this situation the capital cost for purchase and installation becomes part of the fixed capital cost of the process unit. Likewise the related operating costs for producing that particular utility are directly charged to the process unit.

Utilities that would likely be provided in a comprehensive chemical plant complex are shown in

Table 8.3.

Table 8.3. Utilities Provided by Off-Sites for a Plant with Multiple Process Units (Costs Represent Charges for Utilities Delivered to the Battery Limit of a Process)

Utility	Description	Cost $/GJ	Cost $/Common Unit
Air Supply	Pressurized and dried air (add 20% for instrument air)		
	a. 6 barg (90 psig)		$0.49/100 std m^3*
	b. 3.3 barg (50 psig)		$0.35/100 std m^3*
Steam from Boilers	Process steam: latent heat only		
	a. Low pressure (5 barg, 160°C) from HP steam		
	With credit for power	13.28	$27.70/1000 kg
	Without credit for power	14.05	$29.29/1000 kg
	b. Medium pressure (10 barg, 184°C) from HP steam		
	With credit for power	14.19	$28.31/1000 kg
	Without credit for power	14.83	$29.59/1000 kg
	c. High pressure (41 barg, 254°C)	17.70	$29.97/1000 kg
Steam Generated from Process	Estimate savings as avoided cost of burning natural gas in boiler	12.33	
Cooling Tower Water	Processes cooling water: 30°C to 40°C or 45°C	0.354	$14.8/1000 m^3†
Other Water	High-purity water for		
	a. Process use		$0.067/1000 kg
	b. Boiler feed water (available at 115°C)‡		$2.45/1000 kg
	c. Potable (drinking)		$0.26/1000 kg
	d. Deionized water		$1.00/1000 kg
Electrical Substation	Electric Distribution**	16.8	$0.06/kWh
	a. 110 V		
	b. 220 V		
	c. 440 V		
Fuels	a. Fuel oil (no. 2)**	14.2	$549/$m^3$
	b. Natural gas**	11.1§	$0.42/std m^3*
	c. Coal (f.o.b. mine mouth)**	1.72	$41.4/tonne

Refrigeration	a. Moderately low temperature Refrigerated water in at $T = 5°C$ and returned at 15°C	4.43	\$0.185/1000kg
	b. Low temperature Refrigerant available at $T = -20°C$	7.89	
	c. Very low temperature Refrigerant available at $T = -50°C$	13.11	Based on process cooling duty
Thermal Systems	Cost based on thermal efficiency of fired heater using natural gas		
	a. 90% efficient	12.33	Based on process heating duty
	b. 80% efficient	13.88	
Waste Disposal (Solid and Liquid)	a. Nonhazardous		\$36/tonne
	b. Hazardous		\$200–2000/tonne°
Wastewater Treatment	a. Primary (filtration)		\$41/1000 m^3
	b. Secondary (filtration + activated sludge)		\$43/1000 m^3
	c. Tertiary (filtration, activated sludge, and chemical processing)		\$56/1000 m^3

*Standard conditions are 1.013 bar and 15°C.
**These values are used to determine the other utility costs given in this table.
†Based on $\Delta T_{cooling\ water} = 10°C$. Cooling water return temperatures should not exceed 45°C due to excess scaling at higher temperatures.
‡Approximately equal credit is given for condensate returned from exchangers using steam.
§Based on lower heating value of natural gas.
°For hazardous waste, the cost of disposal varies widely. Chemical analyses are required for all materials that cannot be thoroughly identified. This does not include radioactive waste.

8.3.2. Calculation of Utility Costs

The calculation of utility costs can be quite complicated, and the true cost of such streams is often difficult to estimate in a large facility. For estimating operating costs associated with supplying utilities to different processes, the approach taken here is to assume that the capital investment required to build a facility to supply the utility—for example, a cooling tower, a steam boiler, and so forth—has already been made. This would be the case when a grassroots cost has been used for the fixed capital investment. The costs associated with supplying a given utility are then obtained by calculating the operating costs to generate the utility. These are the costs that have been presented in Table 8.3, and the following sections show how these cost estimates were obtained for the major utilities given in the table.

Cooling Tower Water. In most large chemical, petrochemical, and refinery plants, cooling water is supplied to process units from a central facility. This facility consists of a cooling tower (or many towers), water makeup, chemical injection, and the cooling water feed pumps. A typical cooling water facility is shown in Figure 8.2.

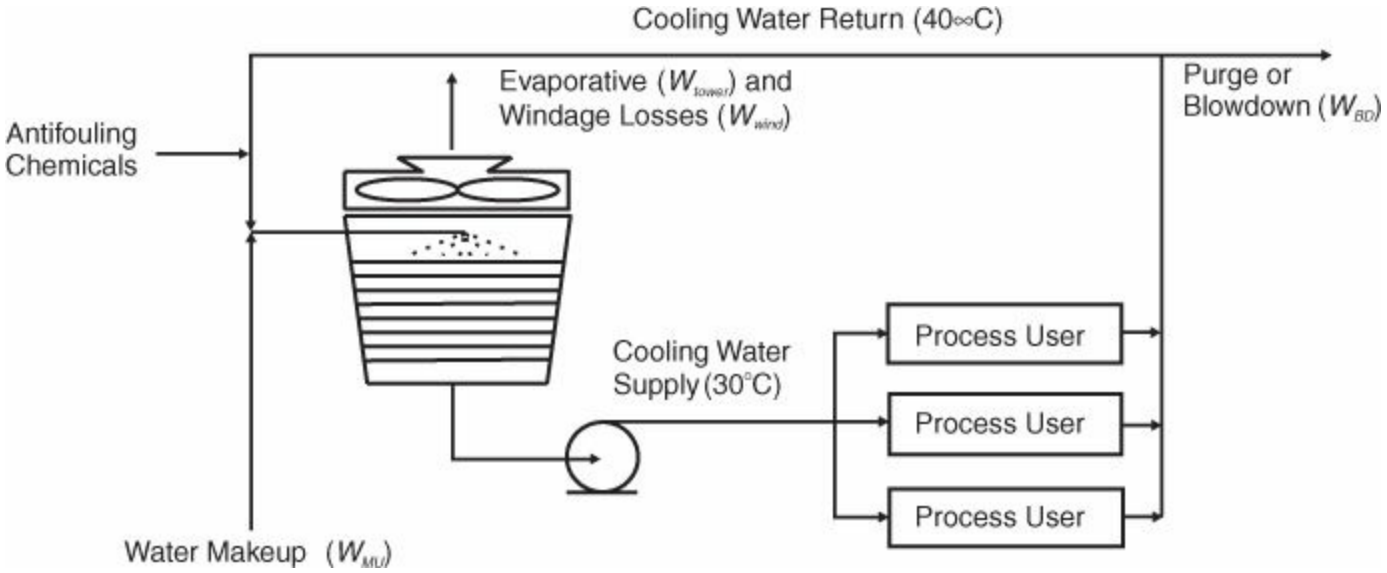


Figure 8.2. Schematic Diagram of Cooling Water Loop

The cooling of the water occurs in the cooling tower where some of the water is evaporated. Adding makeup water to the circulating cooling water stream makes up this loss. Because essentially pure water is evaporated, there is a tendency for inorganic material to accumulate in the circulating loop; therefore, there is a water purge or blowdown from the system. The makeup water stream also accounts for windage or spray losses from the tower and also the water purge. Chemicals are added to reduce the tendency of the water to foul heat exchanger surfaces within the processes. For a detailed discussion and further information regarding the conditioning of water for cooling towers, the reader is referred to Hile et al. [7] and Gibson [8]. From Figure 8.2, the cost to supply process users with cooling water can be estimated if the following are known:

- Total heat load and circulation rate required for process users
- Composition and saturation compositions of inorganic chemicals in the feed water
- Required chemical addition rate
- Desired supply and return temperatures (shown earlier to be 30°C and 40°C, respectively)
- Cost of cooling tower and cooling water pumps
- Costs of supply chemicals, electricity for pumps and cooling tower fans, and makeup water

The estimation of operating costs associated with a typical cooling water system is illustrated in Example 8.3.

Example 8.3.

Estimate the utility cost for producing a circulating cooling water stream using a mechanical draft cooling tower. Consider a basis of 1 GJ/h of energy removal from the process units. Flow of cooling water required to remove this energy = $\dot{m}$ kg/h.

An energy balance gives

$$\dot{m}c_p\Delta T = 1 \times 10^9 \Rightarrow (\dot{m})(4180)(40 - 30) = 41{,}800\,\dot{m} = 1 \times 10^9 \text{ J/h}$$

$$\text{Therefore, } \dot{m} = \frac{1 \times 10^9}{41{,}800} = 23{,}923 \text{ kg/h}$$

Latent heat of water at average temperature of 35°C = 2417 kJ/kg

Amount of water evaporated from tower, W_{tower}

$$W_{tower} = \frac{Heat\ Load}{\Delta H_{vap}} = \frac{1 \times 10^9}{2417 \times 10^3} = 413.7\ \text{kg/h}$$

This is (413.7)(100)/(23,923) = 1.73% of the circulating water flowrate.

Typical windage losses from mechanical draft towers are between 0.1% and 0.3% [9, 10]; use 0.3%.

To calculate the blowdown, the maximum allowable salt (inorganics) concentration factor, s, of the circulating water compared with the makeup water must be known. The definition of s is given in the following equation:

$$s = \frac{\text{concentration salts in cooling water loop}}{\text{concentration salts in makeup water}} = \frac{s_{loop}}{s_{in}}$$

Typical values are between 3 and 7 [9]. Here a value of 5 is assumed. By performing a water and salt balance on the loop shown in Figure 8.2, the following results are obtained:

$$W_{MU} = W_{tower} + W_{wind} + W_{BD}$$

$$s_{in} W_{MU} = s_{loop} W_{wind} + s_{loop} W_{BD}$$

Because $s_{loop} = 5 s_{in}$, it follows that

$$s_{in}(W_{tower} + W_{wind} + W_{BD2}) = s_{loop} W_{wind} + s_{loop} W_{BD}$$

$$W_{BD} = \frac{s_{in} W_{tower} + W_{wind}(s_{in} - s_{loop})}{s_{loop} - s_{in}} = \frac{s_{in} W_{tower}}{s_{loop} - s_{in}} - W_{wind} = \frac{W_{tower}}{4} - W_{wind} = \frac{1.73\%}{4} - 0.3\% = 0.133\%$$

$$W_{MU} = 1.73 + 0.3 + 0.133 = 2.163\% = 517\ \text{kg/h}$$

Pressure drop around the cooling water loop is estimated as follows: ΔP_{loop} = 15 psi (pipe losses) + 5 psi (exchanger losses) + 10 psi (control valve loss) + 8.7 psi of static head (because water must be pumped to top of cooling water tower, estimated to be 20 ft above pump inlet) = 38.7 psi = 266.7 kPa.

Power required for cooling water pumps with a volumetric flowrate $\dot{V}$ assuming an overall efficiency of 75%, is

$$\text{Pump power} = \frac{1}{\varepsilon} \dot{V} \Delta P = \frac{1}{(0.75)} \frac{(23{,}923)}{(1000)(3600)} (266.7) = 2.36\ \text{kW}$$

Power required for fans: From reference [11], the required surface area in the tower = 0.5 ft^2/gpm (this assumes that the design wet-bulb air temperature is 26.7°C [80°F]). From the same reference, the fan horsepower per square foot of tower area is 0.041 hp/ft^2.

$$\text{Power for fan} = \frac{(23{,}923)(2.2048)}{(60)(8.337)} (0.5)(0.041) = (2.16)(0.746) = 1.61\ \text{kW}$$

From a survey of vendors, the cost of chemicals is $0.156/1000 kg of makeup water.

Using an electricity cost of $0.06/kWh and a process water cost of $0.067/1000 kg, the overall cost of the cooling water is given by

Cost of cooling water = cost of electricity + cost of chemicals for makeup water + cost of makeup water

Using the cost values for electricity and process water given in Table 8.3,

$$\text{Cooling water cost} = (0.06)(2.36 + 1.61) + \frac{(517.3)(0.156)}{1000} + \frac{(517.3)(0.067)}{1000}$$

$$= \$0.354/\text{h} = \$0.354/\text{GJ}$$

Clearly, this cost will change depending on the cost of electricity, the cost of chemicals, and the cost of process water.

Refrigeration. The basic refrigeration cycle consists of circulating a working fluid around a loop consisting of a compressor, evaporator, expansion valve or turbine, and condenser. This cycle is shown in Figure 8.3. The phases of the working fluid (L-liquid and V-vapor) are shown on the diagram.

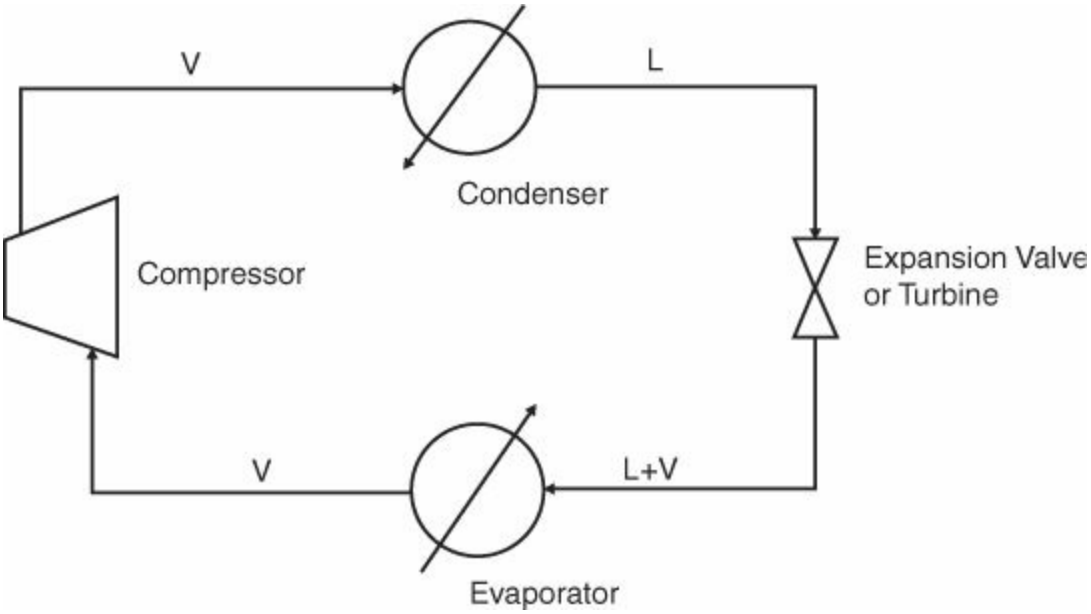


Figure 8.3. Process Flow Diagram for a Simple Refrigeration Cycle

The Carnot efficiency of a mechanical refrigeration system can be expressed by the reversible coefficient of performance, COP_{REV}:

$$COP_{REV} = \frac{\text{evaporator temperature } (T_1)}{\text{temperature difference between condenser and evaporator } (T_2 - T_1)}$$

$$COP \cong \frac{\text{evaporator heat load}}{\text{work required}} \quad \text{or} \quad \text{work required} = \frac{\text{evaporator heat load}}{\text{COP}}$$

Because all the processes for a Carnot engine must be reversible, the COP_{REV} gives the best theoretical performance of a refrigeration system. Thus the net required power (compressor-expansion turbine) will always be greater than that predicted by the equation above using COP_{REV}. Nevertheless, it is clear that as the temperature difference between the evaporator and condenser increases, then the work required per unit of energy removed in the evaporator (refrigerator) increases. Therefore, the operating costs for refrigeration will increase as the temperature at which the refrigeration is required decreases. The condensation of the working fluid will most often be achieved using cooling water, so a reasonable condensing temperature would be 45°C (giving a 5°C approach in the condensing exchanger). Figure 8.4 illustrates the effect of the evaporator temperature on the reversible work required for a given cooling load. This figure gives an approximate guide to the relative cost of refrigeration. The relative costs of refrigeration at different temperatures are

explored in Example 8.4.

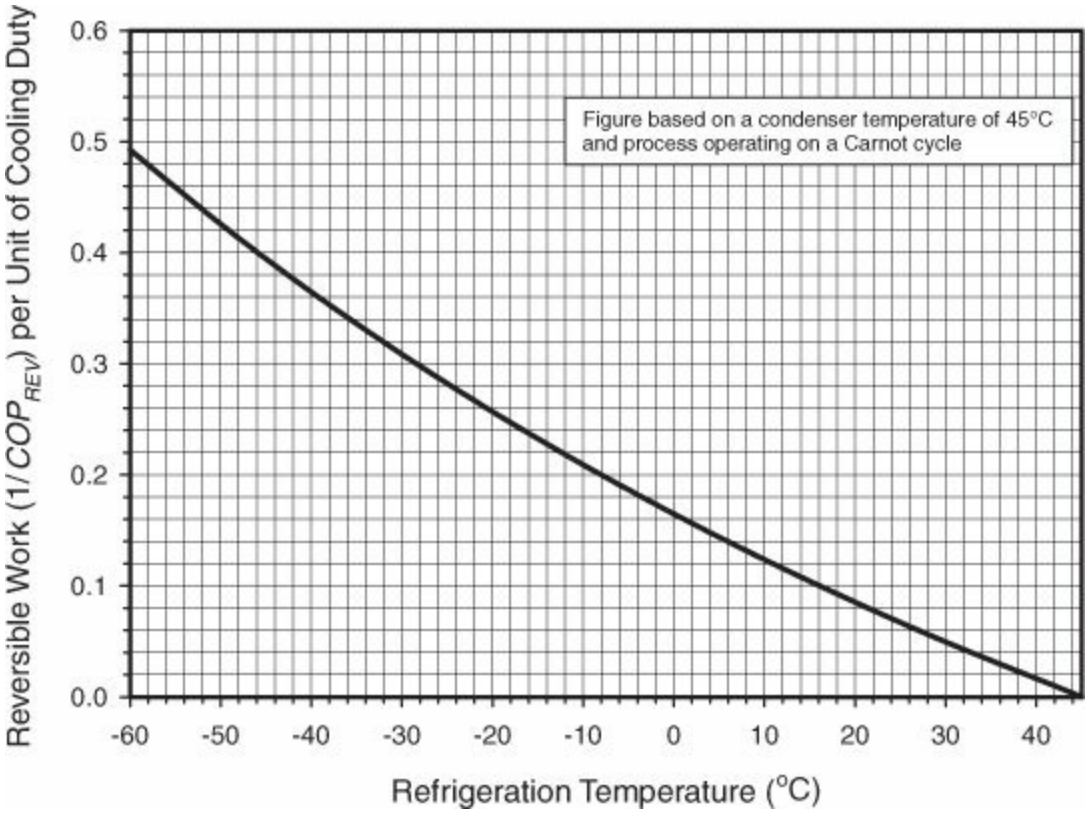


Figure 8.4. Ideal Work for Refrigeration Cycles as a Function of Refrigeration Temperature

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Example 8.4.

Using Figure 8.4, calculate the relative costs of providing refrigeration at 5°C, –20°C, and –50°C. From the figure, the ordinate values are given as follows:

Temperature	$1/COP_{REV}$
5°C	0.144
–20°C	0.257
–50°C	0.426

Therefore, compared with cooling at 5°C, cooling to –20°C is 0.257/0.144 times as expensive, and cooling to –50°C is 0.426/0.144 times as expensive. This analysis assumes that the two refrigeration systems operate equally efficiently with respect to the reversible limit and that the major cost is the power to run the compressors.

In Example 8.5, a real refrigeration system is considered, and operating costs are estimated.

Example 8.5.

Obtain a cost estimate for a refrigerated cooling utility operating at 5°C.

Consider a single-stage refrigeration system to provide refrigeration at 5°C, using 1,1 difluoroethane (R-152a) as the refrigerant. The process flow diagram and operating conditions are given in Figure E8.5 and Table E8.5, respectively.

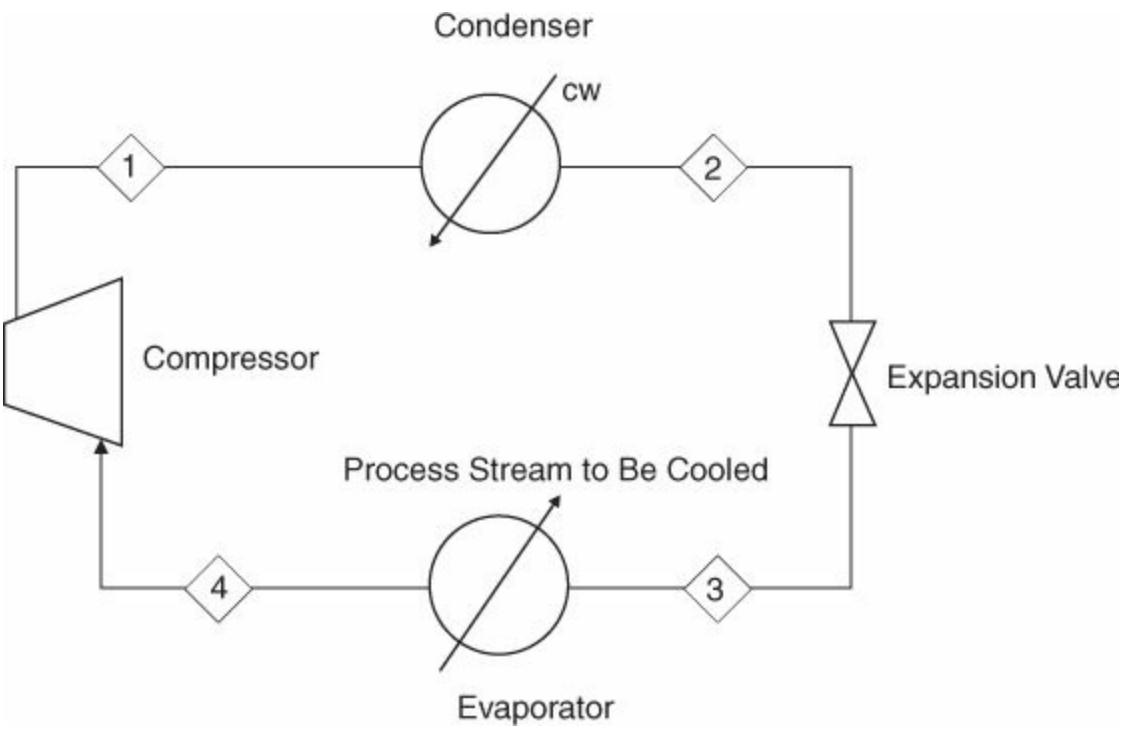


Figure E8.5. Process Flow Diagram for Simple Refrigeration Cycle of Example 8.5

Table E8.5. Stream Conditions for Figure E8.5

	Stream Number			
Condition	**1**	**2**	**3**	**4**
Pressure (bar)	10.9	10.9	3.21	3.21
Temperature (°C)	68.7	45.0	5.0	5.0
Vapor Fraction	1.0	0.0	0.2492	1.0

For the simulation shown, pressure drops across piping and heat exchangers have not been considered. When the circulation rate of R-152a is 65.3 kmol/h, the duty of the evaporator is 1 GJ/h. The compressor is assumed to be 75% efficient and the loads on the equipment are as follows:

Compressor Power = 66.5 kW (at 75% efficiency)

Condenser Duty = 1.24 GJ/h

Evaporator Duty = 1.00 GJ/h

$$\text{Compressor work per unit of cooling} = (66.5)/(1{,}000{,}000/3600) = 0.2394$$

This value compares with 0.144 for the Carnot cycle. The main differences are due to the inefficiencies in the compressor and the use of a throttling valve instead of a turbine.

$$\text{The cost of refrigeration at } 5°C = (66.5)(0.06) + (1.24)(0.354) = 3.99 + 0.44$$
$$= \$4.43/h = \$4.43/GJ$$

Using the results of Example 6.4, the cost of refrigeration at –20°C and –50°C can be predicted as

$$\text{The cost of refrigeration at } -20°C = (4.43)(1.78) = \$7.89/GJ$$
$$\text{The cost of refrigeration at } -50°C = (4.43)(2.96) = \$13.11/GJ$$

For refrigeration systems operating at less than temperatures of approximately –60°C, the simple refrigeration cycle shown in Figures 8.4 and E8.5 is no longer applicable. The main reason for this is

that there are no common refrigerants that can be liquefied at 45°C under reasonable pressures (not excessively high) and still give the desired low temperature in the condenser also at reasonable pressures (not excessively low). For these low-temperature systems, some form of cascaded refrigeration system is required. In such systems, two working fluids are used. The primary fluid provides cooling to the process (at the lowest temperature) and rejects heat to the secondary working fluid that rejects its heat to cooling water at 45°C. A simplified diagram of a cascaded refrigeration system is shown in Figure 8.5.

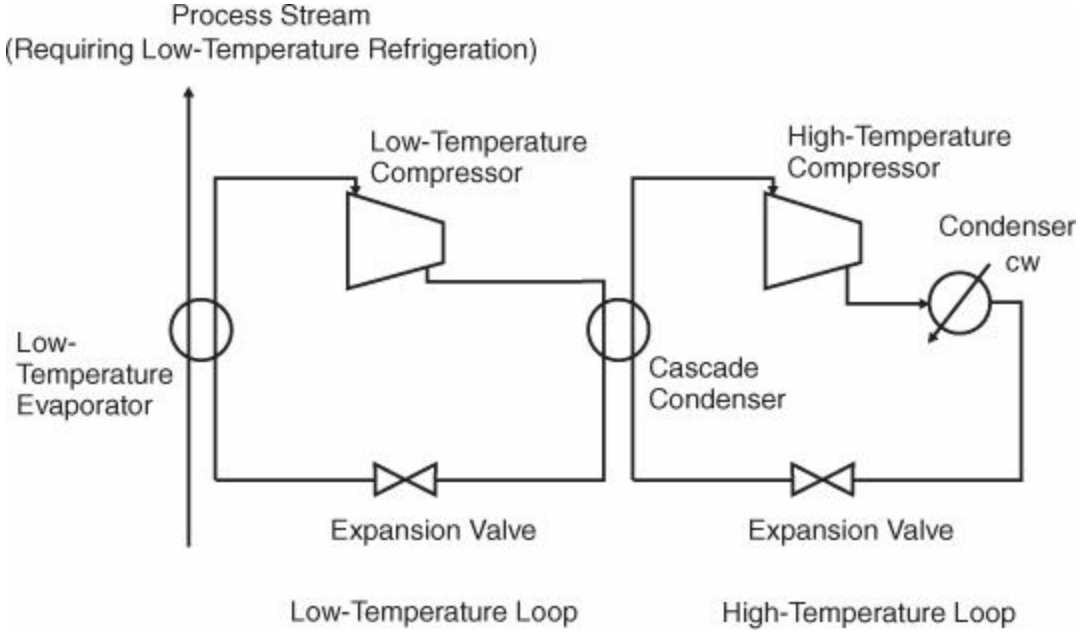


Figure 8.5. Schematic Diagram of a Simple Cascaded Refrigeration System

Steam Production. Steam is produced by the evaporation and superheating of specially treated water. The fuel that is used to supply the energy to produce steam is by far the major operating expense. However, water treatment costs can be substantial depending on the supply water composition and the degree of recovery of condensed steam in process heat exchangers. As shown in Table 8.3, for large chemical plants, steam is often required at several different pressure levels. However, it is often generated at the highest level and then let down to the lower pressure levels through turbines. These turbines produce electricity used in the plant. A typical steam generating facility is shown in Figure 8.6. Because there are losses of steam in the system due to leaks and, more important, due to process users not returning condensate, there is a need to add makeup water. This water is filtered to remove particulates and then treated to reduce the hardness. The latter can be achieved by the addition of chemicals to precipitate magnesium and calcium salts followed by filtration. These salts have **reverse solubility** characteristics and therefore precipitate at high temperatures. Alternatively, an ion-exchange system can be employed. The solids-free, "soft" water is now fed to the steam generating system. The thorough treatment of the water is necessary, because any contaminants entering with the water will ultimately deposit on heat-exchanger surfaces and boiler tubes and cause fouling and other damage. Another important issue is the dissolved oxygen and carbon dioxide that enter with the makeup water. These dissolved gases must be removed in order to eliminate (reduce) corrosion of metal surfaces in the plant. The removal occurs in the deaerator, in which the makeup water is scrubbed with steam to de-gas the water. Oxygen scavengers are also added to the circulating condensate to remove any trace amounts of oxygen in the system. Amines may also be added to the water in order to neutralize any residual carbonic acid formed from dissolved carbon dioxide. Finally, blowdown of water from the water storage tank (situated near the boiler) is

necessary to remove any heavy sludge and light solids that are picked up as steam and condensate circulate through the system [12]. The problems associated with the buildup of chemicals become even more troublesome in high-pressure (> 66 bar) boilers, and several solutions are discussed by Wolfe [13].

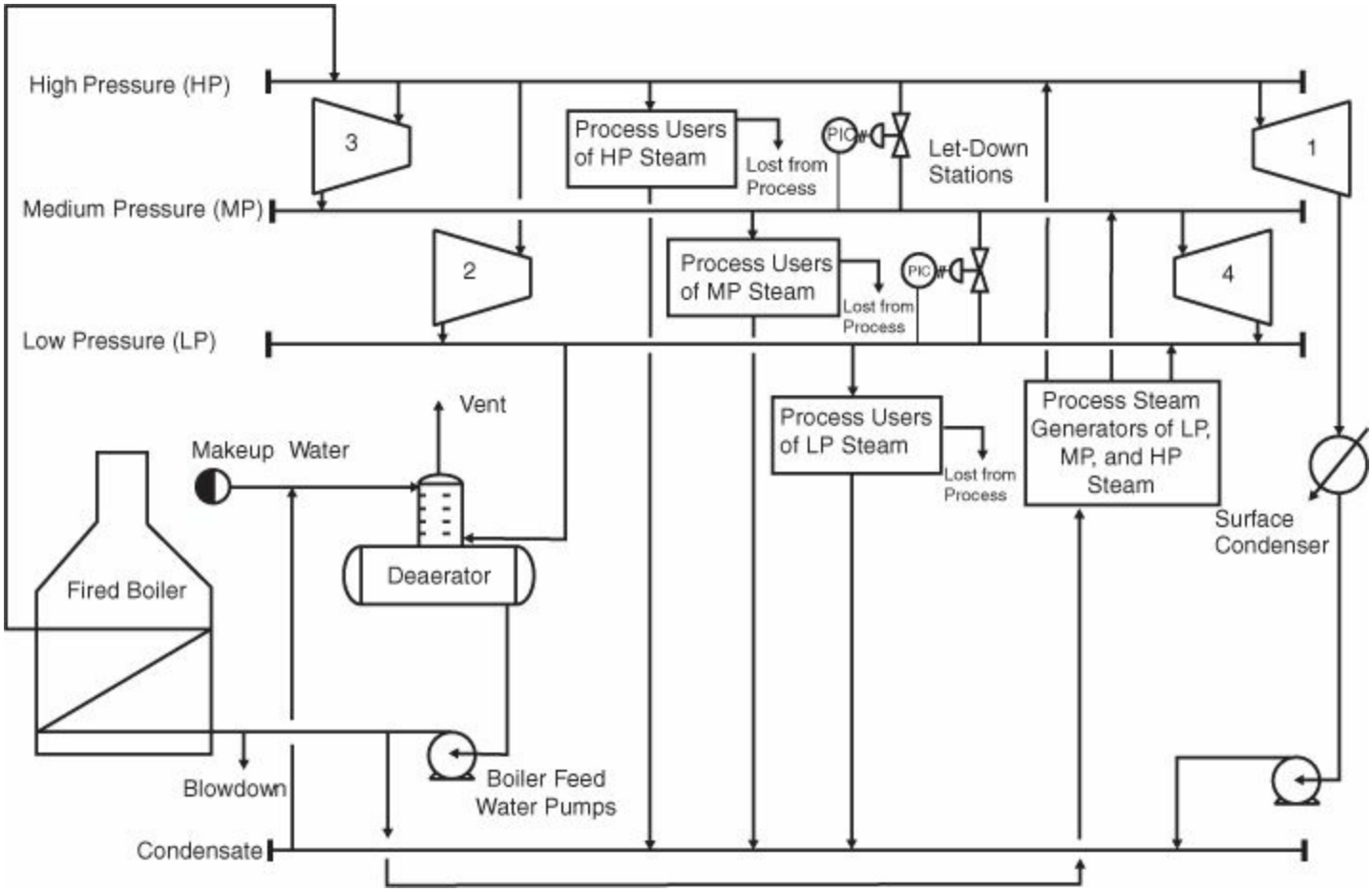


Figure 8.6. Typical Steam Producing System for a Large Chemical Facility

In order to estimate accurately steam generation costs, it is necessary to complete a steam balance on the plant. An algorithm for carrying out a steam balance for a new facility is listed below.

1. Determine the pressure levels for the steam in the plant. These are usually set at around 41.0 barg (600 psig), between 10.0 barg (150 psig) and 15.5 barg (225 psig), and between 3.4 barg (50 psig) and 6.1 barg (90 psig).
2. Determine the total number of process users of the different levels of steam. These numbers become the basis for the steam balance.
3. Determine which of the above users will return condensate to the boiler feed water (bfw) system. *Note:* If live steam injection is required for the process, there will be no condensate returned from this service. In addition, for some small users, condensate return may not be economical.
4. Determine the condensate-return header pressure.
5. Estimate the blowdown losses.
6. Complete a balance on the steam and condensate, and determine the required water makeup to the steam system.
7. Determine the steam generating capacity of the steam boiler. The logic used here is that all steam will be generated at the highest-pressure level and will be let down either through turbines or let-down stations (valves) to the medium- and low-pressure headers. The high-

pressure steam is often generated at 44.3 barg (650 psig) to allow for frictional losses and superheated to 400°C (752°F) to produce more efficient power production in the turbines.

8. Additional power generation may be accomplished by running turbines using the high-pressure steam, by using surface condensers (operating at the cooling water temperature), and by running turbines between the medium- and low-pressure steam headers. All these options are shown in Figure 8.6. In order to balance a plant's electrical and steam needs, the determination of the correct amount of steam to generate is an iterative process.

Clearly the algorithm can become quite complicated. In order to determine a reasonable value or cost for the different steam levels, the approach used here is to assume that all the steam will be generated at the highest pressure level and then let down to the appropriate pressure level through turbines or let-down stations (valves). In the former case, credit will be taken for generating power; in the latter case, credit will not be taken. The procedure for calculating the cost of steam at different pressure levels is given in Example 8.6.

Example 8.6.

Determine the cost of producing high-, medium-, and low-pressure steam using a natural gas fuel source. For medium- and low-pressure steam production, assume that steam is produced at the highest pressure level, and consider both the case when this steam is sent through a turbine to make electricity and when it is simply throttled through a valve.

Again the approach taken here is to assume that the fixed capital investment associated with the initial purchase of the steam generation facilities has been accounted for elsewhere. The analysis given below accounts only for the operating costs associated with steam (and power) production. The source of fuel is assumed to be natural gas that costs $11.10/GJ. See Table 8.3.

High-Pressure Steam (41.0 barg)

Basis is 1000 kg of HP steam generated at 45.3 bar and 400°C ⇒ $h_{44.3\ barg,\ 400°C} = 3204.3$ kJ/kg.

Conditions at the header are 41 bar saturated ($T_{sat} = 254°C$). Note that the steam is generated at a higher pressure and superheated for more efficient expansion, but that desuperheating will be assumed at the process user.

Assume boiler feed water comes from a deaerator that operates at exhaust steam header pressure of 0.7 barg and $T_{sat} = 115°C$ (10 psig) ⇒ $h_{bfw} = 483.0$ kJ/kg.

$$\Delta H_{bfw\text{-}HP\ Steam} = (3204.3 - 483.0) = 2721.3\ \text{kJ/kg}$$

$$\text{Energy required to produce HP steam} = (2721.3)(1000) = 2.721\ \text{GJ}$$

Because this HP steam is superheated, more than 1000 kg of saturated steam can be produced from it. In order to desuperheat this steam, bfw is added to produce saturated steam at 41.0 barg ($h = 2797.6$ kJ/kg). See Figure E8.6.

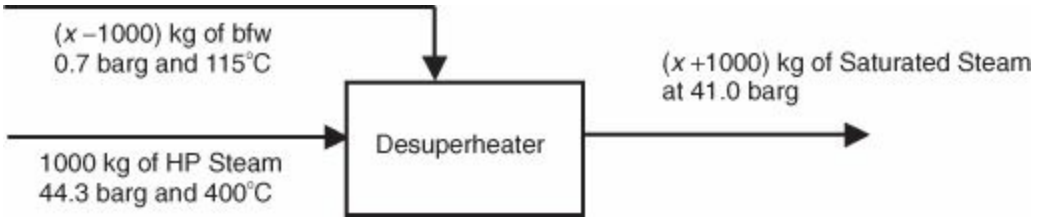


Figure E8.6. Sketch of Desuperheating Process for HP Steam

Let x be the amount of saturated HP steam produced from superheated HP steam; an enthalpy balance gives $(1000)(3204.3) + (x - 1000)(483) = (x)(2797.6) \Rightarrow x = 1175.7$ kg.

The cost of natural gas to produce 1000 kg of sat HP steam (assuming a 90% boiler efficiency) is given by

$$\text{Cost} = \frac{(2.721)}{(0.9)}\frac{(1000)(11.1)}{(1175.7)} = \$28.54$$

Treatment costs for circulating boiler feed water = \$0.15/1000 kg for oxygen scavengers, and so on (average from several vendors).

Boiler feed water cost is based on the assumption that 10% makeup is required.

Cost of electricity to power air blowers supplying combustion air to boiler:

Natural gas usage = 2.721/0.9/1.1757 = 2.572 GJ = (2.572)(6)/(0.23) = 67.1 std m^3 = 67.1/22.4 = 2.99 kmol

Oxygen usage (based on 3% excess over stoichiometric) = (2.99)(2)(1.03) = 6.17 kmol oxygen

This comes from (6.17)/(0.21) = 29.38 kmol of air.

Assume that this air must be raised 0.5 bar to overcome frictional losses in boiler and stack, and assume that the blower is 60% efficient. Therefore,

The electrical usage for blower is 14 kWh/1000 kg of steam produced, giving an electricity cost = (14)(0.06) = \$0.84.

The cost of bfw is based on the water makeup, treatment chemicals, and the thermal energy in the stream.

For a basis of 1000 kg of bfw,

Cost of makeup water = \$0.067

Cost of chemicals for treatment = \$0.15

Energy in bfw = $\dot{m}c_p\Delta T = (1000)(4.18)(115 - 25) = 0.376$ GJ

Value of energy = (\$11.10)(0.376) = \$4.17

bfw cost = 4.17 + 0.067 + 0.15 = \$4.39/1000 kg

Cost of bfw makeup = (0.1)(4.39) = \$0.439

Total cost of HP steam = \$28.54 + \$0.15 + \$0.84 + \$0.439 = \$29.97/1000 kg

Medium-Pressure Steam (10.0 barg)

It is assumed that letting steam down through a turbine from the high-pressure header to the medium-pressure header will generate electrical power.

The theoretical steam requirement (kg steam/kWh) for this situation is found by assuming an isentropic expansion of the steam from the HP condition to the medium-pressure level. From the steam tables, the following information is known:

$$h_{44.3\ barg,\ 400°C} = 3204.3 \text{kJ/kg and } s_{44.3\ barg,\ 400°C} = 6.6953 \text{ kJ/kg K}$$

By interpolating at constant specific entropy, the outlet temperature is calculated as 212°C and the outlet enthalpy = 2851.0 kJ/kg.

$$\Delta h = (3204.3 - 2851.0) = 353.3 \text{ kJ/kg} = \text{theoretical work}$$

Therefore, 1000 kg of HP steam produces 353.3 MJ or 98.14 kWh of electricity.

Assuming a turbine efficiency of 75%, the output power is (0.75)(98.14) = 73.6 kWh.

$$\text{Credit for electricity} = (73.6)(0.06) = \$4.42$$

The actual outlet enthalpy of the steam is 3204.3 – (353.3)(0.75) = 2939.3 kJ/kg. This is still superheated steam. Desuperheating the steam to 10.3 barg and saturated conditions (h = 2779.1 kJ/kg) will generate x kg of MP steam from the 1000 kg of HP steam, where

$$(1000)(2939.3) + (x - 1000)(483.0) = (x)(2779.1) \Rightarrow x = 1069.8 \text{ kg}$$

Therefore, the cost of natural gas to produce 1000 kg of MP steam (assuming a 90% boiler efficiency) is

$$\text{Cost} = \frac{(2.721)}{(0.9)}\frac{(1000)(11.10)}{(1069.8)} = \$31.37$$

The cost of electricity for the blower can be found by using the ratio of the natural gas usage from the high-pressure steam case. Therefore,

$$\text{Cost of electricity} = \frac{(31.37)}{(28.54)}(0.84) = \$0.92$$

Total cost of MP steam (with power production) = \$31.37 – \$4.42 + \$0.92 + \$0.439 = \$28.31/1000 kg

For the case when power production is not implemented, the HP steam is throttled to the pressure of the MP header through a let-down station, which is essentially an irreversible, isentropic process through a valve. The superheated steam is then desuperheated at the process user.

Enthalpy of HP steam (at 44.8 barg and 400°C) = 3204.3 kJ/kg

Enthalpy of saturated MP steam = 2779.1 kJ/kg

Enthalpy of bfw = 483.0 kJ/kg

If x is the amount of saturated MP steam obtained by desuperheating, then an enthalpy balance gives

$$(1000)(3204.3) + (x - 1000)(483) = (x)(2779.1) \Rightarrow x = 1185.2 \text{ kg}$$

Cost of natural gas to produce 1000 kg of sat HP steam (assuming a 90% boiler efficiency) is

$$\text{Cost} = \frac{(2.721)}{(0.9)}\frac{(1000)(11.10)}{(1185.2)} = \$28.32$$

$$\text{Cost of electricity for the air blower} = \frac{(28.32)}{(28.54)}(0.84) = \$0.83$$

$$\text{Total cost of MP steam (without power production)} = \$28.32 + \$0.83 + \$0.439 = \$29.59/1000 \text{ kg}$$

Note: This is almost identical to the cost for HP steam.

Low-Pressure Steam (5.2 barg)

The calculation procedures for evaluating the cost of low-pressure steam are identical to those given above for medium-pressure steam and the results are given below.

Total cost of LP steam (with power production) = \$32.25 – \$5.94 + \$0.95 + \$0.439

= \$27.70/1000 kg

Total cost of LP steam (without power production) = $28.03 + $0.82 + $0.439 = $29.29/1000 kg

Waste Heat Boilers

When steam is generated from within the process—in a waste heat boiler, for example—the savings to the process are usually calculated from the avoided cost of using an equivalent amount of natural gas in the boiler system. If the boiler efficiency is assumed to be 90%, then for every GJ of energy saved by producing steam within a process unit, the boiler facility saves ($11.1)/(0.9) = $12.33 in natural gas costs.

Hot Circulating Heat Transfer Fluids. Again, the greatest cost for these systems is the fuel that is burned to heat the circulating heat-transfer fluid. Typical efficiencies (based on the lower heating value, LHV, of the fuel) for these heaters range from 60% to 82% [1]. With air preheating economizers, the efficiency can be as high as 90%. Example 8.7 illustrates the use of efficiencies in fired heaters.

Example 8.7.

Estimate the utility cost of a heat-transfer medium heated in a fired heater using natural gas as the fuel.

Assuming that the heat-transfer medium is heated in a process heater that is 80% efficient and uses natural gas at $11.10/GJ as the fuel source,

$$\text{Cost of 1 GJ of energy} = (1)(11.10)/(0.80) = \$13.88/\text{GJ}$$

Assuming a 90% efficient heater,

$$\text{Cost of 1 GJ of energy} = (1)(11.10)/(0.9) = \$12.33/\text{GJ}$$

8.4. Raw Material Costs

The cost of raw materials can be estimated by using the current price listed in such publications as the *Chemical Market Reporter* (*CMR*) [14]. A list of common chemicals and their selling price, as of August 2008, are given in Table 8.4. Current raw material and product chemical prices may be obtained from the current issue of the *CMR* [14]. To locate costs for individual items, it is not sufficient to look solely at the current issue, because not all chemicals are listed in each issue. It is necessary to explore several of the most recent issues. In addition, for certain chemicals large seasonal price fluctuations may exist, and it may be advisable to look at the average price over a period of several months.

Table 8.4. Costs of Some Common Chemicals*

Chemical	Cost ($/kg)	Typical Shipping Capacity or Basis for Price
Acetaldehyde	1.003	Railroad Tank Cars
Acetic Acid	0.838	Railroad Tank Cars
Acetone (MMA grade)	1.102	Railroad Tank Cars
Acrylic Acid	1.918	Railroad Tank Cars
Allyl Chloride	1.80†	F.O.B. Gulf Coast
Benzene	0.919	Barge, Gulf Coast
Chlorine	0.284	Railroad Tank Car
Dimethyl Ether	0.841†(2011)	Railroad Tank Car
Ethanol (190 Proof)	1.138	Railroad Tank Car
Ethylbenzene	1.268	Railroad Tank Car, Gulf Coast
Ethylene	1.488	Contract
Ethylene Oxide	1.687	Railroad Tank Car
Formaladehyde/Formalin (37 wt%)		
No-inhibitor	0.838	Railroad Tank Car, Gulf Coast
7% Methanol Inhibitor	0.463	Railroad Tank Car, Gulf Coast
Hydrochloric Acid (23ϒBe)	0.090	Railroad Tank Car, Works
Iso-Butylene	0.706	F.O.B. Works
Iso-Propanol (99%)	1.400	Railroad Tank Car
Maleic Anhydride	1.158	Railroad Tank Car
Methanol	0.672	F.O.B. Gulf Coast
Methyl Ethyl Ketone	1.598	Railroad Tank Car
MTBE	0.609	Barge, F.O.B. Asia
Propylene		
(Polymer Grade)	1.488	F.O.B. Gulf Coast—Spot Price
(Chemical Grade)	1.444	F.O.B. Gulf Coast—Spot Price
Styrene	1.598	F.O.B. Works
Sulfur (Crude)	0.409	Railroad Car
Sulfuric Acid (virgin)	0.078	Railroad Tank Car, Gulf Coast
Toluene	1.033	Barge, Gulf Coast
Mixed Xylenes	0.820	Barge, Gulf Coast
Ortho-Xylene	1.235	Railroad Tank Cars
Para-Xylene	1.488	Railroad Tank Cars
Meta-Xylene	2.910	Railroad Tank Cars

*Unless stated otherwise, these are average values from http://www.icis.com/StaticPages/a-e.htm#top, August 2008.
†Vendor quote.

Another factor that is sometimes overlooked is that often companies will lock onto a selling or purchase price through a short- or long-term contract. Such contracts will often yield prices that are significantly lower than those given in the *CMR*. In addition, in doing economic evaluations for different chemical processes, the purchase and selling price for chemicals will not always be available from the *CMR*. For example, in January 2001, *CMR* stopped publishing the price of

dimethyl ether. Likewise, prices for allyl alcohol have not been published for several years. The prices shown in Table 8.4 were obtained from manufacturers' quotes. When doing economic evaluations for new, existing, or future plants, it is advisable to establish the true selling or purchase price for all raw materials and products. Because the largest operating cost is nearly always the cost of raw materials, it is important to obtain accurate prices if realistic economic evaluations are to be obtained.

8.5. Yearly Costs and Stream Factors

Manufacturing and associated costs are most often reported in terms of $/y. Information on a PFD is most often reported in terms of kg or kmol per hour or per second. In order to calculate the yearly cost of raw materials or utilities, the fraction of time that the plant is operating in a year must be known. This fraction is known as the **stream factor** (SF), where

$$\text{Stream factor (SF)} = \frac{\text{Number of days plant operates per year}}{365} \qquad (8.5)$$

Typical values of the stream factor are in the range of 0.96 to 0.90. Most reliable and well-managed plants will typically shut down for one or two weeks a year for scheduled maintenance, giving an SF = 0.98–0.96. Less reliable processes may require more downtime and hence lower SF values. The stream factor represents the fraction of time that the process unit is on-line and operating at design capacity. When estimating the size of equipment, care must be taken to use the design flowrate for a typical stream day and not a calendar day. Example 8.8 illustrates the use of the stream factor.

Example 8.8.

a. Determine the yearly cost of toluene for the process given in Chapter 1.

b. What is the yearly consumption of toluene?

c. What is the yearly revenue from the sale of benzene?

Assume a stream factor of 0.95, and note that the flowrates given on the PFD are in kilograms per stream hour.

From Table 1.5, flowrate of toluene = 10,000 kg/h (Stream 1)

From Table 1.5, flowrate of benzene = 8210 kg/h (Stream 15)

From Table 8.5, cost of toluene = $0.919/kg

From Table 8.5, cost of benzene = $1.033/kg

a. Yearly cost of toluene = (24)(365)(10,000)(1.033)(0.95) = $85,967,000/y.

b. Yearly consumption of toluene = (24)(365)(10,000)(0.95)/1000 = 83,200 tonne/y.

c. Yearly revenue from benzene sales = (24)(365)(8210)(0.919)(0.95) = $62,790,000/y.

Comparing the results from Parts (a) and (c), it can be seen that with the current prices for these two chemicals it is not economical to produce benzene from toluene. Historically, the price differential between benzene and toluene has been greater than the $0.114/kg shown in Table 8.4, and this is the reason why this process has been used, and is currently being used, to produce benzene. Clearly, if this low price differential were to exist for a long period of time, this process might have to be shut down.

8.6. Estimating Utility Costs from the PFD

Most often, utilities do not directly contact process streams. Instead, they exchange heat energy (fuel gas, steam, cooling water, and boiler feed water) in equipment such as heat exchangers and process heaters, or they supply work (electric power or steam) to pumps, compressors, and other rotating equipment. In most cases, the flowrate can be found either by inspection or by doing a simple heat balance around the equipment.

Steam can be used to drive a piece of rotating equipment such as a compressor. In this case, both the theoretical steam requirement and efficiency are required. Table 8.5 provides the theoretical steam requirements as a function of the steam inlet pressure and the exhaust pressure for steam turbine drives. The mechanical efficiencies of different drives are shown in Figure 8.7, using data from Walas [9].

Table 8.5. Theoretical Steam Requirements (kg steam/kWh)

	Inlet Pressure of Steam (barg) (Superheat in °C)							
	10.0 (sat'd)	13.8 (sat'd)	17.2 50	27.6 170	41.4 145	41.4 185	58.6 165	58.6 205
Exhaust Pressure								
2″ Hg abs	4.77	4.54	4.11	3.34	3.22	3.07	2.98	2.85
4″ Hg abs	5.33	5.04	4.54	3.62	3.47	3.30	3.20	3.05
0 barg	8.79	7.94	6.88	5.08	4.72	4.45	4.22	4.00
0.69 barg	10.87	9.57	8.11	5.77	5.28	4.97	4.67	4.40
2.07 barg	15.24	12.72	10.40	6.91	6.18	5.78	5.35	5.02
3.45 barg	20.86	16.32	12.79	7.97	6.97	6.49	5.93	5.54
4.14 barg	24.45	18.32	14.11	8.50	7.34	6.83	6.20	5.78
4.82 barg	28.80	20.68	15.47	9.05	7.71	7.16	6.45	6.01

From Perry, R. H., and D. W. Green, *Perry's Chemical Engineers' Handbook*, 6th ed., McGraw-Hill, New York, NY, 1984. Reprinted by permission of the McGraw-Hill Companies.

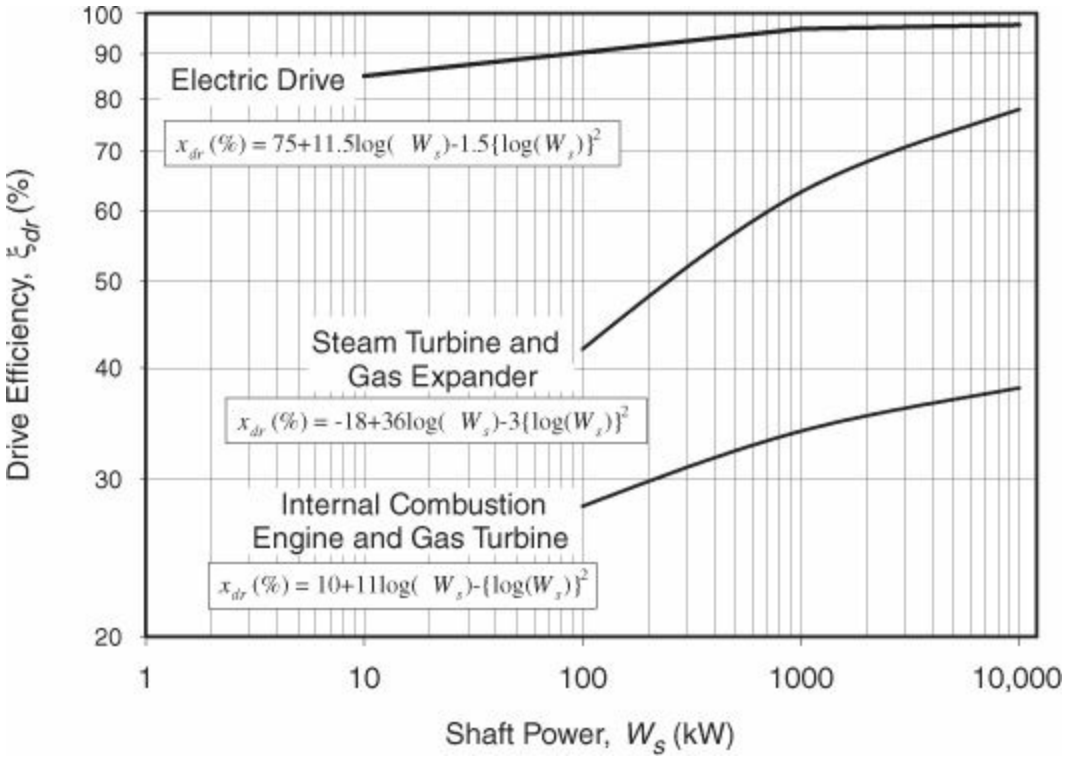


Figure 8.7. Efficiencies for Pumps and Compressor Drives (Data from Walas [9], Chapter 4)

To illustrate the techniques used to estimate the utility flowrates and utility costs for various types of equipment, see Example 8.9.

Example 8.9.

Estimate the quantities and yearly costs of the appropriate utilities for the following pieces of equipment on the toluene hydrodealkylation PFD (Figure 1.5). It is assumed that the stream factor is 0.95 and that all the numbers on the PFD are on a stream time basis. The duty on all of the units can be found in Table 1.7.

a. E-101, Feed Preheater

b. E-102, Reactor Effluent Cooler

c. H-101, Heater

d. C-101, Recycle Gas Compressor, assuming electric drive

e. C-101, Recycle Gas Compressor, assuming steam drive using 10 barg steam discharging to atmospheric pressure

f. P-101, Toluene Feed Pump

Solution

a. E-101: Duty is 15.19 GJ/h. From Table 8.3, Cost of High-Pressure Steam = \$17.70/GJ

Energy Balance: Q = 15.19 GJ/h = $(\dot{m}_{steam})(\Delta H_{vap})$ = $(\dot{m}_{steam})$(1699.3) kJ/kg

$\dot{m}_{steam}$ = 8939 kg/h = 2.48 kg/s

Yearly Cost = $(Q)(C_{steam})(t)$ = (15.19 GJ/h)(\$17.70/GJ)(24)(365)(0.95) = \$2,237,000/y

Alternatively, Yearly Cost = (Yearly flowrate)(Cost per unit mass)

Yearly Cost = (2.48)(3600)(24)(365)(0.95)(29.97/1000) = \$2,227,000/y

(same as above within round-off error)

b. E-102: Duty is 46.66 GJ/h. From Table 8.3, Cost of Cooling Water = \$0.354/GJ

$$Q = 46.66 \text{ GJ/h} = (\dot{m}_{cw})(C_{pcw})(\Delta T_{cw}) = (\dot{m}_{cw})(4.18)(10) = 41.8\ \dot{m}_{cw}$$

$$\dot{m}_{cw} = (46.66)(10^9/41.8)(10^3) = 1{,}116{,}270 \text{ kg/h} = 310 \text{ kg/s}$$

$$\text{Yearly Cost} = (46.66 \text{ GJ/h})(24)(365)(0.95)(\$0.354/\text{GJ}) = \$137{,}000/\text{y}$$

c. H-101: Duty is 27 GJ/h (7510 kW). Assume that an indirect, nonreactive process heater has a thermal efficiency (ξ_{th}) of 90%. From Table 8.3, natural gas costs \$11.10/GJ, and the heating value is 0.0377 GJ/m^3.

$$Q = 27 \text{ GJ/h} = (\dot{v}_{gas})(\Delta H_{natural\ gas})(\text{efficiency}) = (\dot{v}_{gas})(0.0377)(0.9)$$

$$\dot{v}_{gas} = 796 \text{ std m}^3\text{/h } (0.22 \text{ std m}^3\text{/s})$$

$$\text{Yearly Cost} = (27)(11.10)(24)(365)(0.95)/(0.90) = \$2{,}771{,}000/\text{y}$$

d. C-101: Shaft power is 49.1 kW, and from Figure 8.7 the efficiency of an electric drive (ξ_{dr}) is 90%.

$$\text{Electric Power} = P_{dr} = \text{Output power}/\xi_{dr} = (49.1)/(0.90) = 54.6 \text{ kW}$$

$$\text{Yearly Cost} = (54.6)(0.06)(24)(365)(0.95) = \$27{,}200/\text{y}$$

e. Same as Part (d) with steam-driven compressor. For 10 barg steam with exhaust at 0 barg, Table 8.5 provides a steam requirement of 8.79 kg steam/kWh of power. The shaft efficiency is about 35% (extrapolating from Figure 8.7).

$$\text{Steam required by drive} = (49.1)(8.79/0.35) = 1233 \text{ kg/h } (0.34 \text{ kg/s})$$

$$\text{Cost of Steam} = (1233)(24)(365)(0.95)(28.32 \times 10^{-3}) = \$290{,}600/\text{y}$$

f. P-101: Shaft power is 14.2 kW. From Figure 8.7 the efficiency of an electric drive is about 86%.

$$\text{Electric Power} = 14.2/0.86 = 16.5 \text{ kW}$$

$$\text{Yearly Cost} = (16.5)(0.06)(24)(365)(0.95) = \$8240/\text{y}$$

Note: The cost of using steam to power the compressor is much greater than the cost of electricity even though the cost per unit energy is much lower for the steam. The reasons for this are (1) the thermodynamic efficiency is low, and (2) the efficiency of the drive is low for a small compressor. Usually steam drives are used only for compressor duties greater than 100 kW.

8.7. Cost of Treating Liquid and Solid Waste Streams

As environmental regulations continue to tighten, the problems and costs associated with the treatment of waste chemical streams will increase. In recent years there has been a trend to try to reduce or eliminate the volume of these streams through waste minimization strategies. Such strategies involve utilizing alternative process technology or using additional recovery steps in order to reduce or eliminate waste streams. Although waste minimization will become increasingly important in the future, the need to treat waste streams will continue. Some typical costs associated with this treatment are given in Table 8.3, and flowrates can be obtained from the PFD. It is worth noting that the costs associated with the disposal of solid waste streams, especially hazardous wastes, have grown immensely in the past few years, and the values given in Table 8.3 are only approximate average numbers. Escalation of these costs should be done with extreme caution.

8.8. Evaluation of Cost of Manufacture for the Production of Benzene Via the Hydrodealkylation of Toluene

The cost of manufacture for the production of benzene via the toluene HDA process is given in Example 8.10.

Example 8.10.

Calculate the cost of manufacture without depreciation (COM_d) for the toluene hydrodealkylation process using the PFD in Figure 1.5 and the flow table given in Table 1.5.

A utility summary for all the equipment is given in Table E8.10, from which the total yearly utility costs for this process are found:

Steam = \$3,412,000/y

Cooling Water = \$165,000/y

Fuel Gas = \$2,771,000/y

Electricity = \$37,400/y

Total Utilities = \$6,385,000/y

Raw Material Costs from the PFD, Table 8.4, and Example 8.8 are

Toluene = \$85,967,000/y

Hydrogen = \$6,622,000/y (based on a value of \$0.118/std m^3)

Total Raw Materials = \$92,589,000/y

There are no waste streams shown on the PFD, so

Table E8.10. Summary of Utility Requirements for the Equipment in the Toluene Hydrodealkylation Process

Equipment	Electric Power (kW)	Steam High Pressure (kg/s)	Steam Med. Pressure (kg/s)	Steam Low Pressure (kg/s)	Cooling Water (m^3/s)	Fuel Gas (std m^3/s)
E-101	—	2.48	—	—	—	—
E-102	—	—	—	—	0.31	—
E-103	—	—	—	0.14	—	—
E-104	—	—	—	—	0.055	—
E-105	—	—	—	—	0.007	—
E-106	—	—	1.26	—	—	—
H-101	—	—	—	—	—	0.22
C-101	54.5	—	—	—	—	—
P-101	16.5	—	—	—	—	—
P-102	4.0	—	—	—	—	—
Totals	75.0	2.48	1.26	0.14	0.372	0.22
Total yearly cost $/y	37,400	2,227,000	1,069,000	116,000	165,000	2,771,000

Data from Figure 1.5, Table 1.7, and Example 8.9.

Waste Treatment = $0.0/y

From Example 8.2 the cost of operating labor is

$$\boldsymbol{C_{OL} = (14)(59{,}580) = \$834{,}000/y}$$

From Problem 7.21 (using CAPCOST), the fixed capital investment (C_{GR}) for the process is found to be $\$12.5 \times 10^6$.

$$\boldsymbol{FCI = \$12.5 \times 10^6}$$

Finally, using Equation (8.2), the total manufacturing cost is estimated to be

$$COM_d = 0.180FCI_L + 2.73C_{OL} + 1.23(\text{Utilities} + \text{Raw Materials} + \text{Waste Treatment})$$

$$COM_d = (0.180)(12.5 \times 10^6) + 2.73\ (834{,}000) + 1.23\ (6{,}385{,}000 + 92{,}589{,}000 + 0)$$

$$COM_d = \$126.3 \times 10^6/y$$

8.9. Summary

In this chapter, the cost of manufacturing for a chemical process was shown to depend on the fixed capital investment, the cost of operating labor, the cost of utilities, the cost of waste treatment, and the cost of raw materials. In most cases, the cost of raw materials is the biggest cost. Methods to evaluate these different costs were discussed. Specifically, the amount of the raw materials and utilities can be obtained directly from the PFD. The cost of operating labor can be estimated from the number of pieces of equipment given on the PFD. Finally, the fixed capital investment can again be estimated from the PFD using the techniques given in Chapter 7.

What You Should Have Learned

- The primary costs of manufacture for a chemical process are for raw materials, utilities, and waste treatment.
- Other costs of manufacture can be estimated based on the primary manufacturing costs.
- There are resources available to obtain chemical costs and procedures to permit estimation of utility costs.

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Short Answer Questions

1. In the general equation for determining the cost of manufacturing (COM_d), Equation (8.2), one of the terms is $0.180FCI$, where FCI is the fixed capital investment of the plant. "This term is included to cover the interest payment on the loan for the plant." Is this statement true or false? Explain your answer.
2. Why is the number of operators per shift multiplied by approximately 4.5 to obtain the total number of operators required to run the plant?
3. What is a stream factor?

4. When estimating the cost of manufacturing (COM_d) for a chemical process, the overall COM_d may be estimated using only five individual costs. List these five costs.
5. Cooling water is priced on an energy basis: $/GJ. The temperature rise is usually assumed to be 10°C. Does the cooling water cost change if the return temperature changes? Are there any limitations to the return temperature? Explain.
6. In Equation (8.2), the cost of raw materials, C_{RM}, is multiplied by a factor of 1.23. The reason for this is that, in general, the estimated cost of raw materials is expected to be about 20% low and a correction factor of 1.23 is added to adjust for this. Do you agree with this explanation? If you do not, give another reason for using the factor of 1.23.
7. In Equation (8.2), the cost of operating labor, C_{OL}, is multiplied by a factor of 2.73. One reason for this is that the value of C_{OL} includes only plant operators and not supervisory and clerical labor costs. Is this statement true or false? What other factors (if any) account for the multiplication factor of 2.73?
8. Explain the difference between direct costs, fixed costs, and general expenses. Give two examples of each.

Problems

9. You are employed at a chemical company and have recently been transferred from a plant that manufactures synthetic dyes to a new facility that makes specialty additives for the polymer resin industry.
   a. You have been asked to estimate the cost of manufacturing at this new facility. Would you
      i. Use Equation (8.2) to estimate COM_d?
      ii. Use data from the old plant where you worked, because you are very familiar with all the aspects of manufacturing for that process?
      iii. Dig up information on the new process and use these figures?
   b. When would you use a relationship such as Equation (8.2)?
10. When a chemical plant needs steam at multiple pressure levels, it is often economical to generate all the steam at a high pressure and then to let the steam down through pressure-reducing turbines to the desired pressure. This principle is illustrated in Figure 8.6. The downside of this approach is that as the exhaust pressure of the turbine increases, the theoretical (and actual) steam requirements increase, meaning that less energy is extracted. To illustrate this point, do the following:
    a. Estimate the amount of energy extracted from 10,000 kg/h of 58.6 barg steam superheated by 165°C when connected to the following turbines (each 80% efficient):
       i. Exhaust pressure is 4″ Hg absolute.
       ii. Exhaust pressure is 4.82 barg.
    b. Estimate the amount of energy extracted from 10,000 kg/h of saturated, 10.0 barg steam when connected to a turbine (80% efficient) exhausting at 4.82 barg.
    c. Identify the locations of each of the three turbines described above on Figure 8.6.
11. What are the operating costs associated with a typical cooling water system? Based on the

example given in this chapter, answer the following:

a. What percentage of the operating costs is the makeup water?

b. By how much would the cost of cooling water increase if the cost of power (electricity) were to double?

c. By how much would the cost of cooling water increase if the cost of make-up water were to double?

12. Determine the cost of producing a refrigerant stream at –50°C using propane as the working fluid in a noncascaded system. You may wish to refer to Example 8.5 to do this problem. The steps you should follow are as follows:

a. Determine the pressure at which propane can be condensed at 45°C, which assumes that cooling water with a 5°C temperature approach will be used as the condensing medium.

b. Determine the pressure to which the propane must be throttled in order to liquefy it at –50°C.

c. Use the results of Parts (a) and (b) to set the approximate pressure levels in the condenser and evaporator in the refrigeration system.

d. Determine the amount of propane necessary to extract 1 GJ of heat in the evaporator.

e. Assuming a 5 kPa pressure drop in both heat exchangers and that a single-stage compressor is used with an efficiency of 75%, determine the cost of electricity to run the compressor, determine the cooling water cost, and from this determine the cost of providing refrigeration at –50°C using propane as the working fluid.

13. Repeat the process described in Problem 8.12 using a simple refrigeration loop to determine the cost of providing 1 GJ of refrigeration at –50°C using the following working fluids:

a. Propylene

b. Ethane

c. Ammonia

Determine whether any of the working fluids given above cannot be used in a simple (noncascaded) refrigeration loop. For these fluids, would using a cascaded refrigeration system to provide –50°C refrigerant make sense? Explain carefully your answers to these questions.

14. Estimate the cost of operating labor (C_{OL}), the cost of utilities (C_{UT}), and the cost of manufacturing (COM_d) for the ethylbenzene process given in Project B.2 of Appendix B. You must do Problem 7.22 in order to estimate COM_d.

15. Estimate the cost of operating labor (C_{OL}), the cost of utilities (C_{UT}), and the cost of manufacturing (COM_d) for the styrene process given in Project B.3 of Appendix B. You must do Problem 7.23 in order to estimate COM_d.

16. Estimate the cost of operating labor (C_{OL}), the cost of utilities (C_{UT}), and the cost of manufacturing (COM_d) for the drying oil process given in Project B.4 of Appendix B. You must do Problem 7.24 in order to estimate COM_d.

17. Estimate the cost of operating labor (C_{OL}), the cost of utilities (C_{UT}), and the cost of manufacturing (COM_d) for the maleic anhydride process given in Project B.5 of Appendix B. You must do Problem 7.25 in order to estimate COM_d.

18. Estimate the cost of operating labor (C_{OL}), the cost of utilities (C_{UT}), and the cost of manufacturing (COM_d) for the ethylene oxide process given in Project B.6 of Appendix B. You must do Problem 7.26 in order to estimate COM_d.

19. Estimate the cost of operating labor (C_{OL}), the cost of utilities (C_{UT}), and the cost of manufacturing (COM_d) for the formalin process given in Project B.7 of Appendix B. You must do Problem 7.27 in order to estimate COM_d.

Chapter 9. Engineering Economic Analysis

What You Will Learn

- That if money is invested, it grows
- That there are different types of interest
- How to do interest and investment calculations
- That there are different types of cash flow diagrams, which can be used to represent financial transactions
- How to represent financial transactions on a cash flow diagram
- How to include taxation
- What depreciation is, how to calculate it, and how to include it in financial calculations
- What inflation is, and how it is related to interest

The goal of any manufacturing company is to make money. This is realized by producing products with a high market value from raw materials with a low market value. The companies in the chemical process industry produce high-value chemicals from low-value raw materials.

In the previous chapters, a process flow diagram (Chapter 1), an estimate of the capital cost (Chapter 7), and an estimate of operating costs (Chapter 8) were provided for the production of benzene. From this material, an economic evaluation can be carried out to determine

1. Whether the process generates money
2. Whether the process is attractive compared with other processes (such as those for the production of ethylbenzene, ethylene oxide, formalin, and so on, given in Appendix B)

In the next two chapters, the necessary background to perform this economic analysis is provided.

The principles of economic analysis are covered in this chapter. The material presented covers all of the major topics required for completion of the Fundamentals of Engineering (FE) examination. This is the first requirement for becoming a registered professional engineer in the United States.

It is important for you, the graduating student, to understand the principles presented in this chapter at the beginning of your professional career in order to manage your money skillfully. As a result, discussions and examples of personal money management are integrated throughout the chapter.

The evaluation of profitability and comparison of alternatives for proposed projects are covered in Chapter 10.

9.1. Investments and the Time Value of Money

The ability to profit from investing money is the key to our economic system. In this text, investment in terms of personal financing is introduced and then applied to chemical process economics.

There are various ways to distribute one's personal income. The first priority is to maintain a basic (no-frills) standard of living. This includes necessary food, clothing, housing, transportation, and expenses such as taxes imposed by the government. The remaining money, termed *discretionary money*, can then be distributed. It is wise to distribute this money in a manner that will realize both

your short-term and long-term goals.

Generally, there are two classifications for spending discretionary money:

1. Consume money as received. This provides immediate personal gratification and/or satisfaction. Most people experience this use for money early in life.
2. Retain money for future consumption. This is money put aside to meet future needs. These may result from hard-to-predict causes such as sickness and job layoffs or from a more predictable need for long-term retirement income. It is unlikely that you have considered these types of financial needs and you probably have little experience in investing to secure a comfortable lifestyle after you stop working.

There are two approaches to setting money aside for use at a later date:

- **Simple savings:** Put money in a safety deposit box, sugar bowl, or other such container.
- **Investments:** Put money into an investment.

These two approaches are considered in Example 9.1.

Example 9.1.

Upon graduation, you start your first job at $50,000/y. You decide to set aside 10%, or $5000/y, for retirement in 40 years' time, and you assume that you will live 20 years after retiring. You have been offered an investment that will pay you $67,468/y during your retirement years for the money you invest.

a. How much money would you have per year in retirement if you had saved the money, but not invested it, until retirement?

b. How does this compare with the investment plan offered?

c. How much money was produced from the investment?

Solution

a. Money saved: ($5000)(40) = $200,000

Income during retirement: $200,000/20 = $10,000/y

b. Comparison: (Income from savings)/(Income from investments) = $10,000/$67,468 = 0.15

c. Money Produced = Money Received – Money Invested = ($67,468)(20) – $200,000 = $1,149,360

The value of the investment is clear. The income in retirement from savings amounts to only 15% of the investment income. The amount of money provided during retirement, by setting $200,000 aside, was more than a million dollars. It will be shown later that this high return on investment resulted from two factors: the long time period for the investment and the interest rate earned on the savings.

Money, when invested, makes money.

The term *investment* will now be defined.

An **investment** is an agreement between two parties, whereby one party, the **investor,** provides money, P, to a second party, the **producer,** with the expectation that the producer will return money,

F, to the investor at some future specified date, where $F > P$. The terms used in describing the investment are

P: Principal or Present Value

F: Future Value

n: Years between F and P

The amount of money earned from the investment is

$$E = F - P \tag{9.1}$$

The yearly earnings rate is

$$i_s = \frac{E}{Pn} = \frac{(F - P)}{Pn} \tag{9.2}$$

where i_s is termed the simple interest rate.

Equation (9.2) rearranges to

$$\frac{F}{P} = (1 + ni_s) \text{ or, in general, } \frac{F}{P} = f(n,i) \tag{9.3}$$

Example 9.2 illustrates this concept.

Example 9.2.

You decide to put $1000 into a bank that offers a special rate if left in for two years. After two years you will be able to withdraw $1150.

a. Who is the producer?

b. Who is the investor?

c. What are the values of P, F, i_s, and n?

Solution

a. Producer: The bank has to produce $150.00 in interest after two years.

b. Investor: You invest $1000 in an account at the beginning of the two-year period.

c. P = $1000 (given)

F = $1150 (given)

n = 2 years (given)

From Equation (9.2),

i_s = ($1150 – $1000)/($1000)/(2) = 0.075 or 7.5% per year

In Example 9.2, you were the investor and invested in the bank. The bank was the "money producer" and had to return to you more dollars ($1150) than you invested ($1000). This bank transaction is an investment commonly termed as *savings*. In the reverse situation, termed *loan*, the bank becomes the investor. You must produce money during the time of the investment.

Equations (9.1) through (9.3) apply to a single transaction between the investor and the producer that covers n years and uses simple interest. There are other investment schedules and interest formulations in practice; these will be covered later in this chapter.

Figure 9.1 illustrates a possible arrangement to provide the funds necessary to build a new chemical plant such as the one introduced in the narrative in Chapter 1.

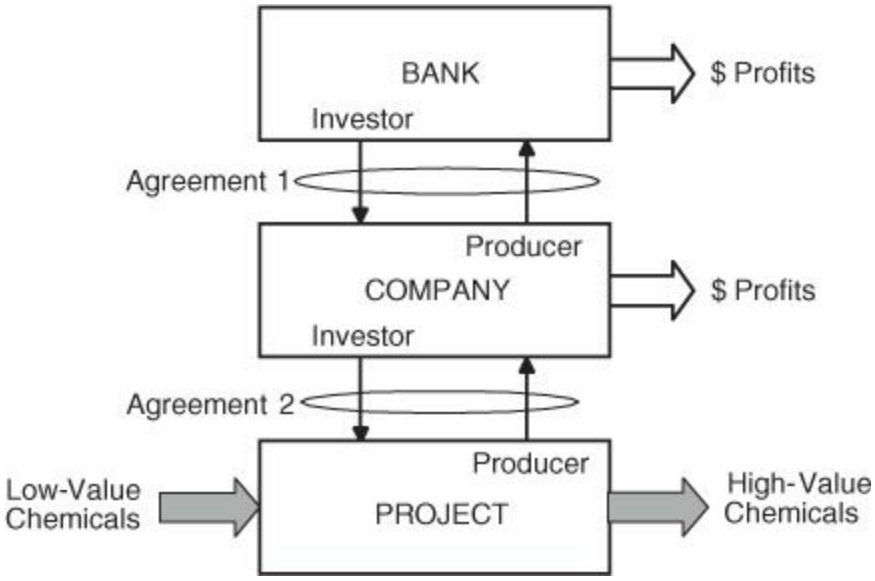


Figure 9.1. A Typical Financing Scheme for a Chemical Plant

In this arrangement, a bank invests in a company, which in turn invests in a project to produce a chemical. There are two agreements in this project (see Figure 9.1).

1. The bank is an investor and the company is the producer.
2. The company is an investor and the project is the producer.

In this illustration, all the money produced in the project is sent to the company. The company pays its investor, the bank, and draws off the rest as profit. The bank also makes a profit from its investment loan to the company. The project is the source of money to provide profits to both the company and the bank. The project converts a low-value, raw chemical into chemicals of higher value. Without the investor, the plant would not be built, and without the plant, there would be no profits for either the company or the bank.

Money is a measure of the value of products and services. The value of a chemical material is the price it can be exchanged for in dollars. Investments may be made in units other than dollars, such as stocks, bonds, grain, oil, or gold. This is often called value, or value added, in describing investments. The term *value* is a general one and, in this case, may be assigned a dollar figure for economic calculations.

Figure 9.1 shows that all profits were produced from an operating plant. The role of engineers in our economy should be clear. This is to ensure efficient production of highvalue products, including current as well as new and improved products.

In almost all cases, the economic analysis of processes will be made from the point of view of the company as the investor in a project. The project may be the construction of a new plant or a modification to an existing plant.

Consider the decisions involved in the investment in a new plant (the project) from the point of view of the company. The company must invest the money to build the plant before any income resulting from production can begin. Once the plant has been built and is operational, it is expected to operate for many years. During this time, the plant produces a profit and the company receives income from its investment. It is necessary to be able to determine whether this future income is sufficiently attractive to make the investment worthwhile.

The **time value of money** refers to a concept that is fundamental to evaluating an investment. This is illustrated in Example 9.3.

Example 9.3.

You estimate that in two years' time you will need $1150 in order to replace the linoleum in your kitchen. Consider two choices:

1. Wait two years to take action.
2. Invest $1000 now (assume that interest is offered by the bank at the same rate as given in Example 9.1).

What would you do (explain your answer)?

Solution

Consider investing the $1000 today because it will provide $1150 in two years. The key is that the dollar I have today is worth 15% more than a dollar I will have in two years' time.

From Example 9.3, it was concluded that today's dollar is worth more than tomorrow's dollar because it can be invested to earn more dollars. This must not be confused with inflation, which erodes purchasing power and is discussed in Section 9.6.

Money today is worth more than money in the future.

In the upcoming sections, it will be found that when comparing capital investments made at different times, the timing of each investment must be considered.

9.2. Different Types of Interest

Two types of interest are used when calculating the future value of an investment. They are referred to as *simple* and *compound interest*. Simple interest calculations are rarely used today. Unless specifically noted, all interest calculations will be carried out using compound interest methods.

9.2.1. Simple Interest

In **simple interest** calculations, the amount of interest paid is based solely on the initial investment.

Interest paid in any year = Pi_s

For an investment period of n years, the total interest paid = $Pi_s\, n$

Total value of investment in n years = $F_n = P + Pi_s n$

$$F_n = P(1 + i_s n) \qquad (9.4)$$

If, instead of setting the earned interest aside, it were reinvested, the total amount of interest earned would be greater. When earned interest is reinvested, the interest is referred to as **compound interest.**

9.2.2. Compound Interest

Let us determine the future value of an investment, F_n, after n years at an interest rate of i per year for an initial investment of P when the interest earned is reinvested each year.

a. At the start, there is the initial investment = P.

b. In year 1, Pi in interest is earned.

For year 2, $P + Pi$ or $P(1 + i)$ is invested.

c. In year 2, $P(1 + i)i$ in interest is earned.

For year 3, $P(1 + i) + P(1 + i)i$, or $P(1 + i)^2$ is invested.

d. In year 3, $P(1 + i)^2 i$ in interest is earned.

For year 4, $P(1 + i)^2 + P(1 + i)^2 i$, or $P(1 + i)^3$ is invested.

e. By induction it is found that after n years the value of the investment is $P(1 + i)^n$.

Thus, for compound interest it can be written

$$F_n = P(1 + i)^n \qquad (9.5)$$

The process can be reversed, and the question can be asked: How much would have to be invested now, P, in order to receive a certain sum, F_n, in n years' time? The solution to this problem is found by rearranging Equation (9.5):

$$P = \frac{F_n}{(1 + i)^n} \qquad (9.6)$$

The use of these equations is illustrated in Examples 9.4, 9.5, and 9.6. The letters *p.a.* following the interest refers to per year (per annum).

Example 9.4.

For an investment of \$500 at an interest rate of 8% p.a. for four years, what would be the future value of this investment, assuming compound interest?

From Equation (9.5) for $P = 500$, $i = 0.08$, and $n = 4$

$F_4 = P(1 + i)^n = 500(1 + 0.08)^4 = \$680.24$

Note: Simple interest would have yielded $F_4 = 500(1 + (4)(0.08)) = \$660$ (\$20.24 less).

Example 9.5.

How much would I need to invest in a savings account yielding 6% interest p.a. to have \$5000 in five years' time?

From Equation (9.6) using $F_5 = \$5000$, $i = 0.06$, and $n = 5$

$P = F_n/(1 + i)^n = 5000/(1.06)^5 = \$3736.29$

If \$3736.29 is invested into the savings account today, the accumulated value will be \$5000 in five years' time.

Example 9.6.

I need to borrow a sum of money (P) and have two loan alternatives.

a. I borrow from my local bank, which will lend me money at an interest rate of 7% p.a. and pay compound interest.

b. I borrow from "Honest Sam," who offers to lend me money at 7.3% p.a. using simple interest.

In both cases, I need the money for three years. How much money would I need in three years to pay off this loan? Consider each option separately.

Bank: From Equation (9.5) for $n = 3$ and $i = 0.07$

$F_3 = (P)(1 + 0.07)^3 = 1.225\ P$

Sam: From Equation (9.4) for $n = 3$ and $i = 7.3$

$F_3 = (P)(1 + (3)(0.073)) = 1.219\ P$

Sam stated a higher interest rate, and yet it is still preferable to borrow the money from Sam because $1.219P < 1.225P$. This is because Sam used simple interest, and the bank used compound interest.

9.2.3. Interest Rates Changing with Time

If there is an investment over a period of years and the interest rate changes each year, then the appropriate calculation for compound interest is given by

$$F_n = P\prod_{j=1}^{n}(1 + i_j) = P(1 + i_1)(1 + i_2)\cdots(1 + i_n) \qquad (9.7)$$

9.3. Time Basis for Compound Interest Calculations

In industrial practice, the length of time assumed when expressing interest rates is one year. However, sometimes terms such as 6% p.a. compounded monthly are used. In this case, the 6% is referred to as a **nominal annual interest rate,** i_{nom}, and the number of compounding periods per year is m (12 in this case). The nominal rate is not used directly in any calculations. The **actual rate** is the interest rate per compounding period, r. The relationship needed to evaluate r is

$$r = \frac{i_{nom}}{m} \qquad (9.8)$$

This is illustrated in Example 9.7.

Example 9.7.

For the case of 12% p.a. compounded monthly, what are m, r, and i_{nom}?

Given: $m = 12$ (months in a year), $i_{nom} = 12\% = 0.12$

From Equation (9.8),

$r = 0.12/12 = 0.01$ (or 1% per month)

9.3.1. Effective Annual Interest Rate

An **effective annual interest rate,** i_{eff}, can be used, which allows interest calculations to be made on an annual basis and gives the same result as using the actual compounding periods. From the value of an investment after one year,

$$F_1 = P(1 + i_{eff}) = P\left(1 + \frac{i_{nom}}{m}\right)^m$$

which, upon rearrangement, gives

$$i_{eff} = \left(1 + \frac{i_{nom}}{m}\right)^m - 1 \qquad (9.9)$$

Effective annual interest rate is illustrated in Example 9.8.

Example 9.8.

What is the effective annual interest rate for a nominal rate of 8% p.a. when compounded monthly?

From Equation (9.9), for $i_{nom} = 0.08$ and $m = 12$,

$i_{eff} = (1 + 0.08/12)^{12} - 1 = 0.083$ (or 8.3 % p.a.)

The effective annual interest rate is greater than the nominal annual rate. This indicates that the effective interest rate will continue to increase as the number of compounding periods per year increases. For the limiting case, interest is compounded continuously.

9.3.2. Continuously Compounded Interest

For the case of continuously compounded interest, Equation (9.9) must be observed as $m \to \infty$:

$$i_{eff} = \lim_{m\to\infty}\left[\left(1 + \frac{i_{nom}}{m}\right)^m - 1\right]$$

Rewriting the left-hand side as $\lim_{m\to\infty}\left[\left\{\left(1 + \frac{i_{nom}}{m}\right)^{\frac{m}{i_{nom}}}\right\}^{i_{nom}} - 1\right]$

and noting that $\lim_{n\to\infty}\left[1 + \frac{x}{n}\right]^{\frac{n}{x}} = e$

it is found that for continuous compounding,

$$i_{eff} = e^{i_{nom}} - 1 \qquad (9.10)$$

Equation (9.10) represents the maximum effective annual interest rate for a given nominal rate.

The method for calculating continuously compounded interest is illustrated in Example 9.9.

Example 9.9.

What is the effective annual interest rate for an investment made at a nominal rate of 8% p.a. compounded continuously?

From Equation (9.10) for $i_{nom} = 0.08$

$i_{eff} = e^{0.08} - 1 = 0.0833$, or 8.33% p.a.

Note: It can be seen by comparison with Example 9.8 that by compounding continuously little was gained over monthly compounding.

In comparing alternatives, the effective annual rate, and not the nominal annual rate of interest, must be used.

9.4. Cash Flow Diagrams

To this point, only an investment made at a single point in time at a known interest rate has been considered, and it was shown how to evaluate the future value of this investment. More complicated

transactions involve several investments and/or payments of differing amounts made at different times. For more complicated investment schemes, careful track must be kept of the amount and time of each transaction. An effective way to track these transactions is to utilize a **cash flow diagram**, or CFD. Such a diagram offers a visual representation of each investment. Figure 9.2 is the cash flow diagram for Example 9.10, which is used to introduce the basic elements of the **discrete CFD**.

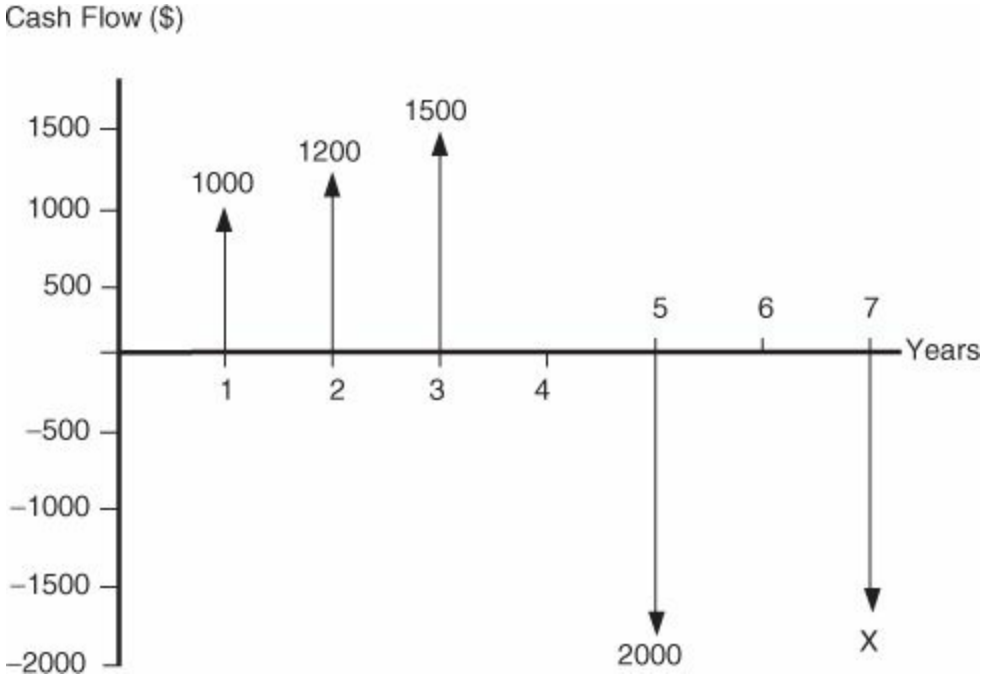


Figure 9.2. An Example of a Representative Discrete Cash Flow Diagram (CFD)

Figure 9.2 shows that cash transactions were made periodically. The values given represent payments made at the end of the year. Figure 9.2 shows that $1000, $1200, and $1500 were received at the end of the first, second, and third year, respectively. In the fifth and seventh year, $2000 and $$X$ were paid out. There were no transactions in the fourth and sixth years.

Each cash flow is represented by a vertical line, with length proportional to the cash value of the transaction. The sign convention uses a downward-pointing arrow when cash flows outward and an upward-pointing arrow representing inward cash flows. When a company invests money in a project, the company CFD shows a negative cash flow (outward flow), and the project CFD shows a positive cash flow (inward flow). Lines are placed periodically in the horizontal direction to represent the time axis. Most frequently, an analysis is performed from the point of view of the investor.

The cash flow diagram shown in Figure 9.2 can be presented in a simplified format, using the following simplifications:

1. The y-axis is not shown.
2. Units of monetary transactions are not given for every event.

In addition to the discrete CFD described above, the same information can be shown in a **cumulative CFD.** This type of CFD presents the accumulated cash flow at the end of each period.

9.4.1. Discrete Cash Flow Diagram

The discrete CFD provides a clear, unambiguous pictorial record of the value, type, and timing of each transaction occurring during the life of a project. In order to avoid making mistakes and save time, it is recommended that prior to doing any calculations, you sketch a cash flow diagram. Examples 9.10 and 9.11 illustrate the use of discrete cash flow diagrams.

Example 9.10.

I borrow \$1000, \$1200, and \$1500 from a bank (at 8% p.a. effective interest rate) at the end of years 1, 2, and 3, respectively. At the end of year 5, I make a payment of \$2000, and at the end of year 7, I pay off the loan in full. The CFD for this exchange from my point of view (producer) is given in Figure E9.10(a).

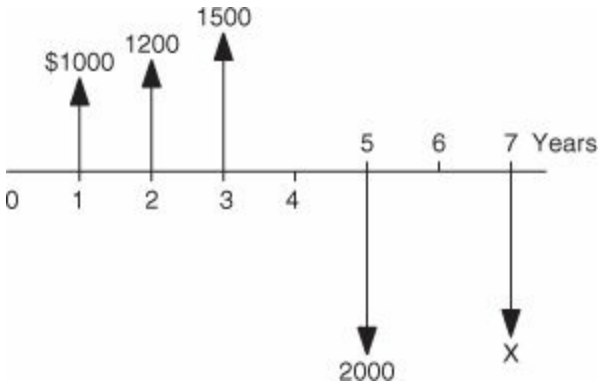


Figure E9.10a. CFD for Example 9.10 from My Perspective

Note: Figure E9.10(a) is the shorthand version of the one presented in Figure 9.2 used to introduce the CFD.

Draw a discrete cash flow diagram for the investor.

The bank represents the investor. From the investor's point of view, the initial three transactions are negative and the last two are positive.

Figure E9.10(b) represents the CFD for the bank. It is the mirror image of the one given in the problem statement.

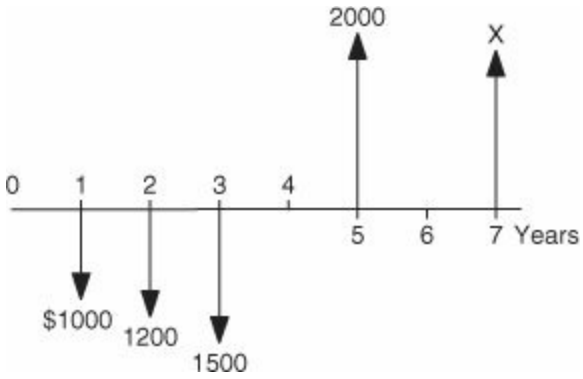


Figure E9.10b. CFD for Example 9.10 from the Bank's Perspective

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The value of *X* in Example 9.10 depends on the interest rate. Its value is a direct result of the time value of money. The effect of interest rate and the calculation of the value of *X* (in Example 9.13) are determined in the next section.

Example 9.11.

You borrow \$10,000 from a bank to buy a new car and agree to make 36 equal monthly payments of \$320 each to repay the loan. Draw the discrete CFD for the investor in this agreement.

The bank is the investor. The discrete CFD for this investment is shown in Figure E9.11.

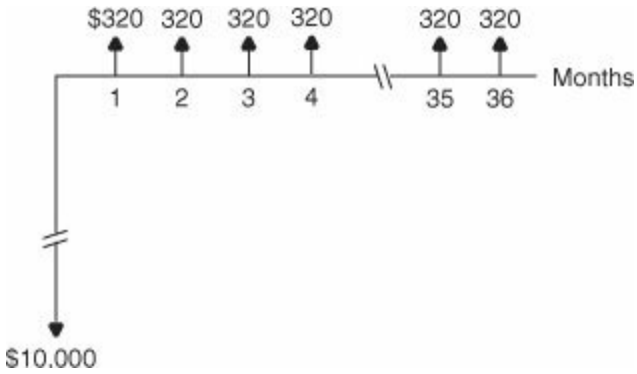


Figure E9.11. CFD for Car Loan Described in Example 9.11

Notes:

1. There is a break in both the time scale and in the investment at time = 0 (the initial investment).
2. From your point of view, the cash flow diagram would be the mirror image of the one shown.

The cash flow diagram constructed in Example 9.11 is typical of those you will encounter throughout this text. The investment (negative cash flow) is made early in the project during design and construction before there is an opportunity for the plant to produce product and generate money to repay the investor. In Example 9.11, payback was made in a series of equal payments over three years to repay the initial investment by the bank. In Section 9.5, you will learn how to calculate the interest rate charged by the bank in this example.

9.4.2. Cumulative Cash Flow Diagram

As the name suggests, the cumulative CFD keeps a running total of the cash flows occurring in a project. To illustrate how to construct a cumulative CFD, consider Example 9.12, which illustrates the cash flows associated with the construction and operation of a new chemical plant.

Example 9.12.

The yearly cash flows estimated for a project involving the construction and operation of a chemical plant producing a new product are provided in the discrete CFD in Figure E9.12a. Using this information, construct a cumulative CFD.

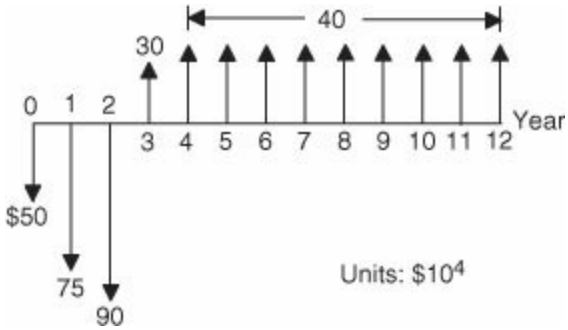


Figure E9.12a. Discrete CFD for Chemical Plant Described in Example 9.12

The numbers shown in Table E9.12 were obtained from this diagram.

Table E9.12. Summary of Discrete and Cumulative Cash Flows in Example 9.12

Year	Cash Flow ($) (from Discrete CFD)	Cumulative Cash Flow (Calculated)
0	–500,000	–500,000
1	–750,000	–1,250,000
2	–900,000	–2,150,000
3	300,000	–1,850,000
4	400,000	–1,450,000
5	400,000	–1,050,000
6	400,000	–650,000
7	400,000	–250,000
8	400,000	150,000
9	400,000	550,000
10	400,000	950,000
11	400,000	1,350,000
12	400,000	1,750,000

The cumulative cash flow diagram is plotted in Figure E9.12b.

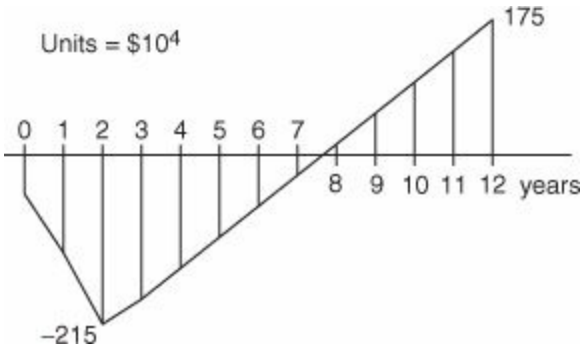


Figure E9.12b. Cumulative CFD for Chemical Plant Described in Example 9.12

9.5. Calculations from Cash Flow Diagrams

To compare investments that take place at different times, it is necessary to account for the time value of money.

> **When cash flows occur at different times, each cash flow must be brought forward (or backward) to the same point in time and then compared.**

The point in time that is chosen is arbitrary. This is illustrated in Example 9.13.

Example 9.13.

The CFD obtained from Example 9.10 (for the borrower) is repeated in Figure E9.13. The interest rate paid on the loan is 8% p.a.

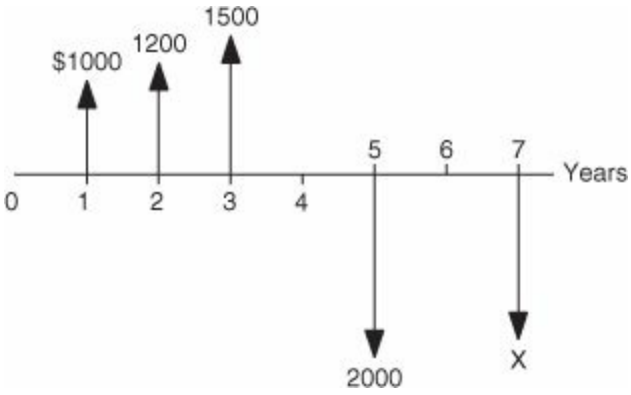


Figure E9.13. CFD for Example 9.13

In year 7, the remaining money owed on the loan is paid off.

a. Determine the amount, X, of the final payment.

b. Compare the value of X with the value that would be owed if there were no interest paid on the loan.

With the final payment at the end of year 7, no money is owed on the loan. If all the positive and negative cash flows adjusted for the time of the transactions are summed, this adjusted sum must equal zero.

The date of the final payment is selected as the base time.

a. From Equation (9.5) for $i = 0.08$ the following is obtained:

For withdrawals:

\$1000 end of year 1: $F_6 = (\$1000)(1 + 0.08)^6 = \$1586.87$

\$1200 end of year 2: $F_5 = (\$1200)(1 + 0.08)^5 = \$1763.19$

\$1500 end of year 3: $F_4 = (\$1500)(1 + 0.08)^4 = \$2040.73$

Total withdrawals = \$5390.79

For repayments:

\$2000 end of year 5: $F_2 = -(\$2000)(1 + 0.08)^2 = -\$2332.80$

\$$X$ end of year 7: $F_0 = -(\$X)(1 + 0.08)^0 = -\$X$

Total repayments = $-\$(2332.80 + X)$

Summing the cash flows and solving for X yields

$0 = \$5390.79 - \$(2332.80 + X)$

$X = \$3057.99 \approx \$3058$

b. For $i = 0.00$

Withdrawals = \$1000 + \$1200 + \$1500 = \$3700

Repayments = $-\$(2000 + X)$

$0 = \$3700 - \$(2000 + X)$

$X = \$1700$

Note: Because of the interest paid to the bank, the borrower repaid a total of \$1358 (\$3058 – \$1700) more than was borrowed from the bank seven years earlier.

To demonstrate that any point in time could be used as a basis, compare the amount repaid based on the end of year 1. Equation (9.6) is used, and all cash flows are moved backward in time (exponents become negative). This gives

$$0 = 1000 + \frac{1200}{1.08} + \frac{1500}{1.08^2} - \frac{2000}{1.08^4} - \frac{X}{1.08^6}$$

and solving for X yields

$$X = (1.08)^6\left[1000 + \frac{1200}{1.08} + \frac{1500}{1.08^2} - \frac{2000}{1.08^4}\right] = \$3058 \text{ (the same answer as before!)}$$

Usually, the desire is to compute investments at the start or at the end of a project, but the conclusions drawn are independent of where that comparison is made.

9.5.1. Annuities—A Uniform Series of Cash Transactions

Problems are often encountered involving a series of uniform cash transactions, each of value A, taking place at the end of each year for n consecutive years. This pattern is called an **annuity**, and the discrete CFD for an annuity is shown in Figure 9.3.

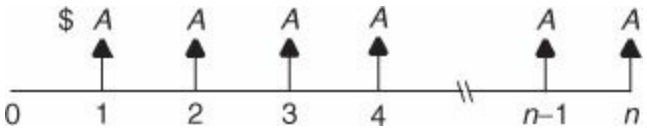


Figure 9.3. A Cash Flow Diagram for an Annuity Transaction

To avoid the need to do a year-by-year analysis like the one in Example 9.13, an equation can be developed to provide the future value of an annuity.

The future value of an annuity at the end of time period n is found by bringing each of the investments forward to time n, as was done in Example 9.13.

$$F_n = A(1+i)^{n-1} + A(1+i)^{n-2} + A(1+i)^{n-3} + \ldots + A$$

This equation is a geometric series of the form $a, ar, ar^2, \ldots, ar^{n-1}$ with sum $S_n = F_n$.

$$S_n = a\left[\frac{r^n - 1}{r - 1}\right]$$

For the present case, $a = A$; $r = 1 + i$; $n = n$. Therefore,

$$F_n = A\left[\frac{(1+i)^n - 1}{i}\right] \qquad (9.11)$$

It is important to notice that Equation (9.11) is correct when the annuity starts at the end of the *first* time period and not at time zero. In the next section, a shorthand notation is provided that will be useful in CFD calculations.

9.5.2. Discount Factors

The shorthand notation for the future value of an annuity starts with Equation (9.11). The term F_n is shortened by simply calling it F, and then dividing through by A yields

$$F/A = [(1+i)^n - 1]/i = f(i, n)$$

This ratio of F/A is a function of i and n—that is, $f(i,n)$. It can be evaluated when both the interest rate, i, and the time duration, n, are known. The value of $f(i,n)$ is referred to as a **discount factor.** If either A or F is known, the remaining unknown can be evaluated.

In general terms, a discount factor is designated as

$$\text{Discount factor for } X/Y = (X/Y, i, n) = f(i, n)$$

Discount factors represent simple ratios and can be multiplied or divided by each other to give additional discount factors. For example, assume that the present worth, P, of an annuity, A, must be known—that is, the discount factor for P/A—but the needed equation is not available. The only available formula containing the annuity term, A, is the one for F/A derived above. The future value, F, can be eliminated, and the present value, P, introduced by multiplying by the ratio of P/F, from Equation 9.6.

$$\text{Discount factor for } P/A = (P/A, i, n)$$
$$= (F/A, i, n)(P/F, i, n)$$

Substituting for F/A and P/F gives

$$P/A = \frac{(1+i)^n - 1}{i}\frac{1}{(1+i)^n}$$
$$= \frac{(1+i)^n - 1}{1}\frac{1}{i(1+i)^n} = (P/A, i, n)$$

Table 9.1 lists the most frequently used discount factors in this text with their common names and corresponding formulae.

Table 9.1. Commonly Used Factors for Cash Flow Diagram Calculations

Conversion	Symbol	Common Name	Eq. No.	Formula
P to F	$(F/P, i, n)$	Single Payment Compound Amount Factor	(9.5)	$(1+i)^n$
F to P	$(P/F, i, n)$	Single Payment Present Worth Factor	(9.6)	$\frac{1}{(1+i)^n}$
A to F	$(F/A, i, n)$	Uniform Series Compound Amount Factor, Future Worth of Annuity	(9.11)	$\frac{(1+i)^n - 1}{i}$
F to A	$(A/F, i, n)$	Sinking Fund Factor	(9.12)	$\frac{i}{(1+i)^n - 1}$
P to A	$(A/P, i, n)$	Capital Recovery Factor	(9.13)	$\frac{i(1+i)^n}{(1+i)^n - 1}$
A to P	$(P/A, i, n)$	Uniform Series Present Worth Factor, Present Worth of Annuity	(9.14)	$\frac{(1+i)^n - 1}{i(1+i)^n}$

The key to performing any economic analysis is the ability to evaluate and compare equivalent investments. In order to understand that the equations presented in Table 9.1 provide a comparison of alternatives, it is suggested to replace the equal sign with the words "is equivalent to." As an example, consider the equation given for the value of an annuity, A, needed to provide a specific future worth, F. From Table 9.1, Equation (9.11) can be expressed as

$$F \text{ (Future value) is equivalent to } \{f(i,n)\ A(\text{Annuity value})\}$$

where

$$f(i,n) = (F/A, i, n)$$

Example 9.14 illustrates a future value calculation.

Example 9.14.

You have just won $2,000,000 in the Texas Lottery as one of seven winners splitting up a jackpot of $14,000,000. It has been announced that each winner will receive $100,000/year for the next 20 years. What is the equivalent present value of your winnings if you have a secure investment opportunity providing 9.5% p.a.?

From Table 9.1, Equation (9.14), for $n = 20$ and $i = 0.075$,

$$P = (\$100{,}000)[(1 + 0.075)^{20} - 1]/[(0.075)(1 + 0.075)^{20}]$$

$$P = \$1{,}019{,}000$$

A present value of $1,019,000 is equivalent to a 20-year annuity of $100,000/y when the effective interest rate is 9.5%.

Examples 9.15 through 9.17 illustrate how to use these discount factors and how to approach problems involving discrete CFDs.

Example 9.15.

Consider Example 9.11, involving a car loan. The discrete CFD from the bank's point of view was shown.

What interest rate is the bank charging for this loan?

You have agreed to make 36 monthly payments of $320. The time selected for evaluation is the time at which the final payment is made. At this time, the loan will be fully paid off. This means that the future value of the $10,000 borrowed is equivalent to a $320 annuity over 36 payments.

$$(\$10{,}000)(F/P, i, n) = (\$320)(F/A, i, n)$$

Substituting the equations for the discount factors given in Table 9.1, with $n = 36$ months, yields

$$0 = -(10{,}000)(1 + i)^{36} + (320)[(1 + i)^{36} - 1]/i$$

This equation cannot be solved explicitly for i. It is solved by plotting the value of the right-hand side of the equation shown above for various interest rates. This equation could also be solved using a numerical technique. From Figure E9.15, the interest rate that gives a value of zero represents the answer. From Figure E9.15 the rate of interest is $i = 0.0079$.

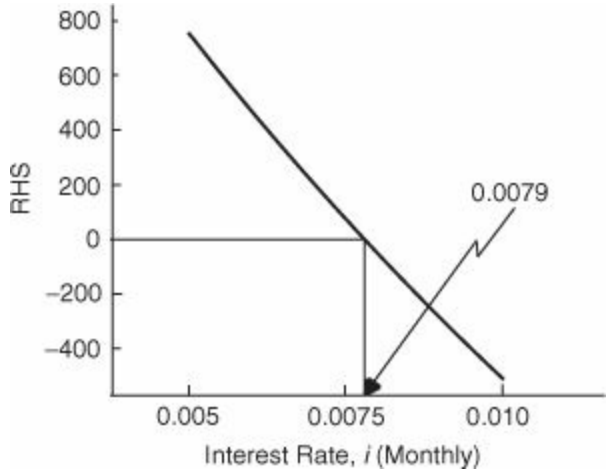


Figure E9.15. Determination of Interest Rate for Example 9.15

The nominal annual interest rate is (12)(0.00786) = 0.095 (9.5%).

Example 9.16.

I invest money in a savings account that pays a nominal interest rate of 6% p.a. compounded monthly. I open the account with a deposit of $1000 and then deposit $50 at the end of each month for a period of two years, followed by a monthly deposit of $100 for the following three years. What will the value of my savings account be at the end of the five-year period?

First, draw a discrete CFD (Figure E9.16).

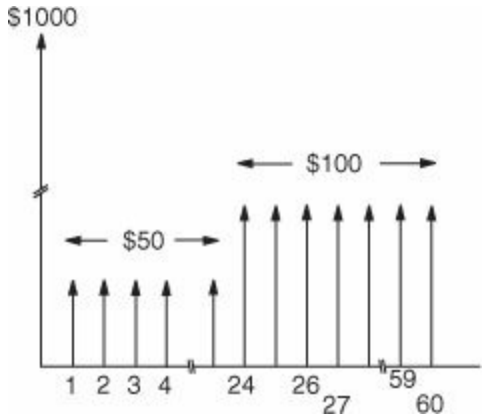


Figure E9.16. Cash Flow Diagram for Example 9.16

Although this CFD looks rather complicated, it can be broken down into three easy sub-problems:

1. The initial investment
2. The 24 monthly investments of $50
3. The 36 monthly investments of $100

Each of these investments is brought forward to the end of month 60.

$F = (\$1000)(F/P, 0.005, 60) + (\$50)(F/A, 0.005, 24)(F/P, 0.005, 36) + (\$100)(F/A, 0.005, 36)$

Note: The effective monthly interest rate is 0.06/12 = 0.005.

$$F = (\$1000)(1.005)^{60} + (\$50)\frac{(1.005^{24} - 1)}{0.005}(1.005)^{36} + (\$100)\frac{(1.005^{36} - 1)}{0.005} = \$6804.16$$

There are many ways to solve most complex problems. No one method is more or less correct than another. For example, the discrete CFD could be considered to be made up of a single investment of $1000 at the start, a $50 monthly annuity for the next 60 months, and another $50 annuity for the last 36 months. Evaluating the future worth of the investment gives

$F = (\$1000)(F/P, 0.005, 60) + (\$50)(F/A, 0.005, 60) + (\$50)(F/A, 0.005, 36)$

$$F = (\$1000)(1.005)^{60} + (\$50)\frac{(1.005^{60} - 1)}{0.005} + (\$50)\frac{(1.005^{36} - 1)}{0.005} = \$6804.16$$

This is the same result as before.

Example 9.17.

In Example 9.1, an investment plan for retirement was introduced. It involved investing $5000/year for 40 years leading to retirement. The plan then provided $67,468/year for 20 years of retirement income.

a. What yearly interest rate was used in this evaluation?

b. How much money was invested in the retirement plan before withdrawals began?

Solution

a. The evaluation is performed in two steps.

Step 1: Find the value of the $5000 annuity investment at the end of the 40 years.

Step 2: Evaluate the interest rate of an annuity that will pay out this amount in 20 years at $67,468/y.

Step 1: From Equation (9.11), Table 9.1, for $A = \$5000$ and $n = 40$,

$$F_{40} = (A)(F/A, n, i) = (\$5000)\,[(1+i)^{40}-1]/i$$

Step 2: From Equation (9.14), Table 9.1, for $A = \$67{,}468$ and $n = 20$,

$$P = (A)(P/A, n, i) = (\$67{,}468)[(1 + i)^{20} - 1]/[(i)(1 + i)^{20}]$$

Set $F_{40} = P$ and solve for i. From Figure E9.17, $i = 0.060$

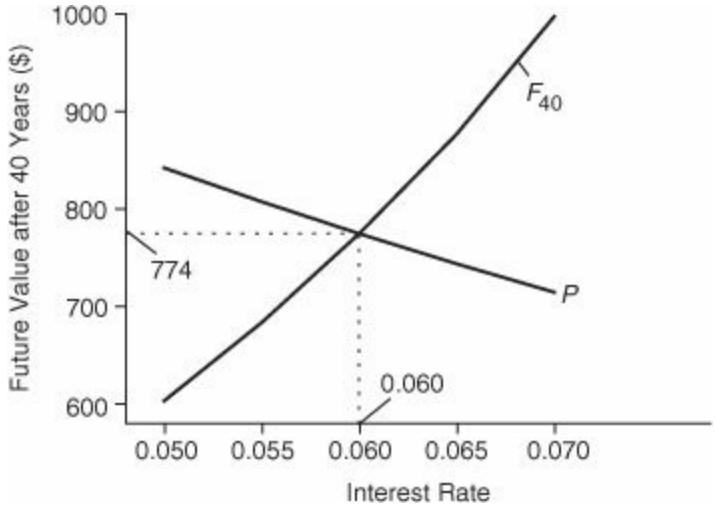


Figure E9.17. Determination of Interest Rate for Example 9.17

b. With $i = 0.060$, from Figure E9.17, $F_{40} = \$774{,}000$

Note: The interest rate of 6.0% p.a. represents a relatively low interest rate, involving small risk.

9.6. Inflation

As a result of inflation, a dollar set aside (not invested) will purchase fewer goods and services in the future than the same dollar would today. In Chapters 7 and 8, it was seen that inflation of equipment, labor, and fuel costs could be tracked by the use of cost indexes.

It is sometimes desirable to express these trends in terms of rates of inflation (f). This can be done using the cost indexes as follows:

$$CEPCI(j + n) = (1 + f)^n\, CEPCI(j) \qquad (9.15)$$

where n = time span in years

f = average inflation rate over the time span

j = arbitrary year

The use of Equation (9.15) to estimate the inflation rate is illustrated in Example 9.18.

Example 9.18.

What was the average rate of inflation for the costs associated with building a chemical plant over the following periods?

a. 1995 through 2001

b. 2001 through 2007

From Table 7.4, the values of the Chemical Engineering Plant Cost Index (*CEPCI*) are

CEPCI (1995) = 381

CEPCI (2001) = 394

CEPCI (2007) = 500

Equation (9.15) yields

a. $394 = (381)(1 + f)^6$,

$f = 0.006$ (0.6% p.a.)

b. $500 = 394\ (1 + f)^6$

$f = 0.049$ (4.9% p.a.)

To understand inflation, it is necessary to distinguish between cash and the purchasing power (for the purchase of goods and services) of cash. Inflation decreases this purchasing power with time. All the previous discussions on *A, P*, and *F* are given in terms of cash and not in terms of the relative purchasing power of this cash. The term *F'* is introduced, which represents the purchasing power of future cash. This purchasing power can be estimated using Equation (9.16).

$$F' = \frac{F}{(1+f)^n} \tag{9.16}$$

Substituting the equation for *F* in terms of *P*, from Equation (9.5), gives

$$F' = P\frac{(1+i)^n}{(1+f)^n} = P\left[\frac{1+i}{1+f}\right]^n \tag{9.17}$$

Equation (9.17) is now written in terms of an effective interest rate, *i'*, which includes the effect of inflation.

$$F' = P(1+i')^n \tag{9.18}$$

By comparing Equation (9.18) with Equation (9.17), it is seen that *i'* is given by

$$i' = \frac{1+i}{1+f} - 1 = \frac{i-f}{1+f} \tag{9.19}$$

For small values of $f < 0.05$, Equation (9.19) can be approximated by

$$i' \approx (i-f) \tag{9.20}$$

Example 9.19 demonstrates the incorporation of inflation into a calculation.

Example 9.19.

In this example, consider the effect of inflation on the purchasing power of the money set aside for retirement in Example 9.17. Previously, the amount of cash available at the time of retirement in 40 years was calculated to be $774,000. This provided an income of $67,468 for 20 years.

a. Assuming an annual inflation rate of 2%, what is the purchasing power of the cash available at

retirement?

b. What is the purchasing power of the retirement income in the first and twentieth years of retirement?

c. How does Part (a) compare with the total annuity payments of $5000/y for 40 years?

Solution

a. Using Equation (9.16) for $f = 0.02$, $n = 40$, and $F = \$774{,}000$,

$$F' = \$774{,}000/(1 + 0.02)^{40} = \$351{,}000$$

b. At the end of the forty-first year (first year of retirement),

Purchasing Power $= \$67{,}468/(1 + 0.02)^{41} = \$29{,}956/y$

At the end of the sixtieth year (twentieth year of retirement),

Purchasing Power $= \$67{,}468/(1 + 0.02)^{60} = \$20{,}563/y$

c. Amount invested = ($5000/y)(40 y) = $200,000, compared with $351,000

Example 9.19 reveals the consequences of inflation. It showed that the actual income received in retirement of $67,468/y had a purchasing power equivalent to between $29,956 and $20,563 at the time the initial investment was made. This does not come close to the $50,000/y base salary at that time. To increase this value, you would have to increase one or more of the following:

a. The amount invested

b. The interest rate for the investment

c. The time over which the investment was made

The effects of inflation should not be overlooked in any decisions involving investments. Because inflation is influenced by politics, future world events, and so on, it is hard to predict. In this book, inflation will not be considered directly, and cash flows will be considered to be in uninflated dollars.

9.7. Depreciation of Capital Investment

When a company builds and operates a chemical process plant, the physical plant (equipment and buildings) associated with the process has a finite life. The value or worth of this physical plant decreases with time. Some of the equipment wears out and has to be replaced during the life of the plant. Even if the equipment is seldom used and is well maintained, it becomes obsolete and of little value. When the plant is closed, the plant equipment can be salvaged and sold for only a fraction of the original cost.

The cash flows associated with the purchase and installation of equipment are expenses that occur before the plant is operational. This results in a negative cash flow on a discrete CFD. When the plant is closed, equipment is salvaged, and this results in a positive cash flow at that time. The difference between these costs represents capital depreciation.

For tax purposes, the government does not allow companies to charge the full costs of the plant as a one-time expense when the plant is built. Instead, it allows only a fraction of the capital depreciation to be charged as an operating expense each year until the total capital depreciation has been charged.

The amount and rate at which equipment may be depreciated are set by the federal government

(Internal Revenue Service of the U.S. Treasury Department). The regulations that cover the capital depreciation change often. Both the current method of depreciation suggested by the IRS and several of the techniques that have been used in the past to depreciate capital investment are presented. Example 9.20 illustrates the need for depreciation of capital.

Example 9.20.

Consider a person who owns a business with the following annual revenue and expenses:

Revenue from sales	$356,000
Rent	($ 22,000)
Employee salaries	($100,000)
Employee benefits	($ 32,000)
Utilities	($ 7000)
Miscellaneous expenses	($ 5000)
Overhead expenses	($ 40,000)
Before-tax profit	$150,000

The owner of the business decides that, in order to improve the manufacturing operation, she must buy a new packing and labeling machine for $100,000, which has a useful operating life of four years and can be sold for $2000 scrap value at that time. This, she estimates, will increase her sales by 5% per year. The only additional cost is an extra $1000/y in utilities. The new, before-tax profit is estimated to be

Before-Tax Profit = $150,000 + 17,800 – 1000 = $166,800/y, or an increase of $16,800/y

Using a before-tax basis, it can be seen that her $100,000 investment yields $16,800/y. The alternative to buying the new machine is to invest money in a mutual fund that yields 10% per year before tax. At face value, the investment in the new machine looks like a winner. However, take a close look at the cash flows for each case (Table E9.20).

Table E9.20. Cash Flows for Both Investment Opportunities

Year	Cash Flow for Investment in Machine (All $ Figures in 1000)	Cash Flow for Investment in Mutual Fund (All $ Figures in 1000)
0	–100	–100
1	16.8	10
2	16.8	11
3	16.8	12.1
4	16.8 + 2.0	13.31 + 100
Total	**–30.8**	**46.41**

Although the yearly return for buying the machine looks much better than that for the investment in the mutual fund, the big difference is that at the end of the fourth year the owner can recover her initial investment from the mutual fund, but the machine is worth only $2000. From this example, it can be seen that the $100,000 – $2000 = $98,000 investment in the machine is really a long-term expense, and the owner should be able to deduct it as a legitimate operating expense. Depreciation is the method that the government allows for businesses to obtain operating expense credits for capital investments.

9.7.1. Fixed Capital, Working Capital, and Land

When the depreciation of capital investment is discussed, care must be taken to distinguish between what can and cannot be depreciated. In general, the total capital investment in a chemical process is made up of two components:

$$\text{Total Capital Investment} = \text{Fixed Capital} + \text{Working Capital} \qquad (9.21)$$

Fixed capital is all the costs associated with building the plant and was covered in Chapter 7 (either total module cost or grassroots cost). The only part of the fixed capital investment that cannot be depreciated is the **land,** which usually represents only a small fraction of the total.

Working capital is the amount of capital required to start up the plant and finance the first few months of operation before revenues from the process start. Typically, this money is used to cover salaries, raw material inventories, and any contingencies. The working capital will be recovered at the end of the project and represents a float of money to get the project started. This concept is similar to that of paying the first and last month's rent on an apartment. The last month's rent is fully recoverable at the end of the lease but must be paid at the beginning. Because the working capital is fully recoverable, it cannot be depreciated. Typical values for the working capital are between 15% and 20% of the fixed capital investment.

9.7.2. Different Types of Depreciation

First the terms that are used to evaluate depreciation are introduced and defined.

Fixed Capital Investment, FCI_L: This represents the fixed capital investment to build the plant minus the cost of land and represents the depreciable capital investment.

Salvage Value, S: This represents the fixed capital investment of the plant, minus the value of the land, evaluated at the end of the plant life. Usually, the equipment salvage (scrap) value represents a small fraction of the initial fixed capital investment. Often the salvage value of the equipment is assumed to be zero.

Life of the Equipment, n: This is specified by the U.S. Internal Revenue Service (IRS). It does not reflect the actual working life of the equipment but rather the time allowed by the IRS for equipment depreciation. Chemical process equipment currently has a depreciation class life of 9.5 years [1].

Total Capital for Depreciation: The total amount of depreciation allowed is the difference between the fixed capital investment and the salvage value.

$$D = FCI_L - S$$

Yearly Depreciation: The amount of depreciation varies from year to year. The amount allowed in the kth year is denoted d_k.

Book Value: This is the amount of the depreciable capital that has not yet been depreciated.

$$BV_k = FCI_L - \sum_1^k d_j$$

A discussion of three representative depreciation methods that have been widely used to determine the depreciation allowed each year is provided. Currently, only the straight-line and double declining balance methods are approved by the IRS. The sum of the years digits method has been used previously and is included here for completeness.

Straight-Line Depreciation Method, *SL*: An equal amount of depreciation is charged each year over the depreciation period allowed. This is shown as

$$d_k^{SL} = \frac{[FCI_L - S]}{n} \tag{9.22}$$

Sum of the Years Digits Depreciation Method, *SOYD*: The formula for calculating the depreciation allowance is as follows:

$$d_k^{SOYD} = \frac{[n + 1 - k][FCI_L - S]}{\frac{n}{2}[n + 1]} \tag{9.23}$$

The method gets its name from the denominator of Equation (9.23), which is equal to the sum of the number of years over which the depreciation is allowed:

$$1 + 2 + 3 \ldots + n = (n)(n + 1)/2$$

For example, if $n = 7$, then the denominator equals 28.

Double Declining Balance Depreciation Method, *DDB*: The formula for calculating the depreciation allowance is as follows:

$$d_k^{DDB} = \frac{2}{n}\left[FCI_L - \sum_{j=0}^{j=k-1} d_j\right] \tag{9.24}$$

In the declining balance method, the amount of depreciation each year is a constant fraction of the book value, BV_{k-1}. The word *double* in *DDB* refers to the factor 2 in Equation (9.24). Values other than 2 are sometimes used; for example, for the 150% declining balance method, 1.5 is substituted for the 2 in Equation (9.24).

In this method, the salvage value does not enter into the calculations. It is not possible, however, to depreciate more than the value of *D*. To avoid this problem, the final year's depreciation is reduced to obtain this limiting value.

Example 9.21 illustrates the use of each of the above formulas to calculate the yearly depreciation allowances.

Example 9.21.

The fixed capital investment (excluding the cost of land) of a new project is estimated to be \$150.0 million, and the salvage value of the plant is \$10.0 million. Assuming a seven-year equipment life, estimate the yearly depreciation allowances using the following:

a. The straight-line method

b. The sum of the years digits method

c. The double declining balance method

It is given that $FCI_L = \$150 \times 10^6$, $S = \$10.0 \times 10^6$, and $n = 7$ years.

Sample calculations for year 2 give the following:

For straight-line depreciation, using Equation (9.22),

$d_2 = (\$150 \times 10^6 - \$10 \times 10^6)/7 = \$20 \times 10^6$

For SOYD depreciation, using Equation (9.23),

$d_2 = (7 + 1 - 2)\ (\$150 \times 10^6 - \$10 \times 10^6)/28 = \$30 \times 10^6$

For double declining balance depreciation, using Equation (9.24),

$d_2 = (2/7)\ (\$150 \times 10^6 - \$42.86 \times 10^6) = \$30.6 \times 10^6$

A summary of all the calculations is given in Table E9.21 and presented graphically in Figure E9.21.

Table E9.21. Calculations and Results for Example 9.21: The Depreciation of Capital Investment for a New Chemical Plant (All Values in 10^7)

Year (k)	d_k^{SL}	d_k^{SOYD}	d_k^{DDB}	Book Value $FCI_L - Sd_k^{DDB}$
0				$(15 - 0) = 15$
1	$\frac{(15-1)}{7} = 2$	$\frac{(7+1-1)(15-1)}{28^*} = 3.5$	$\frac{(2)(15)}{7} = 4.29$	$(15 - 4.29) = 10.71$
2	$\frac{(15-1)}{7} = 2$	$\frac{(7+1-2)(15-1)}{28^*} = 3.0$	$\frac{(2)(10.71)}{7} = 3.06$	$(10.71 - 3.06) = 7.65$
3	$\frac{(15-1)}{7} = 2$	$\frac{(7+1-3)(15-1)}{28^*} = 2.5$	$\frac{(2)(7.65)}{7} = 2.19$	$(7.65 - 2.19) = 5.46$
4	$\frac{(15-1)}{7} = 2$	$\frac{(7+1-4)(15-1)}{28^*} = 2.0$	$\frac{(2)(5.46)}{7} = 1.56$	$(5.46 - 1.56) = 3.90$
5	$\frac{(15-1)}{7} = 2$	$\frac{(7+1-5)(15-1)}{28^*} = 1.5$	$\frac{(2)(3.90)}{7} = 1.11$	$(3.90 - 1.11) = 2.79$
6	$\frac{(15-1)}{7} = 2$	$\frac{(7+1-6)(15-1)}{28^*} = 1.0$	$\frac{(2)(2.79)}{7} = 0.80$	$(2.79 - 0.80) = 1.99$
7	$\frac{(15-1)}{7} = 2$	$\frac{(7+1-7)(15-1)}{28^*} = 0.5$	$1.99 - 1.0 = 0.99^\dagger$	$(1.99 - 0.99) = 1.00$
Total	14.0	14.0	14.0	$1.0 = \text{Salvage Value}^\dagger$

*Sum of digits: $[n + 1]n/2 = [7 + 1]\ 7/2 = 28$

†The depreciation allowance in the final year of the double declining balance method is adjusted to give a final book value equal to the salvage value.

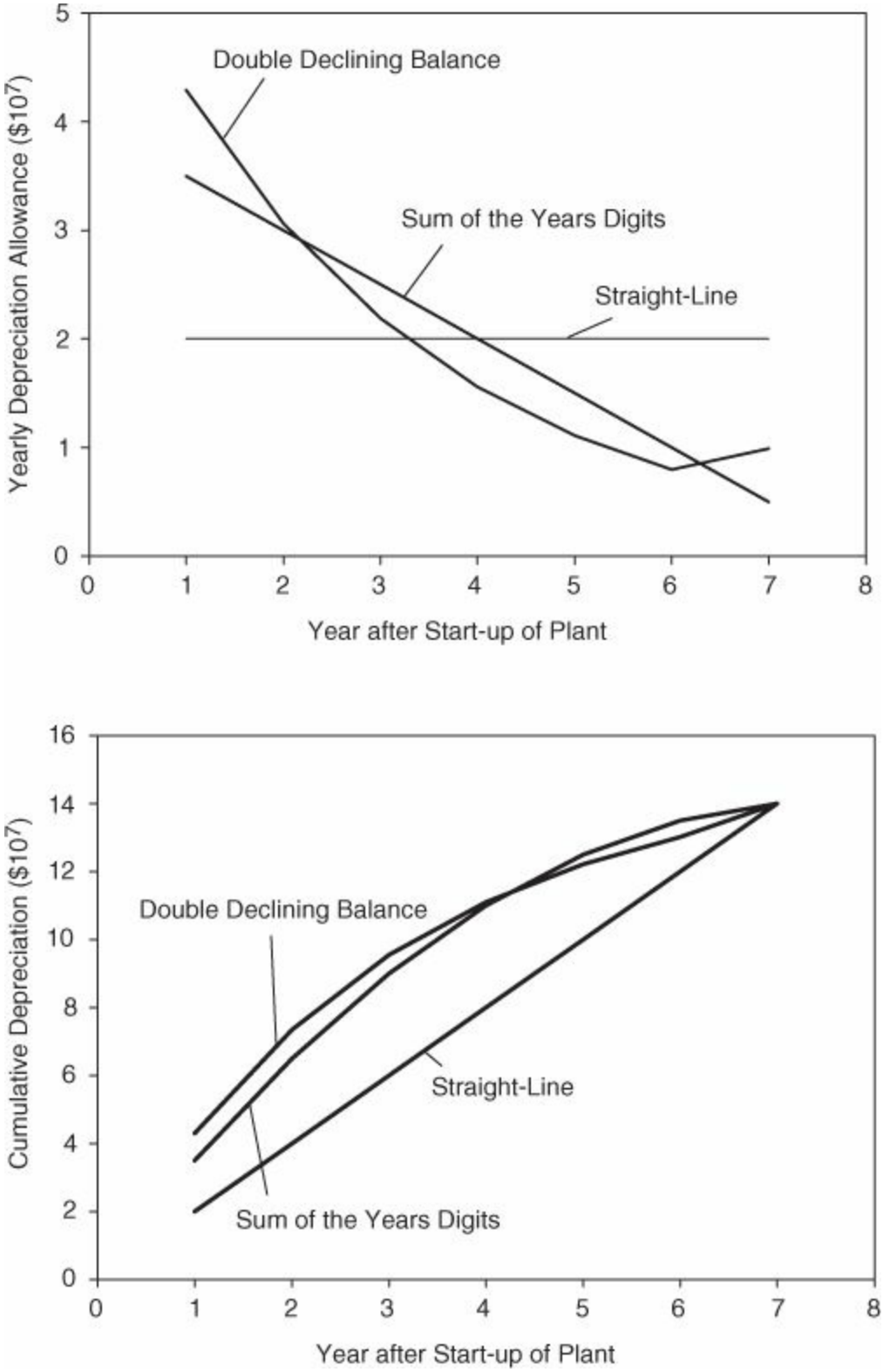


Figure E9.21. Yearly Depreciation Allowances and Cumulative Depreciation Amounts for Example 9.21

From Figure E9.21 it is seen as follows:

1. The depreciation values obtained from the sum of the years digits are similar to those obtained from the double declining balance method.
2. The double declining balance method has the largest depreciation in the early years.
3. The straight-line method represents the slowest depreciation in the early years.

The SOYD and the DDB methods are examples of accelerated depreciation schemes (relative to the straight line). It is shown in Section 9.8 that accelerated depreciation has significant economic

advantages over the straight-line method.

Capital investment can be depreciated only in accordance with current tax regulations.

9.7.3. Current Depreciation Method: Modified Accelerated Cost Recovery System (MACRS)

The current federal tax law is based on MACRS, using a half-year convention. All equipment is assigned a class life, which is the period over which the depreciable portion of the investment may be discounted. Most equipment in a chemical plant has a class life of 9.5 years [1] with no salvage value. This means that the capital investment may be depreciated using a straight-line method over 9.5 years. Alternatively, a MACRS method over a shorter period of time may be used, which is five years for this class life. In general, it is better to depreciate an investment as soon as possible. This is because the more the depreciation is in a given year, the less taxes paid. As shown earlier in this chapter, "money now is worth more than the same amount in the future"; therefore, it is better to pay less in taxes at the beginning of a project than at the end.

The MACRS method uses a double declining balance method and switches to a straight-line method when the straight-line method yields a greater depreciation allowance for that year. The straight-line method is applied to the remaining depreciable capital over the remaining time allowed for depreciation. The half-year convention assumes that the equipment is bought midway through the first year for which depreciation is allowed. In the first year, the depreciation is only half of that for a full year. Likewise in the sixth (and last) year, the depreciation is again for one-half year. The depreciation schedule for equipment with a 9.5-year class life and 5-year recovery period, using the MACRS method, is shown in Table 9.2.

Table 9.2. Depreciation Schedule for MACRS Method for Equipment with a 9.5-Year Class Life and a 5-Year Recovery Period [1]

Year	Depreciation Allowance (% of Capital Investment)
1	20.00
2	32.00
3	19.20
4	11.52
5	11.52
6	5.76

Example 9.22 illustrates the method by which the MACRS depreciation allowances in Table 9.2 are obtained.

Example 9.22.

The basic approach is to use the double declining balance (DDB) method and compare the result with the straight-line (SL) method for the remaining depreciable capital over the remaining period of time. The MACRS method requires depreciation of the total FCI_L, without regard for the salvage value. Calculations are given below, using a basis of $100:

$$\text{For DDB, } d_k^{DDB} = \frac{2}{5}\left[100 - \sum_{j=0}^{k-1} d_j^{DDB}\right]$$

$$\text{For SL, } d_k^{SL} = \frac{\text{undepreciated capital}}{\text{remaining time for depreciation}}$$

k	d_k^{DDB} ← ½ year convention		d_k^{SL} time remaining
1	0.4(100)(0.5) = **20**		
2	0.4(100 – 20) = **32**		(100 – 20)/4.5 = 17.78
3	0.4(100 – 52) = **19.2**	switch to SL	(100 – 52)/3.5 = 13.71
4	0.4(100 – 71.2) = **11.52**	→	(100 – 71.2)/2.5 = **11.52**
5	0.4(100 – 82.72) = 6.91		(100 – 82.72)/1.5 = **11.52**
6		½ year convention →	(0.5)(100 – 94.24)/0.5 = **5.76**

9.8. Taxation, Cash Flow, and Profit

Taxation has a direct impact on the profits realized from building and operating a plant. Tax regulations are complex, and companies have tax accountants and attorneys to ensure compliance and to maximize the benefit from these laws. When individual projects are considered or similar projects are compared, accounting for the effect of taxes is required. Taxation rates for companies and the laws governing taxation change frequently. The current tax rate schedule (as of 2001) is given in Table 9.3.

Table 9.3. Federal Tax Rate Schedule for Corporations [2]

Range of Net Taxable Income	Taxation Rate
> $0 and ≤ $50,000	15%
> $50,000 and ≤ $75,000	$7500 + 25% of amount over $50,000
> $75,000 and ≤ $100,000	$13,750 + 34% of amount over $75,000
> $100,000 and ≤ $335,000	$22,250 + 39% of amount over $100,000
> $335,000 and ≤ $10 million	$113,900 + 34% of amount over $335,000
> $10 million and ≤ $15 million	$3,4000,000 + 35% of amount over $10 million
> $15 million and ≤ $18.333 million	$5,150,000 + 38% of amount over $15 million
> $18.333 million	35%

For most large corporations, the basic federal taxation rate is 35%. In addition, corporations must also pay state, city, and other local taxes. The overall taxation rate is often in the range of 40% to 50%. The taxation rate used in the problems at the back of this chapter will vary and may be as low as 30%. For the economic analysis of a proposed (current) process, clearly it is important to use the correct taxation rate, which will, in turn, depend on the location of the proposed process.

Table 9.4 provides the definition of important terms and equations used to evaluate the cash flow and the profits produced from a project.

Table 9.4. Evaluation of Cash Flows* and Profits* in Terms of Revenue (*R*), Cost of Manufacturing (*COM*), Depreciation (*d*), and Tax Rate (*t*)

	Description	Formula	Equation
Expenses	= Manufacturing Costs + Depreciation	$= COM_d + d$	(9.25)
Income Tax	= (Revenue − Expenses)(Tax Rate)	$= (R - COM_d - d)(t)$	(9.26)
After-Tax (Net) Profit	= Revenue − Expenses − Income Tax	$= (R - COM_d - d)(1 - t)$	(9.27)
After-Tax Cash Flow	= Net Profit + Depreciation	$= (R - COM_d - d)(1 - t) + d$	(9.28)
Variables:			
t	Tax Rate		Constant
COM_d	Cost of Manufacture Excluding Depreciation		(8.2)
d	Depreciation: Depends upon Method Used		(9.22) (9.23)
R	Revenue from Sales		(9.24)

*To obtain before-tax values, set the tax rate (t) to zero.

The equations from Table 9.4 are used in Example 9.23.

Example 9.23.

For the project given in Example 9.21, the manufacturing costs, excluding depreciation, are \$30 million per year, and the revenues from sales are \$75 million per year. Given the depreciation values calculated in Example 9.21, calculate the following for a 10-year period after start-up of the plant:

a. The after-tax profit (net profit)

b. The after-tax cash flow, assuming a taxation rate of 30%

From Equations (9.27) and (9.28) (all numbers are in $\$10^6$),

After-tax profit = $(75 - 30 - d_k)(1 - 0.3) = 31.5 - (0.7)(d_k)$

After-tax cash flow = $(75 - 30 - d_k)(1 - 0.3) + d_k = 31.5 + (0.3)(d_k)$

A sample calculation for year 1 ($k = 1$) is provided:

From Example 9.21, $d_1^{SL} = 20$, $d_1^{SOYD} = 35$, and $d_1^{DDB} = 42.9$

	SL	SOYD	DDB
Profit after Tax	17.5	7.0	1.47
Cash Flow after Tax	37.5	42.0	44.37

The calculations for years 1 through 10 are plotted in Figure E9.23. From this plot, it can be seen that the cash flow at the start of the project is greatest for the DDB method and lowest for the SL method.

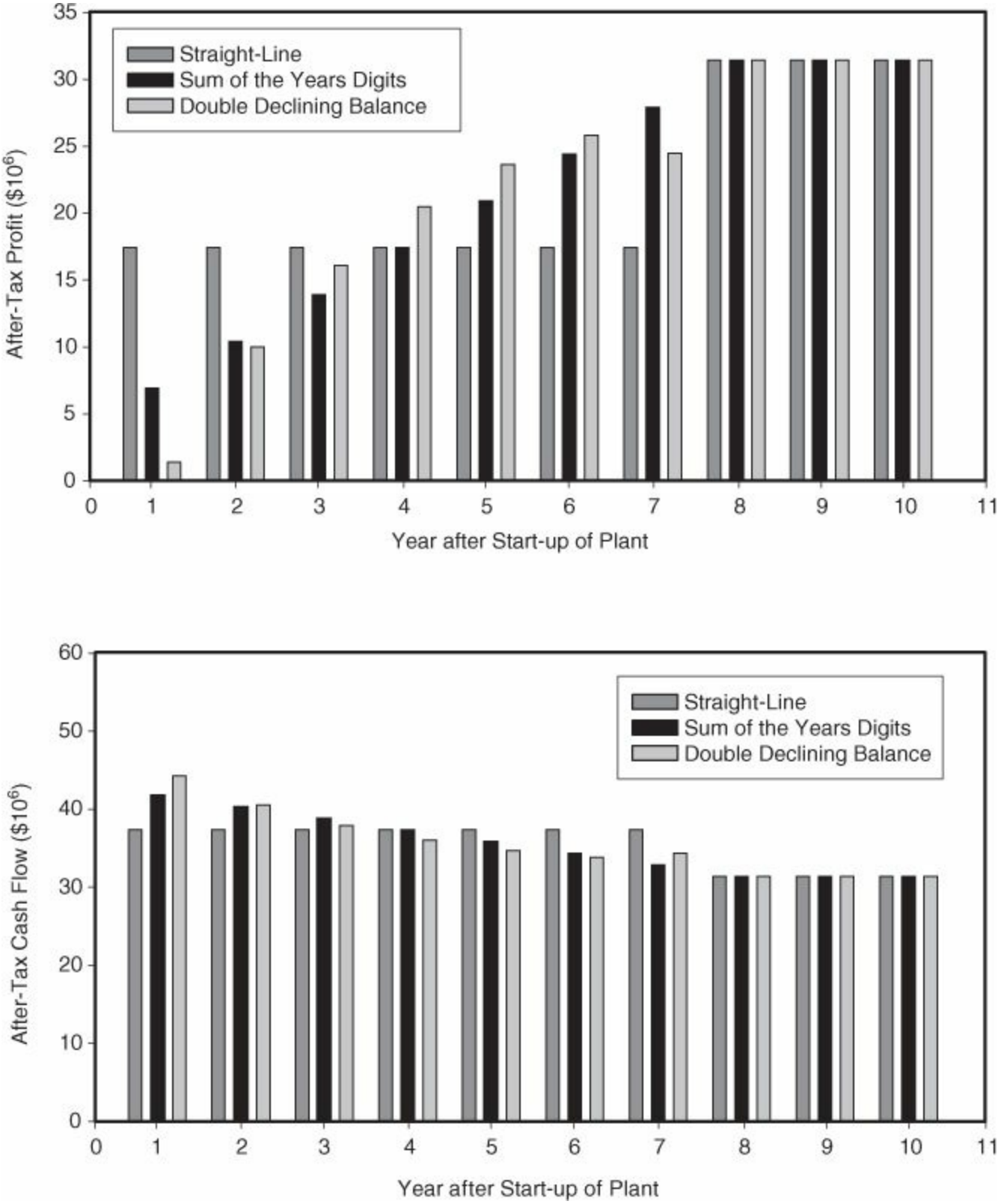


Figure E9.23. Comparison of the After-Tax Profit and Cash Flow Using Different Depreciation Schedules from Example 9.23

The sum of the profits and cash flows over the 10-year period are $217 million and $357 million, respectively. These totals are the same for each of the depreciation schedules used. The difference between the cash flows and the profits is seen to be the depreciation ($357 – 217 = $140 million).

Example 9.23 demonstrated how different depreciation schedules affect the after-tax cash flow. The accelerated schedules for depreciation provided the greatest cash flows in the early years. Because money earned in early years has a greater value than money earned in later years, the accelerated schedule of depreciation is the most desirable alternative.

9.9. Summary

In this chapter, the basics of economic analysis required to evaluate project profitability were covered. The material presented in this chapter is founded on the principle that

Money + Time = More Money

To benefit from this principle, it is necessary to have resources to make an investment and the time to allow the investment to grow. When this principle is applied to chemical processes, the revenue or additional money is generated when low-value materials and services are converted into high-value materials and services.

A central concept identified as the time value of money grows out of this principle. This principle is applied to a wide range of applications, from personal financial management to the analysis of new chemical plants.

The use of cash flow diagrams to visualize the timing of cash flows and to manage cash flows during a project was illustrated. A shorthand notation for the many discount factors involved in economic calculations (factors that account for the time value of money) were introduced to simplify cash flow calculations. Other items necessary for a comprehensive economic evaluation of a chemical plant were covered and included depreciation, taxation, and the evaluation of profit and cash flow.

Applications involving these principles and concepts directly relating to chemical plants will be pursued in Chapter 10.

What You Should Have Learned

- That money today is worth more than money tomorrow
- Simple versus compound interest
- How to calculate the time value of money involving present value, future value, and annuity
- How to represent calculations of the time value of money on a cash flow diagram
- How to include taxation and depreciation
- The significance and impact of inflation

References

1. *How to Depreciate Property*, Publication 946, Department of the Treasury, Internal Revenue Service, December 2000.
2. *Corporations, Property*, Publication 542, Department of the Treasury, Internal Revenue Service, December 2000.

Short Answer Questions

1. What is the difference between simple and compound interest? Provide an example.
2. What is the difference between the nominal annual interest rate and the effective annual interest rate? When are these two rates equal?
3. You work in the summer and receive three large, equal monthly paychecks in June, July, and August. You are living at home, so there are no living expenses. You use this money to pay your

tuition for the next academic year in September and in January. You also use this money to pay monthly living expenses during the academic year, which are assumed to be cash flows once per month from September through May. Illustrate these cash flows on a cash flow diagram.

4. Define the term *annuity*.
5. The current value of the Chemical Engineering Plant Cost Index (*CEPCI*) is 485. If at the same time next year the value has risen to 525, what will be the average inflation rate for the year?
6. Discuss the differences and similarities between interest, inflation, and the time value of money.
7. What term describes the method by which a fixed capital investment can be used to reduce the tax that a company pays?
8. What is depreciation? Explain how it affects the economic analysis of a new chemical process.
9. Why is it advantageous to use an accelerated depreciation schedule?
10. "In general, it is better to depreciate the fixed capital investment as soon as allowable." Give one example of when this statement would not be true.
11. What is the difference between after-tax profit and after-tax cash flow? When are these two quantities the same?

Problems

12. You need to borrow $1000 for an emergency. You have two alternatives. One is to borrow from a bank. The other is to borrow from your childhood friend Greta Ganav, who is in the "private" financing business. Because you and Greta go way back, she will give you her preferred rate, which is $5/week until you pay back the entire loan.
    a. What is Greta's effective annual interest rate?
    b. Your alternative is to borrow from a bank, where the interest is compounded monthly. What nominal interest rate would make you choose the bank over Greta?
    c. If the bank's interest rate is 7% p.a., compounded monthly, how many months would it be until the interest paid to Greta equaled the interest paid to the bank?
13. Consider the following three investment schemes:
    9.5% p.a. (nominal rate) compounded daily
    10.0% p.a. (nominal rate) compounded monthly
    10.5% p.a. (nominal rate) compounded quarterly
    a. Which investment scheme is the most profitable, assuming that the initial investment is the same for each case?
    b. What is the effective annual interest rate of the best scheme?
    c. What is the nominal interest rate of the best scheme when compounded continuously?
14. At an investment seminar that I recently attended, I learned about something called "the Rule of 72." According to the person in charge of the seminar, a good estimate for finding how long it takes for an investment to double is given by the following equation:

$$\text{Number of years to double investment} = \frac{72}{\text{effective annual interest rate (in \%)}}$$

Using what you know about the time value of money, calculate the error in using the above

equation to estimate how long it takes to double an investment made at the following effective annual interest rates: 5%, 7.5%, and 10%.

Express your answers as % error to two significant figures.

Comment on the Rule of 72 and its accuracy for typical financial calculations today.

15. You invested $5000 eight years ago, and you want to determine the value of the investment now, at the end of year 8. During the past eight years, the nominal interest rate has fluctuated as follows:

Year	Nominal Interest Rate (% p.a.)
1	4
2	5
3	7
4	8
5	6
6	4
7	5
8	4

If your investment is compounded daily, how much is it worth today? (Ignore the effect of leap years.)

16. What are the differences between investing $15,000 at 9% p.a. for 15 years when compounded yearly, quarterly, monthly, daily, and continuously? Ignore the effect of leap years.

17. One bank advertises an interest rate on a certificate of deposit (CD) to be 4% compounded daily. Another bank advertises a CD with a 4.1% effective annual rate. In which CD would you invest?

18. You want to begin an investment plan to save for your daughter's college education. Because you believe that your newly born daughter will be a genius (just like you!), you are assuming the cost of an Ivy League education. You plan to put money into an investment account, at the end of each year, for the next 18 years. You believe that you will need about $75,000 per year, each year, 19 through 22 years from now.

a. Draw a discrete cash flow diagram for this situation.

b. How much would you have to invest each year to pay for college and have a zero balance at the end of year 22? The effective annual interest rate of your investment is 8%.

c. What interest rate would be needed if you could invest only $5000/y?

19. You begin an investment plan by putting $10,000 in an account that you assume will earn 8% annually. For the next 25 years, you add $5000 per year. In anticipation of buying a house with a 15-year mortgage, you expect to need a one-time down payment of $55,000 at the end of year 8. You anticipate being able to make the monthly mortgage payment without affecting the yearly contribution to the savings plan.

a. Draw a discrete, nondiscounted cash flow diagram for this situation.

b. Will you have the down payment at the end of year 8?

c. What will be the value of your savings account at the end of year 25?

20. You begin work on June 1 and work until August 31, and receive pay on the last day of the month. Your expenses for these three months are $1500/mo. At the end of September, you make a $7000 payment, and you make an identical payment at the end of January. Your expenses from September 1 through May 31 are $1000/mo.

a. Draw a discrete, nondiscounted cash flow diagram for this situation.

b. If you earn 4% interest, compounded monthly, on the money until it is spent, what monthly salary is required from June 1 through August 31 to break even on May 31?

c. If you earn 4% interest, compounded monthly, on the money until it is spent and the salary is $4000/mo, how much would you have to earn each month from a different job from September through May to break even on May 31?

d. What situation is depicted in this problem?

21. The cash flows for a bank account are described by the discrete CFD in Figure P9.21. The bank account has an effective annual interest rate of 4.5%.

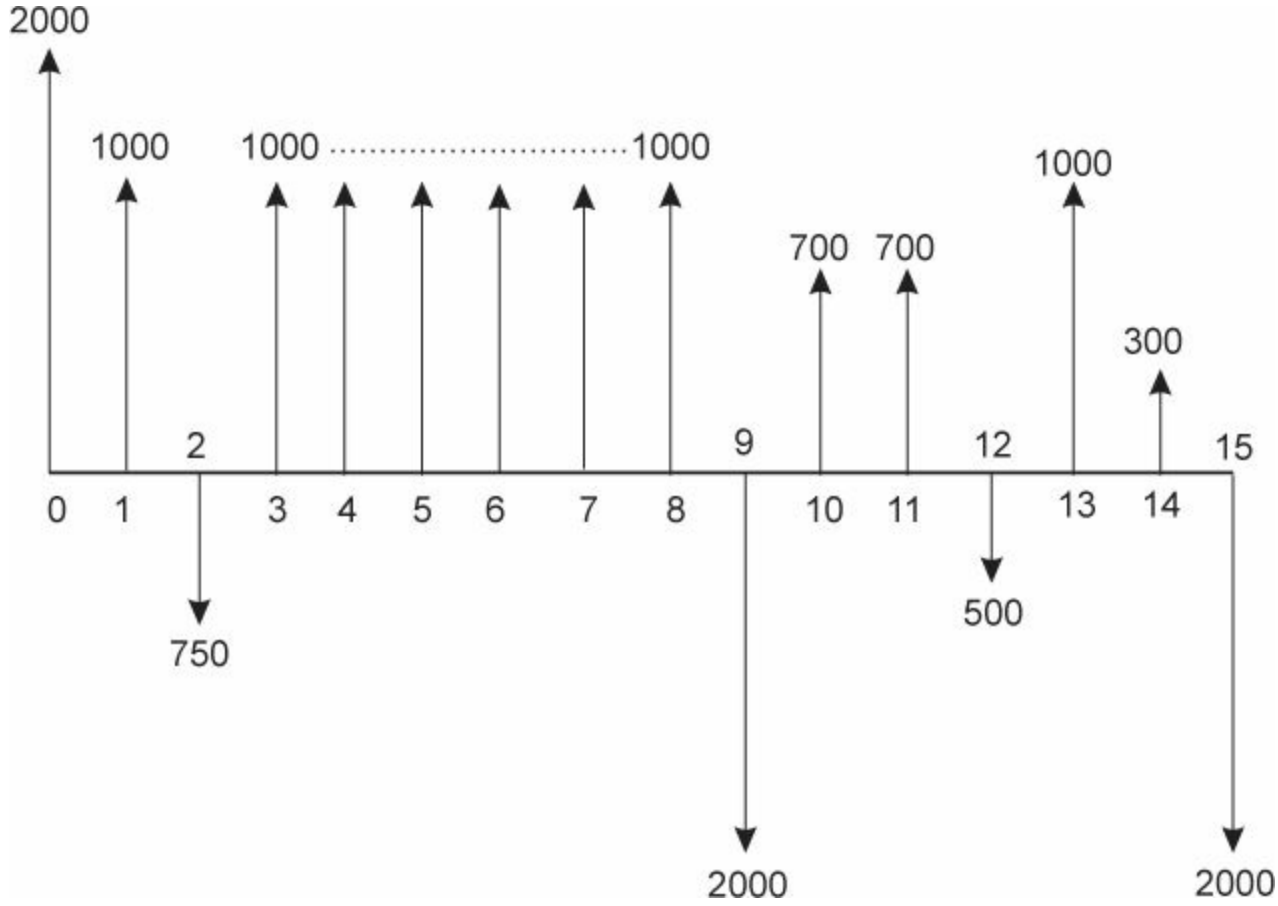


Figure P9.21. Cash Flow Diagram for Problem 9.21.

a. Calculate the future value of all cash flows after 15 years.

b. Calculate the future value of all cash flows after 25 years assuming that there are no more transactions after year 15.

22. You begin to contribute to an investment plan with your company immediately after graduation, when you are 23 years old. Your contribution plus your company's contribution totals $6000/y. Assume that you work for the same company for 40 years.

a. What effective annual interest rate is required for you to have $1 million in 40 years?

b. Repeat Part (a) for $2 million.

c. What is the future value of this investment after 40 years if the effective annual interest rate is 7% p.a.?

23. An IRA is an investment vehicle available to most individuals to save for retirement. The benefit is that the interest is not taxed until you withdraw money, and most retirees are in a lower tax bracket than when they worked. Under current laws, the maximum annual contribution is $5000 until age 50 and $6000 thereafter, including the year one turns 50. Suppose that you make the maximum contribution every year for 40 years, beginning at age 25 until age 65.
    a. What is the future value of this retirement fund after 40 years, assuming an effective annual interest rate of 9%?
    b. What effective annual interest rate is required for the future value of this investment to be $2 million after 40 years?
24. You plan to finance a new car by borrowing $25,000. The interest rate is 7% p.a., compounded monthly. What is your monthly payment for a three-year loan, a four-year loan, and a five-year loan?
25. You have just purchased a new car by borrowing $20,000 for four years. Your monthly payment is $500. What is your nominal interest rate if compounded monthly?
26. You plan to borrow $200,000 to purchase a new house. The nominal interest rate is fixed at 6.5% p.a., compounded monthly.
    a. What is the monthly payment on a 30-year mortgage?
    b. What is the monthly payment on a 15-year mortgage?
    c. What is the difference in the amount of interest paid over the lifetime of each loan?
27. You just borrowed $225,000 to purchase a new house. The monthly payment (before taxes and insurance) is $1791 for the 25-year loan. What is the effective annual interest rate?
28. You just borrowed $250,000 to purchase a new house. The nominal interest rate is 6% p.a., compounded monthly, and the monthly payment is $1612 for the loan. What is the duration of the loan?
29. A home-equity loan involves borrowing against the equity in a house. For example, if your house is valued at $250,000 and you have been paying the mortgage for a sufficient amount of time, you may owe only $150,000 on the mortgage. Therefore, your **equity** in the home is $100,000. You can use the home as collateral for a loan, possibly up to $100,000, depending on the bank's policy. Home-equity loans often have shorter durations than regular mortgages. Suppose that you take a home-equity loan of $50,000 for the down payment on a new house in a new location because you have a new job. When you complete the sale of your old house, the home-equity loan will be paid off at the closing. The home-equity loan terms are a 10-year term at 7% p.a., compounded monthly, but you must also pay 0.05% of the original high-equity loan principal each month. What is the monthly payment?
30. Your company is trying to determine whether to spend $500,000 in process improvements. The projected cash flow increases based on the process improvements are as follows:

Year	Annual Increased Cash Flow ($thousands)
1	25
2	75
3	100
4	125
5	250

The alternative is to do nothing and leave the $500,000 in the investment portfolio earning interest. What interest rate is required in the investment portfolio for the better choice to be to do nothing?

31. It is necessary to evaluate the profitability of proposed improvements to a process prior to obtaining approval to implement changes. For one such process, the capital investment (end of year 0) for the project is $250,000. There is no salvage value. In years 1 and 2, you expect to generate an after-tax revenue from the project of $60,000/y. In years 3–8, you expect to generate an after-tax revenue of $50,000/y. Assume that the investments and cash flows are single transactions occurring at the end of the year. Assume an effective annual interest rate of 9%.
    a. Draw a discrete cash flow diagram for this project.
    b. Draw a cumulative, discounted (to year 0) cash flow diagram for this project.
    c. What is the future value of this project at the end of year 8?
    d. Instead of investing in this project, the $250,000 could remain in the company's portfolio. What rate of return on the portfolio is needed to equal the future value of this project at the end of year 8? Would you invest in the project, or leave the money in the portfolio?
32. In Problem 9.31, the net revenue figures were generated using a taxation rate of 45% and a straight-line depreciation over the eight-year project. Calculate the yearly net revenues if the five-year MACRS depreciation schedule were used.
33. You are evaluating the profitability potential of a process and have the following information. The criterion for profitability is a 15% rate of return over ten operating years. The equipment has zero salvage value at the end of the project.

    Fixed capital investment (including land) in four installments (all values are in millions of dollars as one transaction at the end of the year):

Year 0 land	$10
Year 1 FCI installment 1	$20
Year 2 FCI installment 2	$30
Year 3 FCI installment 3	$20
Start-up capital at end of year 3	$10
Positive cash flow years 4–13	$25

    a. Draw a discrete, discounted cash flow diagram for this process.
    b. Draw a cumulative, discounted cash flow diagram for this process.
    c. What is the present value (at end of year 0) for this process?

d. What is the future value at the end of year 13?

e. What would the effective annual interest rate have to be so that the present value (end of year 0) of this investment is zero? (This interest rate is known as the DCFROR, and it will be discussed in the next chapter.)

f. What is your recommendation regarding this process? Explain.

34. What are the MACRS depreciation allowances for recovery periods of four, six, and nine years?

35. For a new process, the land was purchased for $10 million. The fixed capital investment, paid at the end of year 0, is $165 million. The working capital is $15 million, and the salvage value is $15 million. The estimated revenue from years 1 through 10 is $70 million/y, and the estimated cost of manufacture over the same time period is $25 million/y. The internal hurdle rate (interest rate) is 14% p.a., before taxes, and the taxation rate is 40%.

a. Draw a discrete, nondiscounted cash flow diagram for this process.

b. Determine the yearly depreciation schedule using the five-year MACRS method.

c. Determine the after-tax profit for each year.

d. Determine the after-tax cash flow for each year.

e. Draw a discrete, discounted (to year 0) cash flow diagram for this process.

f. Draw a cumulative, discounted (to year 0) cash flow diagram for this process.

g. What is the present value (year 0) of this process?

Chapter 10. Profitability Analysis

What You Will Learn

- There are different methods for estimating the profitability of a proposed chemical process.
- These methods do not always give the same result.
- Certain methods are more appropriate for specific situations.
- The impact of uncertainty can be included in these profitability estimates using a Monte-Carlo analysis.

This chapter will explain how to apply the techniques of economic analysis developed in Chapter 9. These techniques will be used to assess the profitability of projects involving both capital expenditures and yearly operating costs. A variety of projects will be examined, ranging from large multimillion-dollar ventures to much smaller process improvement projects. Several criteria for profitability will be discussed and applied to the evaluation of process and equipment alternatives. The first concept is the profitability criteria for new large projects.

10.1. A Typical Cash Flow Diagram for a New Project

A typical cumulative, after-tax cash-flow diagram (CFD) for a new project is illustrated in Figure 10.1. It is convenient to relate profitability criteria to the cumulative CFD rather than the discrete CFD. The timing of the different cash flows is explained below.

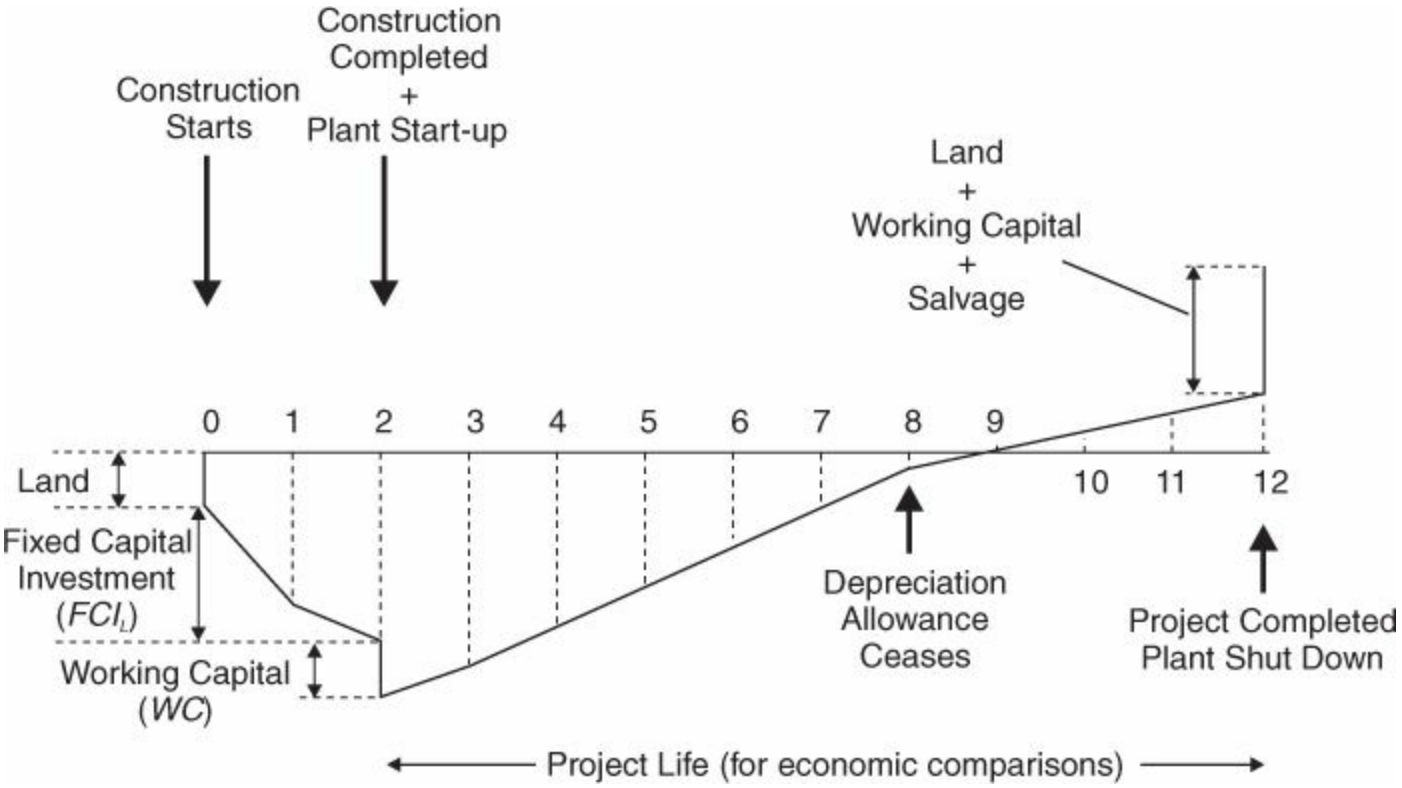


Figure 10.1. A Typical Cumulative Cash Flow Diagram for the Evaluation of a New Project

In the economic analysis of the project, it is assumed that any new land purchases required are done at the start of the project, that is, at time zero. After the decision has been made to build a new chemical plant or expand an existing facility, the construction phase of the project starts. Depending

on the size and scope of the project, this construction may take anywhere from six months to three years to complete. In the example shown in Figure 10.1, a typical value of two years for the time from project initiation to the start-up of the plant has been assumed. Over the two-year construction phase, there is a major capital outlay. This represents the fixed capital expenditures for purchasing and installing the equipment and auxiliary facilities required to run the plant (see Chapter 7). The distribution of this fixed capital investment is usually slightly larger toward the beginning of construction, and this is reflected in Figure 10.1. At the end of the second year, construction is finished and the plant is started. At this point, the additional expenditure for working capital required to float the first few months of operations is shown. This is a one-time expense at the start-up of the plant and will be recovered at the end of the project.

After start-up, the process begins to generate finished products for sale, and the yearly cash flows become positive. This is reflected in the positive slope of the cumulative CFD in Figure 10.1. Usually the revenue for the first year after start-up is less than in subsequent years due to "teething" problems in the plant; this is also reflected in Figure 10.1. The cash flows for the early years of operation are larger than those for later years due to the effect of the depreciation allowance discussed in Chapter 9. The time used for depreciation in Figure 10.1 is six years. The time over which the depreciation is allowed depends on the IRS regulations and the method of depreciation used.

In order to evaluate the profitability of a project, a life for the process must be assumed. This is not usually the working life of the equipment, nor is it the time over which depreciation is allowed. It is a specific length of time over which the profitability of different projects is to be compared. Lives of 10, 12, and 15 years are commonly used for this purpose. It is necessary to standardize the project life when comparing different projects. This is because profitability is directly related to project life, and comparing projects using different lives biases the results.

Usually, chemical processes have anticipated operating lives much greater than ten years. If much of the equipment in a specific process is not expected to last for a ten-year period, then the operating costs for that project should be adjusted. These operating costs should reflect a much higher maintenance cost to include the periodic replacement of equipment necessary for the process to operate the full ten years. A project life of ten years will be used for the examples in the next section.

From Figure 10.1, a steadily rising cumulative cash flow is observed over the ten operating years of the process, that is, years 2 through 12. At the end of the ten years of operation, that is, at the end of year 12, it is assumed that the plant is closed down and that all the equipment is sold for its salvage or scrap value, that the land is also sold, and that the working capital is recovered. This additional cash flow, received on closing down the plant, is shown by the upward-pointing vertical line in year 12. Remember that in reality, the plant will most likely *not* be closed down; it is only assumed that it will be in order to perform the economic analysis.

The question that must now be addressed is how to evaluate the profitability of a new project. Looking at Figure 10.1, it can be seen that at the end of the project the cumulative CFD is positive. Does this mean that the project will be profitable? The answer to this question depends on whether the value of the income earned during the time the plant operated was smaller or greater than the investment made at the beginning of the project. Therefore, the time value of money must be considered when evaluating profitability. The following sections will look at different ways to evaluate project profitability.

10.2. Profitability Criteria for Project Evaluation

There are three bases used for the evaluation of profitability:

1. Time
2. Cash
3. Interest rate

For each of these bases, discounted or nondiscounted techniques may be considered. The nondiscounted techniques do not take into account the time value of money and are *not* recommended for evaluating new, large projects. Traditionally, however, such methods have been and are still used to evaluate smaller projects, such as process improvement schemes. Examples of both types of methods are presented for all the three bases.

10.2.1. Nondiscounted Profitability Criteria

Four nondiscounted profitability criteria are illustrated in Figure 10.2. The graphical interpretation of these profitability criteria is shown in the figure. Each of the four criteria is explained below.

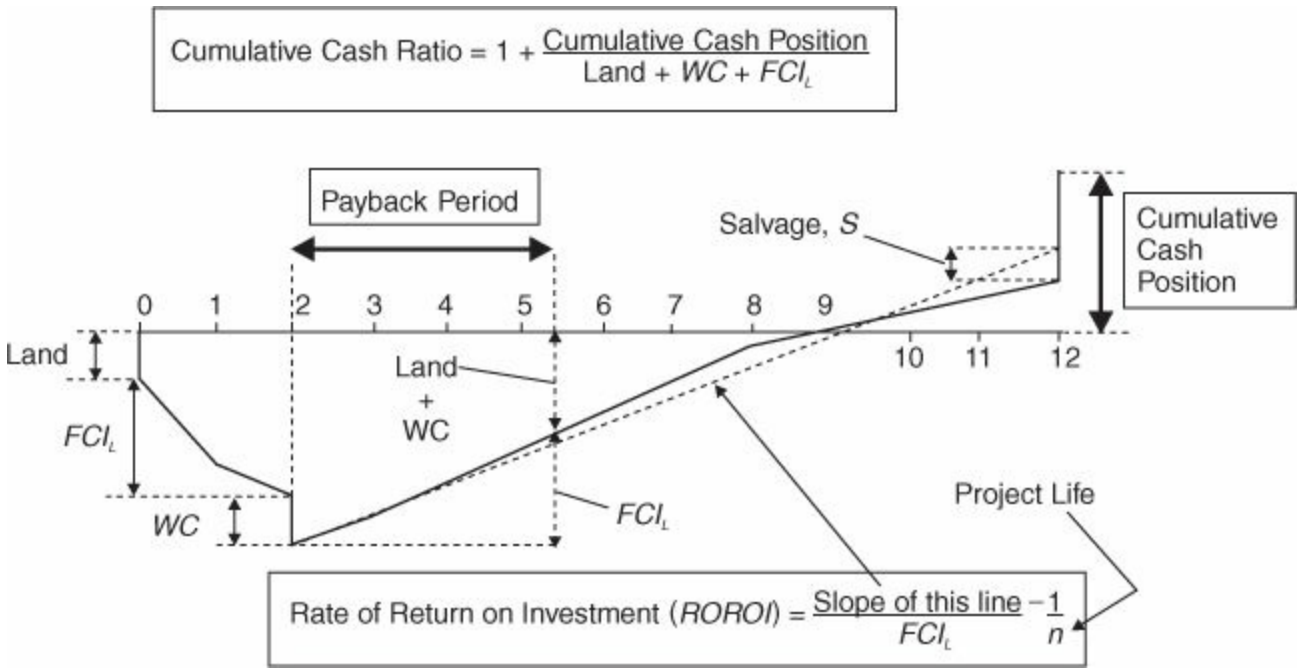


Figure 10.2. Illustration of Nondiscounted Profitability Criteria

Time Criterion. The term used for this criterion is the **payback period (PBP),** also known by a variety of other names, such as payout period, payoff period, and cash recovery period. The payback period is defined as follows:

PBP = Time required, after start-up, to recover the fixed capital investment, FCI_L, for the project

The payback period is shown as a length of time on Figure 10.2. Clearly, the shorter the payback period, the more profitable the project.

Cash Criterion. The criterion used here is the **cumulative cash position (CCP),** which is simply the worth of the project at the end of its life. For criteria using cash or monetary value, it is difficult to compare projects with dissimilar fixed capital investments, and sometimes it is more useful to use the **cumulative cash ratio (CCR),** which is defined as

$$CCR = \frac{\text{Sum of All Positive Cash Flows}}{\text{Sum of All Negative Cash Flows}}$$

The definition effectively gives the cumulative cash position normalized by the initial investment. Projects with cumulative cash ratios greater than one are potentially profitable, whereas those with ratios less than unity cannot be profitable.

Interest Rate Criterion. The criterion used here is called the **rate of return on investment (ROROI)** and represents the nondiscounted rate at which money is made from a fixed capital investment. The definition is given as

$$ROROI = \frac{\text{Average Annual Net Profit}}{\text{Fixed Capital Investment } (FCI_L)}$$

The annual net profit in this definition is an average over the life of the plant after start-up.

The use of fixed capital investment, FCI_L, in the calculations for payback period and rate of return on investment given above seems reasonable, because this is the capital that must be recovered by project revenue. Many alternative definitions for these terms can be found, and sometimes the total capital investment ($FCI_L + WC +$ Land) is used instead of fixed capital investment. When the plant has a salvage value (S), the fixed capital investment minus the salvage value ($FCI_L - S$) could be used instead of FCI_L. However, because the salvage value is usually very small, it is preferable to use FCI_L alone. Example 10.1 is a comprehensive profitability analysis calculation using nondiscounted criteria.

Example 10.1.

A new chemical plant is going to be built and will require the following capital investments (all figures are in $million):

Cost of land, L= $10.0

Total fixed capital investment, FCI_L = $150.0

Fixed capital investment during year 1 = $90.0

Fixed capital investment during year 2 = $60.0

Plant start-up at end of year 2

Working capital = $30.0 at end of year 2

The sales revenues and costs of manufacturing are given below:

Yearly sales revenue (after start-up), R = $75.0 per year

Cost of manufacturing excluding depreciation allowance (after start-up), COM_d = $30.0 per year

Taxation rate, t = 45%

Salvage value of plant, S = $10.0

Depreciation: Use 5-year MACRS.

Assume a project life of 10 years.

Calculate each nondiscounted profitability criterion given in this section for this plant.

The discrete and cumulative nondiscounted cash flows for each year are given in Table E10.1. Using this data, the cumulative cash flow diagram is drawn, as shown in Figure E10.1.

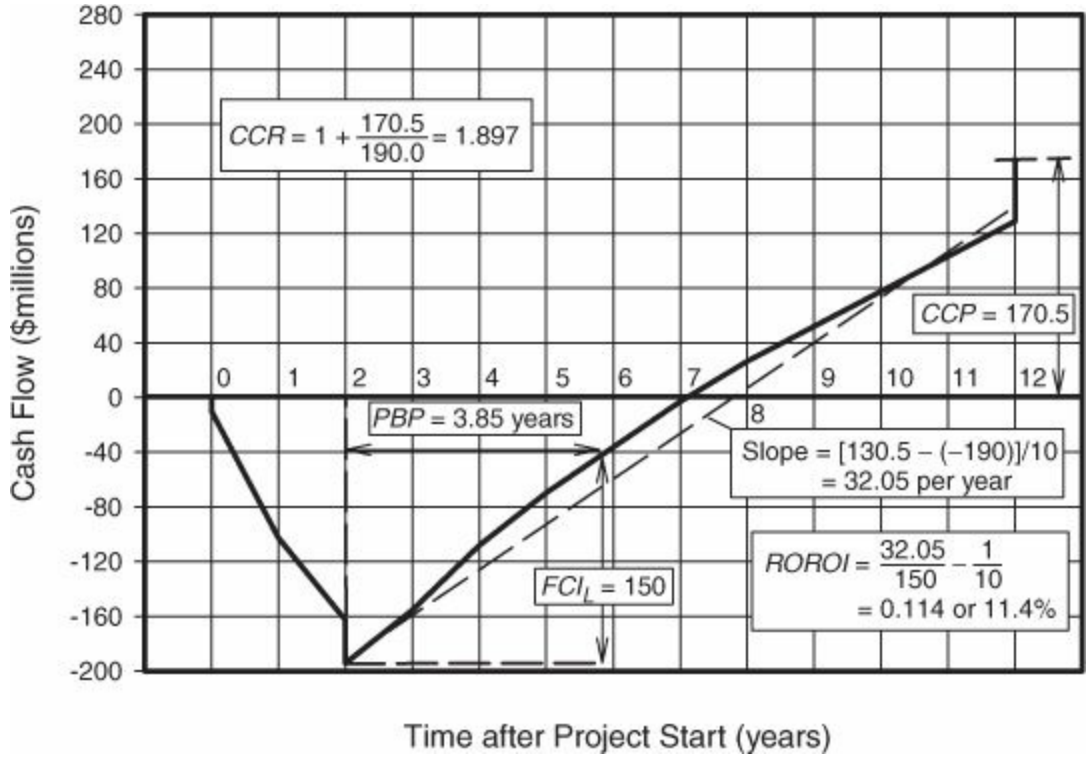


Figure E10.1. Cumulative Cash Flow Diagram for Nondiscounted After-Tax Cash Flows for Example 10.1

The method of evaluation for each of the criteria is given on Figure E10.1 and in Table E10.1.

Table E10.1. Nondiscounted After-Tax Cash Flows for Example 10.1 (All Numbers in 10^6)

End of Year (k)	Investment	d_k	$FCI_L - \Sigma d_k$	R	COM_d	$(R\text{-}COM\text{-}d_k) \times (1\text{-}t) + d_k$	Cash Flow	Cumulative Cash Flow
0	(10)*	—	150.00	—	—	—	(10.00)	(10.00)
1	(90)	—	150.00	—	—	—	(90.00)	(100.00)
2	(60 + 30) = (90)	—	150.00	—	—	—	(90.00)	(190.00)
3	—	30.00	120.00	75	30	38.25	38.25	(151.75)
4	—	48.00	72.00	75	30	46.35	46.35	(105.40)
5	—	28.80	43.20	75	30	37.71	37.71	(67.69)
6	—	17.28	25.92	75	30	32.53	32.53	(35.16)
7	—	17.28	8.64	75	30	32.53	32.53	(2.64)
8	—	8.64	0.00	75	30	28.64	28.64	26.00
9	—	—	0.00	75	30	24.75	24.75	50.75
10	—	—	0.00	75	30	24.75	24.75	75.50
11	—	—	0.00	75	30	24.75	24.75	100.25
12	10 + 30 = 40	—	0.00	85	30	30.25	70.25	170.50

*Numbers in () are negative cash flows.

Nondiscounted Profitability Criteria

Payback Period (PBP)

Land + Working Capital = 10 + 30 = $\$40 \times 10^6$—find time after start-up for which cumulative cash flow = $-\$40 \times 10^6$

PBP = 3 + (−67.69 + 40)/(−67.69 + 35.16) = **3.85 years**

Cumulative Cash Position (CCP) and Cumulative Cash Ratio (CCR)

***CCP* = 170.50×106** and **CCR** = Σ positive cash flows/Σ negative cash flows = (38.25 + 46.35 + 37.71 + ... + 24.75 + 70.25) / (10 + 90 + 90) = **1.897**

Rate of Return on Investment (ROROI)

ROROI = (38.25 + 46.35 + 37.71 + ... + 24.75 + 30.25)/10/150 − 1/10 = **0.114 or 11.4% p.a.**

Payback Period (*PBP*) = 3.85 years

Cumulative Cash Position (CCP) = $\$170.5 \times 10^6$

Cumulative Cash Ratio (CCR) = 1.897

Rate of Return on Investment ($ROROI$) = 11.4%

All these criteria indicate that the project cannot be eliminated as unprofitable. They all fail to take into account the time value of money that is necessary for a thorough measure of profitability. The effects of the time value of money on profitability are considered in the next section.

10.2.2. Discounted Profitability Criteria

The main difference between the nondiscounted and discounted criteria is that for the latter each of the yearly cash flows is discounted back to time zero. The resulting discounted cumulative cash flow diagram is then used to evaluate profitability. The three different types of criteria are:

Time Criterion. The **discounted payback period (DPBP)** is defined in a manner similar to the nondiscounted version given above.

$DPBP$ = Time required, after start-up, to recover the fixed capital investment, FCI_L, required for the project, with all cash flows discounted back to time zero

The project with the shortest discounted payback period is the most desirable.

Cash Criterion. The **discounted cumulative cash position,** more commonly known as the **net present value (NPV)** or **net present worth (NPW)** of the project, is defined as

NPV = Cumulative discounted cash position at the end of the project

Again, the NPV of a project is greatly influenced by the level of fixed capital investment, and a better criterion for comparison of projects with different investment levels may be the **present value ratio (PVR):**

$$PVR = \frac{\text{Present Value of All Positive Cash Flows}}{\text{Present Value of All Negative Cash Flows}}$$

A present value ratio of unity for a project represents a break-even situation. Values greater than unity indicate profitable processes, whereas those less than unity represent unprofitable projects. Example 10.2 continues Example 10.1 using discounted profitability criteria.

Example 10.2.

For the project described in Example 10.1, determine the following discounted profitability criteria:

a. Discounted payback period (DPBP)

b. Net present value (NPV)

c. Present value ratio (PVR)

Assume a discount rate of 0.1 (10% p.a.).

The procedure used is similar to the one used for the nondiscounted evaluation shown in Example 10.1. The discounted cash flows replace actual cash flows. For the discounted case, all the cash flows in Table E10.1 must first be discounted back to the beginning of the project (time = 0). This is done by multiplying each cash flow by the discount factor ($P/F, i, n$), where n is the number of years

after the start of the project. These discounted cash flows are shown along with the cumulative discounted cash flows in Table E10.2.

Table E10.2. Discounted Cash Flows for Example 10.2 (All Numbers in Millions of $)

End of Year	Nondiscounted Cash Flow	Discounted Cash Flow	Cumulative Discounted Cash Flow
0	(10.00)	(10)	(10.00)
1	(90.00)	$(90)/1.1 = (81.82)$	(91.82)
2	(90.00)	$(90)/1.1^2 = (74.38)$	(166.20)
3	38.25	$38.25/1.1^3 = 28.74$	(137.46)
4	46.35	$46.35/1.1^4 = 31.66$	(105.80)
5	37.71	$37.71/1.1^5 = 23.41$	(82.39)
6	32.53	$32.53/1.1^6 = 18.36$	(64.03)
7	32.53	$32.53/1.1^7 = 16.69$	(47.34)
8	28.64	$28.64/1.1^8 = 13.36$	(33.98)
9	24.75	$24.75/1.1^9 = 10.50$	(23.48)
10	24.75	$24.75/1.1^{10} = 9.54$	(13.94)
11	24.75	$24.75/1.1^{11} = 8.67$	(5.26)
12	70.25	$70.25/1.1^{12} = 22.38$	17.12

Discounted Profitability Criteria

Discounted Payback Period (DPBP)

Discounted value of land + working capital = $10 + 30/1.12 = \$34.8 \times 10^6$

Find time after start-up when cumulative cash flow = $-\$34.8 \times 10^6$

DPBP = $5 + (-47.34 + 34.8)/(-47.34 + 33.98)$ = **5.94 y**

Net Present Value (NPV) *and Present Value Ratio (PVR)*

NPV = $17.12 × 10^6

PVR = Σ positive discounted cash flows/Σ negative discounted cash flows = (28.74 + 31.36 + 23.41 + ... + 22.38) / (10 + 81.82 + 74.38)

PVR = (183.31) / (166.2) = 1 + 17.12 / 166.2 = **1.10**

The cumulative discounted cash flows are shown on Figure E10.2, and the calculations are given in Table E10.2. From these sources the profitability criteria are given as

a. Discounted payback period (*DPBP*) = 5.94 years

b. Net present value (*NPV*) = $\$17.12 \times 10^6$

c. Present value ratio (*PVR*) = 1.10

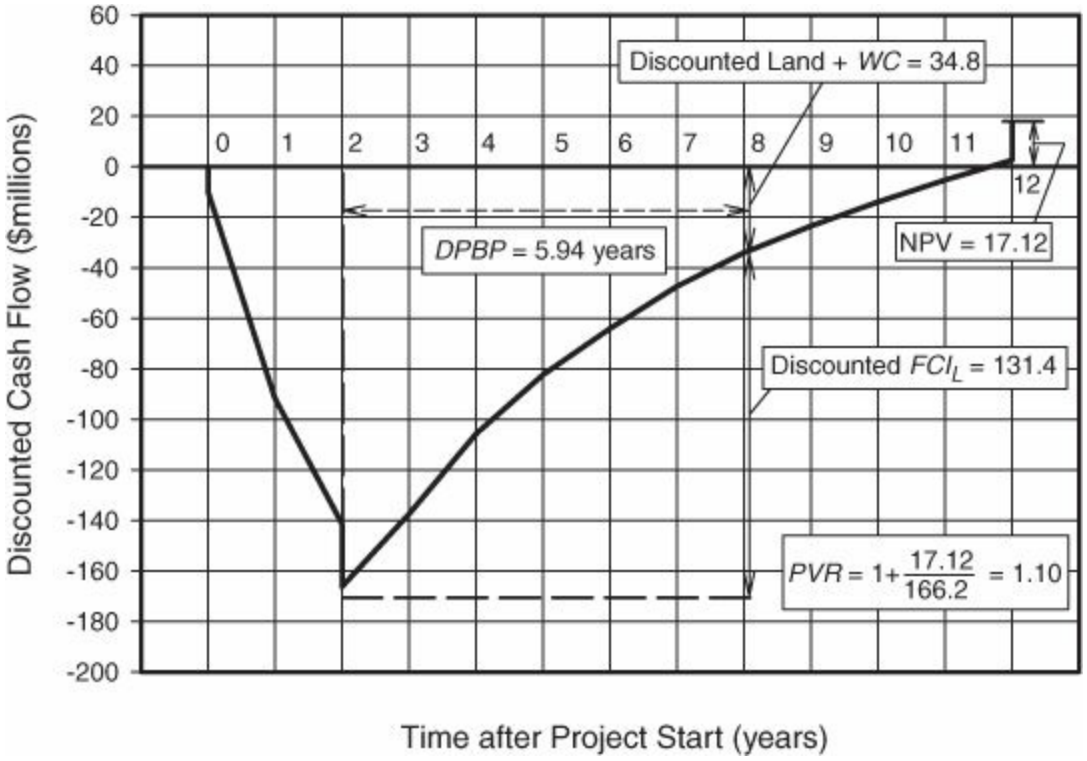


Figure E10.2. Cumulative Cash Flow Diagram for Discounted After-Tax Cash Flows for Example 10.2

These examples illustrate that there are significant effects of discounting the cash flows to account for the time value of money. From these results, the following observations may be made:

1. In terms of the time basis, the payback period increases as the discount rate increases. In the above examples, it increased from 3.85 to 5.94 years.
2. In terms of the cash basis, replacing the cash flow with the discounted cash flow decreases the value at the end of the project. In the above examples, it dropped from $170.5 to $17.12 million.
3. In terms of the cash ratios, discounting the cash flows gives a lower ratio. In the above examples, the ratio dropped from 1.897 to 1.10.

As the discount rate increases, all of the discounted profitability criteria will be reduced.

Interest Rate Criterion. The **discounted cash flow rate of return (DCFROR)** is defined to be the interest rate at which all the cash flows must be discounted in order for the net present value of the project to be equal to zero. Thus,

> DCFROR = Interest or discount rate for which the net present value of the project is equal to zero

Therefore, the DCFROR represents the highest after-tax interest or discount rate at which the project can just break even.

For the discounted payback period and the net present value calculations, the question arises as to what interest rate should be used to discount the cash flows. This “internal” interest rate is usually determined by corporate management and represents the minimum rate of return that the company will accept for any new investment. Many factors influence the determination of this discount interest rate, and for current purposes, it is assumed that it is always given.

It is worth noting that for evaluation of the discounted cash flow rate of return, no interest rate is

required because this is what is calculated. Clearly, if the DCFROR is greater than the internal discount rate, then the project is considered to be profitable. Use of DCFROR as a profitability criterion is illustrated in Example 10.3.

Example 10.3.

For the problem presented in Examples 10.1 and 10.2, determine the discounted cash flow rate of return (DCFROR).

The NPVs for several different discount rates were calculated and the results are shown in Table E10.3.

Table E10.3. NPV for Project in Example 10.1 as a Function of Discount Rate

Interest or Discount Rate	NPV ($million)
0%	170.50
10%	17.12
12%	0.77
13%	−6.32
15%	−18.66
20%	−41.22

The value of the DCFROR is found at NPV = 0. Interpolating from Table E10.3 gives:

$$\frac{(\text{DCFROR} - 12\%)}{(13\% - 12\%)} = \frac{(0 - 0.77)}{(-6.32 - 0.77)} = 0.109$$

Therefore, DCFROR = 12 + 1(0.109) = 12.1%

An alternate method for obtaining the DCFROR is to solve for the value of i in an implicit, nonlinear algebraic expression. This is illustrated in Example 10.4.

Figure 10.3. provides the cumulative discounted cash flow diagram for Example 10.3 for several discount factors. It shows the effect of changing discount factors on the profitability and shape of the curves. It includes a curve for the DCFROR found in Example 10.3. For this case, it can be seen that the NPV for the project is zero. In Example 10.3, if the acceptable rate of return for a company were set at 20%, then the project would not be considered an acceptable investment. This is indicated by a negative NPV for i = 20%.

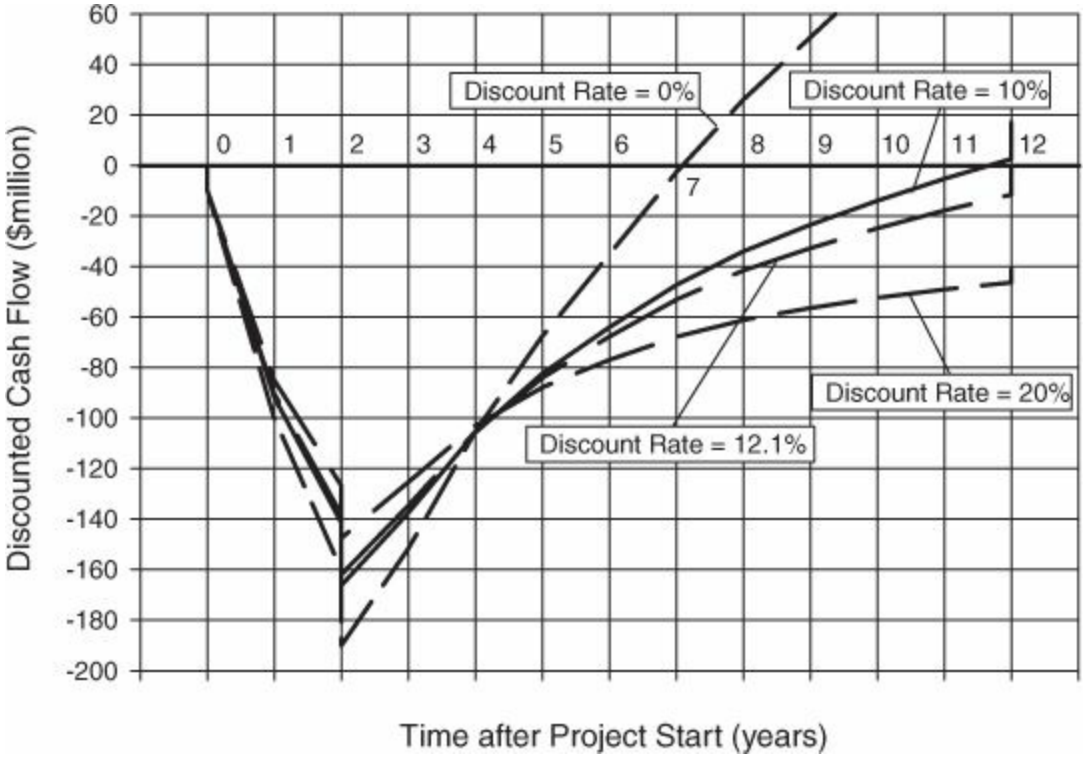


Figure 10.3. Discounted Cumulative Cash Flow Diagrams Using Different Discount Rates for Example 10.3

Each method described above used to gauge the profitability of a project has advantages and disadvantages. For projects having a short life and small discount factors, the effect of discounting is small, and nondiscounted criteria may be used to give an accurate measure of profitability. However, it is fair to say that for large projects involving many millions of dollars of capital investment, discounting techniques should always be used.

Because all the above techniques are commonly used in practice, you must be familiar with and be able to use each technique.

10.3. Comparing Several Large Projects: Incremental Economic Analysis

In this section, comparison and selection among investment alternatives are discussed. When comparing project investments, the DCFROR tells how efficiently money is being used. The higher the DCFROR, the more attractive the individual investment. However, when comparing investment alternatives, it may be better to choose a project that does not have the highest DCFROR. The rationale for comparing projects and choosing the most attractive alternative is discussed in this section.

In order to make a valid decision regarding alternative investments (projects), it is necessary to know a baseline rate of return that must be attained in order for an investment to be attractive. A company that is considering whether to invest in a new project always has the option to reject all alternatives offered and invest the cash (or resources) elsewhere. The baseline or benchmark investment rate is related to these alternative investment opportunities, such as investing in the stock market. Incremental economic analysis is illustrated in Examples 10.4 and 10.5.

Example 10.4.

A company is seeking to invest approximately $\$120 \times 10^6$ in new projects. After extensive research and preliminary design work, three projects have emerged as candidates for construction. The

minimum acceptable internal discount (interest) rate, after tax, has been set at 10%. The after-tax cash-flow information for the three projects using a ten-year operating life is as follows (values in $million):

	Initial Investment	After-Tax Cash Flow in Year i $i = 1$	$i = 2–10$
Project A	$60	$10	$12
Project B	$120	$22	$22
Project C	$100	$12	$20

For this example it is assumed that the costs of land, working capital, and salvage are zero. Furthermore, it is assumed that the initial investment occurs at time = 0, and the yearly annual cash flows occur at the end of each of the ten years of plant operation.

Determine the following:

a. The NPV for each project

b. The DCFROR for each project

For Project A,

$$\text{NPV} = -\$60 + (\$10)(P/F, 0.10, 1) + (\$12)(P/A, 0.10, 9)(P/F, 0.10, 1)$$

$$= -\$60 + \frac{(\$10)}{1.1} + (\$12)\frac{1.1^9 - 1}{(0.1)(1.1^9)}\frac{1}{1.1} = \$11.9$$

The DCFROR is the value of i that results in NPV = 0.

$$NPV = 0 = -\$60 + (\$10)(P/F, i, 1) + (\$12)(P/A, i, 9)(P/F, i, 1)$$

Solving for i yields i = DCFROR = 14.3 %.

Values obtained for NPV and DCFROR are as follows:

	NPV (i = 10%)	DCFROR
Project A	11.9	14.3%
Project B	15.2	12.9%
Project C	15.6	13.3%

Note: Projects A, B, and C are mutually exclusive because investment cannot be made in more than one of them, due to the cap of $\$120 \times 10^6$. The analysis that follows is limited to projects of this type. For the case when projects are not mutually exclusive, the analysis becomes somewhat more involved and is not covered here.

Although all the projects in Example 10.4 showed a positive NPV and a DCFROR of more than 10%, at this point it is not clear how to select the most attractive option with this information. It will be seen later that the choice of the project with the highest NPV will be the most attractive. However, consider the following alternative analysis. If Project B is selected, a total of $\$120 \times 10^6$ is invested and yields 12.9%, whereas the selection of Project A yields 14.3% on the $\$60 \times 10^6$ invested. To compare these two options, a situation in which the same amount is invested in both cases would have to be considered. In Project A, this would mean that $\$60 \times 10^6$ is invested in the project and the remaining $\$60 \times 10^6$ is invested elsewhere, whereas in Project B, a total of $\$120 \times 10^6$ is invested in

the project.

It is necessary in the analysis to be sure that the last dollar invested earns at least 10%. To do this, an incremental analysis must be performed on the cash flows to establish that at least 10% is made on each additional increment of money invested in the project.

Example 10.5.

This is a continuation of Example 10.4.

a. Determine the NPV and the DCFROR for each increment of investment.

b. Recommend the best option.

Solution

a. Project A to Project C:

Incremental investment is $\$40 \times 10^6 = (\$100 - \$60) \times 10^6$.

Incremental cash flow for $i = 1$ is $\$2 \times 10^6/\text{y} = (\$12/\text{y} - \$10/\text{y}) \times 10^6$.

Incremental cash flow for $i = 2$ to 10 is $\$8 \times 10^6/\text{y} = (\$20/\text{y} - \$12/\text{y}) \times 10^6$.

$$NPV = -\$40 \times 10^6 + (\$2 \times 10^6)(P/F, 0.10, 1) + (\$8 \times 10^6)(P/A, 0.10, 9)(P/F, 0.10, 1)$$

$$NPV = \$3.7 \times 10^6$$

Setting NPV = 0 yields DCFROR = 0.119 (11.9%).

Project C to Project B:

Incremental investment is $\$20 \times 10^6 = (\$120 - \$100) \times 10^6$.

Incremental cash flow for $i = 1$ is $\$10 \times 10^6/\text{y} = (\$22/\text{y} - \$12/\text{y}) \times 10^6$.

Incremental cash flow for $i = 2$ to 10 is $\$2 \times 10^6/\text{y} = (\$22/\text{y} - \$20/\text{y}) \times 10^6$.

$$\text{NPV} = -\$0.4 \times 10^6 \text{ and DCFROR} = 0.094 \ (9.4\%)$$

b. It is recommended to move ahead on Project C.

From Example 10.5, it is clear that the rate of return on the $\$20 \times 10^6$ incremental investment required to go from Project C to Project B did not return the 10% required and gave a negative NPV.

The information from Example 10.4 shows that an overall return on investment of more than 10% is obtained for each of the three projects. However, the correct choice, Project C, also has the highest NPV using a discount rate of 10%, and it is this criterion that should be used to compare alternatives.

When comparing mutually exclusive investment alternatives, choose the alternative with the greatest positive net present value.

When carrying out an incremental investment analysis on projects that are mutually exclusive, the following four-step algorithm is recommended:

Step 1: Establish the minimum acceptable rate of return on investment for such projects.

Step 2: Calculate the NPV for each project using the interest rate from Step 1.

Step 3: Eliminate all projects with negative NPV values.

Step 4: Of the remaining projects, select the project with the highest NPV.

10.4. Establishing Acceptable Returns from Investments: The Concept of Risk

Most comparisons of profitability will involve the rate of return of an investment. Company management usually provides several **benchmarks** or **hurdle rates** for acceptable rates of return that must be used in comparing alternatives.

A company vice president (VP) has been asked to recommend which of the following two alternatives to pursue.

> **Option 1:** A new product is to be produced that has never been made before on a large scale. Pilot plant runs have been made and the products sent to potential customers. Many of these customers have expressed an interest in the product but need more material to evaluate it fully. The calculated return on the investment for this new plant is 33%.
>
> **Option 2:** A second plant is to be built in another region of the country to meet increasing demand in the region. The company has a dominant market position for this product. The new facility would be similar to other plants. It would involve more computer control, and attention will be paid to meeting pending changes in environmental regulations. The rate of return is calculated to be 12%.

The recommendation of the VP and the justifications are given below.

Items that favor Option 1 if pursued:

- High return on the investment
- Opens new product possibilities

Items that favor Option 2:

- The market position for Option 2 is well established. The market for the new product has not been fully established.
- The manufacturing costs are well known for Option 2 but are uncertain for the new process because only estimates are available.
- Transportation costs will be less than current values due to the proximity of plant.
- The technology used in Option 2 is mature and well known. For the new process there is no guarantee that it will work.

The closing statement from the VP included the following summary:

> *"We have little choice but to expand our established product line. If we fail to build these new production facilities, our competitors are likely to build a new plant in the region to meet the increasing demand. They could undercut our regional prices, and this would put at risk our market share and dominant market position in the region."*

Clearly, the high return on investment for Option 1 was associated with a high risk. This is usually the case. There are often additional business reasons that must be considered prior to making the final decision. The concern for lost market position is a serious one and weighs heavily in any decision. The relatively low return on investment of 12% given in this example would probably not be very attractive had it not been for this concern. It is the job of company management to weigh all of these

factors, along with the rate of return, in order to make the final decision.

In this chapter, the terms *internal interest/discount rates* and *internal rates of return* are used. This deals with benchmark interest rates that are to be used to make profitability evaluations. There are likely to be different values that reflect dissimilar conditions of risk—that is, the value for mature technology would differ from that for unproven technology. For example, the internal rate of return for mature technology might be set at 12%, whereas that for very new technology might be set at 40%. Using these values the decision by the VP given above seems more reasonable. The analysis of risk is considered in Section 10.7.

10.5. Evaluation of Equipment Alternatives

Often during the design phases of a project, it will be necessary to evaluate different equipment options. Each alternative piece of equipment performs the same process function. However, the capital cost, operating cost, and equipment life may be different for each, and the best choice must be determined using some economic criterion.

Clearly, if there are two pieces of equipment, each with the same expected operating life, that can perform the desired function with the same operating cost, then *common sense* suggests choosing the *less expensive alternative!* When the expected life and operating expenses vary, the selection becomes more difficult. Techniques available to make the selection are discussed in this section.

10.5.1. Equipment with the Same Expected Operating Lives

When the operating costs and initial investments are different but the equipment lives are the same, then the choice should be made based on NPV. The choice with the least negative NPV will be the best choice. Examples 10.6 and 10.7 illustrate evaluation of equipment alternatives.

Example 10.6.

In the final design stage of a project, the question has arisen as to whether to use a water-cooled exchanger or an air-cooled exchanger in the overhead condenser loop of a distillation tower. The information available on the two pieces of equipment is provided as follows:

	Initial Investment	Yearly Operating Cost
Air-cooled	$23,000	$1200
Water-cooled	$12,000	$3300

Both pieces of equipment have service lives of 12 years. For an internal rate of return of 8% p.a., which piece of equipment represents the better choice?

The NPV for each exchanger is evaluated as follows:

$$NPV = -\text{Initial Investment} + (\text{Operating Cost})(P/A, 0.08, 12)$$

	NPV
Air-cooled	–$32,040
Water-cooled	–$36,870

The air-cooled exchanger represents the better choice.

Despite the higher capital investment for the air-cooled exchanger in Example 10.6, it was the recommended alternative. The lower operating cost more than compensated for the higher initial investment.

10.5.2. Equipment with Different Expected Operating Lives

When process units have different expected operating lives, care is required in determining the best choice. In terms of expected equipment life, it is assumed that this is less than the expected working life of the plant. Therefore, during the normal operating life of the plant, it can be expected that the equipment will be replaced at least once. This requires that different profitability criteria be applied. Three commonly used methods are presented to evaluate this situation. (The effect of inflation is not considered in these methods.) All methods consider both the capital and operating cost in minimizing expenses, thereby maximizing profits.

Capitalized Cost Method. In this method, a fund is established for each piece of equipment to be compared. This fund provides the amount of cash that would be needed to

a. Purchase the equipment initially

b. Replace it at the end of its life

c. Continue replacing it forever

The size of the initial fund and the logic behind the capitalized cost method are illustrated in Figure 10.4.

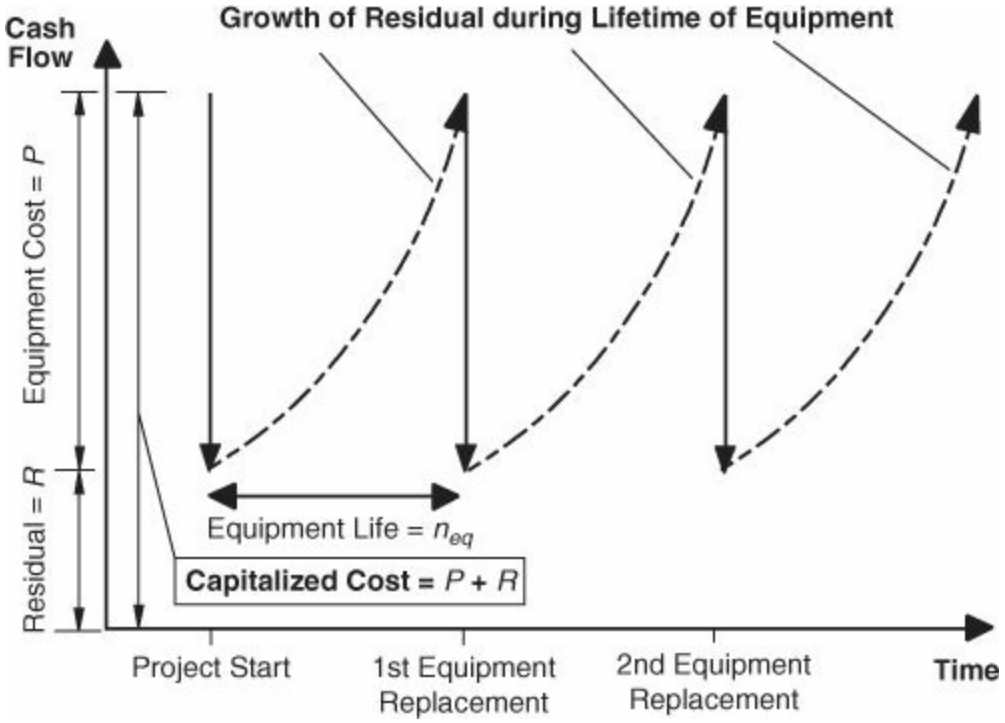


Figure 10.4. An Illustration of the Capitalized Cost Method for the Analysis of Equipment Alternatives

From Figure 10.4, it can be seen that if the equipment replacement cost is P, then the total fund set aside (called the **capitalized cost**) is $P + R$, where R is termed the residual. The purpose of this residual is to earn sufficient interest during the life of the equipment to pay for its replacement. At the end of the equipment life, n_{eq}, the amount of interest earned is P, the equipment replacement cost. As Figure 10.4 shows, replacing the equipment every time it wears out may continue. Referring to Figure 10.4, the equation is developed for the capitalized cost defined as $(P + R)$:

$$R(1+i)^{n_{eq}} - R = P$$

and

$$\text{Capitalized Cost} = P + R = P + \frac{P}{(1+i)^{n_{eq}} - 1} = P\left[\frac{(1+i)^{n_{eq}}}{(1+i)^{n_{eq}} - 1}\right] \qquad (10.1)$$

The term in square brackets in Equation (10.1) is commonly referred to as the **capitalized cost factor.**

The capitalized cost obtained from Equation (10.1) does not include the operating cost and is useful in comparing alternatives only when the operating costs of the alternatives are the same. When operating costs vary, it is necessary to capitalize the operating cost. An equivalent capitalized operating cost that converts the operating cost into an equivalent capital cost is added to the capitalized cost calculated from Equation (10.1) to provide the **equivalent capitalized cost (ECC):**

$$\text{Equivalent Capitalized Cost} = \text{Capitalized Cost} + \text{Capitalized Operating Cost}$$

$$\text{Equivalent Capitalized Cost} = \left[\frac{P(1+i)^{n_{eq}} + YOC(F/A, i, n_{eq})}{(1+i)^{n_{eq}} - 1}\right] \qquad (10.2)$$

This cost considers both the capital cost of equipment and the **yearly operating cost (YOC)** needed to compare alternatives. The extra terms in Equation (10.2) represent the effect of taking the yearly cash flows for operating costs from the residual, *R*.

By using Equation (10.1) or (10.2), it is possible to account correctly for the different operating lives of the equipment by calculating an effective capitalized cost for the equipment and operating cost. Example 10.7 illustrates the use of these equations.

Example 10.7.

During the design of a new project, a decision must be made regarding which type of pump should be used for a corrosive service. The options are as follows:

	Capital Cost	Operating Cost (per Year)	Equipment Life (Years)
Carbon steel pump	$8000	$1800	4
Stainless steel pump	$16,000	$1600	7

Assume a discount rate of 8% p.a.

Using Equation (10.2) for the carbon steel pump,

$$\text{Capitalized Cost} = \frac{(8000)(1.08)^4 + (1800)\dfrac{[1.08^4 - 1]}{0.08}}{1.08^4 - 1} = \$52{,}700$$

For the stainless steel pump,

$$\text{Capitalized Cost} = \frac{(16{,}000)(1.08)^7 + (1600)\dfrac{[1.08^7 - 1]}{0.08}}{1.08^7 - 1} = \$58{,}400$$

The carbon steel pump is recommended because it has the lower capitalized cost.

In Example 10.7, the stainless steel pump costs twice as much as the carbon steel pump and, because of its superior resistance to corrosion, will last nearly twice as long. In addition, the operating cost for the stainless steel pump is lower due to lower maintenance costs. In spite of these advantages, the carbon steel pump was still judged to offer a cost advantage.

Equivalent Annual Operating Cost (EAOC) Method. In the previous method, both capital cost and yearly operating costs were lumped into a single cash fund or equivalent cash amount. An alternative method is to **amortize** (spread out) the capital cost of the equipment over the operating life to establish a yearly cost. This is added to the operating cost to yield the EAOC.

Figure 10.5 illustrates the principles behind this method. From the figure, it can be seen that the cost of the initial purchase will be spread out over the operating life of the equipment. The EAOC is expressed by Equation (10.3).

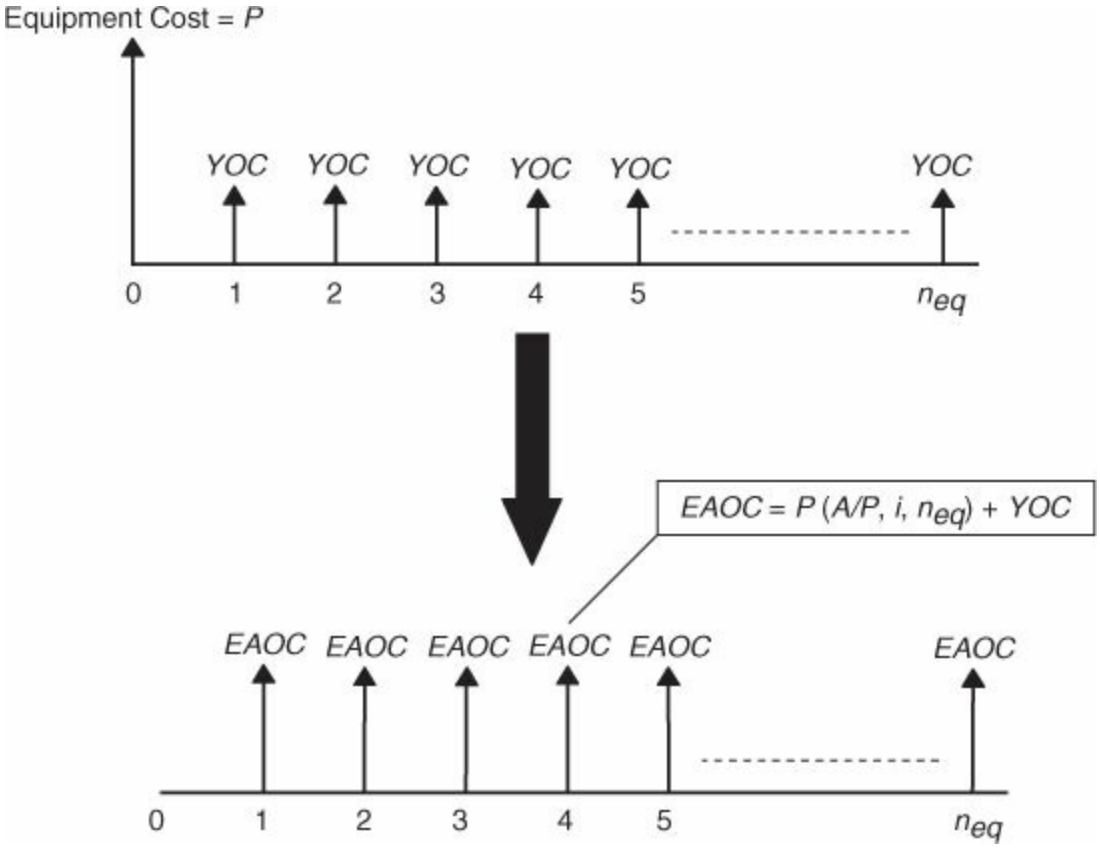


Figure 10.5. Cash Flow Diagrams Illustrating the Concept of Equivalent Annual Operating Cost

$$EAOC = (\text{Capital Investment})(A/P, i, n_{eq}) + YOC \qquad (10.3)$$

Example 10.8 illustrates this method.

Example 10.8.

Compare the stainless steel and carbon steel pumps in Example 10.7 using the EAOC method.

For the carbon steel pump,

$$EAOC = \frac{(8000)(0.08)(1.08)^4}{1.08^4 - 1} + 1800 = \$4220 \text{ per year}$$

For the stainless steel pump,

$$EAOC = \frac{(16{,}000)(0.08)(1.08)^7}{1.08^7 - 1} + 1600 = \$4670 \text{ per year}$$

The carbon steel pump is shown to be the preferred equipment using the EAOC method, as it was in Example 10.7 using the ECC method.

Common Denominator Method. Another method for comparing equipment with unequal operating lives is the **common denominator method.** This method is illustrated in Figure 10.6, in which two pieces of equipment with operating lives of *n* and *m* years are to be compared. This comparison is done over a period of *nm* years during which the first piece of equipment will need *m* replacements and the second will require *n* replacements. Each piece of equipment has an integer number of replacements, and the time over which the comparison is made is the same for both pieces of equipment. For these reasons the comparison can be made using the net present value of each alternative. In general, an integer number of replacements can be made for both pieces of equipment in a time *N*, where *N* is the smallest number into which *m* and *n* are both exactly divisible; that is, *N* is the common denominator. Example 10.9 illustrates this method.

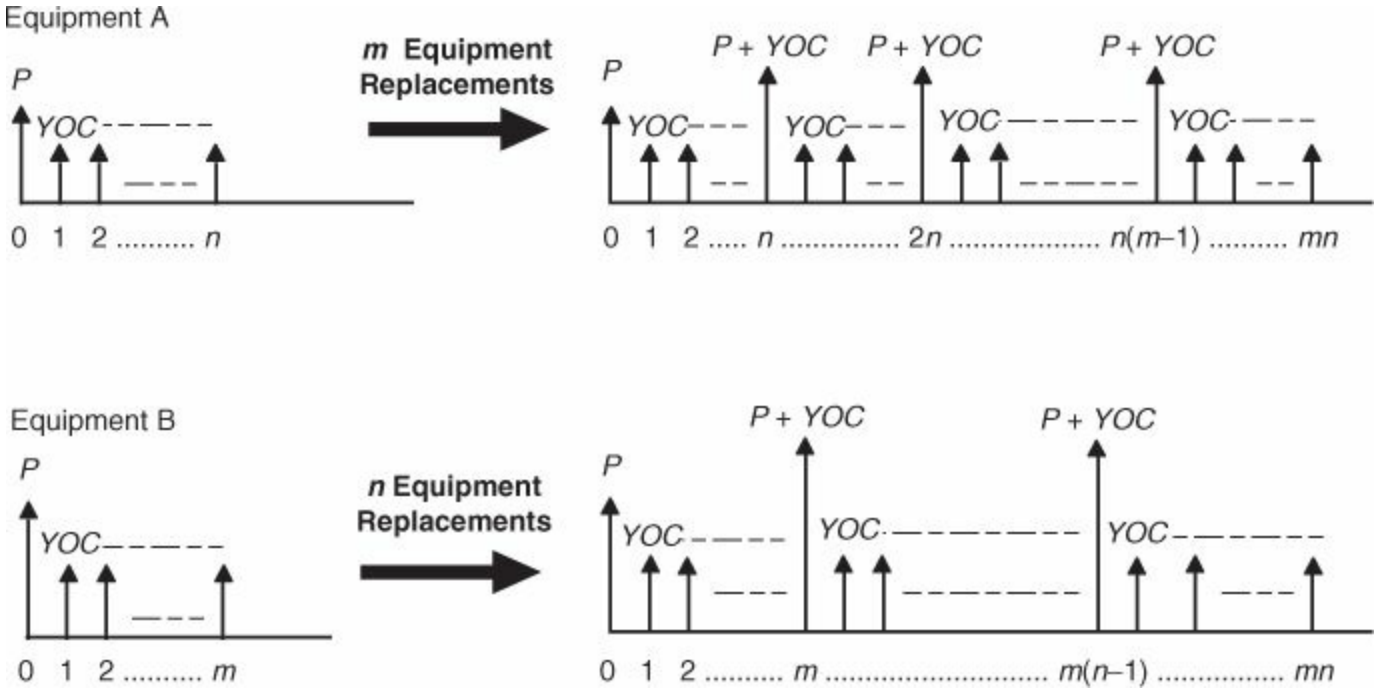


Figure 10.6. An Illustration of the Common Denominator Method for the Analysis of Equipment Alternatives

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Example 10.9.

Compare the two pumps given in Example 10.7 using the common denominator method. The discrete cash flow diagrams for the two pumps are shown in Figure E10.9. The minimum time over which the comparison can be made is 4(7) = 28 years.

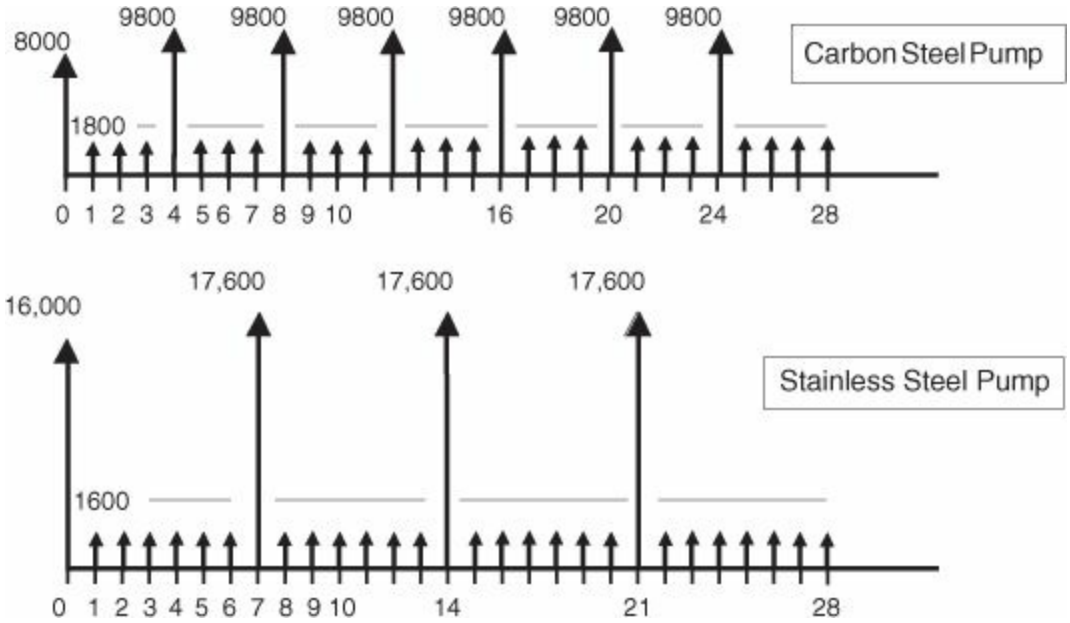


Figure E10.9. Cash Flow Diagrams for the Common Denominator Method Used in Example 10.9

NPV for carbon steel pump:

$$NPV = -(\$8000)(1 + 1.08^{-4} + 1.08^{-8} + 1.08^{-12} + 1.08^{-16} + 1.08^{-20} + 1.08^{-24})$$
$$-(\$1800)(P/A, 0.08, 28)$$
$$= -\$46{,}580$$

NPV for stainless steel pump:

$$NPV = -(\$16{,}000)(1 + 1.08^{-7} + 1.08^{-14} + 1.08^{-21}) - (\$1600)(P/A, 0.08, 28) = -\$51{,}643$$

The carbon steel pump has a less negative NPV and is recommended.

As found for the previous two methods, the common denominator method favors the carbon steel pump.

Choice of Methods. Because all three methods of comparison correctly take into account the time value of money, the results of all the methods are equivalent. In most problems, the common denominator method becomes unwieldy. The use of the EAOC or the capitalized cost methods are favored for these calculations.

10.6. Incremental Analysis for Retrofitting Facilities

This topic involves profitability criteria used for analyzing situations where a piece of equipment is added to an existing facility. The purpose of adding the equipment is to improve the profitability of the process. Such improvements are often referred to as retrofitting. Such retrofits may be extensive—requiring millions of dollars of investment—or small, requiring an investment of only a few thousand dollars.

The decisions involved in retrofitting projects may be of the discrete type, the continuous type, or a combination of both. An example of a discrete decision is whether to add an on-line monitoring and control system to a wastewater stream. The decision is a simple yes or no. An example of a continuous decision is to determine what size of heat recovery system should be added to an existing process heater to improve fuel efficiency. This type of decision would involve sizing the optimum heat exchanger, where the variable of interest (heat-exchanger area) is continuous.

Because retrofit projects are carried out on existing operating plants, it becomes necessary to identify all of the costs and savings associated with the retrofit. When comparing alternative schemes, the focus of attention is on the profitability of the incremental investment required. Simple, discrete choices will be considered in this section. The problem of optimizing a continuous variable is covered in Chapter 14.

The initial step in an incremental analysis of competing alternatives is to identify the potential alternatives to be considered and to specify the increments over which the analysis is to be performed. The first step is to rank the available alternatives by the magnitude of the capital cost. The alternatives will be identified as $A_1, A_2, \ldots, A_n$. There are n possible alternatives. The first alternative, A_1, which is always available, is the "do nothing" option. It requires no capital cost (and achieves no savings). For each of the available alternatives, the project cost (capital cost), PC, and the yearly savings generated (yearly cash flow), YS, must be known.

For larger retrofit projects, discounted profitability criteria should be used. The algorithm to compare alternatives using discounted cash flows follows the same four-step method outlined in Section 10.3. For small retrofit projects, nondiscounted criteria may often be sufficiently accurate for comparing alternatives. Both types of criteria are discussed in the next sections.

10.6.1. Nondiscounted Methods for Incremental Analysis

For nondiscounted analyses, two methods are provided below.

1. Rate of Return on Incremental Investment (ROROII)

$$ROROII = \frac{\text{Incremental Yearly Savings}}{\text{Incremental Investment}}$$

2. Incremental Payback Period (IPBP)

$$IPBP = \frac{\text{Incremental Investment}}{\text{Incremental Yearly Savings}}$$

Examples 10.10–10.12 illustrate the method of comparison of projects using these two criteria.

Example 10.10.

A circulating heating loop for an endothermic reactor has been in operation for several years. Due to an oversight in the design phase, a certain portion of the heating loop piping was left uninsulated. The consequence is a significant energy loss. Two types of insulation can be used to reduce the heat loss. They are both available in two thicknesses. The estimated cost of the insulation and the estimated yearly savings in energy costs are given below. (The ranking has been added to the alternatives and is based on increasing project cost.)

Ranking (Option #)	Alternative Insulation	Project Cost (PC)	Savings Generated by Project (YS)
1	No Insulation	0	0
2	B-1″ Thick	$3000	$1400
3	B-2″ Thick	$5000	$1900
4	A-1″ Thick	$6000	$2000
5	A-2″ Thick	$9700	$2400

Assume an acceptable internal rate of return for a nondiscounted profitability analysis to be 15% (0.15).

a. For the four types of insulation determine the rate of return on incremental investment (ROROII) and the incremental payback period (IPBP).

b. Determine the value of the incremental payback period equivalent to the 15% internal rate of return.

Solution

a. Evaluation of ROROII and IPBP

Option #-Option 1	*ROROII*	*IPBP* (years)
2-1	\$1400/\$3000 = 0.47 (47%)	\$3000/\$1400 = 2.1
3-1	\$1900/\$5000 = 0.38 (38%)	\$5000/\$1900 = 2.6
4-1	\$2000/\$6000 = 0.33 (33%)	\$6000/\$2000 = 3.0
5-1	\$2400/\$9700 = 0.25 (25%)	\$9700/\$2400 = 4.0

b. $IPBP = 1/(ROROII) = 1/0.15 = 6.67$ y

Note that in Part (a) of Example 10.10, the incremental investment and savings are given by the difference between installing the insulation and doing nothing. All of the investments considered in Example 10.10 satisfied the internal benchmark for investment of 15%, which means that the do-nothing option (Option 1) can be discarded. However, which of the remaining options is the best can be determined only by using pairwise comparisons.

Example 10.11.

Which of the options in Example 10.10 is the best based on the nondiscounted ROROII of 15%?

Step 1: Choose Option 2 as the base case, because it has the lowest capital investment.

Step 2: Evaluate incremental investment and incremental savings in going from the base case to the case with the next higher capital investment, Option 3.

Incremental Investment = (\$5000 – \$3000) = \$2000

Incremental Savings = (\$1900/y – \$1400/y) = \$500/y

$ROROII = 500/2000 = 0.4$, or 40%/y

Step 3: Because the result of Step 2 gives an $ROROII > 15\%$, Option 3 is used as the base case and is compared with the option with the next higher capital investment, Option 4.

Incremental Investment = (\$6000 – \$5000) = \$1000

Incremental Savings = (\$2000/y – \$1900/y) = \$100/y

$ROROII = 100/1000 = 0.1$ or 10%/y

Step 4: Because the result of Step 3 gives an $ROROII < 0.15$, Option 4 is rejected and Option 3 is compared with the option with the next higher capital investment, Option 5.

Incremental Investment = (\$9700 – \$5000) = \$4700

Incremental Savings = (\$2400/y – \$1900/y) = \$500/y

$ROROII = 500/4700 = 0.106$, or 10.6%/y

Step 5: Again, the ROROII from Step 4 is less than 15%, and hence Option 5 is rejected. Because Option 3 (Insulation B-2" thick) is the current base case and no more comparisons remain, Option 3 is accepted as the "best option."

It is important to note that in Example 10.11 Options 4 and 5 are rejected even though they give *ROROII* > 15% when compared with the do-nothing option (see Example 10.10). The key here is that in going from Option 3 to either Option 4 or 5 the incremental investment loses money, that is, *ROROII* < 15%.

Example 10.12.

Repeat the comparison of options in Example 10.10 using a nondiscounted incremental payback period of 6.67 years.

The steps are similar to those used in Example 10.11 and are given below without further explanation.

Step 1: (Option 3 – Option 2) *IPBP* = 2000/500 = 4 years < 6.67

Reject Option 2; Option 3 becomes the base case.

Step 2: (Option 4 – Option 3) *IPBP* = 1000/10 = 10 years > 6.67

Reject Option 4.

Step 3: (Option 5 – Option 3) *IPBP* = 4700/500 = 9.4 years > 6.67

Reject Option 5.

Option 3 is the best option.

10.6.2. Discounted Methods for Incremental Analysis

Incremental analyses taking into account the time value of money should always be used when large capital investments are being considered. Comparisons may be made either by discounting the operating costs to yield an equivalent capital investment or by amortizing the initial investment to give an equivalent annual operating cost. Both techniques are considered in the following section, where the effects of depreciation and taxation are ignored in order to keep the analysis simple. However, it is an easy matter to take these effects into account.

Capital Cost Methods. The incremental net present value (INPV) for a project is given by

$$INPV = -PC + YS(P/A, i, n) \tag{10.4}$$

When comparing investment options, a given case option will always be compared with a do-nothing option. Thus, these comparisons may be considered as incremental investments. In order to use INPV, it is necessary to know the internal discount rate and the time over which the comparison is to be made. This method is illustrated in Example 10.13.

Example 10.13.

Based on the information provided in Example 10.10 for an acceptable internal interest rate of 15% and time n = 5 y, determine the most attractive alternative, using the INPV criterion to compare options.

For $i = 0.15$ and $n = 5$ the value for $(P/A, i, n) = 3.352$. (See Equation [9.14].)

Equation (10.4) becomes

$$\text{NPV} = -PC + 3.352\ YS$$

Option	*INPV*
2-1	1693
3-1	1369
4-1	704
5-1	−1655

From the results above, it is clear that Options 2, 3, and 4 are all potentially profitable as $INPV > 0$. However, the best option is Option 2 because it has the highest INPV when compared with the do-nothing case, Option 1. Note that other pairwise comparisons are unnecessary. The option that yields the highest INPV is chosen. The reason that the INPV gives the best option directly is because by knowing i and n, each dollar of incremental investment is correctly accounted for in the calculation of INPV. Thus, if the incremental investment in going from Option A to Option B is profitable, then the INPV will be greater for Option B and vice versa. It should also be pointed out that by using discounting techniques, the best option has changed from Option 3 (in Example 10.11) to Option 2.

Operating Cost Methods. In the previous section, yearly savings were converted to an equivalent present value using the present value of an annuity, and this was measured against the capital cost. An alternative method is to convert all the investments to annual costs using the capital recovery factor and measure them against the yearly savings.

The needed relationship is developed from Equation (10.4), giving

$$INPV/(P/A, i, n) = -PC/(P/A, i, n) + YS$$

It can be seen that the capital recovery factor $(A/P,i,n)$ is the reciprocal of the present worth factor $(P/A,i,n)$. Substituting this relationship and multiplying by −1 gives

$$-(INPV)(A/P, i, n) = (PC)(A/P, i, n) - YS$$

The term on the left is identified as the Equivalent Annual Operating Cost (EAOC). Thus,

$$EAOC = (PC)(A/P, i, n) - YS \qquad (10.5)$$

When an acceptable rate for i and n is substituted, a negative EAOC indicates the investment is acceptable (because a negative cost is the same as a positive savings). Use of EAOC is demonstrated in Example 10.14.

Example 10.14.

Repeat Example 10.13 using *EAOC* in place of *NPV*.

For $i = 0.15$ and $n = 5$ the value for $(A/P, i, n) = 1/3.352$.

Equation (10.5) becomes

$EAOC = PC/3.352 - YS$

Option	*EAOC*
2–1	–505
3–1	–408
4–1	–210
5–1	494

The best alternative is Option 2 because it has the most negative EAOC.

10.7. Evaluation of Risk in Evaluating Profitability

In this section, the concept of risk in the evaluation of profitability is introduced, and the techniques to quantify it are illustrated. Until now, it has been assumed that the financial analysis is essentially deterministic—that is, all factors are known with absolute certainty. Recalling discussions in Chapter 7 regarding the relative error associated with capital cost estimates, it should not be surprising that many of the costs and parameters used in evaluating the profitability of a chemical process are estimates that are subject to error. In fact, nearly all of these factors are subject to change throughout the life of the chemical plant. The question then is not, "Do these parameters change?" but rather, "By how much do they change?" In Table 10.1, due to Humphreys [1], ranges of expected variations for factors that affect the prediction and forecasting of profitability are given. In reviewing the prediction or forecasting of factors affecting the profitability of chemical processes, Humphreys [1] gives the ranges of expected variations shown in Table 10.1.

Table 10.1. Range of Variation of Factors Affecting the Profitability of a Chemical Process

Factor in Profitability Analysis	Probable Variation from Forecasts over 10-year Plant Life, %
Cost of fixed capital investment*	–10 to +25
Construction time	–5 to +50
Start-up costs and time	–10 to +100
Sales volume	–50 to +150
Price of product	–50 to +20
Plant replacement and maintenance costs	–10 to +100
Income tax rate	–5 to +15
Inflation rates	–10 to +100
Interest rates	–50 to + 50
Working capital	–20 to +50
Raw material availability and price	–25 to +50
Salvage value	–100 to +10
Profit	–100 to +10

*For capital cost estimations using CAPCOST, a more realistic range is –20 to +30%

(From *Jelen's Cost and Optimization Engineering*, 3rd ed., by K. K. Humphreys (1991), reproduced by permission of the McGraw-Hill Companies, Inc.)

The most important variable in Table 10.1 is sales volume, with the price of product and raw

material being a close second. Clearly, if market forces were such that it was possible to sell (and hence produce) only 50% of the originally estimated amount of product, then profitability would be affected greatly. Indeed, the process would quite possibly be unprofitable. The problem is that projections of how the variables will vary over the life of the plant are difficult (and sometime impossible) to estimate. Nevertheless, experienced cost estimators often have a feel for the variability of some of these parameters. In addition, marketing and financial specialists within large companies have expertise in forecasting trends in product demand, product price, and raw material costs. In the next section, the effect that supply and demand have on the sales price of a product is investigated. Following this, methods to quantify risk and to predict the range of profitability that can be expected from a process, when uncertainty exists in some of the profitability parameters listed in Table 10.1, will be discussed.

10.7.1. Forecasting Uncertainty in Chemical Processes

In order to be able to predict the way in which the factors in Table 10.1 vary, it is necessary to take historical data along with information about new developments to formulate a model to predict trends in key economic parameters over the projected life of a process. This prediction process is often referred to as forecasting and is, in general, a very inexact science. The purpose of this section is to introduce some concepts that must be considered when quantifying economic projections. A detailed description of the art of economic forecasting is way beyond the scope of this text. Instead, the basic concepts and factors influencing economic parameters are introduced.

Supply and Demand Concepts in Chemical Markets. Economists use microeconomic theory [2] to describe how changes in the supply of and demand for a given product are affected by changes in the market. Only the most basic supply and demand curves, shown in Figure 10.7, are considered here.

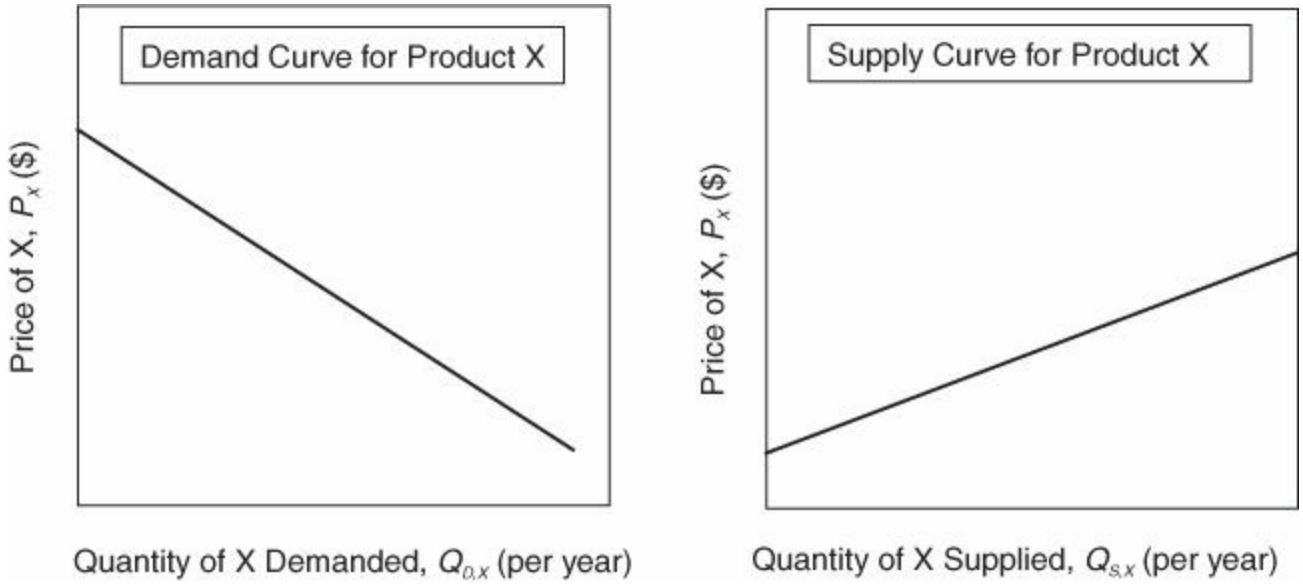


Figure 10.7. Simple Supply and Demand Curves for Product X

The demand curve (on the left) slopes downward and shows the general trend that as the price for commodity X decreases, the demand increases. With very few exceptions, this is always true. Examples of chemical products following this trend are numerous; for example, as the price of gasoline, polyethylene, or fertilizer drops, the demand for these goods increases (all other factors remaining constant). The supply curve (shown on the right) slopes upward and shows the trend that as the price rises, the amount of product X that manufacturers are willing to produce increases. The slope of the supply curve is often positive but may also be negative depending on the product. For

most chemical products, it can be assumed that the slope is positive, and with all other factors remaining constant, the quantity supplied increases as the price for the product increases. Unlike physical laws that govern thermodynamics, heat transfer, and so on, these trends are not absolute. Instead, these trends reflect human nature relating to buying and selling of goods.

When market forces are in equilibrium, the supply and demand for a given product are balanced, and the equilibrium price (P_{eq}) is determined by the intersection of the supply and demand curves, as shown in Figure 10.8.

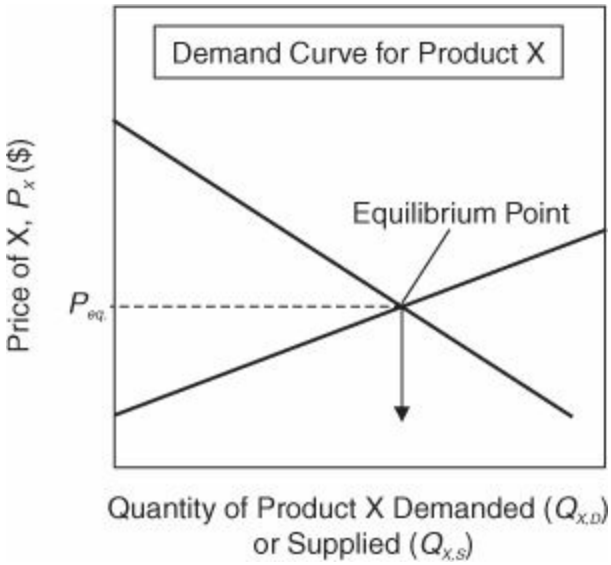


Figure 10.8. Illustration of Market Equilibrium for Product X

There are many factors that can affect the market for product X. Indeed, a market may not be in equilibrium, and, in this case, the market price must be determined in terms of rate equations as opposed to equilibrium relationships. However, for the sake of this simplified discussion, it will be assumed that market equilibrium is always reached. If something changes in the market, either the supply or demand curve (or both) will shift, and a new equilibrium point will be reached. As an example, consider the situation when a large new plant that produces X comes on line. Assuming that nothing else in the market changes, the supply curve will be shifted downward and to the right, which will lead to a lower equilibrium price. This situation is illustrated in Figure 10.9. The intersection of the demand curve and the new supply curve gives rise to the new equilibrium price, $P_{eq,2}$, which is lower than the original equilibrium price, $P_{eq,1}$. The magnitude of the decrease in the equilibrium price depends on the magnitude of the downward shift in the supply curve. If the new plant is large compared with the total current manufacturing capacity for product X, then the decrease in the equilibrium price will be correspondingly large. If this decrease in price is not taken into account in the economic analysis, the projected profitability of the new project will be overestimated, and the decision to invest might be made when the correct decision would be to abandon the project.

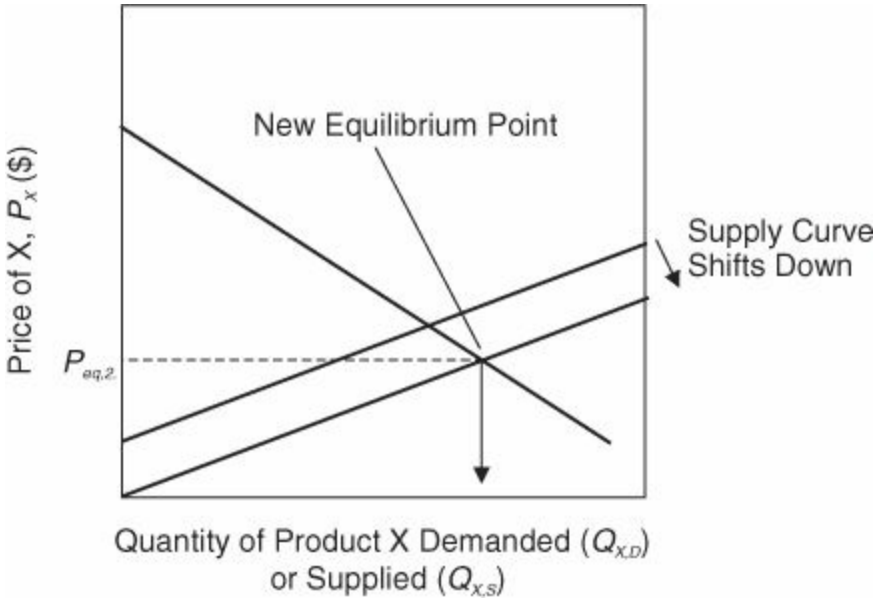


Figure 10.9. Illustration of Market Equilibrium for Product X When a New Plant Comes on Line

The situation is further complicated when competing products are considered. For example, if product Y can be used as a substitute for product X in some applications, then factors that affect Y will also affect X. It is easy to see that quantifying and predicting changes become very difficult. Torries [3] identifies important factors that affect both the shape and relative location of the supply and demand curves. These factors are listed in Table 10.2.

Table 10.2. Factors Affecting the Shape and Relative Location of the Supply and Demand Curves

Factors Influencing Supply	Factors Influencing Demand
Cost and amount of labor	Price of the product
Cost and amount of energy	Price of all substitute products
Cost and amount of raw material	Consumer disposable income
Cost of fixed capital (interest rates) and amount of fixed capital	Consumer tastes
Other miscellaneous factors	Manufacturing technology
	Other miscellaneous factors

(From Torries, T. F., *Evaluating Mineral Projects: Applications and Misconceptions*, by permission of SME, Littleton, CO, 1998; www.smenet.org)

In order to forecast accurately the prices of a product over a 10- or 15-year project, the factors in Table 10.2 need to be predicted. Clearly, even for the most well-known and stable products, this can be a daunting task. An alternative method to quantifying the individual supply and demand curves is to look at historical data for the product of interest.

The examination of historical data is a convenient way to obtain general trends in pricing. Such data represent the change in equilibrium price for a product with time. Often such data fluctuate widely, and although long-term trends may be apparent, predictions for the next one or two years will often be wildly inaccurate. For example, consider the data for average gasoline prices over the period January 1996 to June 2007, as shown in Figure 10.10. The straight line is a regression through the data and represents the best linear fit of the data. If this were the forecast for gasoline prices over this period, it would be a remarkably good prediction. However, even with this predicting line, significant

variations in actual product selling price are noted. The maximum positive and negative deviations are +77¢/gal (+33%) and –54¢/gal (–50%). To illustrate further the effect of these deviations on profitability calculations, consider a new refinery starting production in late 2001. For this new plant, the selling price for its major product (gasoline) over the two-year period after start-up is significantly below that predicted by the trend line. If this refinery were contracted to buy crude oil at a price fixed previously, then the profitability of the plant over this initial two-year period would be severely diminished and it would probably lose money.

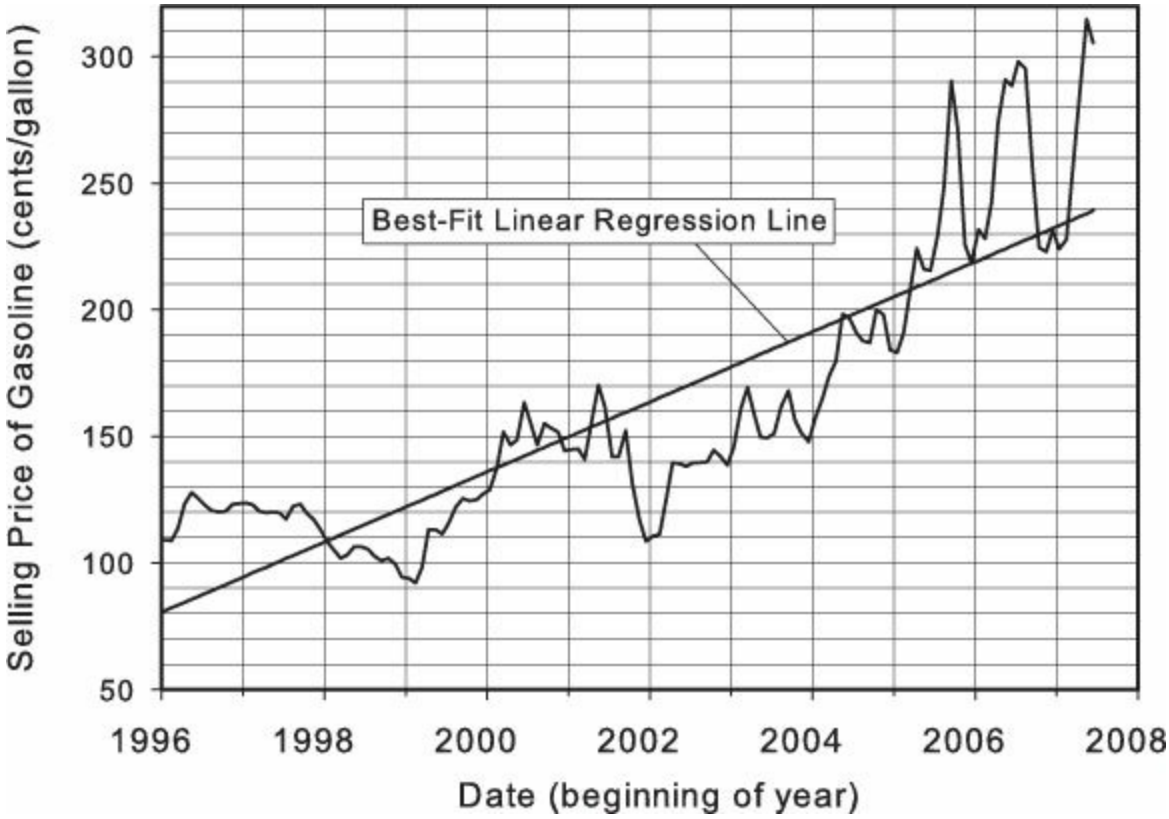


Figure 10.10. Average Price of All Grades of Gasoline over the Period January 1996 to June 2007 (from www.eia.doe.gov)

From the brief discussion given above, it is clear that predicting or forecasting future prices for chemical products is a very inexact and risky business. Perhaps it is best summed up by a quote attributed to "baseball philosopher" Yogi Berra [4]:

"It's tough to make predictions, especially about the future."

In the following section, it will be assumed that such predictions are available and will be used as given, known quantities. The question then is how much meaning can be placed on the results of these predictions when the input data—the basic variability of the parameters—is often poorly known. The answer is that by investigating and looking at how these parameters affect profitability, a better picture of how this variability or uncertainty affects the overall profitability of a project can be obtained. In general, this type of information is much more useful than the single-point estimate of profitability that has been considered up to this point.

10.7.2. Quantifying Risk

It should be noted that the quantification of risk in no way eliminates uncertainty. Rather, by quantifying it, a better feel can be developed for how a project's profitability may vary. Therefore, more informed and rational decisions regarding whether to build a new plant can be made. However,

the ultimate decision to invest in a new chemical process always involves some element of risk.

Scenario Analysis. Returning to Example 10.1 regarding the profitability analysis for a new chemical plant, assume that, as the result of previous experience with similar chemicals and some forecasting of supply and demand for this new product, it is believed that the product price may vary in the range –20% to +5%, the capital investment may vary between –20% and +30%, and the cost of manufacturing may vary in the range –10% to +10%. How can these uncertainties be quantified?

One way to quantify uncertainty is via a **scenario analysis.** In this analysis, the best-and worst-case scenarios are considered and compared with the base case, which has already been calculated. The values for the three parameters for the two cases are given in Table 10.3.

Table 10.3. Values for Uncertain Parameters for the Scenario Analysis (All $ Figures in Millions)

Parameter	Worst Case	Best Case
Revenue, R	–20% = ($75)(0.8) = $60	+5% = ($75)(1.05) = $78.75
Cost of manufacture, COM_d	+10% = ($30)(1.1) = $33	–10% = ($30)(0.9) = $27
Capital investment, FCI_L	+30% = ($150)(1.3) = $195	–20% = ($150)(0.8) = $120

Next, these values are substituted into the spreadsheet shown in Table E10.1, and all the cash flows are discounted back to the start of the project to estimate the NPV. The results of these calculations are shown in Table 10.4.

Table 10.4. Net Present Values (NPVs) for the Scenario Analysis (All $ Figures in Millions)

Case	Net Present Value
Worst Case	–$59.64
Base Case	$17.12
Best Case	$53.62

The results in Table 10.4 show that, in the worst-case scenario, the NPV is very negative and the project will lose money. In the best-case scenario, the NPV is increased over the base case by approximately $45 million. From this result, the decision on whether to go ahead and build the plant is not obvious. On one hand, the process could be highly profitable, but on the other hand, it could lose nearly $73 million over the course of the ten-year plant life. By taking a very conservative philosophy, the results of the worst-case scenario suggest a decision of "do not invest." However, is the worst-case scenario realistic? Most likely, the worst-case (best-case) scenario is unduly pessimistic (optimistic). Consider each of the three parameters in Table 10.3. It will be assumed that the value of the parameter has an equal chance of being at the high, base-case, or low value. Therefore, in terms of probabilities, the chance of the parameter taking each of these values is 1/3, or 33.3%. Because there are three parameters (R, FCI_L, and COM_d), each of which can take one of three values (high, base case, low), there are $3^3 = 27$ combinations as shown in Table 10.5.

Table 10.5. Possible Combinations of Values for Three Parameters

Scenario	R^*	COM_d^*	FCI_L^*	Probability of Occurrence
1	−20%	−10%	−20%	(1/3)(1/3)(1/3) = 1/27
2	−20%	−10%	0%	
3	−20%	−10%	+30%	
4	−20%	0%	−20%	
5	−20%	0%	0%	
6	−20%	0%	+30%	
7	−20%	+10%	−20%	
8	−20%	+10%	0%	
9 (worst)	**-20%**	**+10%**	**+30%**	
10	0%	−10%	−20%	
11	0%	−10%	0%	
12	0%	−10%	+30%	
13	0%	0%	−20%	
14 (base)	**0%**	**0%**	**0%**	
15	0%	0%	+30%	
16	0%	+10%	−20%	
17	0%	+10%	0%	
18	0%	+10%	+30%	
19 (best)	**+5%**	**-10%**	**-20%**	
20	+5%	−10%	0%	
21	+5%	−10%	+30%	
22	+5%	0%	−20%	
23	+5%	0%	0%	
24	+5%	0%	+30%	
25	+5%	+10%	−20%	
26	+5%	+10%	0%	
27	+5%	+10%	+30%	(1/3)(1/3)(1/3) = 1/27

*0% refers to the base-case value.

From Table 10.5, it can be seen that Scenario 9 is the worst case and Scenario 19 is the best case. Either of these two cases has a 1 in 27 (or 3.7%) chance of occurring. Based on this result, it is not very likely that either of these scenarios would occur, and hence care should be taken in evaluating the scenario analysis. This is indeed one of the main shortcomings of the scenario analysis [2]. In reviewing Table 10.5, a better measure of the expected profitability might be the weighted average of all 27 possible outcomes. The idea of weighting results based on the likelihood of occurrence is the basis of the probabilistic approach to quantifying risk that will be discussed shortly. However, before looking at that method, it will be instructive to determine the sensitivity of the profitability of the project to changes in important parameters. Sensitivity analysis is covered in the next section.

Sensitivity Analysis. To a great extent, the risk associated with the variability of a given parameter is dependent on the effect that a change in that parameter has on the profitability criterion of interest. For

the sake of this discussion, the NPV will be used as the measure of profitability. However, this measure could just as easily be the DCFROR, DPEP, or any other profitability criterion discussed in Section 10.2. If it is assumed that the NPV is affected by n parameters ($x_1, x_2, x_3, \ldots, x_n$), then the first-order sensitivity to parameter x_1 is given in mathematical terms by the following quantity:

$$S_1 = \left[\frac{\partial(\text{NPV})}{\partial x_1}\right]_{x_2 x_3, \ldots, x_n} \tag{10.6}$$

where the partial derivative is taken with respect to x_1, while holding all other parameters constant at their mean value. The sensitivity, S_1, is sometimes called a **sensitivity coefficient.** In general, this quantity is too complicated to obtain via analytical differentiation; hence, it is obtained by changing the parameter by a small amount and observing the subsequent change in the NPV, or

$$S_1 \approx \left[\frac{\Delta(\text{NPV})}{\Delta x_1}\right]_{x_2 x_3, \ldots, x_n} \tag{10.7}$$

In Example 10.15, Example 10.1 is revisited to illustrate how the sensitivities of the revenue, cost of manufacturing, and fixed capital investment on the NPV are calculated.

Example 10.15.

For the chemical process considered in Example 10.1, calculate the sensitivity of R, COM_d, and FCI_L and plot these sensitivities with respect to the NPV.

The effect of a 1% change is considered (½% on either side of the base case) in each parameter on the NPV. These results are shown in Table E10.15.

Table E10.15. Calculations for Sensitivity Analysis for Example 10.1 (All $ Figures Are in Millions)

Parameter	Value	NPV	Value	NPV	S_i
x_1 (Revenue, R)	+0.5% ($75.375/y)	$18.17	–0.5% ($74.625/y)	$16.07	$\frac{(18.17-16.07)}{(75.375-74.625)} = \frac{2.1}{0.75} = 2.80$ y
x_2 (COM_d)	+0.5% ($30.150/y)	$16.70	–0.5% ($29.850/y)	$17.54	$\frac{(16.70-17.54)}{(30.15-29.85)} = \frac{-0.84}{0.30} = -2.80$ y
x_3 (FCI_L)	+0.5% ($150.75)	$16.68	–0.5% ($149.25)	$17.56	$\frac{(16.68-17.56)}{(150.75-149.25)} = \frac{-0.88}{1.50} = -0.59$ y

The fact that $S_1 = -S_2$ should not be surprising because, in the calculation of yearly cash flows, whenever R appears COM_d is subtracted from it (see Table E10.1). The changes in NPV for percent changes in each parameter are illustrated in Figure E10.15. The slopes of the lines are not equal to the sensitivities, because the x-axis is the percent change rather than the actual change in the parameter.

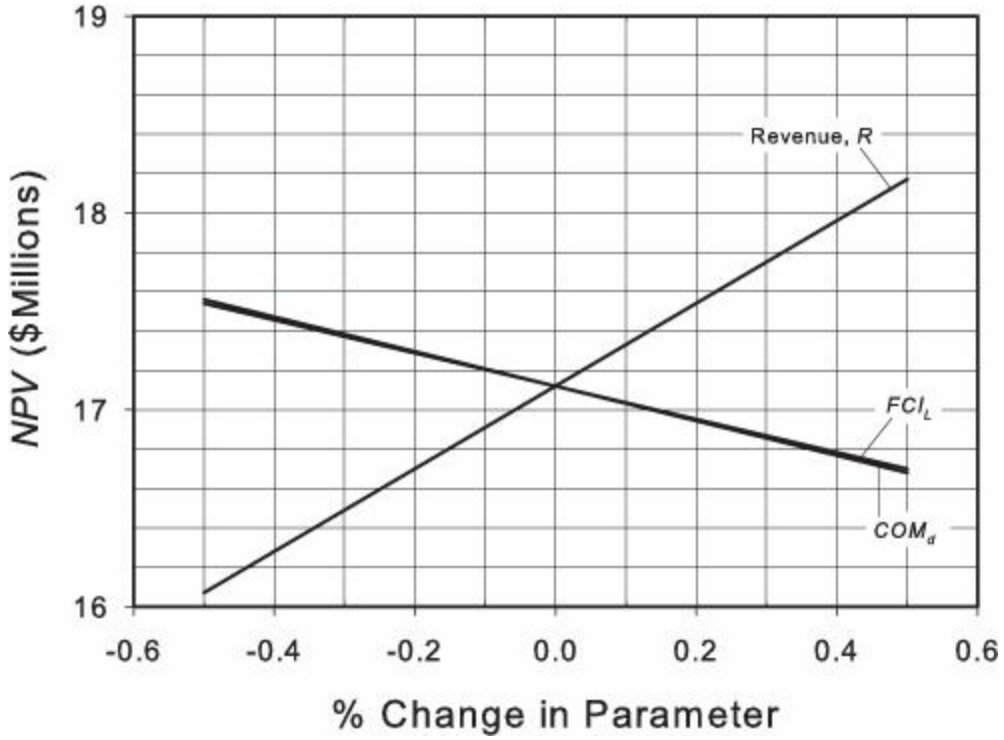


Figure E10.15. Sensitivity Curves for the Parameters Considered in Example 10.15

How can the sensitivity values calculated above be used to estimate changes in the profitability criterion of the process? For small changes in the parameters, it may be assumed that the sensitivities are constant and can be added. Therefore, the change in NPV can be predicted for a set of changes in the parameters using the following formula:

$$\Delta\text{NPV} = S_1\Delta x_1 + S_2\Delta x_2 + \ldots + S_n\Delta x_n \qquad (10.8)$$

Example 10.16 illustrates this concept.

Example 10.16.

What is the change in the NPV for a 2% increase in revenue coupled with a 3% increase in FCI_L?

$$\Delta NPV = S_1\Delta x_1 + S_2\Delta x_2 + S_3\Delta x_3 = (2.80)(0.02)(75)–(2.80)(0)–(0.59)(0.03)(150)$$

$$= \$1.545 \text{ million}$$

A Probabilistic Approach to Quantifying Risk: The Monte-Carlo Method. The basic approach adopted here will involve the following steps:

1. All parameters for which uncertainty is to be quantified are identified.
2. Probability distributions are assigned for all parameters in Step 1.
3. A random number is assigned for each parameter in Step 1.
4. Using the random number from Step 3, the value of the parameter is assigned using the probability distribution (from Step 2) for that parameter.
5. Once values have been assigned to all parameters, these values are used to calculate the profitability (NPV or other criterion) of the project.
6. Steps 3, 4, and 5 are repeated many times (for example, 1000).
7. A histogram and cumulative probability curve for the profitability criteria calculated from Step

6 are created.

8. The results of Step 7 are used to analyze the profitability of the project.

The algorithm described in this eight-step process is best illustrated by means of an example. However, before these steps can be completed, it is necessary to review some basic probability theory.

Probability, Probability Distribution, and Cumulative Distribution Functions. A detailed analysis and description of probability theory are beyond the scope of this book. Instead, some of the basic concepts and simple distributions are presented. The interested reader is referred to Resnick [5], Valle-Riestra [6], and Rose [7] for further coverage of this subject.

For any given parameter for which uncertainty exists (and to which some form of distribution will be assigned), the uncertainty must be described via a probability distribution. The simplest distribution to use is a uniform distribution, which is illustrated in Figure 10.11.

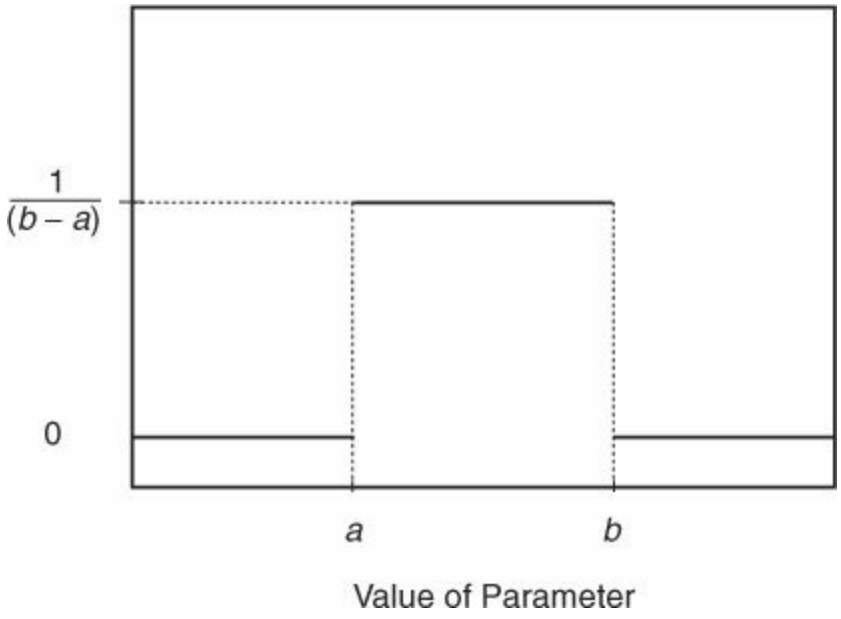


Figure 10.11. Uniform Probability Density Function

From Figure 10.11, the parameter of interest can take on any value between *a* and *b* with equal likelihood. Because the uniform distribution is a probability density function, the area under the curve must equal 1, and hence the value of the frequency (*y*-axis) is equal to $1/(b - a)$. The probability density function can be integrated to give the cumulative probability distribution, which for the uniform distribution is given in Figure 10.12.

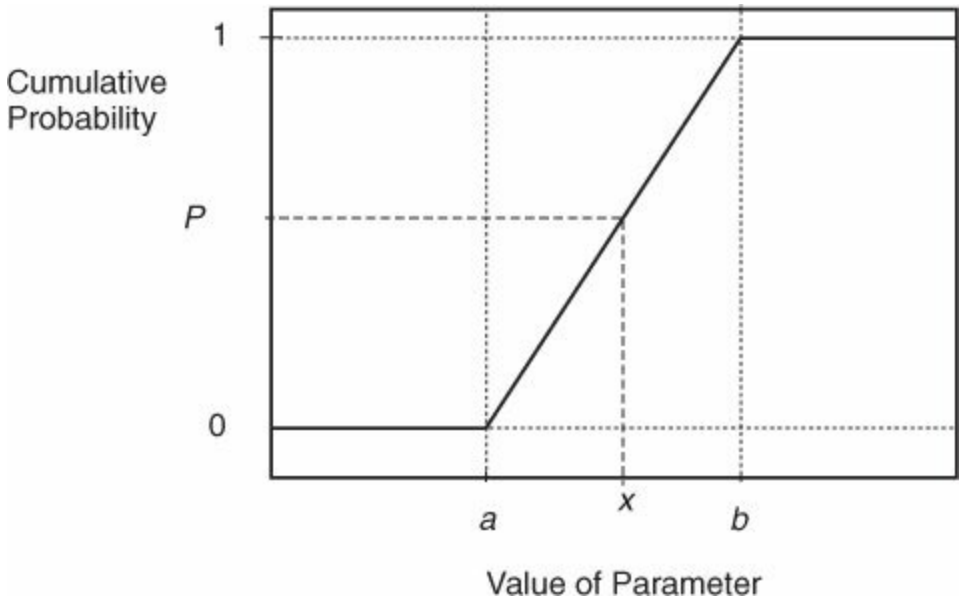


Figure 10.12. Cumulative Probability Distribution for a Uniform Probability Density Function

Figure 10.12 is interpreted by realizing that the probability of the parameter being less than or equal to x is P. Alternatively, a random, uniformly distributed value of the parameter can be assigned by choosing a random number in the range 0 to 1 (on the y-axis) and reading the corresponding value of the parameter, between a and b, on the x-axis. For example, if the random number chosen is P, then, using Figure 10.12, the corresponding value of the parameter is x. Clearly, the shapes of the density function and the corresponding cumulative distribution influence the values of the parameters that are used in the eight-step algorithm. Which probability density function should be used? Clearly, if frequency occurrence data for a given parameter are available, the distribution can be constructed. However, complete information about the way in which a given parameter will vary is often not available. The minimum data set would be the most likely value (b), and estimates of the highest (c) and lowest (a) values that the parameter could reasonably take. With this information, a triangular probability density function or distribution, shown in Figure 10.13, can be constructed. The corresponding cumulative distribution is shown in Figure 10.14. The equations describing these distributions are as follows:

Triangular probability density function:

$$p(x) = \frac{2(x-a)}{(c-a)(b-a)} \quad \text{for } x \le b$$

$$p(x) = \frac{2(c-x)}{(c-a)(c-b)} \quad \text{for } x > b \qquad (10.9)$$

Triangular cumulative probability function:

$$P(x) = \frac{(x-a)^2}{(c-a)(b-a)} \quad \text{for} \quad x \le b$$

$$P(x) = \frac{(b-a)}{(c-a)} + \frac{(x-b)(2c-x-b)}{(c-a)(c-b)} \quad \text{for} \quad x > b \qquad (10.10)$$

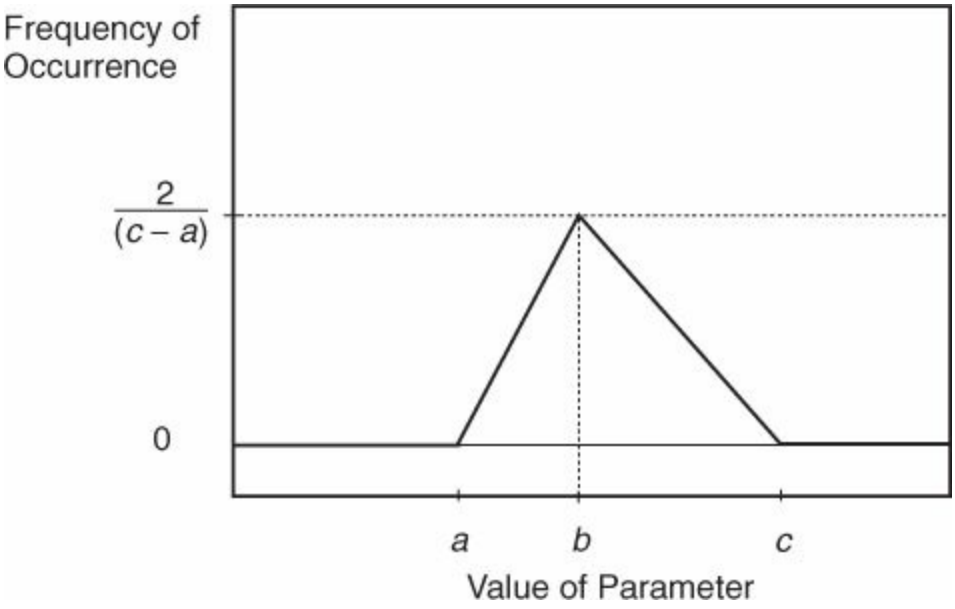


Figure 10.13. Probability Density Function for Triangular Distribution

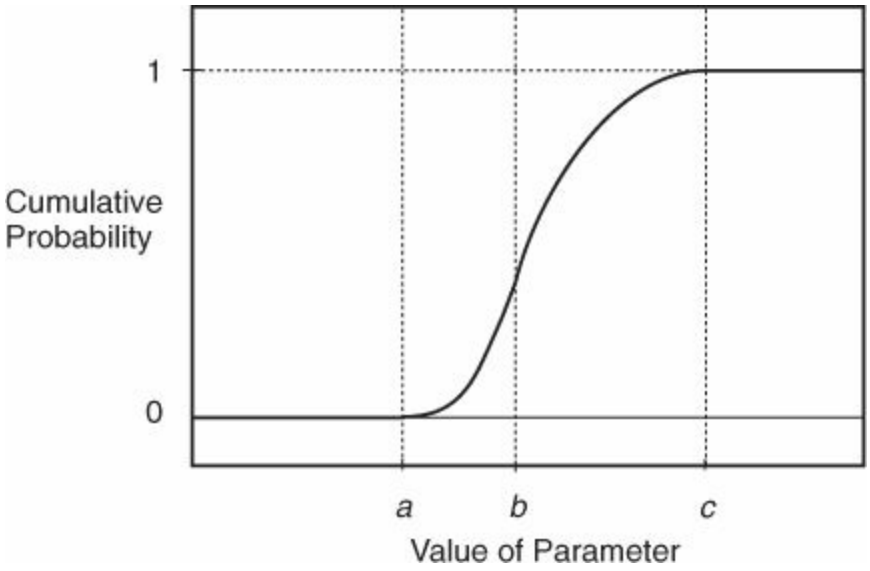


Figure 10.14. Cumulative Probability Function for Triangular Distribution

Clearly, any probability density function and corresponding cumulative probability distribution could be used to describe the uncertainty in the data. Trapezoidal, normal, lognormal, and so on, are used routinely to describe uncertainty in data. However, for simplicity, the following discussions are confined to triangular distributions. The eight-step method for quantifying uncertainty in profitability analysis is illustrated next.

Monte-Carlo Simulation. The Monte-Carlo (M-C) method is simply the concept of assigning probability distributions to parameters, repeatedly choosing variables from these distributions, and using these values to calculate a function dependent on the variables. The resulting distribution of calculated values of the dependent function is the result of the M-C simulation. Therefore, the eight-step procedure is simply a specific case of the M-C method. Each of the eight steps is illustrated using the example discussed previously in the scenario analysis.

Step 1: All the parameters for which uncertainty is to be quantified are identified. Returning to Example 10.1, historical data suggest that there is uncertainty in the predictions for revenue (R), cost of manufacturing (COM_d), and fixed capital investment (FCI_L).

Step 2: Probability distributions are assigned for all parameters in Step 1. All the

uncertainties associated with these parameters are assumed to follow triangular distributions with the properties given in Table 10.6.

Table 10.6. Data for Triangular Distributions for *R*, COM_d, and FCI_L (All $ Figures Are in Millions)

Parameter	Minimum Value (a)	Most Likely Value (b)	Maximum Value (c)
Revenue, *R*	$60.0/y	$75.0/y	$78.75/y
Cost of manufacturing, COM_d	$27.0/y	$30.0/y	$33.0/y
Fixed capital investment, FCI_L	$120.0	$150.0	$195.0

Step 3: A random number is assigned for each parameter in Step 1. First, random numbers between 0 and 1 are chosen for each variable. The easiest way to generate random numbers is to use the Rand( ) function in Microsoft's Excel program or a similar spreadsheet. Tables of random numbers are also available in standard math handbooks [8].

Step 4: Using the random number from Step 3, the value of the parameter is assigned using the probability distribution (from Step 2) for that parameter. With the value of the random number equal to the right-hand side of Equation (10.10) and using the corresponding values of *a, b*, and *c*, this equation is solved for the value of *x*. The value of *x* is the value of the parameter to use in the next step. Table 10.7 illustrates this procedure for *R*, COM_d, and FCI_L.

Table 10.7. Illustration of the Assignment of Random Values to the Parameters *R*, COM_d, and FCI_L (All $ Figures Are in Millions)

Parameter	Random Number	Random Value of Parameter	NPV
Revenue (*R*)	0.3501	$69.92/y	
Cost of manufacturing (COM_d)	0.6498	$30.49/y	$–15.60
Fixed capital investment (FCI_L)	0.9257	$179.16	

To illustrate how the random values for the parameters are obtained, consider the calculation for COM_d. The number 0.6498 was chosen at random from a uniform distribution in the range 0–1 using Microsoft's Excel spreadsheet. This number, along with values of $a = 27$, $b = 30$, and $c = 33$, are then substituted for $P(x)$ in Equation (10.10) to give

$$0.6498 = \frac{(x-27)^2}{(33-27)(30-27)} = \frac{(x-27)^2}{18} \quad \text{for } x \le b$$

$$0.6498 = \frac{(30-27)}{(33-27)} + \frac{(x-30)(2(33)-x-30)}{(33-27)(33-30)} = 0.5 + \frac{(x-30)(36-x)}{18} \quad \text{for } x > b$$

From Equation (10.10), the $P(x)$ value for $x = b$ is given by

$$P(x=30) = \frac{(30-27)^2}{(33-27)(30-27)} = \frac{9}{18} = 0.5$$

Because the value of the random number (0.6498) is greater than 0.5, the form of the equation for $x > b$ must be used. Solving for x yields:

$$0.6498 = 0.5 + \frac{(x-30)(36-x)}{18}$$

$$x^2 - 66x + 1082.6964 = 0$$

$$x = \frac{66 \pm \sqrt{(66^2 - (4)(1)(1082.6964)}}{(2)(1)} = 33 \pm 2.51 = 30.49, \textit{ or } 35.51 \text{ (impossible)}$$

Step 5: Once values have been assigned to all parameters, these values are used to calculate the profitability (NPV or other criterion) of the project. The spreadsheet given in Table E10.1 was used to determine the NPV using the values given in Table 10.7. The NPV is also shown in Table 10.7.

Step 6: Steps 3, 4 and 5 are repeated many times (say, 1000). For the sake of illustration, Steps 3, 4, and 5 were repeated 20 times to yield 20 values of the NPV. These results are summarized in Table 10.8.

Table 10.8. Results of the 20-Point Monte-Carlo Simulation

Run	Rand (1)	R ($/y)	Rand (2)	COM_d ($/y)	Rand (3)	FCI_L ($)	NPV ($)
1	0.3501	69.92	0.6498	30.49	0.9257	179.16	–15.60
2	0.4063	70.69	0.7859	31.04	0.5531	156.16	–1.45
3	0.8232	75.22	0.3046	29.34	0.7073	163.57	11.59
4	0.9691	77.28	0.6164	30.37	0.8207	170.40	10.45
5	0.4418	71.15	0.2386	29.07	0.7273	164.66	–0.34
6	0.7170	74.20	0.9794	32.39	0.8313	171.14	–4.23
7	0.5626	72.58	0.8368	31.29	0.8891	175.65	–8.84
8	0.9854	77.74	0.1836	28.82	0.8136	169.92	16.34
9	0.8200	75.19	0.7440	30.85	0.5268	155.04	12.31
10	0.6319	73.33	0.1320	28.54	0.3863	149.48	16.84
11	0.1712	66.94	0.9465	32.02	0.0406	129.56	0.99
12	0.4966	71.82	0.3921	29.66	0.5993	158.23	4.34
13	0.2781	68.84	0.1474	28.63	0.7533	166.14	–5.76
14	0.2312	68.06	0.4187	29.75	0.5165	154.60	–4.27
15	0.5039	71.90	0.0042	27.28	0.5681	156.82	12.04
16	0.2184	67.84	0.8629	31.43	0.5107	154.36	–9.44
17	0.7971	74.97	0.3452	29.49	0.0789	133.32	28.27
18	0.2068	67.63	0.7975	31.09	0.9803	186.85	–28.20
19	0.8961	76.05	0.5548	30.17	0.1497	138.35	26.43
20	0.4201	70.87	0.2047	28.92	0.5713	156.96	4.50

Step 7: A histogram or cumulative probability curve is created for the values of the profitability criterion calculated from Step 6. Using the data from Table 10.8, a cumulative probability curve is constructed. To do this, the data are ordered from lowest (–28.20) to highest (28.27), and the cumulative probability of the NPV being less than or equal to the value on the x-axis is plotted. The results are shown in Figure 10.15. The dashed line simply connects the 20 data points for this simulation. This line shows several bumps that are due to the small number of simulations. The solid line represents the data for 1000 simulations, and it can be seen that this curve is essentially smooth. The 1000-point simulation was carried out using the CAPCOST software accompanying the text. The use of the software is addressed at the end of this section.

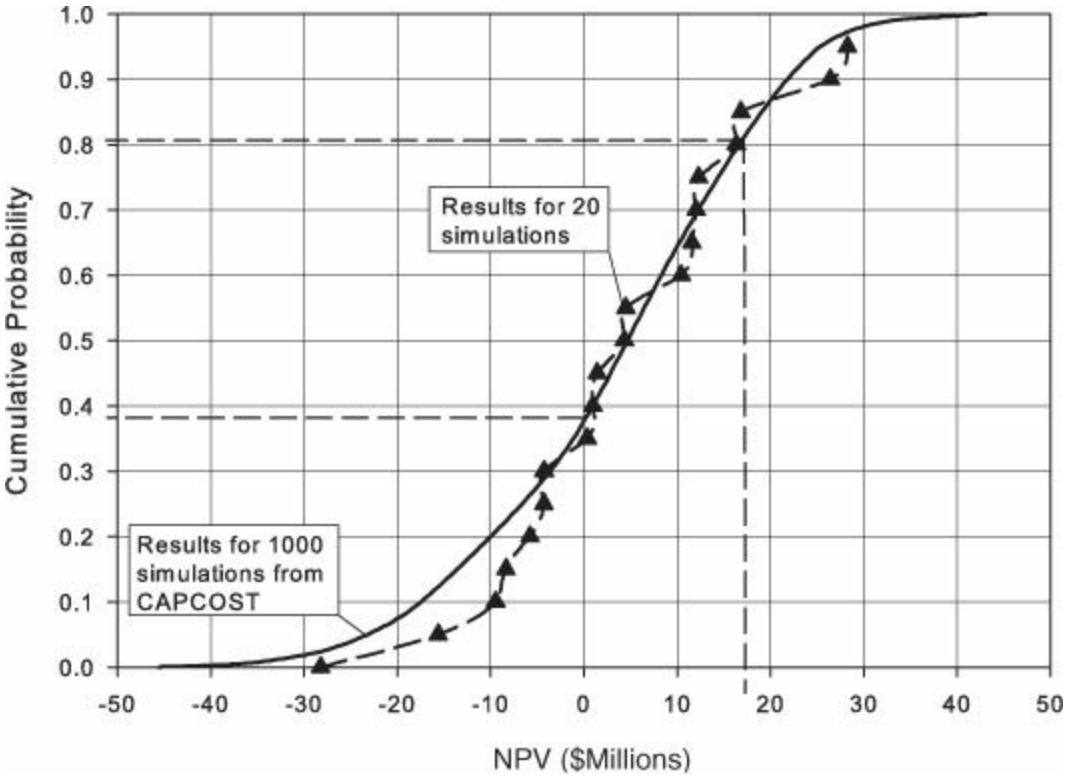


Figure 10.15. Cumulative Probability of NPV for Monte-Carlo Simulation

Step 8: The results of Step 7 are used to analyze the profitability of the project. From Figure 10.15, it can be seen that there is about a 38% chance that the project will not be profitable. The median NPV is about $5 million, and only about 21% of the values calculated lie above $17.12 million, which is the NPV calculated for the base case, using the most likely values of R, COM_d, and FCI_L.

Another way that the data from an M-C analysis can be used is in the comparison of alternatives. For example, consider two competing projects, A and B. A probabilistic analysis of both these projects yields the data shown in Figure 10.16. If only the median profitability is considered, corresponding to a cumulative probability of 0.5, then it might be concluded that Project A is better. Indeed, over a wide range of probabilities Alternative A gives a higher NPV than Alternative B. However, this type of comparison does not give the whole picture. By looking at the low end of NPV predictions, it is found that Project A has a 17% chance of returning a negative NPV compared with Project B, which is predicted to have only a 2% chance of giving a negative NPV. Clearly, the choice regarding Projects A and B must be made taking into account both the probability of success and the magnitude of the profitability. The Monte-Carlo analysis allows a far more complete financial picture to be painted, and the decisions from such information will be more profound having taken more information into account.

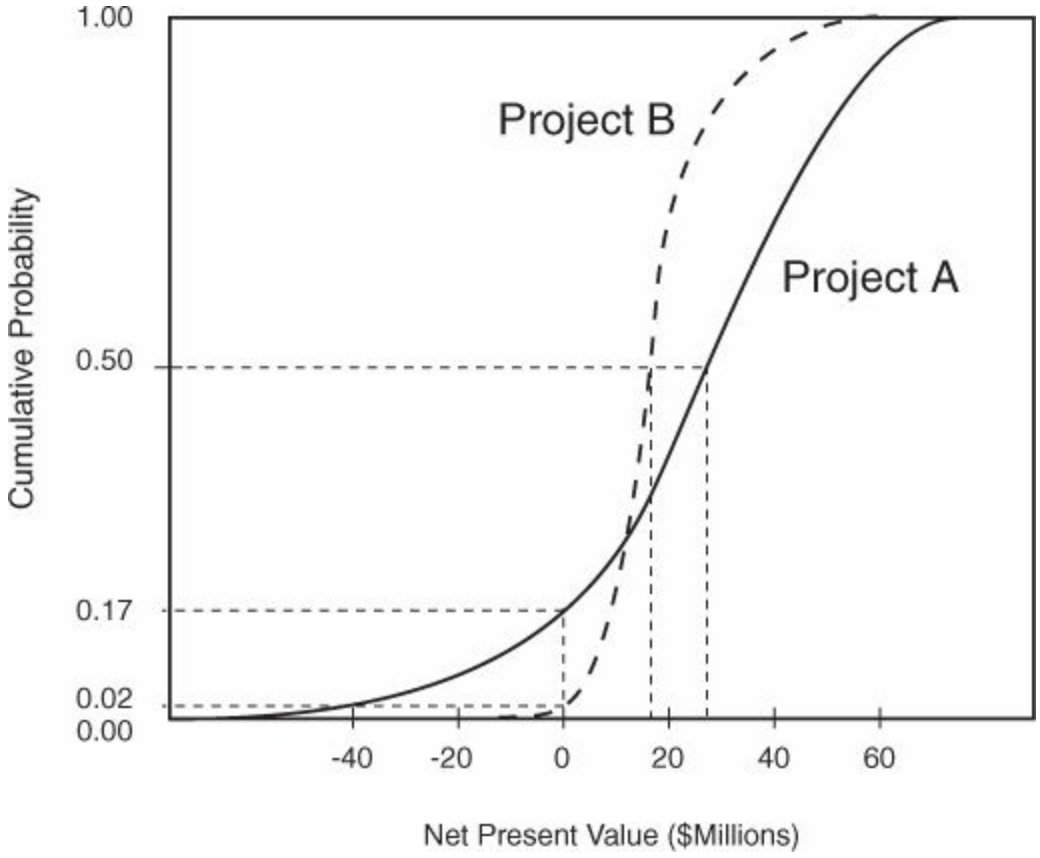


Figure 10.16. A Comparison of the Profitability of Two Projects Showing the NPV with Respect to the Estimated Cumulative Probability from a Monte-Carlo Analysis

Evaluation of the Risks Associated with Using New Technology. To this point, risks associated with predicting the items listed in Table 10.1 have been considered. For example, predictions for the variations associated with the cost of the plant, the cost of manufacturing, and the revenue generated by the plant were made. Then, by using the M-C technique, the relationship given in Figure 10.15 was generated. For processes using new technology, additional risks will be present, but these risks may be impossible to quantify in terms of the parameters given in Table 10.1. One way to take this additional risk into account is to assign a higher acceptable rate of return for projects using new technology compared with those using mature technologies. The effect of using a higher discount rate is to move the curve in Figure 10.15 to the left. This is illustrated in Figure 10.17.

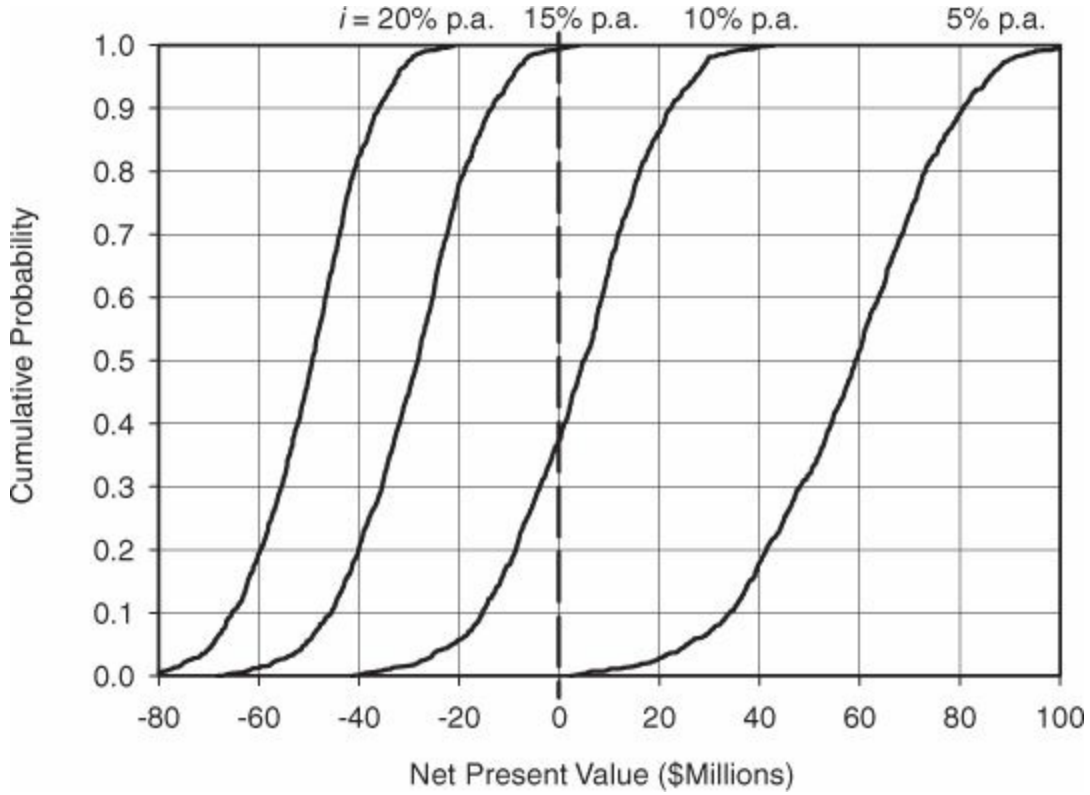


Figure 10.17. The Effect of Interest (Hurdle) Rate on Monte-Carlo Simulations

From this figure, it is apparent that if an acceptable rate of return is 15% p.a., then the project is not acceptable, whereas at a rate of 10% p.a. the project looks quite favorable. It can be argued that using a higher hurdle rate for new processes is unnecessary, because, for a new project, there will be greater ranges in the predictions of the variables, and this automatically makes the project using new technology "riskier," as the effect of broader ranges for variables is to flatten the NPV-probability curve. However, it may be impossible to estimate the effect of the new technology on, for example, the cost of manufacturing or the acceptance of a new product in the market. By specifying a higher acceptable rate of return on the investment for these projects, the interpretation between projects using new and old technologies is clear and unambiguous.

Monte-Carlo Analysis Using CAPCOST. The CAPCOST program introduced in Chapter 7 includes spreadsheets for estimating the cash flows of a project and the evaluation of profitability criteria such as NPV and DCFROR. In addition, a Monte-Carlo simulation has also been included that allows the following variables to be investigated:

- FCI_L
- Price of product
- Working capital
- Income tax rate
- Interest rate
- Raw material price
- Salvage value

By specifying the ranges over which these terms are likely to vary, a Monte-Carlo analysis for a given problem can be achieved. Distributions of criteria such as NPV and DPBP are automatically given. The reader should consult the help file on the accompanying CD for a tutorial on the use of this

software.

10.8. Profit Margin Analysis

All the techniques that have been discussed in this chapter use the fixed capital cost and the operating costs in order to evaluate the profitability of a process. Clearly, the accuracy of such predictions will depend on the accuracy of the estimates for the different costs. When screening alternative processes, it is sometimes useful to evaluate the difference between the revenue from the sale of products and the cost of raw materials. This difference is called the **profit margin** or sometimes just the margin.

$$\text{Profit Margin} = \Sigma(\text{Revenue Products}) - \Sigma(\text{Cost of Raw Materials}) \qquad (10.11)$$

If the profit margin is negative, the process will not be profitable. This is because no capital cost, utility costs, and other ancillary operating costs have been taken into account. A positive profit margin does not guarantee that the process will be profitable but does suggest that further investigation may be warranted. Therefore, the profit margin is a useful, but limited, tool for the initial screening of process alternatives. This is illustrated in Example 10.17.

Example 10.17.

Consider the maleic anhydride process shown in Appendix B.5. Estimate the profit margin for this process using the costs of raw materials and products from Table 8.4.

From Tables 8.4 and B.4 the following flowrates and costs are found:

Cost of benzene = \$0.919/kg

Cost of maleic anhydride = \$1.158/kg

Feed rate of benzene to process (Stream 1, Figure B.4.1) = 3304 kg/h

Product rate of maleic anhydride (Stream 13, Figure B.4.1) = (24.8)(98.058) = 2432 kg/h

Profit Margin = (2432)(1.) – (3304)(0.919) = – \$220.12/h or – \$220.12/(2432)

= – \$0.091/kg of maleic anhydride

Clearly, from an analysis of the profit margin, further investigation of the maleic anhydride process is not warranted.

10.9. Summary

In this chapter, the basics of profitability analysis for projects involving large capital expenditures were covered. The concepts of nondiscounted and discounted profitability criteria were introduced, as were the three bases for these criteria: time, money, and interest rate.

How to choose the economically optimum piece of equipment among a group of alternatives using the capitalized cost, the equivalent annual operating cost, and the common denominator methods was demonstrated.

The concept of incremental economic analysis was introduced and applied to an example involving large capital budgets and also to a retrofit project. It was shown that both the net present value (NPV) and the equivalent annual operating cost (EAOC) methods were particularly useful when comparing alternatives using discounted cash flows.

Finally, the concept of assigning probabilities to variables in order to quantify risk was discussed. The Monte-Carlo technique was introduced, and its application to simulate the cumulative

distribution of net present values of a project was described. The interpretation of results from this technique was presented. Finally, the simulation of risk and the analysis of data using the CAPCOST package was illustrated by an example.

What You Should Have Learned

- There are discounted (including the time value of money) and nondiscounted methods (which do not include the time value of money) for estimating profitability, which may give different results.
- There are time-based, cash-based, and interest-rate-based methods for estimating profitability, which usually give the same result within the same discounted or nondiscounted category.
- Incremental analysis is needed when comparing alternatives that require different amounts of capital expenditures.
- NPV, EAOC, and DCFROR tend to give the most reliable results.
- Monte-Carlo analysis can be used to include the effect of parameter uncertainty in the NPV, EAOC, and DCFROR.

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Short Answer Questions

1. The evaluation of a project requiring a large capital investment has yielded an NPV (net present value) of $\$20 \times 10^6$. If the internal hurdle rate for this project was set at 10% p.a., will the DCFROR (discounted cash flow rate of return) be greater or less than 10%? Explain.
2. The following are results of a recent evaluation of two projects. Which would you choose? Defend your choice. Your opportunity cost for capital is 15%.

	NPV	DCFROR
Project A	10	55%
Project B	10,000	16%

3. Explain the concept of an incremental economic analysis.
4. When comparing two pieces of equipment for a given service, if each piece of equipment has the same life and each costs the same, would the amount of maintenance required for the equipment be an important factor? Why?
5. What economic criterion would you use to choose the best piece of equipment among three alternatives, each with a different operating cost, capital cost, and equipment life?
6. Do you agree with the statement "Monte-Carlo simulation enables the design engineer to eliminate risk in economic analysis"? Please explain your answer.
7. In evaluating a large project, what are the advantages and disadvantages of probabilistic analysis?

Problems

For the following problems, unless stated otherwise, you may assume that the cost of land, L, and the salvage value, S, of the plant are both zero.

8. The projected costs for a new plant are given below (all numbers are in $\$10^6$).

   Land cost = \$7.5

   Fixed capital investment = \$120 (\$60 at end of year 1, \$39.60 at end of year 2, and \$20.40 at end of year 3)

   Working capital = \$35 (at start-up)

   Start-up at end of year 3

   Revenue from sales = \$52

   Cost of manufacturing (without depreciation) = \$18

   Tax rate = 40%

   Depreciation method = Current MACRS over 5 years

   Length of time over which profitability is to be assessed = 10 years after start-up

   Internal rate of return = 9.5% p.a.

   For this project, do the following:

   a. Draw a cumulative (nondiscounted) after-tax cash flow diagram.

   b. From Part (a), calculate the following nondiscounted profitability criteria for the project:

      (i) Cumulative cash position and cumulative cash ratio

      (ii) Payback period

      (iii) Rate of return on investment

   c. Draw a cumulative (discounted) after-tax cash flow diagram.

   d. From Part (c), calculate the following discounted profitability criteria for the project:

      (i) Net present value and net present value ratio

      (ii) Discounted payback period

(iii) Discounted cash flow rate of return (DCFROR)

9. Repeat Problem 10.8 using a straight-line depreciation method over 7 years. Compare the results with those obtained in Problem 10.8. Which depreciation method would you use?

10. The following expenses and revenues have been estimated for a new project:

Revenues from sales = $\$4.1 \times 10^6$/y

Cost of manufacturing (excluding depreciation) = $\$1.9 \times 10^6$/y

Taxation rate = 40%

Fixed capital investment = $\$7.7 \times 10^6$

(two payments of $\$5 \times 10^6$ and $\$2.7 \times 10^6$ at the end of years 1 and 2, respectively)

Start-up at the end of year 2

Working capital = $\$2 \times 10^6$ at the end of year 2

Land cost = $\$0.8 \times 10^6$ at the beginning of the project (time = 0)

Project life (for economic evaluation) = 10 y after start-up

For this project, estimate the NPV of the project assuming an after-tax internal hurdle rate of 11% p.a., using the following depreciation schedules:

a. MACRS method for 5 years

b. Straight-line depreciation with an equipment life (for depreciation) of 9.5 years Comment on the effect of discounting on the overall profitability of large capital projects.

11. In reviewing current operating processes, the company accountant has provided you with the following information about a small chemical process that was built ten years ago.

Capital investment = $\$30 \times 10^6$ ($\$10 \times 10^6$ at the end of year 1, $\$15 \times 10^6$ at the end of year 2, $\$5 \times 10^6$ at the end of year 3. Working capital = $\$10 \times 10^6$)

Year after Start-up	Yearly After-Tax Cash Flow ($\$10^6$/y)
1	7.015
2	6.206
3	6.295
4	6.852
5	6.859
6	7.218
7	5.954
8	5.459
9	5.789
10	5.898

Over the last ten years, the average (after-tax) return on investment that non-process projects have yielded is 10%.

a. What is the DCFROR for this project over the last 12 years? (Ignore land and working capital costs.)

b. In retrospect, was the decision to build this plant a good one?

12. The after-tax cash flows for a new chemical process are shown in Table P10.12. Using these data, calculate the following:
    a. Payback period (PBP)
    b. Cumulative cash position (CCP) and cumulative cash ratio (CCR)
    c. Rate of return on investment (ROROI)
    d. Discounted payback period (DPBP)
    e. Net present value (NPV)
    f. Discounted cash flow rate of return (DCFROR)

Table P10.12. Nondiscounted Cash Flow Calculations for Problem 10.12 (All Figures Are in $Millions)

End of Year	Capital Investment	Depreciation Allowance	Revenue from Sales	Total Annual Costs	Net Profit	Income Tax	Net Profit after Tax	After-Tax Cash Flow
0	(10)*,**	—	—	—	—	—	—	(10)
1	(25)	—	—	—	—	—	—	(25)
2	(20)	—	—	—	—	—	—	(20)
3	(15 + 20)†,‡	—	—	—	—	—	—	(35)
4		8.57	60	50	10	3.80	6.20	14.77
5	—	8.57	120	92	28	10.64	17.36	25.93
6	—	8.57	120	47	73	27.74	45.26	53.83
7	—	8.57	120	50	70	26.80	43.40	51.97
8	—	8.57	120	60	60	22.80	37.20	45.77
9	—	8.57	120	51	69	26.22	42.78	51.35
10	—	—	120	40	80	30.40	49.60	58.17
11	—	—	120	40	80	30.40	49.60	49.60
12		—	120	40	80	30.40	49.60	49.60
13	50	—	120	40	80	30.40	49.60	49.60

*Numbers in ( ) represent negative values.
**Land cost = 0 .
†Plant started up at end of year 3.
‡Working capital = 50.

Use a 10% discount rate for Parts (d) and (e).

13. From the data given in Table P10.12, determine the following information regarding the calculations performed for this analysis:
    a. What taxation rate was assumed?
    b. What was the total fixed capital investment?
    c. What method of depreciation was used?
    d. What was the cost of manufacturing, not including depreciation?

14. Consider the following two new chemical plants, each with an initial fixed capital investment (year 0) of $\$15 \times 10^6$. Their cash flows are as follows:

Year	Process 1 ($million/y)	Process 2 ($million/y)
1	3.0	5.0
2	8.0	5.0
3	7.0	5.0
4	5.0	5.0
5	2.0	5.0

a. Calculate the NPV of both plants for interest rates of 6% and 18%. Which plant do you recommend? Explain your results.

b. Calculate the DCFROR for each plant. Which plant do you recommend?

c. Calculate the nondiscounted payback period (PBP) for each plant. Which plant do you recommend?

d. Explain any differences in your answers to Parts (a), (b), and (c).

15. In a design, you have the choice of purchasing one of the following batch reactors:

Costs	A	B	C
Material of Construction	CS	SS	Hastalloy
Installed Cost	$15,000	$25,000	$40,000
Equipment Life	3 y	5 y	7 y
Yearly Maintenance Cost	$4000	$3000	$2000

If the internal rate of return for such comparisons is 9% p.a., which of the alternatives is least costly?

16. Two pieces of equipment are being considered for an identical service. The installed costs and yearly operating costs associated with each piece of equipment are as follows:

Costs	A	B
Installed Cost	$5000	$10,000
Operating Cost	$2000/y	$1000/y
Equipment Life	5 y	7 y

a. If the internal hurdle rate for comparison of alternatives is set at 15% p.a., which piece of equipment do you recommend be purchased?

b. Above what internal hurdle rate would you recommend Project A?

17. Your company is considering modifying an existing distillation column. A new reboiler and condenser will be required, along with several other peripherals. The equipment lists are as follows:

Option 1

Equipment	Installed Cost ($)	Operating Cost ($/y)	Equipment Life (y)
Condenser	50,000	7000	10
Reboiler	75,000	5000	15
Reflux Pump	7500	8000	10
Reflux Drum	12,500	—	10
Piping	8000	—	15
Valves	6500	—	10

Option 2

Equipment	Installed Cost ($)	Operating Cost ($/y)	Equipment Life (y)
Condenser	75,000	4000	15
Reboiler	75,000	5000	15
Reflux Pump	10,500	5000	15
Reflux Drum	14,500	—	15
Piping	8000	—	15
Valves	6500	—	10

The internal hurdle rate for comparison of investments is set at 12% p.a. Which option do you recommend?

18. Because of corrosion, the feed pump to a batch reactor must be replaced every three years. What is the capitalized cost of the pump?

Data:

Purchased cost of pump = $35,000

Installation cost = 75% of purchased cost

Internal hurdle rate = 10% p.a.

19. Three alternative pieces of equipment are being considered for solids separation from a liquid slurry:

Equipment Type	Capital Investment ($)	Operating Cost ($/y)	Service Life (y)
Rotary Vacuum Filter	15,000	3000	6
Filter Press	10,000	5000	8
Hydrocyclone and Centrifuge	25,000	2000	10

If the internal hurdle rate for this project is 11% p.a., which alternative do you recommend?

20. A change in air pollution control equipment is being considered. A baghouse filter is being considered to replace an existing electrostatic precipitator. Consider the costs and savings for the project in the following data:

Cost of new baghouse filter = $250,000

Projected utility savings = $70,000/y

Time over which cost comparison should be made = 7 years

Internal hurdle rate = 7% p.a.

Should the baghouse filter be purchased and installed?

21. In considering investments in large capital projects, a company is deciding in which of the following projects it will invest:

(All Values in $million)	Project A	Project B	Project C
Capital Required (in year 0)	80	100	120
After-tax, yearly cash flow (years 1–10)	11	14	16

The company can always invest its money in long-term bonds that currently yield 5.5% p.a. (after tax). In which, if any, of the projects should the company invest if the capital ceiling for investment is $250 million and a project life of 10 years is assumed? Would you argue to raise the investment ceiling?

22. Because you live in a southern, warm-weather climate, your electricity bill is very large for about eight months of the year due to the need for air conditioning. You have been approached by an agency that would like to assist you in installing solar panels to provide electricity to run your air conditioning. You were also considering adding additional insulation to your house. You also have the option of doing nothing. Which of the following options would you choose based on the given data?

a. Do nothing.

b. Install only the solar collector.

c. Install only the insulation.

d. Install both the solar collector and the insulation.

Data (all figures in $thousands)

Purchase and installation cost of solar collector	25
Purchase and installation of insulation	5
Current cooling bill	2.5/y
Expected savings from insulation alone	0.9/y
Expected savings from solar collector alone	2.0/y
Expected savings from insulation and solar collector	2.5/y
Other maintenance on house	2.0/y
Assessed value of house (2007)	300
Interest rate of savings if do not spend money	6.5% p.a.
Number of years assumed lifetime of insulation and solar collector	15

If there were a tax credit for installing the solar collector in the year in which it was installed, how much of a tax credit (in % of initial investment) would be required to make the solar collector alone a worthwhile investment?

23. You have been asked to evaluate several investment opportunities for the biotechnology company for which you work. These potential investments concern a new process to manufacture a new, genetically engineered pharmaceutical. The financial information on the process alternatives are as follows:

Case	Capital Investment ($million)	Yearly, After-Tax Cash Flow ($million/y)
Base	75	19
Alternative 1	15	3
Alternative 2	25	5
Alternative 3	30	7

For the alternatives, the capital investment and the yearly after-tax cash flows are incremental to the base case. The assumed plant life is 12 years, and all of the capital investment occurs at time = 0.

a. If an acceptable, nondiscounted rate of return on investment (ROROI) is 25% p.a., which is the best option?

b. If an acceptable, after-tax, discounted rate of return is 15% p.a., which option is the best?

24. Your company is considering investing in a process improvement that would require an initial capital investment of $500,000. The projected increases in revenue over the next seven years are as follows:

Year	Incremental Revenue ($thousand/y)
1	100
2	90
3	90
4	85
5	80
6	80
7	75

a. The company can always leave the capital investment in the stock portfolio, which is projected to yield 8% p.a. over the next seven years. What should the company do?

b. What is the break-even rate of return between the process improvement and doing nothing?

c. If the capital investment could be changed without changing the incremental revenues, what capital investment changes this investment from being profitable (not profitable) to being not profitable (profitable)?

25. During the design of a new process to manufacture nanocomposites, several alternative waste treatment processes are being considered. The base case is the main waste treatment process, and the options are modifications to the base case. Not all options are compatible with each other, and the economic data on the only possible combinations are as follows:

Case	Capital Investment ($million)	Annual, After-Tax Cash Flow ($thousand/y)
Base	5.0	750
Base + option 1	5.1	770
Base + option 1 + option 2	5.3	790
Base + option 3	5.2	782
Base + option 1 + option 3	5.4	810

The nondiscounted, internal hurdle rate for investment is 14% p.a., after tax. Which waste treatment process do you recommend?

26. The installation of a new heat exchanger is proposed for the batch crystallization step in an existing pharmaceutical manufacturing process. The heat exchanger costs $49,600 (installed) and saves $8000/y in operating costs. Is this a good investment based on a before-tax analysis?

Data:

Internal hurdle rate = 12% p.a. (after tax)

Taxation rate = 40%

5-year MACRS depreciation used

Service life of heat exchanger = 12 y

27. A process for the fabrication of microelectronic components has been designed. The required before-tax return on investment is 18% p.a., and the equipment life is assumed to be eight years.

	Base-Case Design	Alternative 1	Alternative 2
Capital Investment ($million)	21	—	—
Additional Investment ($million)	—	2.15	1.35
Product Revenue ($million/y)	12	12	12
Raw Material Costs ($million/y)	5.1	5.1	5.1
Other Operating Costs ($million/y)	0.35	0.27	0.31

a. Do you recommend construction of the base-case process?

b. Do you recommend including either of the process alternatives?

c. Suppose there were another alternative, compatible with either of the previous alternatives, requiring an additional $3.26 million capital investment. What savings in operating cost would be required to make this alternative economically attractive?

28. A new pharmaceutical plant is expected to cost (FCI_L) $25 million, and the revenue (R) from the sale of products is expected to be $10 million/y for the first four years of operation and $15 million/y thereafter. The cost of manufacturing without depreciation (COM_d) is projected to be $4 million/y for the first four years and $6 million/y thereafter. The cost of land (at the end of year zero) is $3 million, the working capital at start-up (which occurs at the end of year 2) is $3 million, and the fixed capital investment is assumed to be paid out as $15 million at the end of year 1 and $10 million at the end of year 2. Yearly income starts in year 3, and the plant life is ten years after start-up. The before-tax criterion for profitability is 17%. Assume the plant has no

salvage value, but that the cost of land and the working capital are recovered at the end of the project life.

a. Draw a labeled, discrete, nondiscounted cash flow diagram for this project.

b. Draw a labeled, cumulative, discounted (to year zero) cash flow diagram for this project.

c. What is the NPV for this project? Do you recommend construction of this plant?

29. How much would you need to save annually to be willing to invest $1.75 million in a process improvement? The internal hurdle rate for process improvements is 18% before taxes over eight years.

30. How much would you be willing to invest in a process improvement to save $2.25 million/y? The internal hurdle rate for process improvements is 15% before taxes over six years.

31. You can invest $5.1 million in a process improvement to save $0.9 million/y. What internal hurdle rate would make this an attractive option? The assumed lifetime for these improvements is nine years.

32. Recommend whether your company should invest in the following process: The internal hurdle rate is 17% p.a., before taxes, over an operating lifetime of 12 years. The fixed capital investment is made in two installments: $5 million at time zero and $3 million at the end of year 1. At the end of year 1, $1 million in working capital is required. For the remainder of the project lifetime, $2 million in income is realized.

33. You are considering two possible modifications to an existing microelectronics facility. The criterion for profitability is 18% p.a. over six years. All values are in $million.

	Alternative 1	Alternative 2
Project Cost	2.25	3.45
Yearly Savings	0.65	0.75

a. What do you recommend based on a nondiscounted ROROII analysis?

b. What do you recommend based on an INPV analysis?

c. Based on the results of Parts (a) and (b), what do you recommend?

34. A new biotech plant is expected to cost (FCI_L) $20 million, with $10 million paid at the beginning of the project and $10 million paid at the end of year 1. There is no land cost because the land is already owned. The annual profit, before taxes, is $4 million and the working capital at start-up (which occurs at the end of year 1) is $1 million, The plant life is 10 years after start-up. The before-tax criterion for profitability is 12%. Assume that the plant has no salvage value, and that the working capital is recovered at the end of the project life.

a. Draw a labeled, discrete, nondiscounted cash flow diagram for this project.

b. Draw a labeled, cumulative, discounted (to year zero) cash flow diagram for this project.

c. What is the NPV for this project? Do you recommend construction of this plant?

d. What would the annual profit, before taxes, have to be for the NPV to be $2 million?

e. The plant is built and has been operational for several years. It has been suggested that $3 million be spent on plant modifications that will save money. Your job is to analyze the suggestion. The criterion for plant modifications is a 16% before-tax return over five years. How much annual savings are required before you would recommend in favor of investing in

the modification?

35. You are responsible for equipment selection for a new micro-fiber process. A batch blending tank is required for corrosive service. You are considering three alternatives:

Alternative	Material	Cost ($thousand)	Maintenance Cost ($thousand/y)	Equipment Life (y)
A	Carbon Steel	5	5.5	3
B	Ni Alloy	15	3.5	5
C	Hastalloy	23	2.5	9

The after-tax internal hurdle rate is 14% p.a. Which alternative do you recommend?

36. In an already operational pharmaceutical plant, you are considering three alternative solvent-recovery systems to replace an existing combustion process. The internal hurdle rate is 15% after taxes over eight years. Which alternative do you recommend?

Alternative	Total Module Cost of System ($thousands)	Natural Gas Savings ($thousand/y)	Savings in Solvent Cost ($thousand/y)	Net Maintenance Savings ($thousand/y)
A	88	15	25	33
B	125	15	45	25
C	250	15	75	18

37. A condenser using refrigerated water is being considered for the recovery of a solvent used in a pharmaceutical coating operation. The amount of solvent recovered from the gas stream is a function of the temperature to which it is cooled. Three cases, each using a different exchanger and a different amount of refrigerated water, are to be considered. Data for the process cases are given in the table.

Case	Installed Cost of Exchanger ($)	Cost of Refrigerated Water ($/y)	Value of Acetone Recovered ($/y)
A	103,700	15,000	32,500
B	162,400	30,000	65,000
C	216,100	34,500	74,750

a. If the nondiscounted hurdle rate for projects is set at 15% p.a., which case do you recommend?

b. If the discounted hurdle rate is set at 5% p.a. and the project life is set at 7 years, which case do you recommend?

c. How does your result from Part (b) change if the project life were changed to 15 years?

d. How does your result from Part (b) change if the project life were changed to 5 years?

38. For Problem 10.8, uncertainties associated with predicting the revenues and cost of manufacturing are estimated to be as follows:

Revenue: Expected range of variation from base case, low = \$45 million, high = \$53.5 million

COM_d: Expected range of variation from base case, low = \$16 million, high = \$21.5 million

Using the above information, evaluate the expected distribution of NPVs and DCFRORs for the project. Would this analysis change your decision compared to that for the base case?

39. Calculate the lowest and highest NPVs that are possible for Problem 10.38. Compare these values with the distribution of NPVs from Problem 10.38. What are the probabilities of getting an NPV within \$5 million of these values?

40. Perform a Monte-Carlo analysis on Problem 10.10, using the following ranges for uncertain variables (all figures in \$millions):

	Low	High
FCI_L	6.6	9.3
Revenues	3.5	4.5
Interest rate (%)	9.5	12.0
COM_d	1.7	2.5

What do you conclude? *Hint*: When using the CAPCOST program, set the equation for $COM_d = C_{raw\ materials}$ and input the variability in COM_d as a variability in the cost of raw materials.

41. You are considering buying a house with a mortgage of \$250,000. The current interest rates for a mortgage loan for a 15-year period are 7.5% p.a. fixed or 6.75% p.a. variable. Based on historical data, the variation in the variable rate is thought to be from a low of 6.0% to a high of 8.5%, with the most likely value as 7.25%. The variable interest rate is fixed at the beginning of each year. Answer the following questions:

    a. What are the maximum and minimum yearly payments that would be expected if the variable interest option is chosen? For simplicity assume that the compounding period is one year.

    b. Set up a Monte-Carlo simulation by picking 20 random numbers and using these to choose the variable interest rate for each of the 20 years of the loan.

    c. Calculate the yearly payments for each year using the data from Part (b). *Hint*: You should keep track of the interest paid on the loan and the remaining principal. The remaining principal is used to calculate the new yearly payment with the new yearly interest rate.

42. Perform a Monte-Carlo simulation on Example 10.1 for the following conditions. Show that the variation in the NPV is the same as shown in Figure 10.15. To which variable is the NPV more sensitive?

	Low	High
FCI_L	–20%	35%
Product Price	–25%	10%
Raw Material Price	–10%	25%

Note: Because the Monte-Carlo method is based on the generation of random numbers, no two simulations will be exactly the same. Therefore, you may see some small differences between your results and those shown in Figure 10.15.

43. A product is to be produced in a batch process. The estimated fixed capital investment is \$5

million. The estimated raw materials cost is $100,000/batch, the estimated utility costs are $60,000/batch, and the estimated waste treatment cost is $23,000/batch. The revenue is predicted to be $220,000/batch. An initial scheduling scenario suggests that it will be possible to produce 22 batches/y. The internal hurdle rate is 15% p.a. before taxes over 10 years.

a. Is this process profitable?

b. What is the minimum number of batches/y that would have to be produced to make the process profitable?

c. If 26 batches/y is the maximum that can be produced, what is the rate of return on the process?

44. Three different products are manufactured in an existing batch process. The details are as follows:

Product	kg/batch	Product Value ($/kg)	Batches/y
A	5000	7.5	20
B	2500	6.25	13
C	4000	5.75	16

The cost of manufacturing is $0.95 million/y. The demand for these products is increasing, and the crystallization step has been determined to be the bottleneck to increasing the capacity. It is desired to add 25% capacity to this process. The internal hurdle rate for process improvements is 17% p.a. over five years.

a. If a new batch crystallizer, which allows for a 25% capacity increase, costs $750,000, do you recommend this process improvement?

b. Capital funds are tight, and it has been determined that the maximum investment possible is $600,000, resulting in a smaller new crystallizer. Using this crystallizer, identical profitability as found in Part (a) has been determined. Determine what capacity increase results from purchasing the smaller crystallizer.

c. Suppose that it is now possible to purchase the $750,000 crystallizer, thereby increasing capacity by 25%. However, the purchase of this crystallizer requires that the DCFROR (for this incremental investment) be at least 40% over five years. Is this DCFROR reached?

45. A batch process runs on a zero-wait-time schedule (see Chapter 3). It has been determined that a 20% increase in capacity is possible if three equally sized storage tanks are purchased, and the processing schedule is altered appropriately. The cost of manufacture is $1.5 million/y with revenues of $2.75 million/y. The internal hurdle rate for process improvements is 20% p.a. over six years.

a. If each tank costs $1.7 million, do you recommend the investment?

b. What is the maximum cost per storage tank that will meet the profitability criterion and result in a 20% increase in capacity?

c. Suppose that storage tanks each cost $2.0 million but still result in a 20% increase in capacity. What is the DCFROR for the recommended process improvement?

Section III: Synthesis and Optimization of Chemical Processes

In this section, the problems of how to create, simulate, and optimize a process and how to develop a process flow diagram (PFD) are addressed. In order to create a PFD, a considerable amount of information needs to be gathered. This includes reaction kinetics, thermodynamic property data, required purity for products and by-products, types of separations to be used in the process, reactor type, range of conditions for the reaction, and many others. Once this information has been gathered, it must be synthesized into a working process. In order to accommodate the synthesis of information, the chemical engineer relies on solving material balances, energy balances, and equilibrium relationships using a process simulator. The basic data required to perform a simulation of a process are covered, and other aspects of using a process simulator are discussed. Once the PFD has been simulated, the optimization of the process can proceed. In general, process optimization involves both parametric and topological changes, and both these aspects are discussed.

Advanced topics in steady-state and dynamic simulation are covered, and the role and importance of the control system in obtaining stable dynamic simulations are discussed. The regulation of process conditions and the various control strategies used in process plants along with an introduction to digital control logic are covered.

All this material is treated in the following chapters:

Chapter 11: Utilizing Experience-Based Principles to Confirm the Suitability of a Process Design

When designing a process, the experienced engineer will often have a good idea as to how large a given piece of equipment needs to be or how many stages a given separation will require. Such information is invaluable in the early stages of design to check the reasonableness of the results of rigorous calculations. To assist the inexperienced engineer, a series of heuristics or guidelines for different equipment is presented in the form of tables.

Chapter 12: Synthesis of the PFD from the Generic BFD

The information required to obtain a base-case process flow diagram is discussed and categorized into the six basic elements of the generic block flow process diagram. The need to obtain reaction kinetics, thermodynamic data, and alternative separation methods is discussed in the context of building a base-case process. Special emphasis is placed on alternative distillation schemes and the sequencing of columns needed for such separations.

Chapter 13: Synthesis of a Process Using a Simulator and Simulator Troubleshooting

The structure of a typical process simulator and the basic process information required to simulate a process are discussed. The various types of equipment that can be simulated, and the differences between alternative modules used to simulate similar process equipment, are reviewed. The importance of choosing the correct thermodynamic package for physical property estimation is emphasized, and strategies to eliminate errors and solve simulation problems are presented. Finally, some advanced techniques for evaluating and implementing thermodynamic models for electrolyte systems and systems involving solid compounds are covered.

Chapter 14: Process Optimization

Basic definitions used to describe optimization problems are presented. The need to look at both topological changes in the flowsheet (rearrangement of equipment) and parametric changes (varying temperature, pressure, etc.) is emphasized. Strategies for both types of optimization are included. A section on batch systems, including batch scheduling and optimal batch cycle times, is included.

Chapter 15: Pinch Technology

The concepts of pinch technology as applied to the design of new heat- and mass-exchange networks are presented. The design of the network requiring the minimum utility consumption and the minimum number of exchangers is developed for a given minimum temperature or concentration approach. The temperature- and concentration-interval diagrams, the cascade diagram, and the cumulative enthalpy and cumulative mass-exchange diagrams are presented. The identification of the pinch point and its role in the design of the exchanger network are discussed. Finally, the estimation of the heat-exchanger network surface area for a given approach temperature and the effect of operating pressure and materials of construction on the optimum, minimum temperature approach are discussed.

Chapter 16: Advanced Topics Using Steady-State Simulators

The material from Chapter 13 is expanded to include the advanced topics of convergence, optimization, and sensitivity studies. The various numerical techniques used in the common process simulators to converge large, complicated, and highly coupled process flowsheets are discussed and compared to show which techniques are preferred for different classes of problems.

Chapter 17: Using Dynamic Simulators in Process Design

The transient response to process disturbances is covered in this chapter. The differences between steady-state and dynamic simulators are discussed, and a brief review of the numerical techniques required to solve the latter is given. The importance of the control system for stable converged dynamic simulations is emphasized with several examples.

Chapter 18: Regulation and Control of Chemical Processes with Applications Using Commercial Software

Using examples from earlier chapters in this section, it is shown how a deviation in output from a piece of equipment can be controlled by altering an input. This is different from, and complementary to, what is treated in a typical process control class. The concepts behind different advanced control strategies and the fundamentals of digital control logic are discussed. Finally, how the elements of dynamic modeling, control structure, and digital logic are combined in the design of an operator training simulator (OTS) is covered.

Chapter 11. Utilizing Experience-Based Principles to Confirm the Suitability of a Process Design

What You Will Learn

- There are experienced-based heuristics that can be used to estimate unknown parameters and validate calculated parameters used to design a chemical process.

Experienced chemical engineers possess the skills necessary to perform detailed and accurate calculations for the design, analysis, and operation of equipment and chemical processes. In addition, these engineers will have formulated a number of experienced-based shortcut calculation methods and guidelines useful for the following:

1. Checking new process designs
2. Providing equipment size and performance estimates
3. Helping troubleshoot problems with operating systems
4. Verifying that the results of computer calculations and simulations are reasonable
5. Providing reasonable initial values for input into a process simulator required to achieve program convergence
6. Obtaining approximate costs for process units
7. Developing preliminary process layouts

These shortcut methods are forms of heuristics that are helpful to the practicing engineer. All heuristics are, in the final analysis, fallible and sometimes difficult to justify. They are merely plausible aids or directions toward the solution of a problem [1]. Especially for the heuristics described in this chapter, the four characteristics of any heuristic should be kept in mind:

1. A heuristic does not guarantee a solution.
2. It may contradict other heuristics.
3. It can reduce the time to solve a problem.
4. Its acceptance depends on the immediate context instead of on an absolute standard.

The fact that one cannot precisely follow all heuristics all the time is to be expected, as it is with any set of technical heuristics. However, despite the limitations of heuristics, they are nevertheless valuable guides for the process engineer.

In Chapter 6, process units and stream conditions that were identified as areas of special concern were analyzed. These areas were highlighted in a series of informational tables. In this chapter, the analysis of chemical processes will be completed by checking the equipment parameters and stream conditions in the PFD for agreement with observations and experiences in similar applications.

The required information to start an analysis is provided in a series of **informational tables** containing shortcut calculation techniques. In this chapter, the use of these resources is demonstrated by checking the conditions given in the basic toluene hydrodealkylation PFD.

11.1. The Role of Experience in the Design Process

The following short narrative illustrates a situation that could be encountered early in your career as an engineer.

> *You are given an assignment that involves writing a report that is to be completed and presented in two weeks. You work diligently and feel confident you have come up with a respectable solution. You present the written report personally to your director (boss), who asks you to summarize only your final conclusions. Immediately after you provide this information, your boss declares that "your results must be wrong" and returns your report unopened and unread.*
>
> *You return to your desk angry. Your comprehensive and well-written report was not even opened and read. Your boss did not tell you what was wrong, and you did not receive any "partial credit" for all your work. After a while, you cool off and review your report. You find that you had made a "simple" error, causing your answer to be off by an order of magnitude. You correct the error and turn in a revised report.*
>
> *What remains is the nagging question, "How could your boss know you made an error without having reviewed your report or asking any questions?"*

The answer to this nagging question is probably a direct result of your director's experience with a similar problem or knowledge of some guideline that contradicted your answer. The ability of your boss to transfer personal experience to new situations is one reason why he or she was promoted to that position.

It is important to be able to apply knowledge gained through experience to future problems.

11.1.1. Introduction to Technical Heuristics and Shortcut Methods

A **heuristic** is a statement concerning equipment sizes, operating conditions, and equipment performance that reduces the need for calculations. A **shortcut method** replaces the need for extensive calculations in order to evaluate equipment sizes, operating conditions, and equipment performance. These are referred to as "back-of-the-envelope calculations." In this text, both of these experience-based tools are referred to as guidelines or heuristics.

The guidelines provided in this chapter are limited to materials specifically covered in this text (including problems at the end of the chapters). All such material is likely to be familiar to final-year B.S. chemical engineering students and new graduates as a result of their education. Upon entering the work force, engineers will develop guidelines that apply specifically to their area of responsibility.

Guidelines and heuristics must be applied with an understanding of their limitations. In most cases, a novice chemical engineer should have sufficient background to apply the rules provided in this text.

The narrative started earlier is now revisited. The assignment remains the same; however, the approach to solving the problem changes.

> *Before submitting your report, you apply a heuristic that highlights an inconsistency in your initial results. You then review your calculations, find the error, and make corrections before submitting your report. Consider two possible responses to this report:*
>
> 1. *Your boss accepts the report and notes that the report appears to be excellent and he or*

she looks forward to reading it.

2. *Your boss expresses concern and returns the report as before. In this case, you have a reasoned response available. You show that your solution is consistent with the heuristic you used to check your work. With this supporting evidence your boss would have to rethink his or her response and provide you with an explanation regarding his or her concern.*

In either case, your work will have made a good impression.

Guidelines and heuristics are frequently used to make quick estimates during meetings and conferences and are valuable in refreshing one's memory with important information.

11.1.2. Maximizing the Benefits Obtained from Experience

No printed article, lecture, or text is a substitute for the perceptions resulting from experience. An engineer must be capable of transferring knowledge gained from one or more experiences to resolve future problems successfully.

To benefit fully from experience, it is important to make a conscious effort to use each new experience to build a foundation upon which to increase your ability to handle and to solve new problems.

An experienced engineer retains a body of information, made up largely of heuristics and shortcut calculation methods, that is available to help solve new problems.

The process by which an engineer uses information and creates new heuristics consists of three steps. These three steps are predict, authenticate, and re-evaluate, and they form the basis of the **PAR** process. The elements of this process are presented in Table 11.1, which illustrates the steps used in the PAR process.

Table 11.1. PAR Process to Maximize Benefits of Experience: *Predict, Authenticate, Reevaluate*

1. **Predict:** This is a precondition of the PAR process. It represents your best prediction of the solution. It often involves making assumptions and applying heuristics based on experience. Calculations should be limited to back-of-the-envelope or shortcut techniques.
2. **Authenticate/Analyze:** In this step, you seek out equations and relationships, do research relative to the problem, and perform the calculations that lead toward a solution. The ability to carry out this activity provides a necessary but not sufficient condition to be an engineer. When possible, information from actual operations is included in order to achieve the best possible solution.
3. **Reevaluate/Rethink:** The best possible solution from Step 2 is compared with the predicted solution in Step 1. When the prediction is not acceptable, it is necessary to correct the reasoning that led to the poor prediction. It becomes necessary to remove, revise, and replace assumptions made in Step 1. This is the critical step in learning from experience.

Example 11.1.

Evaluate the film heat transfer coefficient for water at 93°C (200°F) flowing at 3.05 m/s (10 ft/s)

inside a 38 mm (1.5 in) diameter tube. From previous experience, you know that the film heat transfer coefficient for water, at 21°C (70°F) and 1.83 m/s (6 ft/s), in these tubes is 5250 W/m^2°C. Follow the PAR process to establish the heat transfer coefficient at the new conditions.

Step 1—Predict: Assume that the velocity and temperature have no effect. Predicted Heat Transfer Coefficient = 5250 W/m^2°C

Step 2—Authenticate/Analyze: Using the properties given below, it is found that the Reynolds number for the water in the tubes is

$$\mathrm{Re} = u\rho D_{pipe}/\mu = (1.83)(997.4)(1.5)(0.0254)/(9.8 \times 10^{-4}) = 71 \times 10^3 \rightarrow \text{Turbulent Flow}$$

Use the Sieder-Tate equation [2] to check the prediction:

$$hD/k = (0.023)(Du\rho/\mu)^{0.8}(C_p\mu/k)^{1/3} \qquad (11.1)$$

Property	21°C (70°F)	93°C (200°F)	Ratio of (New/Old)
ρ (kg/m^3)	997.4	963.2	0.966
k (W/m°C)	0.604	0.678	1.12
C_p (kJ/kg°C)	4.19	4.20	1.00
μ (kg/m/s)	9.8×10^{-4}	3.06×10^{-4}	0.312

Take the ratio of Equation (11.1) for the two conditions given above, and rearrange and substitute numerical values. Using ’ to identify the new condition at 93°C,

$$h'/h = (D/D)^{0.2}(u'/u)^{0.8}(\rho'/\rho)^{0.8}(\mu/\mu')^{0.47}(C_p'/C_p)^{0.33}(k'/k)^{0.67} \qquad (11.2)$$

$$= (1)(1.50)(0.973)(1.73)(1.00)(1.08) = 2.725 \qquad (11.3)$$

$$h' = (2.725)(5250)\ \text{W/m}^2\text{°C} = 14{,}300\ \text{W/m}^2\text{°C}$$

The initial assumption that the velocity and temperature do not have a significant effect is incorrect. Equation (11.3) reveals a velocity effect of a factor of 1.5 and a viscosity effect of a factor of 1.73. All other factors are close to 1.0.

Step 3—Reevaluate/Rethink: The original assumptions that velocity and temperature had no effect on the heat transfer coefficient have been rejected. Improved assumptions for future predictions are as follows:

1. The temperature effect on viscosity must be evaluated.
2. The effects of temperature on C_p, ρ, and k are negligible.
3. Pipe diameter has a small effect on h (all other things being equal).
4. Results are limited to the range where the Sieder-Tate equation is valid.

With these assumptions, the values for water at 21°C are substituted into Equation (11.2). This creates a useful heuristic for evaluating the heat transfer coefficients for water.

$$h'(\text{W/m}^2\text{°C}) = 125u'^{0.8}/\mu'^{0.47} \text{ for } u'(\text{m/s}),\ \mu'\ (\text{kg/m/s})$$

Although it takes longer to obtain a solution when you start to apply the PAR process, the development of the heuristic and the addition of a more in-depth understanding of the factors that are important offer substantial long-term advantages.

There are hundreds of heuristics covering areas in chemical engineering—some general, and others

specific to a given application, process, or material. The next section presents a number of these rules that can be used to make predictions to start the PAR analysis.

11.2. Presentation of Tables of Technical Heuristics and Guidelines

A number of these guidelines are provided in this section. The information given is limited to operations most frequently encountered in this text. Most of the information was extracted from a collection presented in Walas [3]. In addition, this excellent reference also includes additional guidelines for the following equipment:

1. Conveyors for particulate solids
2. Cooling towers
3. Crystallization from solution
4. Disintegration
5. Drying of solids
6. Evaporators
7. Size separation of particles

The heuristics or rules are contained in a number of tables and apply to operating conditions that are most often encountered. The information provided is used in Example 11.2 and should be used to work problems at the end of the chapter and to check information on any PFD.

Example 11.2.

Refer to the information given in Chapter 1 for the toluene hydrodealkylation process, namely, Figure 1.7 and Tables 1.5 and 1.7. Using the information provided in the tables in this chapter, estimate the size of the equipment and other operating parameters for the following units:

a. V-102
b. E-105
c. P-101
d. C-101
e. T-101
f. H-101

Compare your findings with the information given in Chapter 1.

a. V-102 High-Pressure Phase Separator

From Table 11.6, the following heuristics are used:

Rule 3 → Vertical vessel

Rule 4 → L/D between 2.5 and 5 with optimum at 3.0

Rule 5 → Liquid holdup time is 5 min based on 1/2 volume of vessel

Rule 9 → Gas velocity u is given by

$$u = k\sqrt{\frac{\rho_l}{\rho_v} - 1} \text{ m/s}$$

where $k = 0.0305$ for vessels without mesh entrainers

Rule 12 → Good performance obtained at 30%–100% of u from Rule 9; typical value is 75%

From Table 1.5,

Vapor flow = Stream 8 = 9200 kg/h, $P = 23.9$ bar, $T = 38°C$

Liquid flow = Streams 17 + 18 = 11,570 kg/h, $P = 2.8$ bar, $T = 38°C$

$\rho_v = 8$ kg/m^3 and $\rho_l = 850$ kg/m^3 (estimated from Table 1.7)

From Rule 9, $u = 0.0305[850/8 - 1]^{0.5} = 0.313$ m/s

Use $u_{act} = (0.75)(0.313) = 0.23$ m/s

Now mass flowrate of vapor = $u\rho_v \pi D^2/4 = 9200/3600 = 2.56$ kg/s

Solving for D, $D = 1.33$ m

From Rule 5, the volume of liquid = $0.5\ L\pi D^2/4 = 0.726L$ m^3

5 min of liquid flow = $(5)(60)(11{,}570)/850/3600 = 1.13$ m^3

Equating the two results above, $L = 1.56$ m

From Rule 4, L/D should be in the range 2.5 to 5. For this case $L/D = 1.56/1.33 = 1.17$

Because this is out of range, change to $L = 2.5D = 3.3$ m.

Heuristics from Table 11.6 suggest that V-102 should be a vertical vessel with $D = 1.33$ m, $L = 3.3$ m

From Table 1.7, the actual V-102 is a vertical vessel with $D = 1.1$ m, $L = 3.5$ m

It should be concluded that the design of V-102 given in Chapter 1 is consistent with the heuristics given in Table 11.6. The small differences in L and D are to be expected in a comparison such as this one.

b. E-105 Product Cooler

From Table 11.11 use the following heuristics:

Rule 1: Set $F = 0.9$

Rule 6: min. $\Delta T = 10°C$

Rule 7: Water enters at 30°C and leaves at 40°C

Rule 8: $U = 850$ W/m^2°C

It is observed immediately from Table 1.5 and Figure 1.5 that Rule 6 has been violated because $\Delta T_{min} = 8°C$.

For the moment, ignore this and return to the heuristic analysis:

$\Delta T_{lm} = [(105 - 40) - (38 - 30)]/\ln[(105 - 40)/(38 - 30)] = 27.2°C$

$Q = 1085$ MJ/h = 301 kW (from Table 1.7)

$A = Q/U\Delta T_{lm}F = (301{,}000)/(850)/(27.2)/(0.90) = 14.46$ m^2

From Rule 9, Table 11.11, this heat exchanger should be a double-pipe or multiple-pipe design.

Comparing this analysis with the information in Table 1.7 shows

Heuristic: Double-pipe design, area = 14.5 m^2

Table 1.7: Multiple-pipe design, area = 12 m^2

Again, the heuristic analysis is close to the actual design. The fact that the minimum approach temperature of 10°C has been violated should not cause too much concern, because the actual minimum approach is only 8°C and the heat exchanger is quite small, suggesting that a little extra area (due to a smaller overall temperature driving force) is not very costly.

c. P-101

From Table 11.9, use the following heuristics:

Rule 1: Power(kW) = (1.67)[Flow(m^3/min)]ΔP(bar)/ε

Rules 4–7: Type of pump based on head

From Figure 1.5 and Tables 1.5 and 1.7,

Flowrate (Stream 2) = 13,300 kg/h

Density of fluid = 870 kg/m^3

ΔP = 25.8 – 1.2 = 24.6 bar = 288 m of liquid (head = $\Delta P/\rho g$)

Volumetric flowrate = (13,300)/(60)/(870) = 0.255 m^3/min

Fluid pumping power = (1.67)(0.255)(24.6) = 10.5 kW

From Rules 4–7, pump choices are multistage centrifugal, rotary, and reciprocating. Choose reciprocating to be consistent with Table 1.7. Typical ε = 0.75.

Power (shaft power) = 10.5/0.75 = 14.0 kW → compares with 14.2 kW from Table 1.7.

d. C-101

From Table 11.10, use the following heuristics:

Rule 2: $W_{rev\ adiab} = mz_1RT_1[(P_2/P_1)^a - 1]/a$

From Table 1.7, flow = 6770 kg/h, T_1 = 38°C = 311 K, mw = 8.45, P_1 = 23.9 bar, P_2 = 25.5

k = 1.41 (assume) and a = 0.2908

m = (6770)/(3600)/(8.45) = 0.223 kmol/s

$W_{rev\ adiab}$ = (223)(1.0)(8.314)(311){ $(25.5/23.9)^{0.2908}$ – 1)/0.2908 = 37.7 kW using a compressor efficiency of 75%

W_{actual} = (37.7)/(0.75) = 50.3 kW → This checks with the shaft power requirement given in Table 1.7.

e. T-101

From Table 11.13, use the following heuristics:

Rule 5: Optimum reflux in the range of 1.2–1.5R_{min}

Rule 6: Optimum number of stages approximately 2N_{min}

Rule 7: $N_{min} = \ln\{ [x/(1-x)]_{ovhd}/[x/(1-x)]_{bot}\}/\ln \alpha$

Rule 8: $R_{min} = \{F/D\}/(\alpha - 1)$

Rule 9: Use a safety factor of 10% on number of trays.

Rule 14: L_{max} = 53 m and $L/D < 30$

From Table 11.14, use the following heuristics:

Rule 2: $F_s = u\rho_v^{0.5} = 1.2 \rightarrow 1.5 \text{m/s}(\text{kg/m}^3)^{0.5}$

Rule 3: $\Delta P_{tray} = 0.007$ bar

Rule 4: $\varepsilon_{tray} = 60 - 90$ %

$x_{ovhd} = 0.9962$, $x_{ovhd} = 0.0308$, $\alpha_{ovhd} = 2.44$, $\alpha_{bot} = 2.13$, $\alpha_{geom\ ave} = (\alpha_{ovhd}\alpha_{bot})^{0.5} = 2.28$

$N_{min} = \ln\{[0.9962/(1 - 0.9962)]/[0.0308/(1 - 0.0308)]\}/\ln(2.28) = 10.9$

$R_{min} = \{142.2/105.6\}/(2.28 - 1) = 1.05$

Range of $R = (1.2 \rightarrow 1.5)R_{min} = 1.26 \rightarrow 1.58$

$N_{theoretical} \approx (2)(10.9) = 21.8$

$\varepsilon_{tray} = 0.6$

$N_{actual} \approx (21.6/0.6)(1.1) = 40$ trays

$\rho_v = 6.1$ kg/m^3

$u = (1.2 \rightarrow 1.5)/6.1^{0.5} = 0.49 \rightarrow 0.60$ m/s

Vapor flowrate (Stream 13) = 22,700 kg/h

Vol. flowrate, $v = 1.03$ m^3/s

$D_{tower} = [4v/\pi u]^{0.5} = [(4)(1.03)/(3.142)/(0.49 \rightarrow 0.60)]^{0.5} = 1.64 - 1.48$ m

$\Delta P_{tower} = (N_{actual})(\Delta P_{tray}) = (40)(0.007) = 0.28$ bar

A comparison of the actual equipment design and the predictions of the heuristic methods are given below.

	From Tables 1.5 and 1.7 and Figure 1.5	From Heuristics
Tower diameter	1.5 m	1.48 → 1.64 m
Reflux ratio, R	1.75	1.26 →1.58
Number of trays	42	40
Pressure drop, ΔP_{tower}	0.30 bar	0.28 bar

f. H-101

From Table 11.11, use the following heuristics:

Rule 13: Equal heat transfer in radiant and convective sections

Radiant rate = 37.6 kW/m^2, convective rate = 12.5 kW/m^2

Duty = 27,040 MJ/h = 7511 kW

Area radiant section = (0.5)(7511)/(37.6) = 99.9 m^2 (106.8 m^2 in Table 1.7)

Area convective section = (0.5)(7511)/(12.5) = 300.4 m^2 (320.2 m^2 in Table 1.7)

From the earlier worked examples, it is clear that the sizing of the equipment in Table 1.7 agrees well with the predictions of the heuristics presented in this chapter. Exact agreement is not to be expected. Instead, the heuristics should be used to check calculations performed using more rigorous methods and to flag any inconsistencies.

11.3. Summary

In this chapter, a number of heuristics have been introduced that allow the reasonableness of the results of engineering calculations to be checked. These heuristics or guidelines cannot be used to determine absolutely whether a particular answer is correct or incorrect. However, they are useful guides that allow the engineer to flag possible errors and help focus attention on areas of the process that may require special attention. Several heuristics, provided in the tables at the end of this chapter, were used to check the designs provided in Table 1.5 for the toluene hydrodealkylation process.

List of Informational Tables

Table	Description
11.2(a)	Physical Property Heuristics
11.2(b)	Typical Physical Property Variations with Temperature and Pressure
11.3	Capacities of Process Units in Common Usage
11.4	Effect of Typical Materials of Construction on Product Color, Corrosion, Abrasion, and Catalytic Effects
11.5	Heuristics for Drivers and Power Recovery Equipment
11.6	Heuristics for Process Vessels (Drums)
11.7	Heuristics for Vessels (Pressure and Storage)
11.8	Heuristics for Piping
11.9	Heuristics for Pumps
11.10	Heuristics for Compressors, Fans, Blowers, and Vacuum Pumps
11.11	Heuristics for Heat Exchangers
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11.13	Heuristics for Towers (Distillation and Gas Absorption)
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11.16	Heuristics for Liquid-Liquid Extraction
11.17	Heuristics for Reactors
11.18	Heuristics for Refrigeration and Utility Specifications

Table 11.2(a) Physical Property Heuristics

	Units	Liquids	Liquids	Gases	Gases	Gases
		Water	Organic Material	Steam	Air	Organic Material
Heat capacity	kJ/kg°C	4.2	1.0–2.5	2.0	1.0	2.0–4.0
Density	kg/m^3	1000	700–1500		1.29@STP	
Latent heat	kJ/kg	1200–2100	200–1000			
Thermal conductivity	W/m°C	0.55–0.70	0.10–0.20	0.025–0.07	0.025–0.05	0.02–0.06
Viscosity	kg/m s	0°C 1.8×10^{-3}	Wide Range	$10–30 \times 10^{-6}$	$20–50 \times 10^{-6}$	$10–30 \times 10^{-6}$
		50°C 5.7×10^{-4}				
		100°C 2.8×10^{-4}				
		200°C 1.4×10^{-4}				
Prandtl no.		1–15	10–1000	1.0	0.7	0.7–0.8

Table 11.2(b) Typical Physical Property Variations with Temperature and Pressure

	Liquids	Liquids	Gases	Gases
Property	Temperature	Pressure	Temperature	Pressure
Density	$\rho_l \propto (T_c - T)^{0.3}$	Negligible	$\rho_g = MW.P/ZRT$	$\rho_g = MW.P/ZRT$
Viscosity	$\mu_l = Ae^{B/T}$	Negligible	$\mu_g \propto \frac{T^{1.5}}{(T + 1.47T_b)}$	Significant only for $P > 10$ bar
Vapor pressure	$P^* = ae^{b/(T+c)}$	—	—	—

T is temperature (K), T_c is the critical temperature (K), T_b is the normal boiling point (K), MW is molecular weight, P is pressure, Z is compressibility, R is the gas constant, and P^* is the vapor pressure.

Table 11.3. Capacities of Process Units in Common Usage[a]

Process Unit	Capacity Unit	Max. Value	Min. Value	Comment
Horizontal vessel	Pressure (bar)	400	Vacuum	*L/D* typically 2–5, see Table 11.6.
	Temper. (°C)	400[b]	−200	
	Height (m)	10	2	
	Diameter (m)	2	0.3	
	L/D	5	2	
Vertical vessel	Pressure (bar)	400	400	*L/D* typically 2–5, see Table 11.6.
	Temper. (°C)	400[b]	−200	
	Height (m)	10	2	
	Diameter (m)	2	0.3	
	L/D	5	2	
Towers	Pressure (bar)	400	Vacuum	Normal Limits
	Temper. (°C)	400[b]	−200	Diameter *L/D*
	Height (m)	50	2	0.5 3.0–40[c]
	Diameter (m)	4	0.3	1.0 2.5–30[c]
	L/D	30	2	2.0 1.6–23[c]
				4.0 1.8–13[c]
Pumps				
Reciprocating	Power[d](kW)	250	< 0.1	
	Pressure (bar)	1000		
Rotary and positive Displacement	Power[d](kW)	150	< 0.1	
	Pressure (bar)	300		
Centrifugal	Power[d](kW)	250	< 0.1	
	Pressure (bar)	300		
Compressors				
Axial, centrifugal + recipr.	Power[d](kW)	8000	50	
Rotary	Power[d](kW)	1000	50	
Drives for Compressors				
Electric	Power[e](kW)	15,000	< 1	
Steam turbine	Power[e](kW)	15,000	100	
Gas turbine	Power[e](kW)	15,000	10	
Internal combustion eng.	Power[e](kW)	15,000	10	
Process heaters	Duty (MJ/h)	500,000	10,000	Duties different for reactive heaters/furnaces.
Heat exchangers	Area (m^2)	1000	10	For area < 10 m^2 use
	Tube dia. (m)	0.0254	0.019	double pipe exchanger.
	Length (m)	6.5	2.5	
	Pressure (bar)	150	Vacuum	For 150 < *P* < 400 bar
	Temp. (°C)	400[b]	−200	need special design.

[a]Most of the limits for equipment sizes shown here correspond to the limits used in the costing program (CAPCOST) introduced in Chapter 7.
[b]Maximum temperature and pressure are related to the materials of construction and may differ from values shown here.
[c]For 20 < *L/D* < 30 special design may be required. Diameters up to 9 m possible but greater than 4 m must be fabricated on site.
[d]Power values refer to fluid/pumping power.
[e]Power values refer to shaft power.

Table 11.4. Effect of Typical Materials of Construction on Product Color, Corrosion,[a] Abrasion, and Catalytic Effects

Metals		
Material	***Advantages***	***Disadvantages***
Carbon steel	Low cost, readily available, resists abrasion, standard fabrication, resists alkali	Poor resistance to acids and strong alkali, often causes discoloration and contamination
Stainless steel	Resists most acids, reduces discoloration, available with a variety of alloys, abrasion less than mild steel	Not resistant to chlorides, more expensive, fabrication more difficult, alloy materials may have catalytic effects
Monel-Nickel	Little discoloration, contamination, resistant to chlorides	Not resistant to oxidizing environments, expensive
Hasteloy	Improved over Monel-Nickel	More expensive than Monel-Nickel
Other exotic metals	Improves specific properties	Can be very high cost
Nonmetals		
Material	***Advantages***	***Disadvantages***
Glass	Useful in laboratory and batch systems, low diffusion at walls	Fragile, not resistant to high alkali, poor heat transfer, poor abrasion resistance
Plastics	Good at low temperature, large variety to select from with various characteristics, easy to fabricate, seldom discolors, low cost	Poor at high temperature, low strength, not resistant to high-alkali conditions, low heat transfer. Minor catalytic effects possible
Ceramics	Withstands high temperatures, variety of formulations available, modest cost	Poor abrasion properties, high diffusion at walls (in particular hydrogen), low heat transfer, may encourage catalytic reactions

[a]In addition, see Chapter 7 for preliminary selection of materials of construction.

Table 11.5. Heuristics for Drivers and Power Recovery Equipment

1. Efficiency is greater for larger machines. Electric motors are 85%–95%; steam turbines are 42%–78%; gas engines and turbines are 28%–38% efficient (see Figure 8.7).
2. For less than 74.6 kW (100 hp), electric motors are used almost exclusively. They are made for services up to 14,900 kW (20,000 hp).
3. Steam turbines are competitive higher than 76.6 kW (100 hp). They are speed controllable. They are frequently used as spares in case of power failure.
4. Combustion engines and turbines are restricted to mobile and remote locations.
5. Gas expanders for power recovery may be justified at capacities of several hundred horsepower; otherwise any pressure reduction in process is done with throttling valves.
6. The following useful definitions are given:

$$\text{Shaft power} = \frac{\text{theoretical power to pump fluid (liquid or gas)}}{\text{efficiency of pump or compressor, } \varepsilon_{sh}}$$

$$\text{Drive power} = \frac{\text{shaft power}}{\text{efficiency of drive, } \varepsilon_{dr}}$$

$$\text{Overall efficiency} = \varepsilon_{ov} = \varepsilon_{sh}\,\varepsilon_{dr}$$

ε_{dr} values are given in this table and Figure 8.7.

ε_{sh} values are given in Tables 11.9 and 11.10. Usually ε_{sh} are given on PFD.

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Table 11.6. Heuristics for Process Vessels (Drums)

1. Drums are relatively small vessels that provide surge capacity or separation of entrained phases.
2. Liquid drums are usually horizontal.
3. Gas-liquid phase separators are usually vertical.
4. Optimum ratio of length to diameter = 3, but the range 2.5 to 5 is common.
5. Holdup time is 5 min for half-full reflux drums and gas/liquid separators, 5–10 min for a product feeding another tower.
6. In drums feeding a furnace, 30 min for half-full drum is allowed.
7. Knockout drums placed ahead of compressors should hold no less than 10 times the liquid volume passing per minute.
8. Liquid-liquid separations are designed for settling velocity of 0.085–0.127 cm/s (2–3 in/min).
9. Gas velocity in gas/liquid separators, $u = k\sqrt{\rho_l/\rho_v - 1}$ m/s (ft/sec) $k = 0.11$ (0.35) for systems with mesh deentrainer, and $k = 0.0305$ (0.1) without mesh deentrainer.
10. Entrainment removal of 99% is attained with 10.2–30.5 cm (4–12 in) mesh pad thickness; 15.25 cm (6 in) thickness is popular.
11. For vertical pads, the value of the coefficient in Step 9 is reduced by a factor of 2/3.
12. Good performance can be expected at velocities of 30%–100% of those calculated with the given k; 75% is popular.
13. Disengaging spaces of 15.2–45.7 cm (6–18 in) ahead of the pad and 30.5 cm (12 in) above the pad are suitable.
14. Cyclone separators can be designed for 95% collection at 5 μm particles, but usually only droplets greater than 50 μm need be removed.

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Table 11.7. Heuristics for Vessels (Pressure and Storage)

Pressure Vessels

1. Design temperature between −30°C and 345°C is 25°C above maximum operating temperature; higher safety margins are used outside the given temperature range.
2. The design pressure is 10% or 0.69–1.7 bar (10–25 psi) over the max. operating pressure, whichever is greater. The max. operating pressure, in turn, is taken as 1.7 bar (25 psi) above the normal operation.
3. Design pressures of vessels operating at 0–0.69 bar (0–10 psig) and 95–540°C (200–1000°F) are 2.76 barg (40 psig).
4. For vacuum operation, design pressures are 1 barg (15 psig) and full vacuum.
5. Minimum wall thickness for rigidity: 6.4 mm (0.25 in) for 1.07 m (42 in) dia. and less than 8.1 mm (0.32 in) for 1.07–1.52 m (42–60 in) dia., and 11.7 mm (0.38 in) for more than 1.52 m (60 in) dia.
6. Corrosion allowance 8.9 mm (0.35 in) for known corrosive conditions, 3.8 mm (0.15 in) for noncorrosive streams, and 1.5 mm (0.06 in) for steam drums and air receivers.
7. Allowable working stresses are one-fourth of the ultimate strength of the material.
8. Maximum allowable stress depends sharply on temperature.

Temperature: (°F)		−20 to 650	750	850	1000
(°C)		(−30 to 345)	400	455	540
Low alloy steel SA 203	(psi)	18,759	15,650	9950	2500
	(bar)	1290	1070	686	273
Type 302 stainless steel	(psi)	18,750	18,750	15,950	6250
	(bar)	1290	1290	1100	431

Storage Vessels

1. For less than 3.8 m^3 (1000 gal), use vertical tanks on legs.
2. Between 3.8 and 38 m^3 (1000 and 10,000 gal), use horizontal tanks on concrete supports.
3. Beyond 38 m^3 (10,000 gal) use vertical tanks on concrete pads.
4. Liquids subject to breathing losses may be stored in tanks with floating or expansion roofs for conservation.
5. Freeboard is 15% below 1.9 m^3 (500 gal) and 10% above 1.9 m^3 (500 gal) capacity.
6. Thirty-day capacity often is specified for raw materials and products but depends on connecting transportation equipment schedules.
7. Capacities of storage tanks are at least 1.5 times the size of connecting transportation equipment, for instance, 28.4 m^3 (7500 gal) tanker trucks, 130 m^3 (34,500 gal) rail cars, and virtually unlimited barge and tanker capacities.

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Table 11.8. Heuristics for Piping

1. Line velocities (u) and pressure drop (ΔP): (a) For liquid pump discharge: $u = (5 + D/3)$ ft/sec and $\Delta P = 2.0$ psi/100 ft; (b) For liquid pump suction: $u = (1.3 + D/6)$ ft/sec and $\Delta P = 0.4$ psi/100 ft; (c) For steam or gas flow: $u = 20D$ ft/sec and $\Delta P = 0.5$ psi/100 ft, D = diameter of pipe in inches.
2. Gas/steam line velocities = 61 m/s (200 ft/sec), and pressure drop = 0.1 bar/100 m (0.5 psi/100 ft).
3. In preliminary estimates set line pressure drops for an equivalent length of 30 m (100 ft) of pipe between each piece of equipment.
4. Control valves require at least 0.69 bar (10 psi) drop for good control.
5. Globe valves are used for gases, control, and wherever tight shutoff is required. Gate valves for most other services.
6. Screwed fittings are used only on sizes 3.8 cm (1.5 in) or less; otherwise, flanges or welding used.
7. Flanges and fittings are rated for 10, 20, 40, 103, 175 bar (150, 300, 600, 1500, or 2500 psig).
8. Approximate schedule number required = 1000 P/S, where P is the internal pressure in psig and S is the allowable working stress [about 690 bar (10,000 psi)] for A120 carbon steel at 260° (500°F). Schedule 40 is most common.

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Table 11.9. Heuristics for Pumps

1. Power for pumping liquids: kW = (1.67)[Flow(m^3/min)][ΔP(bar)]/ε [hp = Flow(gpm) ΔP(psi)/1714/ε] ε = Fractional Efficiency = ε_{sh} (see Table 11.5).
2. Net positive suction head (NPSH) of a pump must be in excess of a certain number, depending upon the kind of pumps and the conditions, if damage is to be avoided. $NPSH$ = (pressure at the eye of the impeller − vapor pressure)/(ρg). Common range is 1.2–6.1 m of liquid (4–20 ft).
3. Specific speed N_s = (rpm)(gpm)$^{0.5}$/(head in feet)$^{0.75}$. Pump may be damaged if certain limits on N_s are exceeded, and the efficiency is best in some ranges.
4. Centrifugal pumps: Single stage for 0.057–18.9 m^3/min (15–5000 gpm), 152 m (500 ft) maximum head; multistage for 0.076–41.6 m^3/min (20–11,000 gpm), 1675 m (5500 ft) maximum head. Efficiency 45% at 0.378 m^3/min (100 gpm), 70% at 1.89 m^3/min (500 gpm), 80% at 37.8 m^3/min (10,000 gpm).
5. Axial pumps for 0.076–378 m^3/min (20–100,000 gpm), 12 m (40 ft) head, 65–85% efficiency.
6. Rotary pumps for 0.00378–18.9 m^3/min (1–5000 gpm), 15,200 m (50,000 ft head), 50–80% efficiency.
7. Reciprocating pumps for 0.0378–37.8 m^3/min (10–10,000 gpm), 300 km (1,000,000 ft) head max. Efficiency 70% at 7.46 kW (10 hp), 85% at 37.3 kW (50 hp), and 90% at 373 kW (500 hp).

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Table 11.10. Heuristics for Compressors, Fans, Blowers, and Vacuum Pumps

1. Fans are used to raise the pressure about 3% {12 in (30 cm) water}, blowers to raise less than 2.75 barg (40 psig), and compressors to higher pressures, although the blower range is commonly included in the compressor range.
2. Theoretical reversible adiabatic power = $mz_1RT_1[(\{P_2/P_1\}^a - 1)]/a$
   where T_1 is inlet temperature, R = gas constant, z_1 = compressibility, m = molar flow rate, $a = (k-1)/k$ and $k = C_p/C_v$.
   Values of R: = 8.314 J/mol K = 1.987 Btu/lbmol R = 0.7302 atm ft^3/lbmol R
3. Outlet temperature for reversible adiabatic process $T_2 = T_1\ (P_2/P_1)^a$.
4. Exit temperatures should not exceed 167–204°C (350–400°F); for diatomic gases ($C_p/C_v = 1.4$). This corresponds to a compression ratio of about 4.
5. Compression ratio should be about the same in each stage of a multistage unit, ratio = $(P_n/P_1)^{1/n}$, with n stages.
6. Efficiencies of reciprocating compressors: 65% at compression ratios of 1.5, 75% at 2.0, and 80–85% at 3–6.
7. Efficiencies of large centrifugal compressors, 2.83–47.2 m^3/s (6000–100,000 acfm) at suction, are 76–78%.
8. For vacuum pumps use the following:

Reciprocating piston type	Down to 1 Torr
Rotary piston type	Down to 0.001 Torr
Two-lobe rotary type	Down to 0.0001 Torr
Steam jet ejectors	1-stage down to 100 Torr
	3-stage down to 1 Torr
	5-stage down to 0.05 Torr

9. A three-stage ejector needs 100 kg steam/kg air to maintain a pressure of 1 Torr.
10. In-leakage of air to evacuated equipment depends on the absolute pressure, Torr, and the volume of the equipment, V in m^3 (ft^3) according to $W = kV^{2/3}$ kg/h (lb/hr) with k = 0.98 (0.2) when P > 90 Torr, k = 0.39 (0.08) between 3 and 20 Torr, and k = 0.12 (0.025) at less than 1 Torr.

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Table 11.11. Heuristics for Heat Exchangers

1. For conservative estimate set $F = 0.9$ for shell-and-tube exchangers with no phase changes, $q = UAF\Delta T_{lm}$. When ΔT at exchanger ends differ greatly, then check F, and reconfigure if F is less than 0.85.
2. Standard tubes are 1.9 cm (3/4 in) OD, on a 2.54 cm (1 in) triangle spacing, 4.9 m (16 ft) long.

   A shell 30 cm (1 ft) dia. accommodates 9.3 m^2 (100 ft^2)
   60 cm (2 ft) dia. accommodates 37.2 m^2 (400 ft^2)
   90 cm (3 ft) dia. accommodates 102 m^2 (1100 ft^2)
3. Tube side is for corrosive, fouling, scaling, and high-pressure fluids.
4. Shell side is for viscous and condensing fluids.
5. Pressure drops are 0.1 bar (1.5 psi) for boiling and 0.2–0.62 bar (3–9 psi) for other services.
6. Minimum temperature approach is 10°C (20°F) for fluids and 5°C (10°F) for refrigerants.
7. Cooling water inlet is 30°C (90°F), maximum outlet 45°C (115°F).
8. Heat transfer coefficients for estimating purposes, W/m^2°C (Btu/hr ft^2°F): water to liquid, 850 (150); condensers, 850 (150); liquid to liquid, 280 (50); liquid to gas, 60 (10); gas to gas 30 (5); reboiler 1140 (200). Maximum flux in reboiler 31.5 kW/m^2 (10,000 Btu/hr ft^2).

   When phase changes occur, use a zoned analysis with appropriate coefficient for each zone.
9. Double pipe exchanger is competitive at duties requiring 9.3–18.6 m^2 (100–200 ft^2).
10. Compact (plate and fin) exchangers have 1150 m^2/m^3 (350 ft^2/ft^3), and about 4 times the heat transfer per cut of shell-and-tube units.
11. Plate and frame exchangers are suited to high-sanitation services and are 25–50% cheaper in stainless steel construction than shell-and-tube units.
12. Air coolers: Tubes are 0.75–1.0 in. OD, total finned surface 15–20 m^2/m^2 (ft^2/ft^2 bare surface), U = 450–570 W/m^2°C (80–100 Btu/hr ft^2 (bare surface) °F). Minimum approach temperature = 22°C (40°F). Fan input power = 1.4–3.6 kW/(MJ/h) [2–5 hp/(1000 Btu/hr)].
13. Fired heaters: Radiant rate, 37.6 kW/m^2 (12,000 Btu/hr ft^2); convection rate, 12.5 kW/m^2 (4000 Btu/hr ft^2); cold oil tube velocity = 1.8 m/s (6 ft/sec); approximately equal transfer in the two sections; thermal efficiency 70–90% based on lower heating value; flue gas temperature 140–195°C (250–350°F) above feed inlet; stack gas temperature 345–510°C (650–950°F).

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Table 11.12. Heuristics for Thermal Insulation

1. Up to 345°C (650°F), 85% magnesia is used.
2. Up to 870–1040°C (1600–1900°F), a mixture of asbestos and diatomaceous earth is used.
3. Ceramic (refractory) linings at higher temperature.
4. Cryogenic equipment −130°C (−200°F) employs insulation with fine pores of trapped air, e.g., Perlite.
5. Optimal thickness varies with temperature: 1.27 cm (0.5 in) at 95°C (200°F), 2.54 cm (1.0 in) at 200°C (400°F), 3.2 cm (1.25 in) at 315°C (600°F).
6. Under windy conditions 12.1 km/h (7.5 miles/hr), 10–20% greater thickness of insulation is justified.

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Table 11.13. Heuristics for Towers (Distillation and Gas Absorption)

1. Distillation is usually the most economical method for separating liquids, superior to extraction, absorption crystallization, or others.
2. For ideal mixtures, relative volatility is the ratio of vapor pressures $\alpha_{12} = P_1^*/P_2^*$.
3. Tower operating pressure is most often determined by the temperature of the condensing media, 38–50°C (100–120°F) if cooling water is used, or by the maximum allowable reboiler temperature to avoid chemical decomposition/degradation.
4. Sequencing of columns for separating multicomponent mixtures:[a]
   a. Perform the easiest separation first, that is, the one least demanding of trays and reflux, and leave the most difficult to the last.
   b. When neither relative volatility nor feed composition varies widely, remove components one by one as overhead products.
   c. When the adjacent ordered components in the feed vary widely in relative volatility, sequence the splits in order of decreasing volatility.
   d. When the concentrations in the feed vary widely but the relative volatilities do not, remove the components in order of decreasing concentration.
5. Economical optimum reflux ratio is in the range of 1.2 to 1.5 times the minimum reflux ratio, R_{min}.
6. The economically optimum number of theoretical trays is near twice the minimum value N_{min}.
7. The minimum number of trays is found with the Fenske-Underwood equation
   $N_{min} = \ln\{[x/(1-x)]_{ovhd}/[x/(1-x)]_{btms}\}/\ln \alpha$.

8. Minimum reflux for binary or pseudobinary mixtures is given by the following when separation is essentially complete ($x_D \approx 1$) and D/F is the ratio of overhead product to feed rate:

   $R_{min} D/F = 1/(\alpha - 1)$, when feed is at the bubble point

   $(R_{min} + 1)\ D/F = \alpha/(\alpha - 1)$, when feed is at the dew point

9. A safety factor of 10% of the number of trays calculated by the best means is advisable.
10. Reflux pumps are made at least 10% oversize.
11. The optimum value of the Kremser absorption factor $A = (L/mV)$ is in the range of 1.25 to 2.0.
12. Reflux drums usually are horizontal, with a liquid holdup of 5 min half-full. A takeoff pot for a second liquid phase, such as water in hydrocarbon systems, is sized for a linear velocity of that phase of 1.3 m/s (0.5 ft/sec), minimum diameter is 0.4 m (16 in).
13. For towers about 0.9 m (3 ft) dia., add 1.2 m (4 ft) at the top for vapor disengagement, and 1.8 m (6 ft) at bottom for liquid level and reboiler return.
14. Limit the tower height to about 53 m (175 ft) max. because of wind load and foundation considerations. An additional criterion is that L/D be less than 30 ($20 < L/D < 30$ often will require special design).

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[a]Additional information on sequencing is given in Table 12.2.

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Table 11.14. Heuristics for Tray Towers (Distillation and Gas Absorption)

1. For reasons of accessibility, tray spacings are made 0.5–0.6 m (20–24 in).
2. Peak efficiency of trays is at values of the vapor factor $F_s = u\rho^{0.5}$ in the range of 1.2–1.5 m/s $\{kg/m^3\}^{0.5}$ [1–1.2 ft/s $\{lb/ft^3\}^{0.5}$]. This range of F_s establishes the diameter of the tower. Roughly, linear velocities are 0.6 m/s (2 ft/sec) at moderate pressures, and 1.8 m/s (6 ft/sec) in vacuum.
3. Pressure drop per tray is on the order of 7.6 cm (3 in) of water or 0.007 bar (0.1 psi).
4. Tray efficiencies for distillation of light hydrocarbons and aqueous solutions are 60–90%; for gas absorption and stripping, 10–20%.
5. Sieve trays have holes 0.6–0.7 cm (0.25–0.5 in) dia., area being 10% of the active cross section.
6. Valve trays have holes 3.8 cm (1.5 in) dia. each provided with a liftable cap, 130–150 caps/m^2 (12–14 caps/ft^2) of active cross section. Valve trays are usually cheaper than sieve trays.
7. Bubblecap trays are used only when a liquid level must be maintained at low turndown ratio; they can be designed for lower pressure drop than either sieve or valve trays.
8. Weir heights are 5 cm (2 in), weir lengths are about 75% of tray diameter, liquid rate—a maximum of 1.2 m^3/min m of weir (8 gpm/in of weir); multipass arrangements are used at higher liquid rates.

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Table 11.15. Heuristics for Packed Towers (Distillation and Gas Absorption)

1. Structured and random packings are suitable for packed towers less than 0.9 m (3 ft) when low pressure drop is required.
2. Replacing trays with packing allows greater throughput and separation in existing tower shells.
3. For gas rates of 14.2 m^3/min (500 ft^3/min), use 2.5 cm (1 in) packing; for 56.6 m^3/min (2000 ft^3/min) or more, use 5 cm (2 in) packing.
4. Ratio of tower diameter to packing diameter should be >15:1.
5. Because of deformability, plastic packing is limited to 3–4 m (10–15 ft) and metal to 6.0–7.6 m (20–25 ft) unsupported depth.
6. Liquid distributors are required every 5–10 tower diameters with pall rings, and at least every 6.5 m (20 ft) for other types of dumped packing.
7. Number of liquid distributors should be >32–55/m^2 (3–5/ft^2) in towers greater than 0.9 m (3 ft) diameter, and more numerous in smaller columns.
8. Packed towers should operate near 70% of flooding (evaluated from Sherwood and Lobo correlation).
9. Height equivalent to theoretical stage (HETS) for vapor-liquid contacting is 0.4–0.56 m (1.3–1.8 ft) for 2.5 cm (1 in) pall rings, and 0.76–0.9 m. (2.5–3.0 ft) for 5 cm (2 in) pall rings.
10. Generalized pressure drops

	Design Pressure Drops (cm of H_2O/m of packing)	Design Pressure Drops (inches of H_2O/ft of packing)
Absorbers and regenerators (nonfoaming systems)	2.1–3.3	0.25–0.40
Absorbers and regenerators	0.8–2.1	0.10–0.25
Atmospheric/pressure stills and fractionators	3.3–6.7	0.40–0.80
Vacuum stills and fractionators	0.8–3.3	0.10–0.40
Maximum value	8.33	1.0

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Table 11.16. Heuristics for Liquid-Liquid Extraction

1. The dispersed phase should be the one with the higher volumetric flowrate except in equipment subject to back-mixing, where it should be the one with the smaller volumetric rate. It should be the phase that wets material of construction less well. Because the holdup of continuous phase is greater, that phase should be made up of the less expensive or less hazardous material.
2. There are no known commercial applications of reflux to extraction processes, although the theory is favorable.
3. Mixer-settler arrangements are limited to at most five stages. Mixing is accomplished with rotating impellers or circulation pumps. Settlers are designed on the assumption that droplet sizes are about 150 μm dia. In open vessels, residence times of 30–60 min or superficial velocities of 0.15–0.46 m/min (0.5–1.5 ft/min) are provided in settlers. Extraction stage efficiencies commonly are taken as 80%.
4. Spray towers as tall as 6–12 m (20–40 ft) cannot be depended on to function as more than a single stage.
5. Packed towers are employed when 5–10 stages suffice. Pall rings 2.5–3.8 cm (1–1.5 in) size are best. Dispersed phase loadings should not exceed 10.2 $m^3/min\ m^2$ (25 $gal/min\ ft^2$). HETS of 1.5–3.0 m (5–10 ft) may be realized. The dispersed phase must be redistributed every 1.5–2.1 m (5–7 ft). Packed towers are not satisfactory when the surface tension is more than 10 dyne/cm.
6. Sieve tray towers have holes of only 3–8 mm dia. Velocities through the holes are kept less than 0.24 m/s (0.8 ft/sec) to avoid formation of small drops. Redispersion of either phase at each tray can be designed for. Tray spacings are 15.2 to 60 cm (6 to 24 in). Tray efficiencies are in the range of 20%–30%.
7. Pulsed packed and sieve tray towers may operate at frequencies of 90 cycles/min and amplitudes of 6–25 mm. In large-diameter towers, HETS of about 1 m have been observed. Surface tensions as high as 30–40 dyne/cm have no adverse effect.
8. Reciprocating tray towers can have holes 1.5 cm (9/16 in) dia., 50–60% open area, stroke length 1.9 cm (0.75 in), 100–150 strokes/min, plate spacing normally 5 cm (2 in) but in the range of 2.5–15 cm (1–6 in). In a 76 cm (30 in) diameter tower, HETS is 50–65 cm (20–25 in) and throughput is 13.7 $m^3/min\ m^2$ (2000 $gal/hr\ ft^2$). Power requirements are much less than that of pulsed towers.
9. Rotating disk contactors or other rotary agitated towers realize HETS in the range of 0.1–0.5 m (0.33–1.64 ft). The especially efficient Kuhni with perforated disks of 40% free cross section has HETS of 0.2 m (0.66 ft) and a capacity of 50 $m^3/m^2\ h$ (164 $ft^3/ft^2\ hr$).

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Table 11.17. Heuristics for Reactors

1. The rate of reaction in every instance must be established in the laboratory, and the residence time or space velocity and product distribution eventually must be found from a pilot plant.
2. Dimensions of catalyst particles are 0.1 mm (0.004 in) in fluidized beds, 1 mm in slurry beds, and 2–5 mm (0.078–0.197 in) in fixed beds.
3. The optimum proportions of stirred tank reactors are with liquid level equal to the tank diameter, but at high pressures slimmer proportions are economical.
4. Power input to a homogeneous reaction stirred tank is 0.1–0.3 kW/m^3 (0.5–1.5 hp/1000 gal), but three times this amount when heat is to be transferred.
5. Ideal CSTR (continuous stirred tank reactor) behavior is approached when the mean residence time is 5 to 10 times the length needed to achieve homogeneity, which is accomplished with 500–2000 revolutions of a properly designed stirrer.
6. Batch reactions are conducted in stirred tanks for small daily production rates or when the reaction times are long or when some condition such as feed rate or temperature must be programmed in some way.
7. Relatively slow reactions of liquids and slurries are conducted in continuous stirred tanks. A battery of four or five in series is most economical.
8. Tubular flow reactors are suited to high production rates at short residence times (seconds or minutes) and when substantial heat transfer is needed. Embedded tubes or shell-and-tube construction then is used.
9. In granular catalyst packed reactors, the residence time distribution is often no better than that of a five-stage CSTR battery.
10. For conversion less than about 95% of equilibrium, the performance of a five-stage CSTR battery approaches plug flow.
11. The effect of temperature on chemical reaction rate is to double the rate every 10°C.
12. The rate of reaction in a heterogeneous system is more often controlled by the rate of heat or mass transfer than by the chemical reaction kinetics.
13. The value of a catalyst may be to improve selectivity more than to improve the overall reaction rate.

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Table 11.18. Heuristics for Refrigeration and Utility Specifications

1. A ton of refrigeration is the removal of 12,700 kJ/h (12,000 Btu/hr) of heat.
2. At various temperature levels: −18 to −10°C (0 to 50°F), chilled brine and glycol solutions; −45 to −10°C (−50 to −40°F), ammonia, freon, butane; −100 to −45°C (−150 to −50°F) ethane or propane.
3. Compression refrigeration with 38°C (100°F) condenser requires kW/tonne (hp/ton) at various temperature levels; 0.93 (1.24) at −7°C (20°F); 1.31 (1.75) at −18°C (0°F); 2.3 (3.1) at −40°C (−40°F); 3.9 (5.2) at −62°C (−80°F).
4. At less than −62°C (−80°F), cascades of two or three refrigerants are used.
5. In single-stage compression, the compression ratio is limited to 4.
6. In multistage compression, economy is improved with interstage flashing and recycling, so-called economizer operation.
7. Absorption refrigeration: ammonia to −34°C (−30°F); lithium bromide to 7°C (+45°F) is economical when waste steam is available at 0.9 barg (12 psig).
8. Steam: 1–2 barg (15–30 psig), 121–135°C (250–275°F); 10 barg (150 psig), 186°C (366°F); 27.6 barg (400 psig), 231°C (448°F); 41.3 barg (600 psig), 252°C (488°F) or with 55–85°C (100–150°F) superheat.
9. Cooling water: For design of cooling tower use supply at 27–32°C (80–90°F) from cooling tower, return at 45–52°C (115–125°F); return seawater at 43°C (110°F); return tempered water or steam condensate above 52°C (125°F).
10. Cooling air supply at 29–35°C (85–95°F); temperature approach to process, 22°C (40°F).
11. Compressed air 3.1 (45), 10.3 (150), 20.6 (300), or 30.9 barg (450 psi) levels.
12. Instrument air at 3.1 barg (45 psig), −18°C (0°F) dew point.
13. Fuels: gas of 37,200 kJ/m^3 (1000 Btu/SCF) at 0.35–0.69 barg (5–10 psig), or up to 1.73 barg (25 psig) for some types of burners; liquid at 39.8 GJ/m^3 (6 million Btu/bbl).
14. Heat transfer fluids: petroleum oils less than 315°C (600°F), Dowtherms less than 400°C (750°F), fused salts less than 600°C (1100°F), direct fire or electricity above 450°F.
15. Electricity: 0.75–74.7 kW. (1–100 hp), 220–550 V; 149–1864 kW (200–2500 hp), 2300–4000 V.

(Adapted from S. M. Walas, *Chemical Process Equipment: Selection and Design,* Stoneham, MA: Butterworth, 1988. Copyright © 1988 by Butterworth Publishers, adapted by permission of Butterworth Publishers, Stoneham, MA. All rights reserved)

What You Should Have Learned

- This chapter is a resource of experienced-based heuristics that can be used to estimate unknown parameters and validate calculated parameters used to design a chemical process.

References

1. Koen, B. V., *Definition of the Engineering Method* (Washington, DC: American Society for Engineering Education, 1985).
2. Sieder, E. N., and G. E. Tate, "Heat Transfer and Pressure Drop of Liquids in Tubes," *Ind. Eng. Chem.* 28 (1936): 1429–1435.
3. Walas, S. M., *Chemical Process Equipment: Selection and Design* (Stoneham, MA: Butterworth, 1988).

Problems

1. For the ethylbenzene process shown in Appendix B, check the design specifications for the following three pieces of equipment against the appropriate heuristics: P-301, V-302, T-302. Comment on any significant differences that you find.
2. For the styrene process shown in Appendix B, check the design specifications for the following three pieces of equipment against the appropriate heuristics: E-401, C-401, T-402. Comment on any significant differences that you find.
3. For the drying oil process shown in Appendix B, check the design specifications for the following three pieces of equipment against the appropriate heuristics: V-501, P-501, H-501. Comment on any significant differences that you find.

Chapter 12. Synthesis of the PFD from the Generic BFD

What You Will Learn

- Design of a chemical process usually starts with a block flow diagram.
- Additional information is required to build a process flow diagram from a block flow diagram.
- There is a logical order to the synthesis of a chemical process from its component sections.

The evolutionary procedure to create a full PFD (as presented in Chapter 1) from the generic block flow process diagram (GBFD) (Chapter 2) is described in this chapter. This full PFD truly defines the process in a chemical engineering sense and is the starting point for chemical and other engineers to design the machines, structures, and electrical/electronic components needed to make the chemical engineer's vision a reality.

This crucial step in the design of the chemical plant involves all subareas of chemical engineering: reaction engineering, thermodynamics, process control, unit operations and transport, and material and energy balances. Each is applied to put details into the six general sections of the GBFD—reactor feed preparation, reactor, separator feed preparation, separator, recycle, and environmental control.

In this synthesis, the broader context of the project (e.g., environmental concerns, customer expectations, return on investment) is integrated with the important details such as the type of heat transfer medium or the number of stages in a column. It is crucial to consider as many alternatives as possible in the early stages to try to avoid becoming trapped in a suboptimal design.

> **It is a common human trait to resist change more strongly as more effort is expended on a task, design, or product. This is described as not wanting to abandon the "investment" in the activity.**

12.1. Information Needs and Sources

Before the detailed synthesis of the PFD can be completed, basic physical property and kinetics information are needed. It is assumed here that the very basic chemistry of the desired reaction is known, that is, what main feed materials go to what main product. Before PFD synthesis can begin, the marketing engineers have identified a market need for a specific product, and the chemists have identified at least one way to produce the chemical in the laboratory. Even the marketing and chemistry information, however, will need to be refined. Flowsheet synthesis will uncover the need for more detailed data on the reaction rate, temperature and pressure effects, and market values of products of different purities.

12.1.1. Interactions with Other Engineers and Scientists

Teams of engineers work on the development of the process. For example, the marketing department will find the customer for the plant's product, and product specifications will be identified. Many chemical engineers are employed as marketing engineers, and they will understand that product purity affects product price, often dramatically so. However, the details of this interplay can be determined

only by the process design engineers as the PFD is being developed; only through discussions and negotiations with customers can the marketing engineer determine the relationship between product purity and the product value (i.e., maximum selling price) to the customer.

Similarly, there may be more than one chemical pathway to the product. Pathways of greatest interest to the chemical engineer are not necessarily those of greatest interest to the chemist. The abilities to use impure feed materials and to avoid the production of by-products reduce costs but may not be of interest to a chemist. The costs of small-lot, high-purity laboratory reagents may not even qualitatively correlate to those of multiple tank-car, industrial-grade raw materials. Isothermal operation of small laboratory reactors is common but essentially impossible to achieve on a large scale. It is more economical per unit volume to maintain high pressures on the plant scale than it is in the lab. Simple batch operations are common in laboratory work, but, at plant scale, sophisticated optimization of scheduling, ramp rates, cycle sequencing, and choice of operating mode (batch, semibatch, continuous) is vital. Thus, the chemical process design engineer must be in touch with the chemist to make sure that expensive constraints or conditions suggested by laboratory studies are truly needed.

12.1.2. Reaction Kinetics Data

Before reactor design can begin, the kinetics of the main reaction must be known. However, a knowledge of the kinetics of unwanted side reactions is also crucial to the development of PFD **structure** or **topology** (number and position of recycle streams; types, numbers, and locations of separators; batch or continuous operating modes; sterilization operations needed for aseptic operation). Knowledge of detailed reaction pathways, elementary reactions, and unstable reaction intermediates is not required. Rather, the chemical process design engineer needs to know the rate of reaction (main and by-product reactions) as a function of temperature, pressure, and composition. The greater the range of these independent variables, the better the design can be.

For some common homogeneous reactions, kinetics are available [1, 2, 3]. However, most commercial reactions involve catalysts. The competitive advantage of the company is often the result of a unique catalyst. Thus, kinetics data for catalyzed reactions are not as readily available in open literature but should be available within the company files or must be obtained from experiments. One source of kinetics data for catalytic reactions is the patent literature. The goal of someone writing a patent application, however, is to present as little data as possible about the invention while obtaining the broadest possible protection. This is why patent information is often cryptic. However, this information is often sufficient to develop a base-case PFD. The key data to obtain from the patent are the inlet composition, temperature, pressure, outlet composition, and space time. If the data are for varying compositions, one can develop crude kinetics rate expressions. If the data are for more than one temperature, an activation energy can be determined. These data reduction procedures are described in undergraduate textbooks on reaction engineering [4, 5].

Without kinetics data, a preliminary PFD and cost analysis can still be done [6]. In this type of analysis, the differing process configurations and costs for different assumed reaction rates provide estimates of the value of a potential catalyst. If doubling the reaction rate reduces the cost of manufacture by $1 million per year, for example, the value of catalysis research to increase the reaction rate (all other things being equal) is clear. As a guideline, the economic breakpoint is often a catalyst productivity to desired product of ~0.10 kg product per kg catalyst per hour [7]. Another guide is that activation energies are usually between 40 and 200 kJ/mol.

12.1.3. Physical Property Data

In addition to kinetics data, physical property data are required for determining material and energy balances, as well as for sizing of heat exchangers, pumps and compressors, and separation units. These data are, in general, easier to obtain and, when necessary, easier than kinetics data to estimate.

For the material and energy balances, pure-component heat capacity and density data are needed. These are among the most widely measured data and are available on process simulators for several thousand substances. (See Chapter 13 for details of process simulators.) There are also reasonably accurate group-contribution techniques for use when no data are available [8]. The enthalpies of mixtures require an accurate equation of state for gases and nonionic liquids. The equations of state available on process simulators are accurate enough for these systems. However, additional heat of solution data are needed for electrolyte solutions, and these data may not be as readily available. For these systems, care should be taken to use accurate experimental data, because estimation techniques are not as well defined (see Chapter 13 for additional information on electrolyte systems).

The design of heat exchangers and the determination of pressure drops across units require thermal conductivity and viscosity data. These data are usually available (often in the databanks of process simulators) and, if unavailable, can be estimated by group-contribution techniques [8].

The most crucial and least available physical property data are for phase equilibrium. Most separators are based on equilibrium stages; thus, these data are usually needed for a process design. For vapor-liquid equilibrium, such as for distillation, either (1) a single equation of state for both phases or (2) a combination of vapor-phase equation of state, pure-component vapor pressure, and liquid-state activity-coefficient model is required. The choice of thermodynamics package for process simulators is explained in Section 13.4. The key experimentally determined mixture parameters for either equations of state or activity-coefficient models are called **BIPs** (**binary interaction parameters**), and they have great effect on the design of separation units. A poor estimation of them (e.g., assuming them to be zero!) can lead to severely flawed designs. The solubilities of noncondensables in the liquid phase are also essential but difficult to estimate.

12.2. Reactor Section

For a process with a reactor, often the synthesis of the PFD begins with the reactor section of the GBFD. (See Chapter 23.) A base-case reactor configuration is chosen according to the procedures described in reaction engineering textbooks. This configuration (e.g., plug flow, CSTR, batch, semibatch, adiabatic, isothermal) is used at some base conditions (temperature, pressure, feed composition) and some preliminary base specification (e.g., 60% conversion) to calculate the outlet composition, pressure, and temperature. The goal at this stage is to develop a feasible PFD for the process. Optimization of the PFD can begin only after a suitable base case is developed. If there are obvious choices that improve the process (such as using a fluidized bed instead of a packed-bed reactor, or batch operation instead of continuous), these choices are made at this stage; however, these choices should be revisited later.

To enable later optimization, the general effects of varying the feed conditions should be investigated at this point by using the trend prediction approach of Chapter 20. A list of possible reactor configurations should also be developed. These choices often have dramatic effects on the other parts of the GBFD. The earlier these effects are understood, the better the final design will be.

At this stage, the utility needs of the reactor should be considered. If heating or cooling is required,

the design of an entire additional system may be required. The choice of heating or cooling medium must be made based on strategies described in Chapter 15, the heuristics presented in Chapter 11, and the costs of these utilities.

The trade-offs of different catalysts, parallel versus series reactors, and conversion versus selectivity should be considered, even though the optimization of these choices occurs after the base case is developed. Again, early identification of alternatives improves later detailed optimization.

Once the base-case reactor configuration is chosen, the duties of the reactor feed preparation and separator feed preparation units are partially determined.

For the reactor, important questions to be considered include the following:

1. *In what phase does the reaction take place (liquid, vapor, mixed, etc.)?* The answer will affect the reactor feed section. For example, if the reaction is in the vapor phase it will determine whether a vaporizer or fired heater is required upstream of the reactor when the feed to the plant is liquid.
2. *What are the required temperature and pressure ranges for the reactor?* If the pressure is higher than the feed pressure, pumps or compressors are needed in the reactor feed preparation section. If the required reactor feed temperature is greater than approximately 250°C, a fired heater is probably necessary.
3. *Is the reaction kinetically or equilibrium controlled?* The answer affects both the maximum single-pass conversion and the reactor configuration. The majority of gas-and liquid-phase reactions in the CPI are kinetically controlled. The most notable exceptions are the formation of methanol from synthesis gas, synthesis of ammonia from nitrogen and hydrogen, and the production of hydrogen via the water-gas shift reaction.
4. *Does the reaction require a solid catalyst, or is it homogeneous?* This difference dramatically affects the reactor configuration. For enzymes immobilized on particles, for example, a fluidized bed reactor or packed-bed reactor could be considered, depending on stability of the enzyme and mass-transfer requirements. The immobilization may also impart some temperature stability to the enzyme, which provides additional flexibility in reactor configuration and operating conditions.
5. *Is the main reaction exothermic or endothermic, and is a large amount of heat exchange required?* Again, the reactor configuration is strongly affected by the heat transfer requirements. For mildly exothermic or endothermic gas-phase reactions, multiple packed beds of catalyst or shell-and-tube reactors (catalyst in tubes) are common. For highly exothermic gas-phase reactions, heat transfer is the dominant concern, and fluidized beds or shell-and-tube reactors with catalyst dilution (with inert particles) are used. For liquid-phase reactions, temperature control can be achieved by pumping the reacting mixture through external heat exchangers (for example, in Figure B.11.1). For some highly exothermic reactions, part of the reacting mixture is vaporized to help regulate the temperature. The vapor is subsequently condensed and returned to the reactor. External jackets and internal heat transfer tubes, plates, or coils may also be provided for temperature control of liquid-phase reactions. (See Chapters 18 and 23.)
6. *What side reactions occur, and what is the selectivity of the desired reaction?* The formation of unwanted by-products may significantly complicate the separation sequence. This is especially important if these by-products are formed in large quantities and are to be purified for sale. For high-selectivity reactions, it may be more economical to dispose of by-products as

waste or to burn them (if they have high heating values), which simplifies the separation section. However, for environmental reasons, great emphasis is placed on producing either salable by-products or none at all.

7. *What is the approximate single-pass conversion?* The final single-pass conversion is determined from detailed parametric optimizations (Chapter 14); however, the range of feasible single-pass conversions affects the structure of the separations section. If extremely high single-pass conversions are possible (e.g., greater than ~98%), it may not be economical to separate and recycle the small amounts of unreacted feed materials. In this case, the feed materials become the impurities in the product, up to the allowable concentration.
8. *For gas-phase oxidations, should the reactor feed be outside the explosive limits?* For example, there are many reactions that involve the partial oxidation of hydrocarbons (see the CD for acrylic acid production in Appendix B and phthalic anhydride production in Appendix C). Air or oxygen is fed to a reactor along with hydrocarbons at high temperature. The potential for explosion from rapid, uncontrolled oxidation (ignition) is possible whenever the mixture is within its explosive limits. (Note that the explosive limits widen significantly with increase in temperature.) An inherently safe design would require operation outside these limits. Often, steam is added both as a diluent and to provide thermal ballast for highly exothermic reactions —for example, in the acrylic acid reactor (Figure B.9.1).

12.3. Separator Section

After the reactor section, the separator section should be studied. The composition of the separator feed is that of the reactor effluent, and the goal of the separator section is to produce a product of acceptable purity, a recycle stream of unreacted feed materials, and a stream or streams of by-products. The ideal separator used in the GBFD represents a process target, but it generally represents a process of infinite cost. Therefore, one step is to "de-tune" the separation to a reasonable level. However, before doing that, one must decide what the by-product streams will be. There may be salable by-products, in which case a purity specification is required from the marketing department. For many organic chemical plants, one by-product stream is a mixture of combustible gases or liquids that are then used as fuel. There may also be a waste stream (often a dilute aqueous stream) to be treated downstream; however, this is an increasingly less desirable process feature.

Prior to enactment of current environmental regulations, it was generally thought to be less expensive to treat waste streams with so-called end-of-pipe operations. That is, one produced, concentrated, and disposed of the waste in an acceptable manner. As regulations evolved, the strategy of pollution prevention or green engineering has led to both better environmental performance and reduced costs. More details are given in Chapter 27, but the overall strategy is to minimize wastes at their source or to turn them into salable products.

The separation section then generally accepts one stream from the pre-separation unit and produces product, by-product, and (sometimes) waste streams. In the development of the PFD, one must consider the most inclusive or flexible topology so that choices can be made in the optimization step. Thus, each type of stream should be included in the base case.

Next, the minimum number of simple separation units must be determined. Although there are single units that produce multiple output streams (such as a petroleum refining pipe still with many side draws), most units accept a single inlet stream and produce two outlet streams. For such simple separators, at least $(N - 1)$ units are needed, where N is the number of outlet streams (products, by-

products, and waste). There are two types of questions to answer concerning these units in the separation section: (1) What types of units should be used? and (2) How should the units be sequenced?

12.3.1. General Guidelines for Choosing Separation Operations

There are general guidelines concerning choice of separation unit. Table 12.1 gives a set of rules for the most common choices of separation units on process simulators.

Table 12.1. Guidelines for Choosing Separation Units

- Use distillation as a first choice for separation of fluids when purity of both products is required.
- Use gas absorption to remove one trace component from a gas stream.
- Consider adsorption to remove trace impurities from gas or liquid streams.
- Consider pressure-swing adsorption to purify gas streams, especially when one of the components has a cryogenic boiling point.
- Consider membranes to separate gases of cryogenic boiling point and relatively low flowrates.
- Choose an alternative to distillation if the boiling points are very close or if the heats of vaporization are very high.
- Consider extraction as a choice to purify a liquid from another liquid.
- Use crystallization to separate two solids or to purify a solid from a liquid solution.
- Use evaporation to concentrate a solution of a solid in a liquid.
- Use centrifugation to concentrate a solid from a slurry.
- Use filtration to remove a solid in almost dry form from a slurry.
- Use screening to separate solids of different particle size.
- Use float/sink to separate solids of different density from a mixture of pure particles.
- Consider reverse osmosis to purify a liquid from a solution of dissolved solids.
- Use leaching to remove a solid from a solid mixture.
- Consider chromatography for final purification of high-value products (such as proteins) from dilute streams.

For a base case, it is essential that the separation technique chosen be reasonable, but it is not necessary that it be the best.

For sequencing of the separation units, there is another set of guidelines, given in Table 12.2. In the base case, it is often helpful to consider the same type of separator for each unit. During optimization, one can compare different separator types for the different duties. Again, some separators can do multiple separations in one unit, but these can be found during optimization. Additional heuristics for separation unit sequencing are given in Table 11.13 and in reference [9].

Table 12.2. Guidelines for Sequencing Separation Units

- Remove the largest product stream first. This makes all of the subsequent separation units smaller.
- For distillation, remove the product with the highest heat of vaporization first, if possible. This reduces the heating/cooling duties of subsequent units.

- Do not recombine separated streams. (This may seem obvious, but it is often disobeyed.)
- Do the easy separations first.
- Do not waste raw materials, and do not overpurify streams based on their uses.
- Remove hazardous or corrosive materials first.
- Use the less expensive, cruder separation technique first (e.g., liquid-liquid extraction before chromatography).

As with all sets of heuristics, these can be mutually contradictory. However, in the initial topology of the separation section, the main goal is to follow as many of these heuristics as possible.

Beyond these general guidelines, beware of azeotropes and multiple phases in equilibrium, especially when water and organics are present. Special techniques are available to deal with these problems, some of which are discussed later. On the other hand, if a single-stage flash will do the separation, do not use a column with reflux.

For the separation section, other important questions to be considered include the following:

1. *What are the product specifications for all products?* Product specifications are developed to satisfy customers who will use these products in their own processes. The most common specification is a minimum concentration of the main constituent, such as 99.5 wt%. Maximum impurity levels for specific contaminants may also be specified, as well as requirements for specific physical properties such as color, odor, and specific gravity. A single separation technique may not be sufficient to meet all the required product specifications, as demonstrated in Example 12.1.

Example 12.1.

In the production of benzene via the hydrodealkylation of toluene, it is necessary to produce a benzene product stream that contains >99.5 wt% benzene that is water white in color (i.e., absolutely clear). If the feed toluene to the process contains a small amount of color, determine a preliminary separation scheme to produce the desired benzene product.

As a guide, look at the toluene hydrodealkylation process shown in Figure 1.5. Because the volatilities of toluene and benzene are significantly different, the main purification step (the separation of benzene from toluene) can be accomplished using distillation, which is consistent with Figure 1.5. However, it has been found that the compound causing the discoloration of the toluene is equally soluble in benzene and toluene, causing the benzene product to be discolored. It is further found by laboratory testing that the benzene product can be decolorized by passing it through a bed of activated carbon. Thus, a second separation step, consisting of an activated carbon adsorber, will be added to the process to decolorize the benzene product.

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2. *Are any of the products heat sensitive?* If any of the products or by-products are heat sensitive (i.e., they decompose, deactivate, or polymerize at elevated temperatures), the conditions used in the separations section may have to be adjusted, as in Example 12.2.

Example 12.2.

It is known that acrylic acid starts to polymerize at 90°C when it is in a concentrated form. Acrylic acid must be separated from acetic acid to produce the required purity product, and the volatilities of

both acids are significantly different. This points to distillation as the separation method. The normal boiling points of acrylic acid and acetic acid are 140°C and 118°C, respectively. How should the separation be accomplished to avoid degradation of the acrylic acid product?

The distillation column must be run under vacuum to avoid the problem of acrylic acid degradation. The pressure should be set so that the bottom temperature of the column is less than 90°C. From Figure B.9.1 and Table B.9.1, it can be seen that a column pressure of 0.16 bar at the bottom can accomplish the desired separation without exceeding 90°C.

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3. *Are any of the products, by-products, or impurities hazardous?* Because separation between components is never perfect, small quantities of toxic or hazardous components may be present in product, fuel, or waste streams. Additional purification or subsequent processing of these streams may be required, depending on their end use.

12.3.2. Sequencing of Distillation Columns for Simple Distillation

Because distillation is still the prevalent separation operation in the chemical industry, it will now be discussed in more detail. **Simple distillation** can be defined as distillation of components without the presence of any thermodynamic anomalies. The most apparent thermodynamic anomaly in distillation systems is an azeotrope. Azeotropic distillation is discussed in the next section. The remainder of this section is for simple distillation.

As stated earlier, as a general guideline, a minimum of $N - 1$ separators are needed to separate N components, and this guideline also applies to distillation systems. Therefore, one distillation column is required to purify both components from a two-component feed. This is the type of problem most often studied in separation classes. To purify a three-component feed into three "pure" components, two distillation columns are required. However, there are two possible sequences, and these are illustrated in Figures 12.1(a) and 12.1(b). Ultimately, the choice of sequence depends upon the economics. However, the results of the economic analysis often follow the guidelines in Table 12.2. For example, if the heavy component (C) is water, it should be removed first due to its high heat of vaporization, so the sequence in Figure 12.1(b) is likely to be more economical for such a situation. This is because the heating and cooling duties in the second column are reduced significantly if the water is removed first. The sequence in Figure 12.1(b) is also likely to be a better choice if component C is present in the largest amount, or if component C is the only corrosive component. This is because in the former case, the second column will be smaller, and in the latter case, the second column may not need the expensive materials of construction needed in the first column.

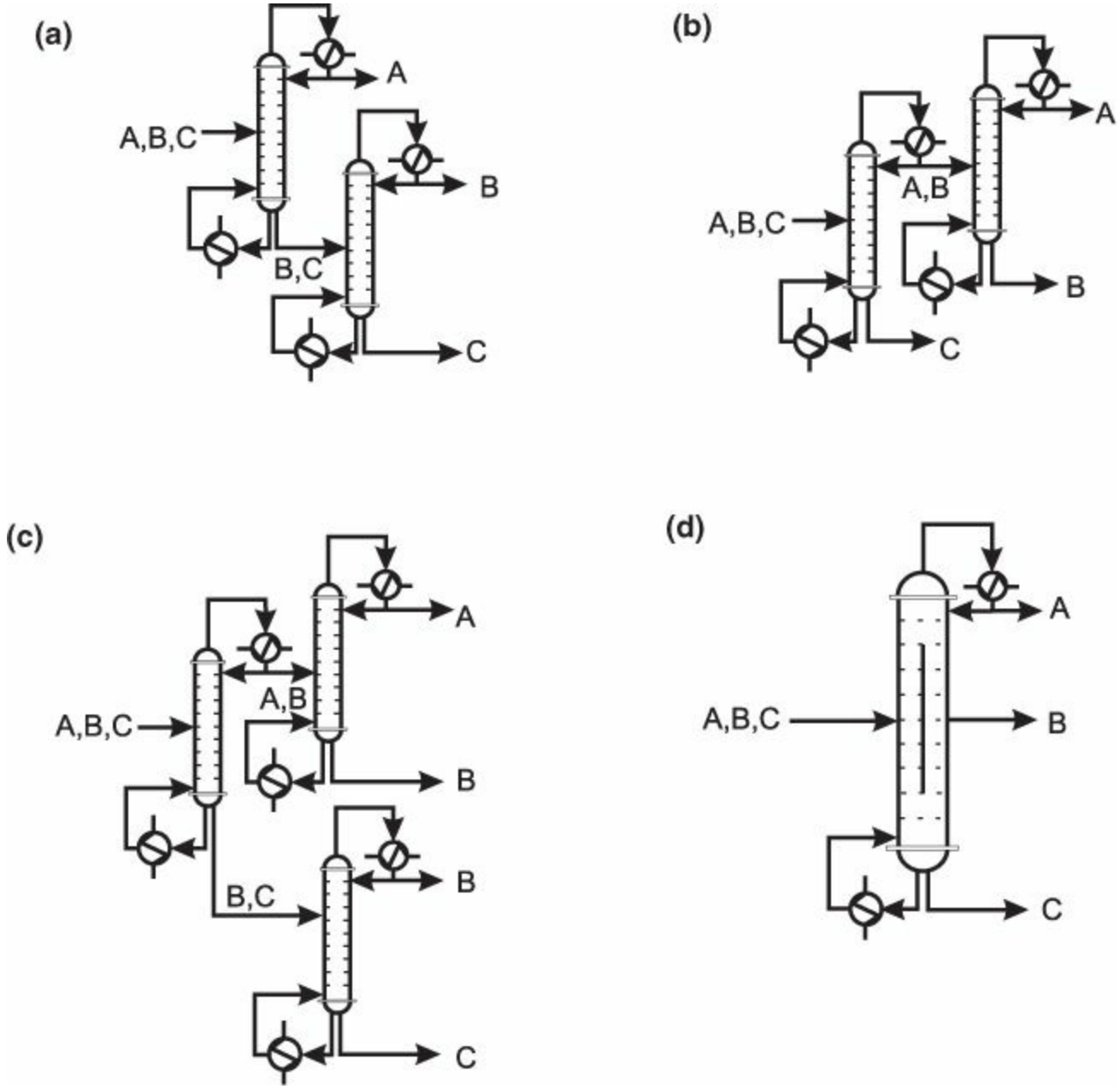


Figure 12.1. Column Arrangements for Simple Distillation of Three Component Feed

It must be understood that more than $N-1$ distillation columns are permissible. There are cases that have been reported where the sequence in Figure 12.1(c) is actually more economical than either of the sequences in Figures 12.1(a) and 12.1(b). This occurs because the sequence in Figure 12.1(c) has lower utility costs that offset the capital cost of the extra column and peripherals [10]. Actually, the sequence represented in Figure 12.1(c) can be accomplished in one column, a partitioned column with a vertical baffle, as illustrated in Figure 12.1(d) [10]. The presence of the vertical baffle makes the column behave like the three columns in Figure 12.1(c). The lesson learned here is that distillation practice can be very different from distillation theory. Textbooks usually state unequivocally that $N-1$ distillation columns are required for separation of N components. However, the two examples presented here demonstrate that distillation practice does not always conform to theory.

Other distillation column configurations are possible [11–13]. In these references, there are column configurations known as Petlyuk-type columns. It should be noted that even though the configuration in Figure 12.1(c) looks like a Petlyuk–type II column, it is not, due to the presence of a reboiler and a condenser on the first column, units that are not present in the Petlyuk–type II column.

Figures 12.1(a) and 12.1(b) show the two theoretical simple sequences possible for separating three

components in simple distillation. As the number of components increases, so does the number of alternative simple sequences. The number of alternative simple sequences, S, for an N-component feed stream is given by [14]

$$S = \frac{[2(N-1)]!}{N!(N-1)!} \qquad (12.1)$$

There are other column arrangements possible for simple distillation. Some of these are illustrated in Figure 12.2. Figure 12.2(a) illustrates distillation with a side stream. It must be understood that in a typical distillation column, a side stream does not contain a pure component; it contains a mixture. In certain petroleum refining operations, side streams are common because a mixture is the desired product. Sometimes a side stream is withdrawn because it contains a maximum concentration of a third component—for example, in the purification of argon from air.

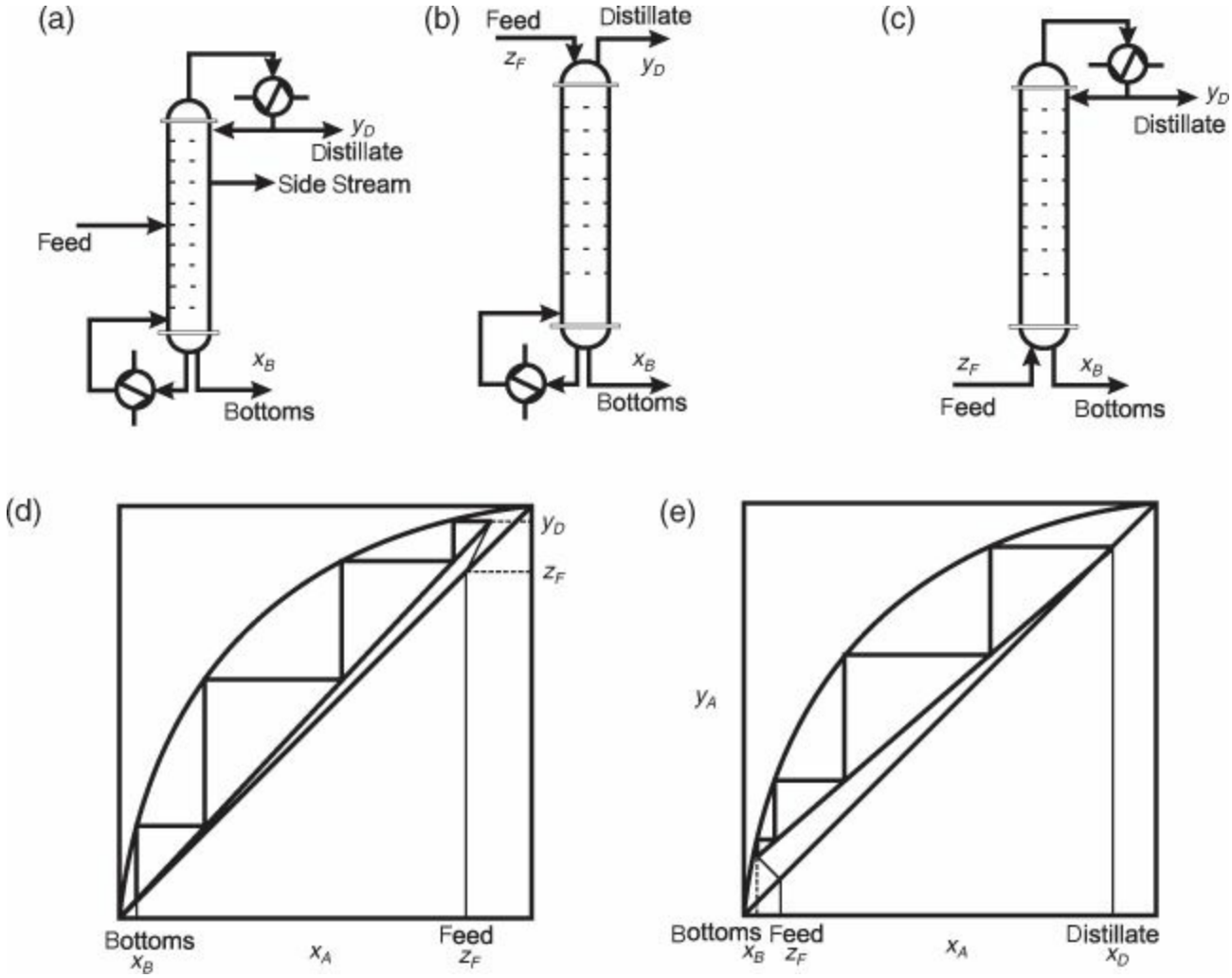


Figure 12.2. Other Distillation Column Arrangements for Simple Distillation

Figure 12.2(a) should not be confused with Figure 12.1(d), because the presence of the vertical baffle in the latter makes that column behave differently. Figure 12.2(b) represents a stripping column (sometimes called a reboiled absorber), and Figure 12.2(c) represents a rectifying column. A stripping column is used when the light components are very dilute and when they need not be purified. A rectifying column is used when the heavy components are very dilute and need not be purified. The performance of the stripping and rectifying columns can be understood from their McCabe-Thiele representations, shown in Figures 12.2(d) and 12.2(e), respectively.

12.3.3. Azeotropic Distillation

Distillation involving azeotropes does not conform to the guidelines discussed in Section 12.3.2. This

is best illustrated by examining the thermodynamic behavior of a binary homogeneous azeotrope, illustrated in Figure 12.3. Clearly, no McCabe-Thiele construction can be made to produce two pure products from the indicated feed. The heavy component can be purified, but an infinite number of stages above the feed would be required just to approach the azeotropic concentration, (x_{az}, y_{az}), the point where the equilibrium curve crosses the 45° line. There are minimum- and maximum-boiling azeotropes, although minimum-boiling azeotropes (where the azeotrope is at a lower temperature than either pure-component boiling point) are more common. Minimum-boiling azeotropes arise from repulsive forces between molecules. One way of thinking about azeotropes is that the volatility switches. In Figure 12.3, Component A is more volatile when it is present below the azeotropic composition, but Component B is more volatile when Component A is present above the azeotropic composition. Given that simple distillation exploits the difference in volatility between components, it is easy to understand how the switch in volatility makes simple distillation impossible.

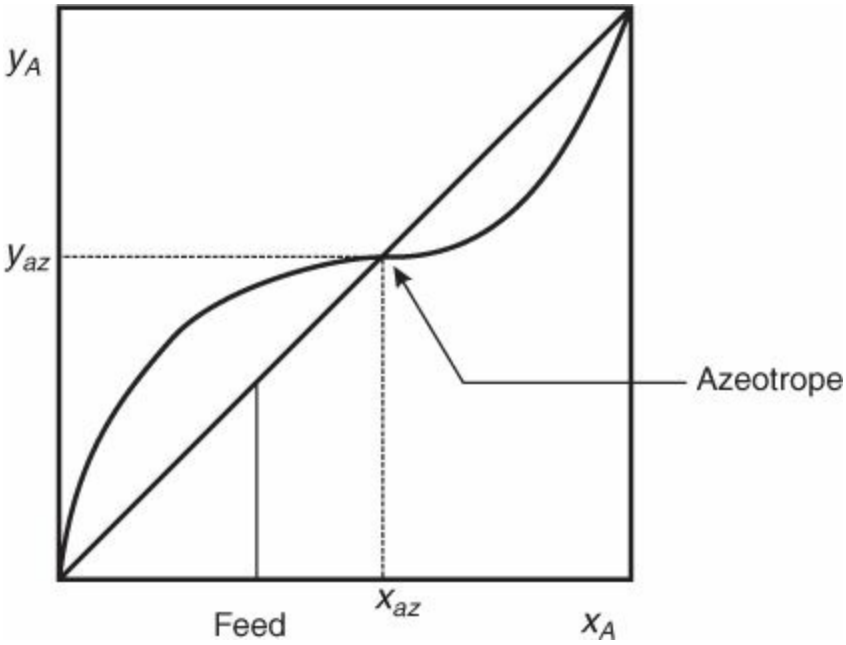


Figure 12.3. *X-Y* Diagram for Component A Forming a Minimum-Boiling, Binary Azeotrope with Component B (Constant Pressure)

In the next section, methods for accomplishing distillation-based separations in the presence of azeotropes for binary systems are discussed. In the subsequent section, methods for azeotropic distillation involving three components are discussed.

Binary Systems. The methods used to distill beyond azeotropes in binary systems are illustrated using McCabe-Thiele diagrams. Four of the more popular methods are discussed here. A more complete discussion is available in any standard separations textbook [15].

The more popular methods for breaking binary azeotropes include the following:

1. One distillation column allows separation close to the azeotrope, and then a different separation method is used to complete the purification (Figure 12.4[a]).

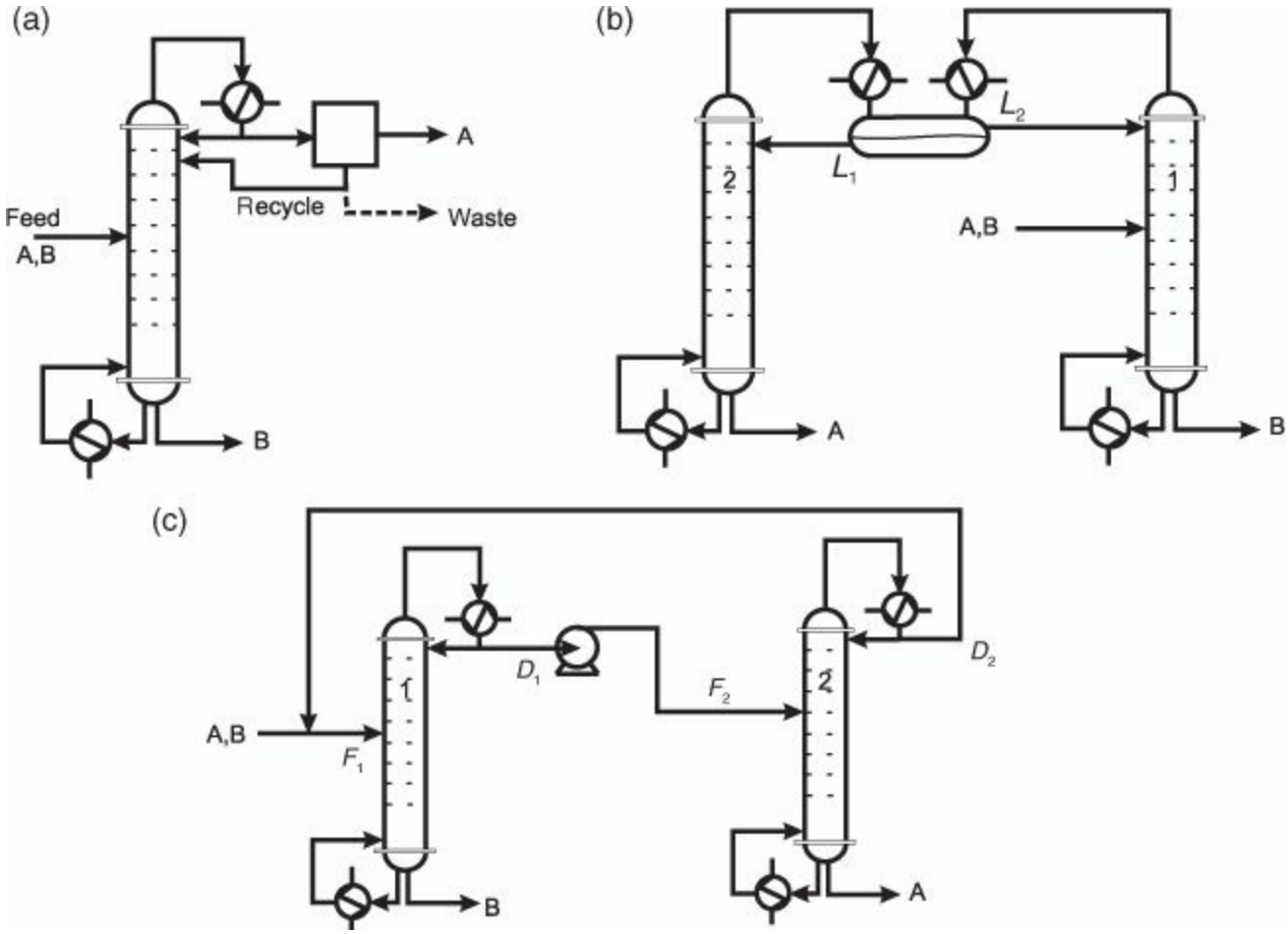


Figure 12.4. Distillation Arrangements to Separate Binary Azeotropes

2. If the azeotrope is a binary, heterogeneous azeotrope, that means there is a region where the two components form two mutually immiscible liquid phases (both in equilibrium with the azeotropic vapor composition, which is between the two liquid compositions), and hence a phase separator and a second column are added. The phase separator provides one phase on the other side of the azeotrope from the feed, so that phase can be purified by distillation in a second column (Figure 12.4[b]).
3. If the azeotrope concentration is pressure sensitive, one column is used to distill close to the azeotrope. One "pure" component is produced from the bottom of this first column. Then the pressure of the distillate is raised so that the azeotropic composition is now below the distillate composition. Then a second column is used to purify the second component. Because the volatility switches as the azeotrope is crossed, the second component is in the bottom stream of the second column (Figure 12.4[c]). This particular sequence assumes that the azeotrope is less concentrated in A at higher pressures.
4. A third component can be added to change the phase behavior. This method is discussed in the next section.

The first alternative is illustrated in Figure 12.4(a). Here, a distillation column is used that will provide "pure" B in the bottoms and a near-azeotropic mixture in the distillate. The McCabe-Thiele construction for this distillation column is illustrated in Figure 12.5(a). Then a different type of separation is used to purify Component A (not shown on the McCabe-Thiele diagram). The impure stream from the second separator should be recycled, if possible; however, treatment as a waste stream is also possible. The recycle stream will most likely be fed to a different tray from the feed stream, because distillation column feeds should always be near the point in the column with the same

concentration as the feed stream.

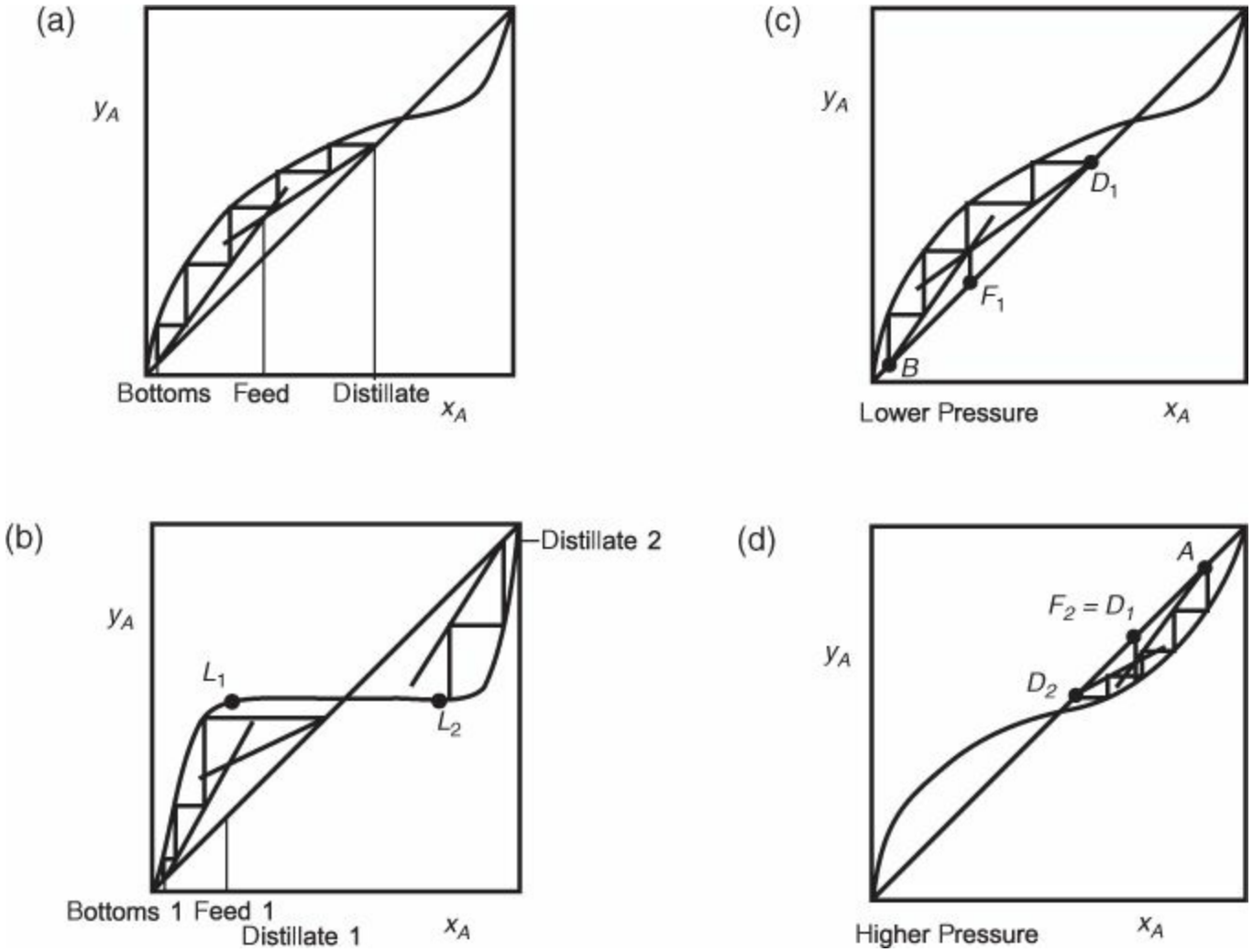


Figure 12.5. McCabe-Thiele Diagrams for Distillation Arrangements in Figure 12.4

An example of this situation is the ethanol-water system, which has a binary azeotrope in the 90–95 mol% ethanol range (depending on system pressure). A relatively recent method for purifying ethanol beyond the azeotropic composition is **pervaporation** [16]. The following question may arise when considering this method: Why not just use pervaporation (or whatever second separation method is possible) for the entire separation? The answer is that, even with volatile energy prices, the relatively low cost of energy makes distillation a very economical separation method [16]. In most cases, an arrangement like Figure 12.4(a) is far less expensive than using the second separation method alone. This is because separations such as distillation are very economical for producing relatively pure products from roughly equal mixtures. Obtaining ultrapure products from distillation can have unfavorable economics, because large numbers of trays are required for very high purity (think about the McCabe-Thiele construction). Separations like pervaporation (or any membrane separation) have much more favorable economics when removing a dilute component from a relatively pure component. They are also economically unattractive for large processing volumes. Therefore, the combination of distillation and another separation like pervaporation usually provides the economic optimum.

In cases where the two components being distilled form an azeotrope with two immiscible liquid phases, the method illustrated in Figure 12.4(b) can be used to obtain two “pure” components. The McCabe-Thiele diagram is shown in Figure 12.5(b). A characteristic of the equilibrium in this system is the horizontal segment of the equilibrium curve, which is caused by the phase separation into immiscible phases. The equilibrium between the two phases is illustrated by the ends of the

horizontal segment of the equilibrium curve marked by L_1 and L_2. Therefore, in one column, the feed is distilled to near-azeotropic conditions, and "pure" component B is in the bottom stream. The impure distillate is condensed and sent to a phase separator. One immiscible phase is on the other side of the azeotrope, and it is sent to a second column to purify component A in the bottom stream. The impure distillate from the second column is condensed and sent to the phase separator. It is important to understand that this method works only for systems exhibiting this type of azeotropic phase behavior.

If a binary azeotrope is pressure sensitive, the method illustrated in Figure 12.4(c) can be used to produce two "pure" products. The McCabe-Thiele construction is illustrated in Figures 12.5(c) and 12.5(d). In this illustration, increasing the system pressure lowers the azeotropic composition of A. The McCabe-Thiele construction in Figure 12.5(d) is at a higher pressure than that in Figure 12.5(c). Therefore, for the case illustrated, the feed is distilled in one column to produce "pure" B and a near-azeotropic distillate (D_1). This distillate is then pumped to a higher pressure, which lowers the azeotropic composition. At a suitable pressure, the distillate from the first column is now above the azeotropic composition, and a second column is then used to purify A. "Pure" A is the bottoms product of the second column because of the reversal in volatilities caused by the azeotrope. The near-azeotropic distillate (D_2) is recycled to the first column.

A related method for pressure-sensitive azeotropes is to run only one column at vacuum conditions. If the equilibrium behavior is favorable, the azeotrope will be at a mole fraction of A approaching unity. Depending on the desired purity of component A, the maximum possible distillate composition may be sufficient.

It is important to remember that pressure-swing methods are applicable only when the azeotropic composition is highly pressure sensitive. Although there are examples of this behavior, it is actually quite rare.

Azeotropes in Ternary Systems. In binary systems, the McCabe-Thiele method provides a conceptual representation of the distillation process. In ternary systems, there is a method that provides a similar conceptual representation. It is called the **boundary value design method (BVDM),** and it is particularly useful for conceptualizing azeotropic distillation in ternary systems. This method is introduced here; however, the reader seeking a more in-depth treatment of this method and all aspects of azeotropic distillation should consult the definitive reference in the field [17].

In the BVDM, ternary distillation is represented on a right-triangular diagram just as binary distillation is represented on a rectangular plot in the McCabe-Thiele method. Each point on the right-triangular diagram represents the mole fraction of each of the three components on a tray. For example, in Figure 12.6(b), the vertex labeled B is the origin of a rectangular coordinate system. At that point, the mole fractions of A and C are zero, and the mole fraction of B is obtained by subtraction from 1. Hence, the mole fraction of B at the origin is 1. Consider any other point on the diagram, point p, as illustrated. The mole fractions of C and A are obtained using the horizontal and vertical coordinates, respectively, based on B as the origin. The mole fraction of B is obtained by subtraction of the mole fractions of A and C from 1.

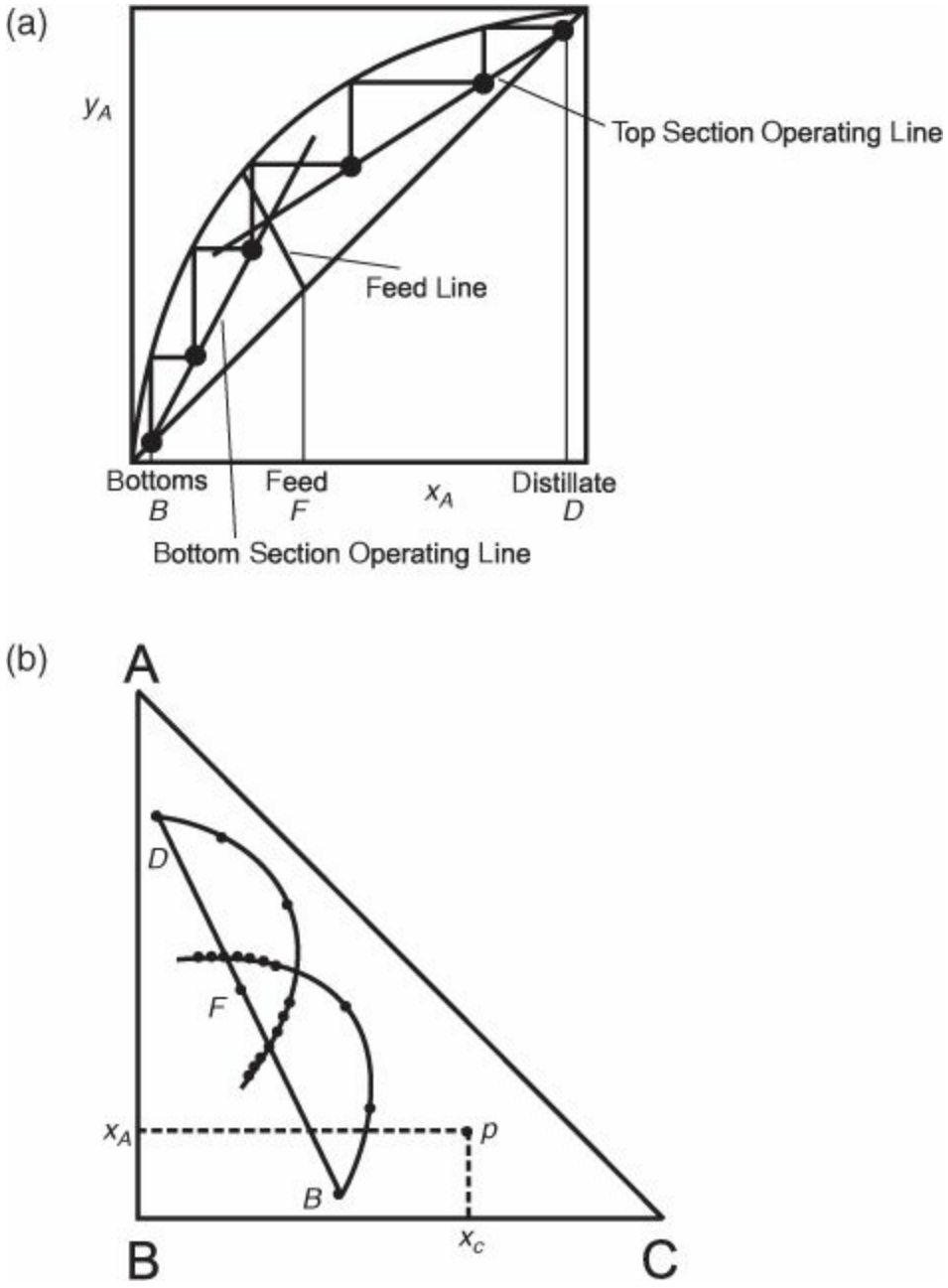


Figure 12.6. Comparison of McCabe-Thiele for Binary Distillation (a) and Triangular Diagram for Ternary Distillation (b)

For a simple ternary distillation process, a curve can be drawn by connecting the compositions on each stage. This is equivalent to the operating line in the McCabe-Thiele method. This is illustrated in Figure 12.6. It is observed that the curves for the rectifying and stripping section intersect. This intersection implies a feasible distillation process, just as intersection of the operating lines for rectifying and stripping implies a feasible binary distillation on the McCabe-Thiele diagram. If the curves do not intersect, then the distillation operation is not feasible.

Each point shown on the curves on the triangular diagram is analogous to the highlighted points on the McCabe-Thiele diagram, where the stepping process intersects the operating lines. In the McCabe-Thiele method, the optimum feed location is determined by the intersection of the operating lines. It is possible to place the feed in a different location; however, the optimum location minimizes the number of stages required. For simple ternary distillation, the feed tray is fixed at the point of intersection of the rectifying and stripping curves on the triangular diagram. To trace the tray-to-tray compositions, one follows a curve for one section and then switches to the curve for the other section at the intersection of the curves. The closely spaced points not in the range of operation are those

analogous to the points on a McCabe-Thiele diagram obtained by not switching operating lines in the stepping process and pinching as the equilibrium curve is approached.

It is also observed that the feed point lies on a straight line connecting the distillate and bottoms product concentrations. This is a consequence of the lever rule and is similar to the representation of mixing and separation processes on triangular diagrams in extraction processes [18, 19]. The line connecting points D, F, and B is a representation of the overall material balance on the column. As a consequence of the requirement of the overall material balance, for a column (with only one feed and without side streams) to be feasible, the points D, F, and B must lie on the same straight line.

Instead of using the equilibrium curve, as is done in the McCabe-Thiele diagram, on a triangular diagram, a residue curve is used. A **residue curve** is a plot of the composition of the liquid residue in a single-stage batch equilibrium still with time at a given pressure (Figure 12.7). In a batch still, as the still pot is heated, the more volatile components are boiled off, and the concentration of the less volatile components increases with time in the still pot. The equation used to calculate the residue curve is the unsteady material balance on the still pot for each component *i*.

$$\frac{dx_i}{dt} = (x_i - y_i)\left(\frac{-d\ell nN}{dt}\right) \tag{12.2}$$

$$y_i = K_i x_i \tag{12.3}$$

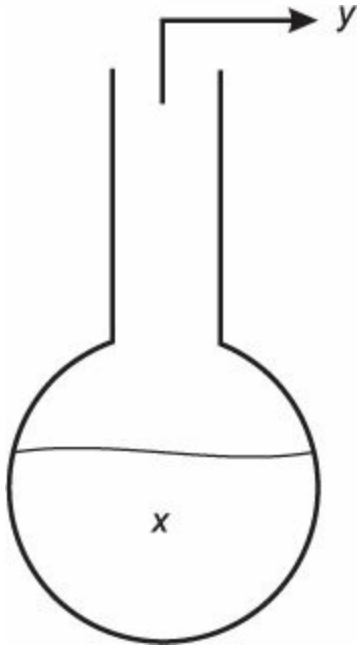


Figure 12.7. Batch Distillation

where *N* is the total moles of liquid in the pot and the form of *K* depends on the thermodynamics used to represent the phase equilibrium (i.e., Raoult's Law, equation of state, fugacity, activity-coefficient model, etc.). Most process simulation packages have utilities to perform this calculation, plot the result, and export the data.

Because the more volatile components are being removed with time, the temperature in the still pot increases with time. The residue curves represent this fact with an arrow in the direction of increasing temperature. It is also true that residue curves never cross. Points on the residue curve map are defined as follows:

Stable node: Arrows on all curves point toward this point (highest temperature).

Unstable node: Arrows on all curves point away from this point (lowest temperature).

Saddle point: Arrows point both toward and away from this point (intermediate

temperature).

Figure 12.8 shows the residue curve map for a ternary system without azeotropes. Note that the curves seeming to emanate from the A vertex actually represent initial still pot compositions of nearly pure A with an infinitesimal amount of B (the curve on the A-B line), with infinitesimal amounts of both B and C in differing ratios (the interior curves), or with an infinitesimal amount of C (the A-C line). Each point anywhere on the triangular diagram is at a different temperature. Because the diagram represents liquid compositions, the temperature is the bubble point of the mixture at the given pressure. Therefore, the vertices of the triangular diagram are at the boiling points of the pure components. In Figure 12.8, Component A is the most volatile, and Component C is the least volatile. In the discussion that follows, the convention of decreasing volatility for components A-B-C will be followed.

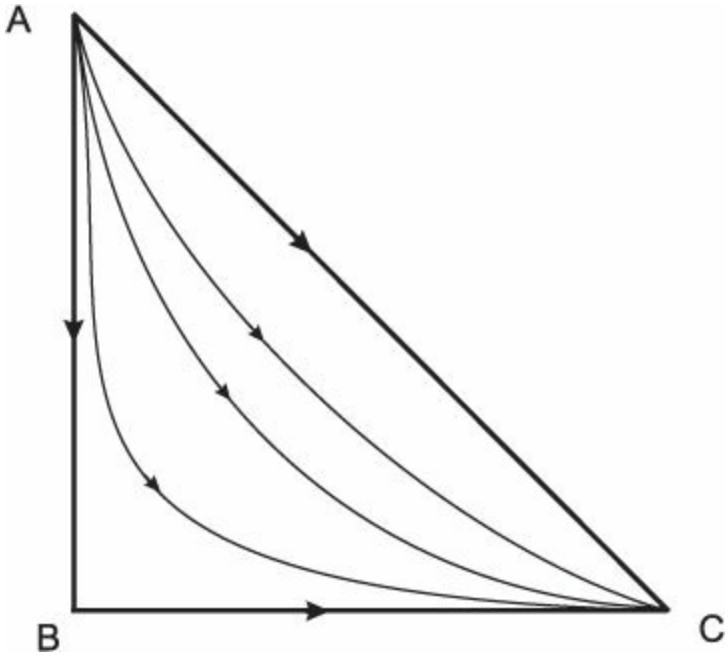


Figure 12.8. Residue Curve Map for Ternary System without Azeotrope

There are many possible representations of azeotropes on triangular diagrams. Four are shown in Figure 12.9. In Figure 12.9(a), there is a binary, minimum-boiling azeotrope between Components A and B. In Figure 12.9(b), there is a binary, minimum-boiling azeotrope between Components B and C that boils above pure Component A. In Figure 12.9(c), there is a binary, minimum-boiling azeotrope between Components A and C that boils below pure Component A. In Figure 12.9(d), there are two binary, minimum-boiling azeotropes. One is between Components A and B that boils below pure Component A, and the other is between Components A and C that also boils below pure Component A.

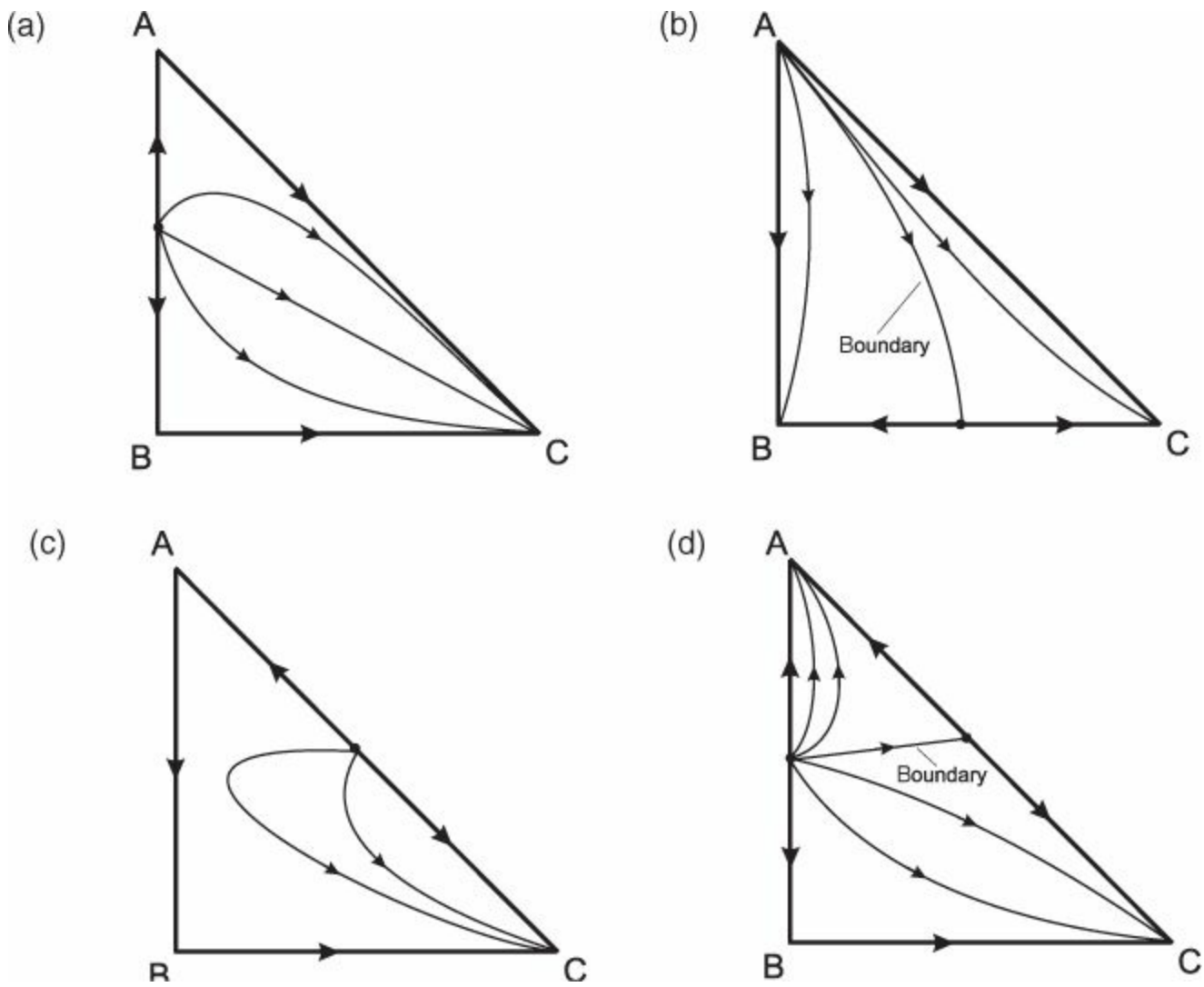


Figure 12.9. Some Possible Azeotropic Situations for Ternary Systems

There are three key rules to using residue curves to conceptualize distillation processes:

1. Because the temperature increases from top to bottom in a distillation column, the time variable can be replaced with a height variable in Equation (12.2). This is true only for a packed column; however, the equivalence of a certain column height and a tray (HETP, height equivalent to a theoretical plate) makes generalization to tray columns possible.
2. The residue curve is the composition profile in a continuous, packed distillation column at total reflux.
3. The BVDM (residue curves on triangular diagrams) is useful only for conceptualization, not numerical calculations, in contrast with the McCabe-Thiele method, which can be used for numerical calculations.

Therefore, to represent a feasible distillation process qualitatively, the second point combined with the material balance criterion illustrated in Figure 12.6 (feed, distillate, and bottoms product must lie on the same straight line) means that *there must be a straight line connecting the feed, distillate, and bottoms that intersects the same residue curve, with one end at the distillate and the other end at the bottoms*. It must be remembered that there are an infinite number of residue curves on a triangular plot, even though only two or three are actually drawn. Figure 12.10 shows examples of feasible and nonfeasible distillation processes. Figure 12.10(a) is for a system without azeotropes, and Figure 12.10(b) is for a system with a minimum-boiling azeotrope between Components A and B.

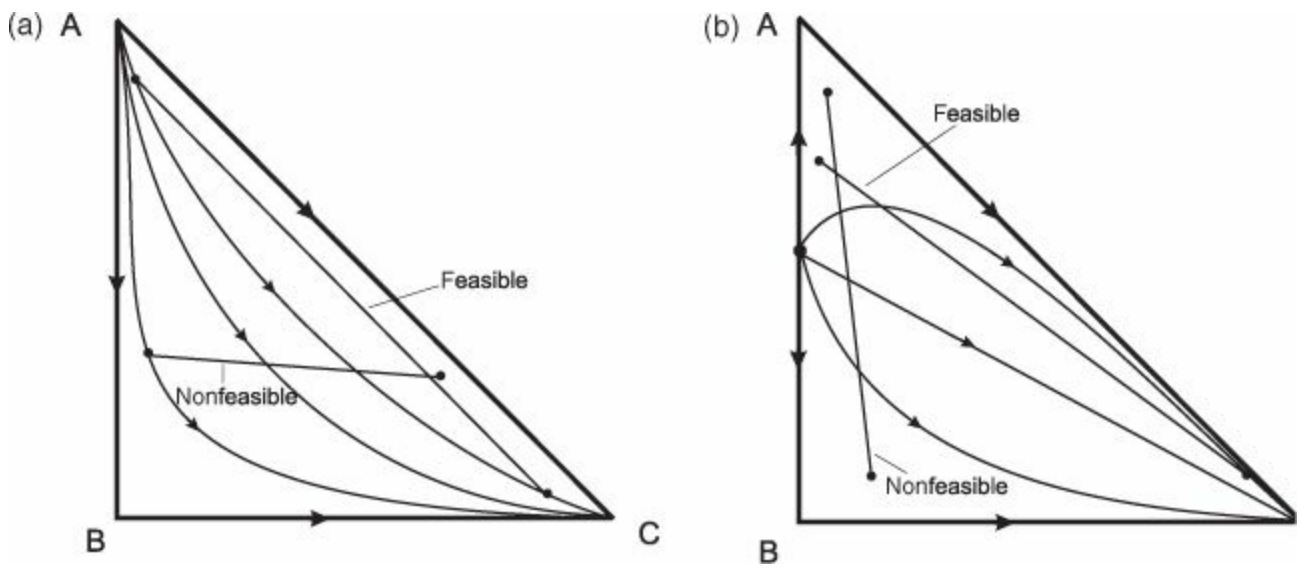


Figure 12.10. Feasible and Nonfeasible Distillation Processes

In the preceding section, a method for breaking binary azeotropes was mentioned that involved adding a third component to break the azeotrope. A key question is how to pick the added component. One answer is to pick an intermediate-boiling component that does not create a new azeotrope and has a residue curve map without any boundaries like Figure 12.9(c). The distillation column sequence and the representation of the sequence on the boundary value diagram are shown in Figure 12.11. The residue curve map suggests a feasible, intermediate-boiling component to break the azeotrope and also suggests the method for column sequencing and recycles to accomplish the separation. It should be noted that finding an intermediate-boiling component to break an azeotrope can be a difficult task given the narrow boiling point range required. Quite often, high-boiling components are used to break azeotropes. One of the most common examples is the use of ethylene glycol to break the ethanol-water azeotrope. An analysis of this situation is beyond the scope of this discussion. However, it is important to mention that the details of the boundary value design method require that the high-boiling component be added as a separate feed to the column and not be mixed with the process stream feed [17].

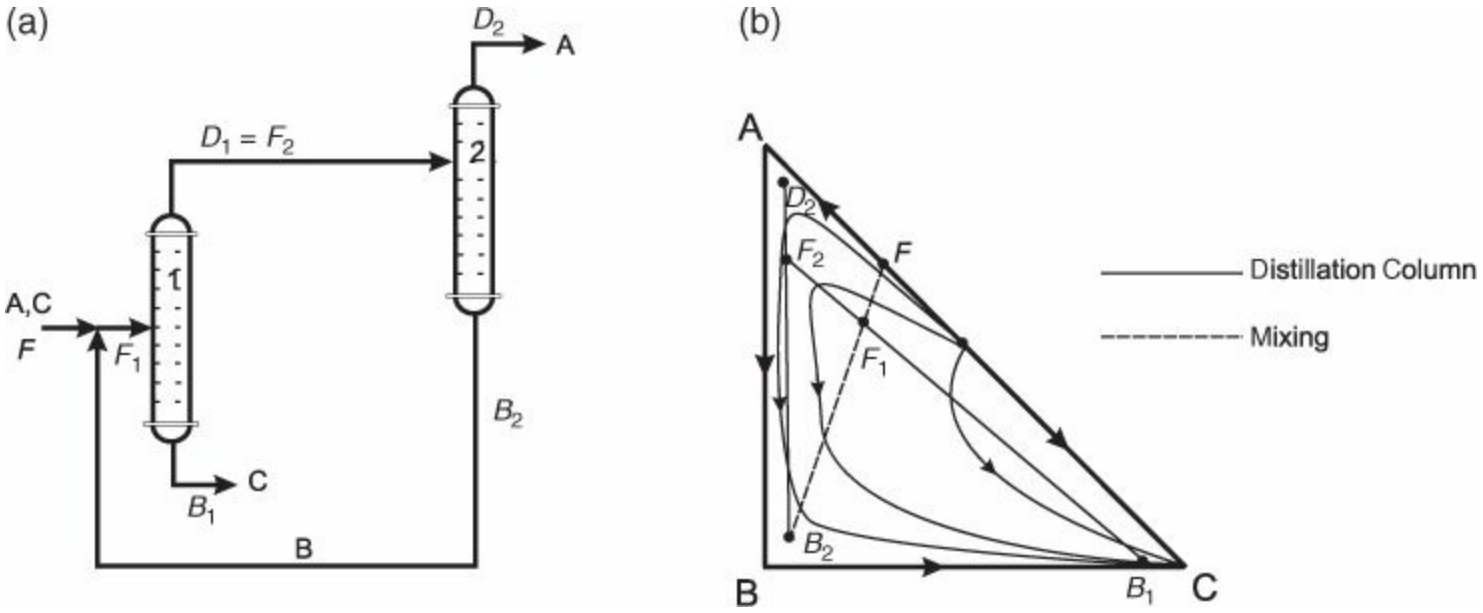


Figure 12.11. Method for Breaking Binary Azeotrope Using Intermedate-Boiling Entrainer

On residue curve maps, a **boundary** is defined as the curve that separates two regions within which simple distillation is possible. In Figure 12.9, plots (b) and (d) have boundaries. A boundary separates two regions with residue curves not having the same starting and ending point. Therefore,

plots (a) and (c) have no boundary. No simple distillation process in a single column may cross a straight boundary. Also, if a boundary is straight, the product streams from a multiple-column arrangement may not cross the boundary.

When the boundary is curved, there are more options for separation sequences. This is because the only requirement is that the distillate and bottoms product from a column be in the same region. The feed can lie in a different region. Also, if a boundary is curved, the product streams from a multiple-column arrangement may lie in a region across the boundary. Therefore, a column such as the one illustrated in Figure 12.12 is feasible. Example 12.3 shows how this feature can be exploited.

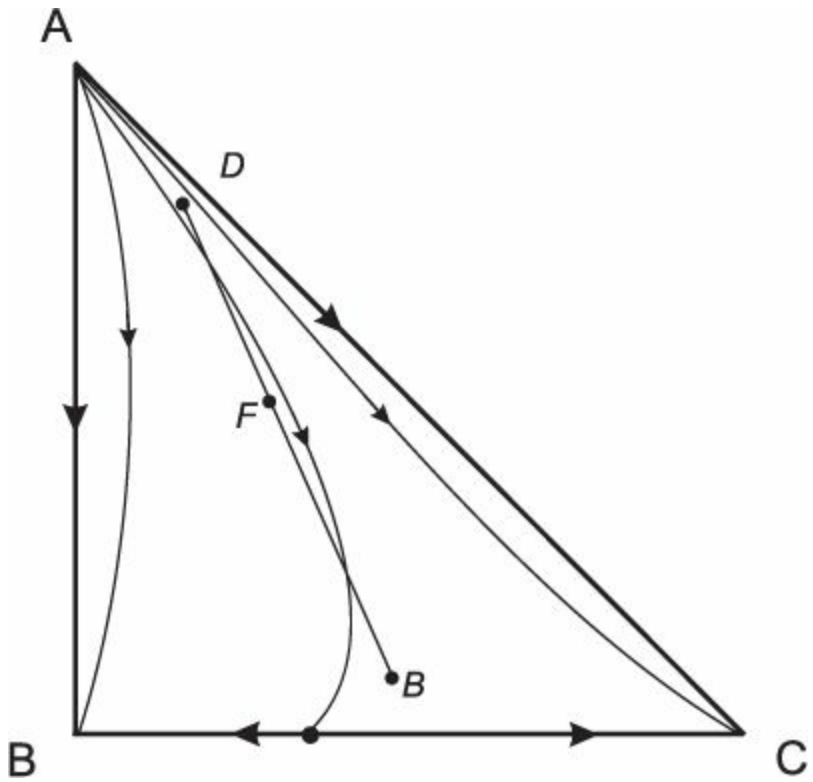


Figure 12.12. Feasible Column Operation with Curved Boundary

Example 12.3.

For the system illustrated in Figure 12.9(b), with a feed mixture of B and C (denoted *F*), conceptualize a distillation sequence that produces "pure" B and C using a light entrainer, A.

One possible sequence is illustrated in Figure E12.3.

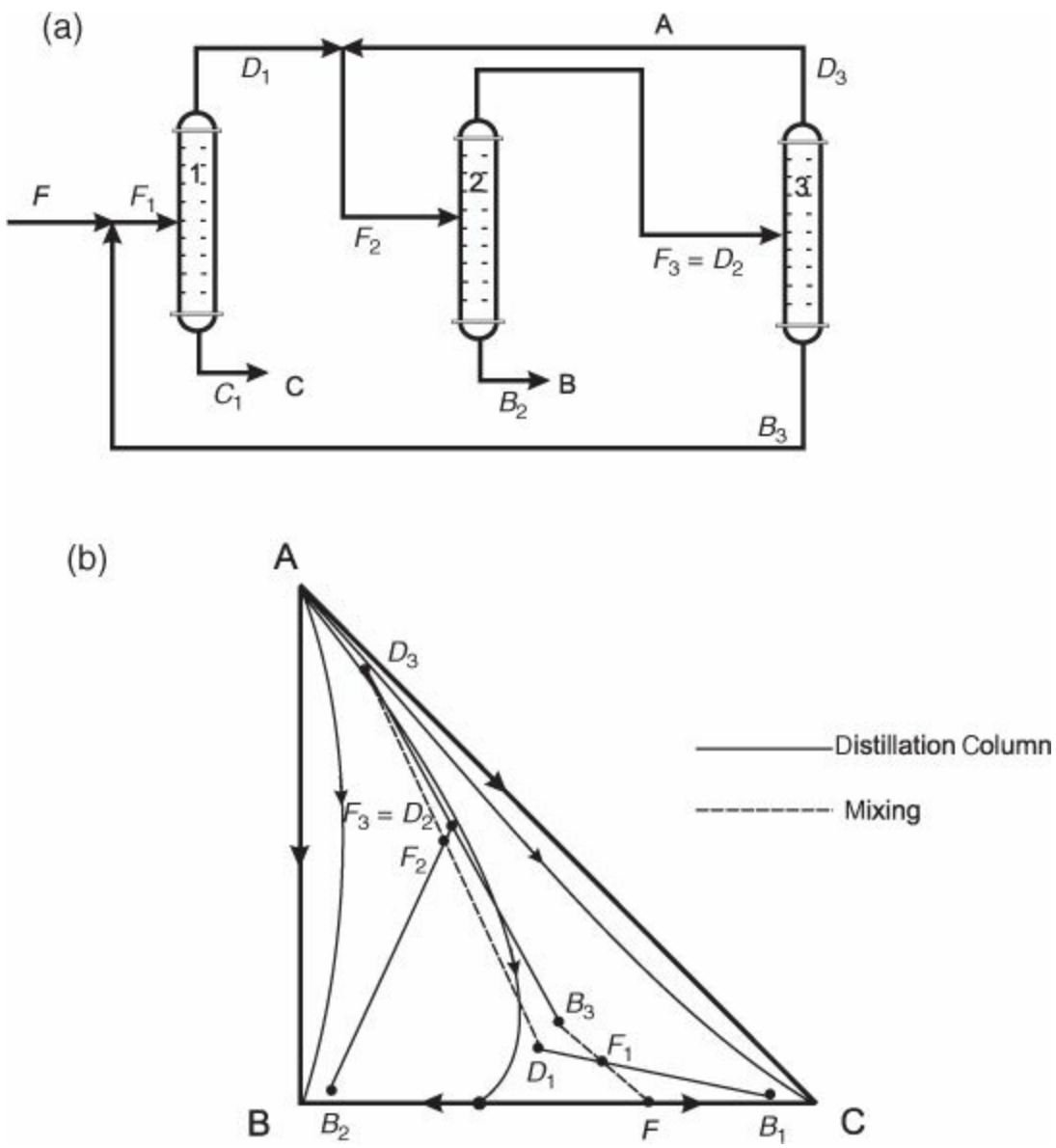


Figure E12.3. Process Configuration and Residue Curve Map for Example 12.3

It is also observed that the distillate D_3 is not very pure. This is because of the layout of the residue curves. Therefore, another feature of the residue curves map is that it suggests when concentration of a component is possible and when it is not possible to achieve a high-purity product.

In summary, the BVDM or residue curve plots can be used to conceptualize feasible distillation sequences. It is particularly useful for azeotropic systems involving three components, either when there are three components in the feed or when an entrainer is added to break a binary azeotrope. This method has only been introduced in this section, so care must be taken when applying this method without additional reading. Reference [17] is suggested for further reading.

12.4. Reactor Feed Preparation and Separator Feed Preparation Sections

The purpose of these sections is to match the temperature and pressure desired for the inlet streams to the reactor section and to the separation section. If the reactor operates at high temperature (a common occurrence because this increases reaction rate), the reactor feed preparation and separator feed preparation sections are often combined in a single process-process heat exchanger. Such heat integration can be built into the base-case flowsheet, but, if not, it should be caught during the heat integration step of optimization (see Chapter 15).

Pressure may also need to be increased for the reactor (or, infrequently, decreased), and this requires a pump for liquids or a compressor for gases. When there is a choice, pumps are preferable to compressors, because the operating, capital, and maintenance costs are all lower for pumps. If pressure is reduced between the reactor and the separator sections (or anywhere else in the process), an expander can be considered (for gases), but often it is not economical both because of its high cost and also because it reduces the controllability of the process. A valve allows control at a modest cost, but energy is not recovered.

In these temperature and pressure matching sections, the lowest-cost utility should always be used. For heating the feed to an exothermic reaction, heat integration can be used with the reactor effluent. For low-temperature heating, low-pressure steam or another low-temperature utility is used. For safety reasons, exothermic reactions (when reactor runaway is possible) should be run, with the reactor feed coming in at a temperature high enough to ensure a significant reaction rate. This avoids the buildup of large inventories of unreacted feed materials, which can happen if cold material enters the reactor and quenches the reaction. When sufficient heat is later provided, the entire contents of the reactor could react very rapidly, a process called ignition.

When possible, consider operation between 1 and 10 bar. High pressures increase pumping, compression, and capital costs, whereas low pressures tend to increase the size and cost of vessels. The temperature of the feed to the separation unit (at least for the base case) is usually set between the boiling points of the top and bottoms product for distillation, or based on similar considerations for the other separation options.

12.5. Recycle Section

This section is relatively straightforward. The stream or streams of unreacted raw materials are sent back to the reactor to reduce feed costs, to reduce impurities in the product, or to improve the operation of the process. If the conditions of the recycle streams are close to those of the raw material feed, then the recycle stream should mix with the raw materials prior to the reactor feed preparation section. Otherwise, any heating/cooling or pressure increase/decrease should be done separately. Thus, the recycle stream is combined with the raw material streams when they are all at a similar temperature. Example 12.4 involves a recycle in a biochemical process.

Example 12.4.

A recycle is used to return enzyme to the reactor. What particular concerns must be addressed in the recyle section?

The enzyme must be protected from deactivation and from degradation by microbes during the recyle, which might include storage times between batches. The recycle must be maintained in aseptic conditions, at the appropriate temperature and pH.

12.6. Environmental Control Section

As stated previously and in Chapter 27, this section should be eliminated or minimized through pollution prevention and green engineering. However, especially if the contaminant has little or no value if concentrated, there will be relatively dilute waste streams generated and sent to the environmental control section. Here, they are concentrated (by the separation techniques discussed earlier) and then disposed of (by incineration, neutralization, oxidation, burial, or other means). The

keys are to concentrate the waste and to make it benign.

12.7. Major Process Control Loops

During the initial synthesis of the PFD, the major control loops are developed. These control loops affect more than just one unit of a process. For example, the level control in the condensate tank of a distillation column is necessary for plant operation. On the other hand, a reactor temperature controller that changes the flowrate of molten salt through the cooling tubes of a reactor is a major loop and should be shown on the PFD.

It is through the early development of major control loops that significant design improvements can be made. In the high-temperature exothermic reactor, for example, failure to consider the control loop might lead one to propose an integrated heat-exchanger network that is difficult or impossible to control.

Beyond the importance of the control loops in maintaining steady-state material balance control, assurance of product purity, and safety, they provide focal points for the optimization that will follow the initial PFD synthesis. As described in Chapter 14, the controlled variables are the variables for which there is a choice. The best values of these variables are found through optimization. These loops also provide early clues to the flexibility of the process operation. For example, if the feed to the reactor is cut in half, less heat needs to be removed. Therefore, there must be an increase in the temperature of the cooling medium, which occurs when the coolant flowrate is reduced. Process control can be both very difficult and extremely important in biological processes, as demonstrated in Example 12.5.

Example 12.5.

In biological waste treatment, microbes that eat the waste and produce benign products are used. In one class of such processes, called **activated sludge,** the culture is separated from reactor output and recycled. What specfic process control issues arise in such a process?

The culture must maintain sufficient activity throughout the recycle. The recycle conditions may become nutrient poor if nearly all the waste nutrient is consumed, leading to loss of activity. The activity of the culture might be adversely affected by upsets in the feed conditions to the reactor, such as pH extremes or high concentrations of compounds toxic to the culture. Therefore, feed-forward control using measurements of the feed conditions should be considered, as well as control of a reserve of the culture to be used in case an uncontrolled process upset leads to culture death. Immediate, on-line analysis of culture activity is difficult, but off-line measurements can be incorporated into the control scheme.

12.8. Flow Summary Table

The format for the flow summary table is given in Chapter 1. Each of the conditions (temperature, pressure, flowrate, composition, and phase) should be estimated early in the flowsheet development. All are needed to get preliminary costs, for example. Even estimates based on perfect separations can provide sufficient data to estimate the cost of a recycle versus the value of burning the impure, unreacted feed material as a fuel.

Completeness of the estimates, not their accuracy, is important at this stage. For example, an early determination of phase (solid versus liquid versus gas) is needed to help choose a separation scheme

or reaction type (see Table 12.1).

12.9. Major Equipment Summary Table

Chapter 1 explains the requirements of a major equipment summary table. In the context of initial PFD development, the process of creating the table forces the process design engineer to question the size (and cost) of various units for which there may well be other options. If, early on, one must specify a large compressor, for example, the process can be changed to a lower pressure or it can be modified to use liquid pumping followed by vaporization rather than vaporization followed by compression. The early consideration of materials of construction provides the clue that normal temperatures and pressures usually result in less expensive materials.

12.10. Summary

The inclusion of enough detail and the freedom to look at the big picture without the burden of excessive detail are the keys to successful PFD synthesis. One must remain fully aware of the broadest goals of the project while looking for early changes in the structure of the flowsheet that can make significant improvements. Particular attention must be paid to the separations and reactor sections. The formation of azeotropes between components to be separated greatly affects the separation sequence. These must be identified early in the synthesis.

The beginning of the process is the generic block flow process diagram. Although the flow summary table at this stage is based on crude assumptions and the equipment summary table is far from the final equipment specifications, they help keep the chemical engineer cognizant of key choices that need to be made.

What You Should Have Learned

- To synthesize a process flow diagram from a block flow diagram, the following key information is needed:
  - Physical property data
  - Reaction kinetics
- The reactor section and the separation section are synthesized first.
- The reactor feed preparation section and the separator feed preparation section are synthesized either along with or immediately following their corresponding sections.
- If needed, the recycle section is synthesized next.
- The final items synthesized are the environmental control section and the major control loops.

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Problems

1. Choose one of the cases from Appendix B. Identify

a. All required physical property data

b. Sources for all data needed but not provided

2. Search the patent literature for kinetics information for one of the processes in Appendix B. Convert the provided data to a form suitable for use on a process simulator.

3. Develop five heuristics for reactor design.

4. For design of an exothermic reactor with cooling, one needs to choose an approach temperature (the nominal temperature difference between the reaction zone and the cooling medium). One engineer claims that the temperature difference across the tube walls should be as small as possible. Another claims that a large temperature difference is better for heat transfer.

   a. Describe the advantages and disadvantages of these two choices from the point of view of capital costs.

   b. Describe the advantages and disadvantages of these two choices from the point of view of operating costs.

   c. Describe the advantages and disadvantages of these two choices from the point of view of operability of the process.

5. Are there any safety considerations in the choice of heat transfer driving force (ΔT) in Problem 12.4? Explain.

6. From the flowsheets in Appendices B and C, identify four examples of each of the following types of recycles described in this chapter:

   a. Recycles that reduce feed costs

   b. Recycles that reduce impurities in products

7. Recycles are also used for the following purposes. Identify four examples of each.

   a. Heat removal

   b. Flowrate control

   c. Improvement of separation

   d. Reduction of utility requirements

8. From your previous courses and experience, identify four process recycle streams that serve different purposes from those identified in Problem 12.7 (a)–(d).

9. What information is needed about the available utilities before a choice between them can be made for a specific heating duty?

10. Take a flowsheet for one of the processes in Appendix B and identify the reactor feed preparation, reactor, separator feed preparation, separator, recycle, and environmental control sections. Is there any ambiguity concerning the demarcation of these sections? Explain.

11. How many simple distillation columns are required to purify a stream containing four components into four “pure” products? Sketch all possible sequences.

12. How many simple distillation columns are required to purify a stream containing five components into five “pure” products? Sketch all possible sequences.

13. Illustrate a system (PFD and McCabe-Thiele diagrams) to purify two components (A and B) from a binary, homogeneous, minimum-boiling azeotrope that is pressure sensitive. The feed concentration of A is greater than the azeotropic composition at the pressure of the column

receiving the feed. The azeotropic composition of A decreases with increasing pressure.

14. In the production of dimethyl carbonate from methanol, it is necessary to separate methanol from formal (also known as methylal—$C_3H_8O_2$). However, an azeotrope exists between these two components. Using a process simulator, examine the equilibrium curves (*x*-*y* plots) between 100 kPa and 1000 kPa to determine a strategy for purifying these two components. Compare your results for the following thermodynamic packages for the *K*-value:
    a. Ideal
    b. NRTL
    c. UNIFAC
    d. SRK

    What do you learn from this comparison?
15. In the production of diethyl ether, it is necessary to purify a stream of equimolar diethyl ether and water that is available at 1500 kPa. Suggest a method for achieving this separation. Use the UNIQUAC model for the *K*-value. Would your answer be different if, for example, only 99 mol% purity were needed instead of 99.9 mol%? What do you learn and how does your answer change if the four models for *K*-values in Problem 12.14 are used? What do you learn from this comparison?
16. In the production of diethyl ether, assume that it is necessary to purify a stream at 1500 kPa containing 75 mol% diethyl ether, 20 mol% ethanol, and 5 mol% dimethyl ether. Assume that the UNIQUAC model adequately predicts the thermodynamics of this system.
    a. Use the residue curve plotting routine on your simulator to plot the residue curves.
    b. Suggest a method for separating this mixture into three relatively pure components.
    c. How would your answer to Part (b) change if the stream contained 85 mol% diethyl ether, 10 mol% ethanol, and 5 mol% dimethyl ether?
    d. Examine the effect of changing the pressure of the distillation columns. Suggest a much simpler method for achieving the necessary separation.
17. When your parents or grandparents were in college, it was not uncommon to "borrow" some "pure" ethanol (grain alcohol) from the university to add to a party punch. However, because of the azeotrope between ethanol and water, "pure" ethanol is not easy to manufacture. At that time, it was not uncommon for benzene to be added as an entrainer to break the azeotrope. Of course, this means that all "pure" ethanol contained trace amounts of benzene, which was later identified as a carcinogen. By plotting both residue curves and *TPxy* diagrams for the ethanol-water system, suggest a method for purifying ethanol by adding benzene as an entrainer. Assume that the UNIQUAC model applies and that the feed stream of ethanol and water is equimolar and at atmospheric pressure.
18. Does Equation (12.1) give the number of alternative sequences for separation processes other than distillation? If so, give two examples. If not, why not?
19. What constraints on the separation process and on the sequence are assumed in the derivation of Equation (12.1)?
20. Figure 12.1(d) shows a nonsimple separation unit. When one says that the minimum number of simple separation units is $(N - 1)$, these nonsimple units are not considered. Identify four other

examples of nonsimple separation units. For each, discuss how it might affect

a. Capital cost

b. Operability and safety

c. Operating costs

21. Does Equation (12.1) apply to batch or semibatch separation processes? Why or why not?

22. The residue curve map of Figure 12.9(a) shows that batch distillation of a mixture at the azeotropic composition for the system (A+B) with a small amount of C added will result in a very pure liquid C residue in the still. Is this a good separation unit choice to obtain "pure" C? Analyze the advantages and disadvantages.

23. On a residue curve map, will the composition of a ternary, minimum-boiling azeotrope always be a stable node, an unstable node, a saddle point, or none of the above?

24. As noted in Section 12.1.1, laboratory studies often involve batch or semi-batch reactors for convenience. Develop four heuristics for choosing whether to use batch, semibatch, or continuous reactors for the commercial plant.

25. Semibatch or batch reactors are common in biochemical operations. What characteristics of biological systems, materials, and products lead to the choice of batch over continuous reactors? To what extent do these characteristics also lead to unsteady operations of other GBFD sections?

a. Reactor feed preparation

b. Separator feed preparation

c. Separator

d. Recycle

e. Environmental control

26. The unique characteristics of an azeotrope make it ideal for some applications. Find three applications of azeotropic products. How is the production of an azeotropic composition different from the production of "pure" A and B when (A+B) forms an azeotrope? Does the process differ for a minimum-boiling and a maximum-boiling azeotrope?

27. For biological systems (which often have a very narrow range of acceptable temperatures), describe the advantages and disadvantages of large and small ΔT's in reactor temperature control systems.

28. Biological systems often require sterilization as a step before inoculation with the appropriate microbial culture. Sterilization can be considered a reaction process in which organisms are killed, often through cell lysis, using thermal or chemical routes. Consider both batch and continuous sterilization. Which has advantages for sterilizing process equipment? Which has advantages for sterilizing reactor feedstock? (*Note*: For some biochemical processes, sterilization is neither required nor desired, e.g., waste treatment.)

Chapter 13. Synthesis of a Process Using a Simulator and Simulator Troubleshooting

What You Will Learn

- Process simulators are used in the design of chemical processes.
- All process simulators contain the same basic algorithms and require the same information, but they all have different user interfaces.
- The correct choice of thermodynamics package is crucial for accurate simulations of chemical processes.
- Simulation of highly nonideal vapor-liquid equilibrium is supported by all process simulators.
- Using solid components requires careful evaluation and implementation.

The advancement in computer-aided process simulation over the past generation has been nothing short of spectacular. Until the late 1970s, it was rare for a graduating chemical engineer to have any experience in using a chemical process simulator. Most material and energy balances were still done by hand by teams of engineers. The rigorous simulation of multistaged separation equipment and complicated reactors was generally unheard of, and the design of such equipment was achieved by a combination of simplified analyses, shortcut methods, and years of experience. In the present day, however, companies now expect their junior engineers to be conversant with a wide variety of computer programs, especially a process simulator.

To some extent, the knowledge base required to simulate successfully a chemical process will depend on the simulator used. Currently there are several process simulators on the market, for example, CHEMCAD, Aspen Plus, HYSYS, PRO/II, and SuperPro Designer. Many of these companies advertise their product in the trade magazines—for example, *Chemical Engineering*, *Chemical Engineering Progress*, *Hydrocarbon Processing*, or *The Chemical Engineer*—and on the Internet. A process simulator typically handles batch, semibatch, and continuous processes, although the extent of integration of the batch and continuous processes in a single PFD varies among the various popular simulators. The availability of such powerful software is a great asset to the experienced process engineer, but such sophisticated tools can be potentially dangerous in the hands of the neophyte engineer. The bottom line in doing any process simulation is that you, the engineer, are still responsible for analyzing the results from the computer. The purpose of this chapter is not to act as a primer for one or all of these products. Rather, the general approach to setting up processes is emphasized, and the aim is to highlight some of the more common problems that process simulator users encounter and to offer solutions to these problems. In addition, two sections have been included at the end of this chapter on electrolyte systems and solids modeling. Electrolyte systems play a key role in many processes. These systems can be modeled in current process simulators reasonably accurately without significant effort. Many process simulators now also have the capability to model solids. This helps to integrate the unit operations involving solids with the rest of the plant without major simplifications.

13.1. The Structure of a Process Simulator

The six main features of all process simulators are illustrated in the left-hand column of Figure 13.1. These elements are:

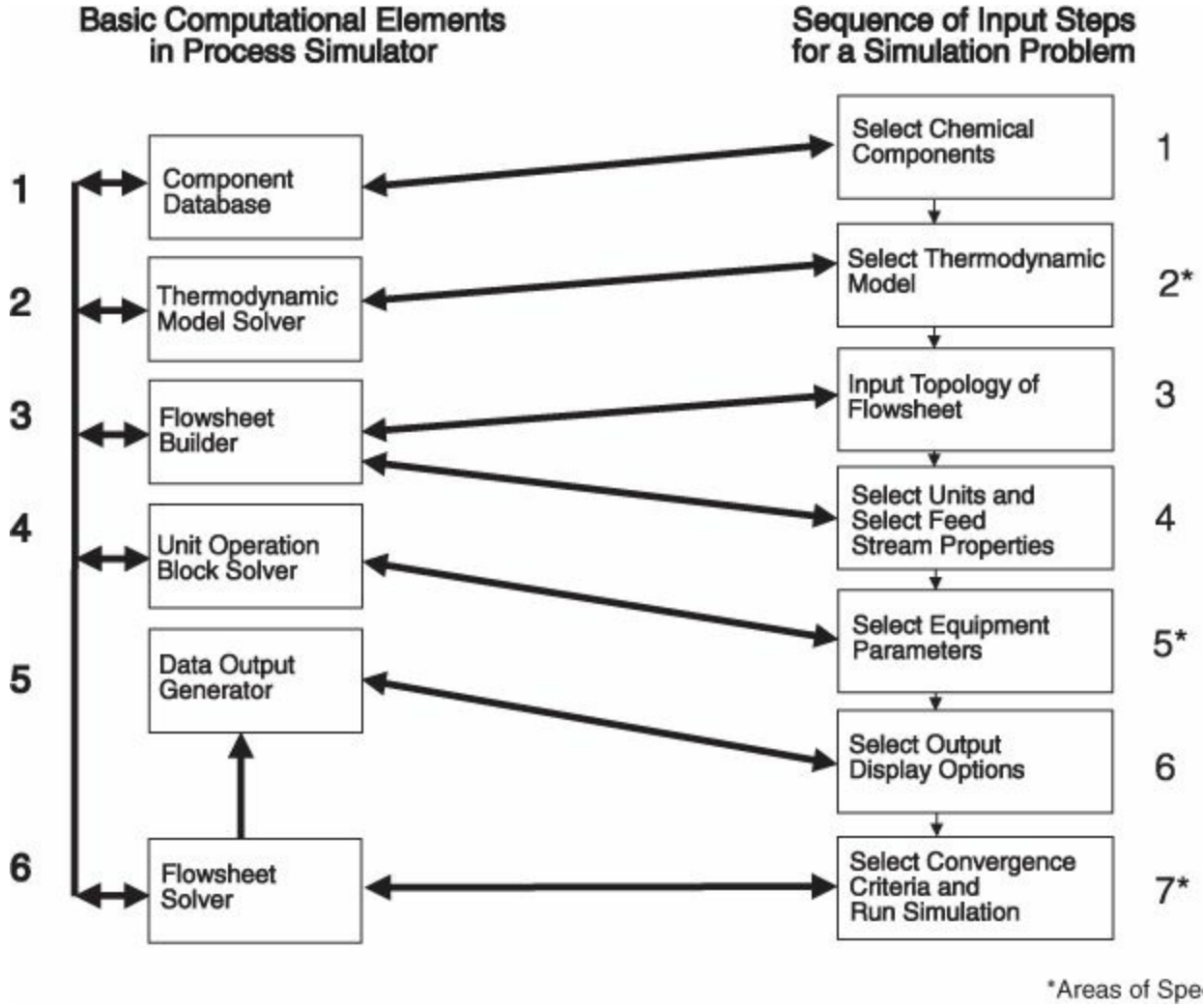


Figure 13.1. Relationship between Basic Computational Elements and Required Input to Solve a Process Simulation Problem

1. **Component Database:** This contains the constants required to calculate the physical properties from the thermodynamic models.
2. **Thermodynamic Model Solver:** A variety of options for vapor-liquid (VLE) and liquid-liquid (LLE) equilibrium, enthalpy calculations, and other thermodynamic property estimations are available.
3. **Flowsheet Builder:** This part of the simulator keeps track of the flow of streams and equipment in the process being simulated. This information can be both input and displayed graphically.
4. **Unit Operation Block Solver:** Computational blocks or modules are available that allow energy and material balances and some design calculations to be performed for a wide variety of process equipment.
5. **Data Output Generator:** This part of the program serves to customize the results of the simulation in terms of an output report. Often, graphical displays of tower profiles, heating curves, and a variety of other useful process data can be produced.
6. **Flowsheet Solver:** This portion of the simulator controls the sequence of the calculations and the overall convergence of the simulation.

There are several other elements commonly found in process simulators that are not shown in Figure

13.1. For example, there are file control options, the option to use different engineering units, possibly some additional features associated with regressing data for thermodynamic models, and so on. The availability of these other options is dependent on the simulator used and will not be discussed further.

Also shown on the right-hand side of the diagram in Figure 13.1 are the seven general steps to setting up a process simulation problem. The general sequence of events that a user should follow in order to set up a problem on a simulator is as follows:

1. Select all of the chemical components that are required in the process from the component database.
2. Select the thermodynamic models required for the simulation. These may be different for different pieces of equipment. For example, to simulate correctly a liquid-liquid extractor, it is necessary to use a thermodynamic model that can predict liquid-phase activity coefficients and the existence of two liquid phases. However, for a pump in the same process, a less sophisticated model could be used.
3. Select the topology of the flowsheet to be simulated by specifying the input and output streams for each piece of equipment.
4. Select the properties (temperature, pressure, flowrate, vapor fraction, and composition) of the feed streams to the process.
5. Select the equipment specifications (parameters) for each piece of equipment in the process.
6. Select the way in which the results are to be displayed.
7. Select the convergence method and run the simulation.

Step 3 is achieved by constructing the flowsheet using equipment icons and connecting the icons with process streams. Sometimes, it is convenient to carry out this step first.

The interaction between the elements and steps and the general flow of information is shown by the lines on the diagram. Of the seven input steps given above, Steps 2, 5, and 7 are the cause of most problems associated with running process simulations. These areas will be covered in more detail in the following sections. However, before these topics are covered, it is worth looking at the basic solution algorithms used in process simulators.

There are basically three types of solution algorithm for process simulators [1]: sequential modular, equation solving (simultaneous nonmodular), and simultaneous modular.

In the **sequential modular** approach, the equations describing the performance of equipment units are grouped together and solved in modules—that is, the process is solved equipment piece by equipment piece. In the equation solving, or **simultaneous nonmodular,** technique, all the relationships for the process are written out together and then the resulting matrix of nonlinear simultaneous equations is solved to yield the solution. This technique is very efficient in terms of computation time but requires a lot of time to set up and is unwieldy. The final technique is the **simultaneous modular** approach, which combines the modularizing of the equations relating to specific equipment with the efficient solution algorithms for the simultaneous equation solving technique.

Of these three types, the sequential modular algorithm is by far the most widely used. In the sequential modular method, each piece of equipment is solved in sequence, starting with the first, followed by the second, and so on. It is assumed that all the input information required to solve each piece of equipment has been provided (see Section 13.2.5). Therefore, the output from a given piece of

equipment, along with specific information on the equipment, becomes the input to the next piece of equipment in the process. Clearly, for a process without recycle streams, this method requires only one flowsheet iteration to produce a converged solution. The term **flowsheet iteration** means that each piece of equipment is solved only once. However, there may be many iterations for any one given piece of equipment, and batch units require time–series calculations to match the required scheduling of operations for the given unit. This concept is illustrated in Figure 13.2.

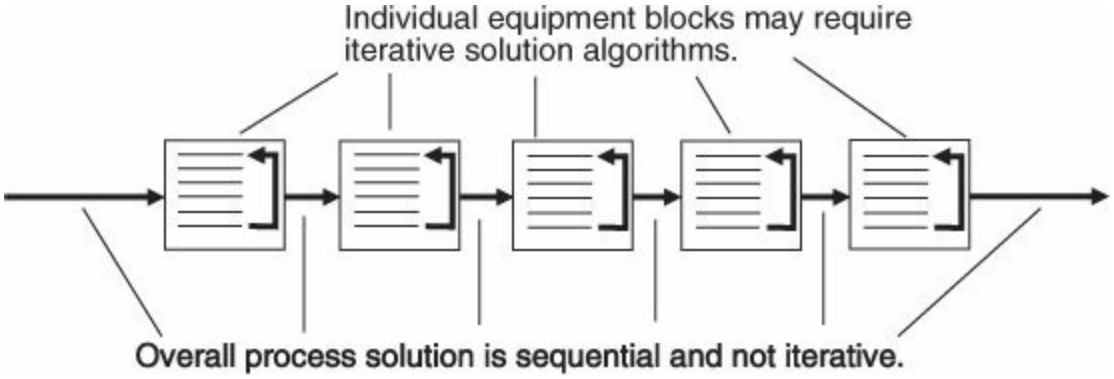


Figure 13.2. Solution Sequence Using Sequential Modular Simulator for a Process Containing No Recycles

The solution sequence for flowsheets containing recycle streams is more complicated, as shown in Figure 13.3. Figure 13.3(a) shows that the first equipment in the recycle loop (C) has an unknown feed stream (r). Thus, before Equipment C can be solved, some estimate of Stream r must be made. This leads to the concept of tear streams. A **tear stream,** as the name suggests, is a stream that is torn or broken. If the flowsheet in Figure 13.3(b) is considered, with the recycle stream torn, it can be seen, provided information is supplied about Stream r2, the input to Equipment C, that the flowsheet can be solved all the way around to Stream r1 using the sequential modular algorithm. Then compare Streams r1 and r2. If they agree within some specified tolerance, then there is a converged solution. If they do not agree, then Stream r2 is modified and the process simulation is repeated until convergence is obtained. The splitting or tearing of recycle streams allows the sequential modular technique to handle recycles. The convergence criterion and the method by which Stream r2 is modified can be varied, and multivariable successive substitution, Wegstein, and Newton-Raphson techniques [2, 3] are all commonly used for the recycle loop convergence. Usually, the simulator will identify the recycle loops and automatically pick streams to tear and a method of convergence. The tearing of streams and method of convergence can also be controlled by the user, but this is not recommended for the novice. Note that heat integration (Chapter 15) introduces recycle streams.

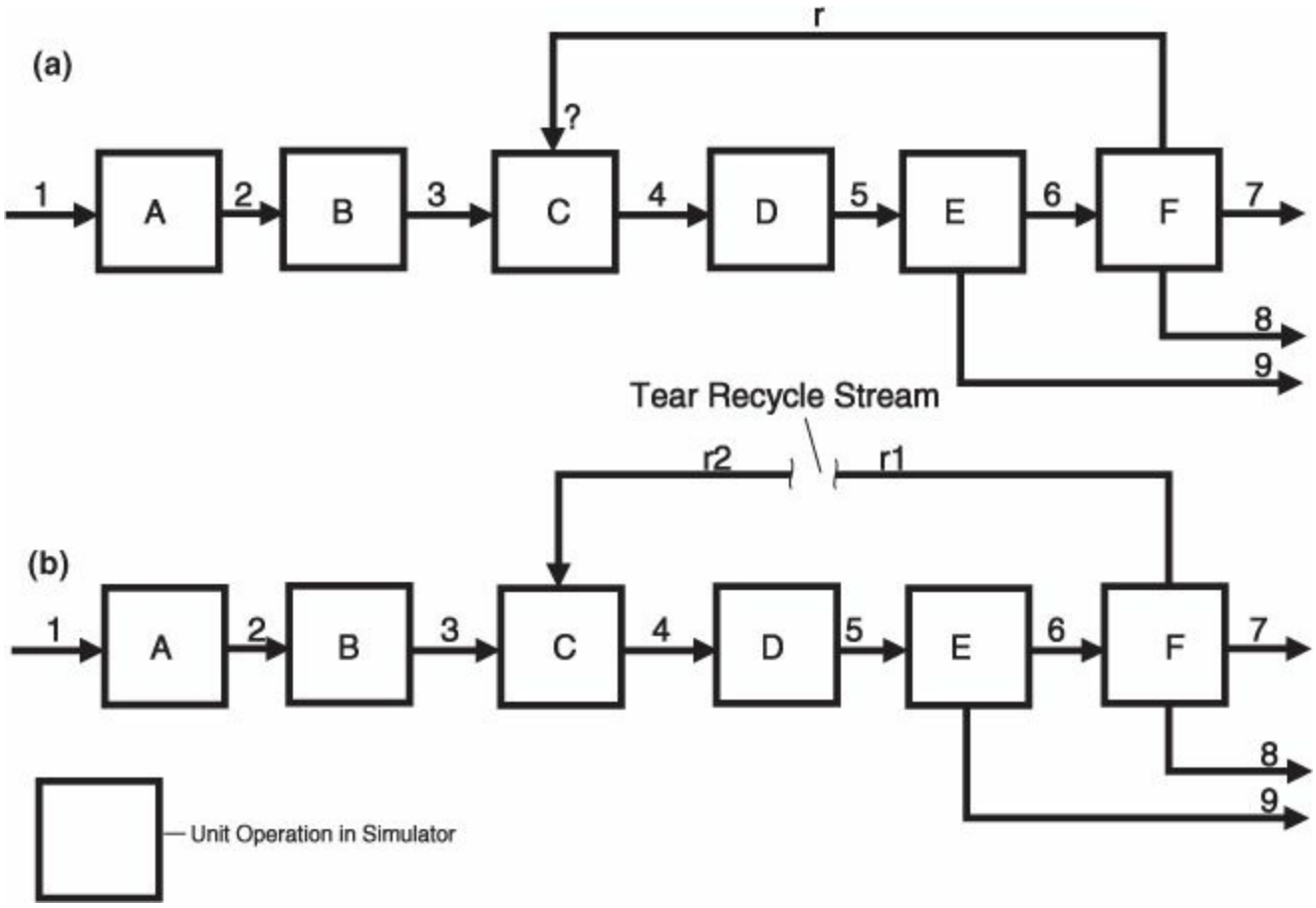


Figure 13.3. The Use of Tear Streams to Solve Problems with Recycles Using the Sequential Modular Algorithm

13.2. Information Required to Complete a Process Simulation: Input Data

Referring back to Figure 13.1, each input block is considered separately. The input data for the blocks without asterisks (1, 3, 4, and 6) are quite straightforward and require little explanation. The remaining blocks (2, 5, and 7) are often the source of problems, and these are treated in more detail.

13.2.1. Selection of Chemical Components

Usually, the first step in setting up a simulation of a chemical process is to select which chemical components are going to be used. The simulator will have a databank of many components (more than a thousand chemical compounds are commonly included in these databanks). It is important to remember that all components—inerts, reactants, products, by-products, utilities, and waste chemicals—should be identified. If the chemicals that you need are not available in the databank, then there are usually several ways that you can add components *(user-added components*) to your simulation. How to input data for user-added components is simulator specific, and the simulator user manual should be consulted.

13.2.2. Selection of Physical Property Models

Selecting the best physical property model is an extremely important part of any simulation. If the wrong property package or model is used, the simulated results will not be accurate and cannot be trusted. The choice of models is often overlooked by the novice, causing many simulation problems down the road. Simulators use both pure component and mixture properties. These range from molecular weight to activity-coefficient models. Transport properties (viscosity, thermal conductivity, diffusivity), thermodynamic properties (enthalpy, fugacity, *K*-factors, critical constants),

and other properties (density, molecular weight, surface tension) are all important.

The physical property options are labeled as “thermo,” “fluid package,” “property package,” or “databank” in common process simulators. There are pure-component and mixture sections, as well as a databank. For temperature-dependent properties, different functional forms are used (from extended Antoine equation to polynomial to hyperbolic trigonometric functions). The equation appears on the physical property screen or in the help utility.

For pure-component properties, the simulator has information in its databank for hundreds of compounds. Some simulators offer a choice between DIPPR and proprietary databanks. These are largely the same, but the proprietary databank may contain additional components, petroleum cuts, electrolytes, and so on. DIPPR is the Design Institute for Physical Property Research (a part of AIChE), and sharing of process data across different simulators (e.g., Aspen Plus, CHEMCAD, HYSYS, PRO/II, SuperPro Designer) can be enhanced by using that databank. (Note that some proprietary databanks may not be supplied in the academic versions of these simulators.) All simulators also have built-in procedures to estimate pure-component properties from group-contribution and other techniques. The details of these techniques are covered in standard chemical engineering thermodynamics texts [4, 5, 6] and are not described here. However, one must be aware of any such estimations made by the simulator. Any estimation, by definition, increases the uncertainty in the results of the simulation. The entry in the databank for each component should indicate estimations. For example, many long-chain hydrocarbons have no experimental critical point because they decompose at relatively low temperatures. However, because critical temperatures and pressures are needed for most thermodynamic models, they must be estimated. Although these estimations allow the use of equation-of-state and some other models, one must never assume that these are experimental data.

Heat capacities, densities, and critical constants are the most important pure-component data for simulation. The transport and other properties are used in equipment sizing calculations. The techniques used in the simulators are no more accurate than those covered in transport, thermodynamics, unit operations, and separations courses—they are just easier to apply.

Even though simple mass and energy balances cannot be done by the simulator without the above-mentioned pure-component properties, often the most influential decision in a simulation is the choice of a model to predict phase equilibria. Several of the popular simulators have **expert systems** to help the user select the appropriate model for the system. The expert system determines the range (usually with additional user input) of operating temperatures and pressures covered by the simulation and, with data on the components to be used, makes an informed guess of the thermodynamic models that will be best for the process being simulated. The word *expert* should not be taken too seriously! The expert-system choice is only a first guess. Additionally, the model chosen may not be best for a given piece of equipment. A moderately complex simulation will use at least two different thermodynamic packages for different parts of the flowsheet.

Due to the importance of thermodynamic model selection and the many problems that the wrong selection leads to, a separate section (Section 13.4) is dedicated to this subject. An example of how the wrong thermodynamic package can cause serious errors is given in Example 13.1.

Example 13.1.

Consider the HCl absorber (T-602) in the separation section of the allyl chloride process, Figure C.3

(Appendix C, on the CD). This equipment is shown in Figure E13.1. The function of the absorber is to contact countercurrently Stream 10a, containing mainly propylene and hydrogen chloride, with water, Stream 11. The HCl is highly soluble in water and is almost completely absorbed to form 32 wt% hydrochloric acid, Stream 12. The gas leaving the top of the absorber, Stream 13, is almost pure propylene, which is cleaned and then recycled.

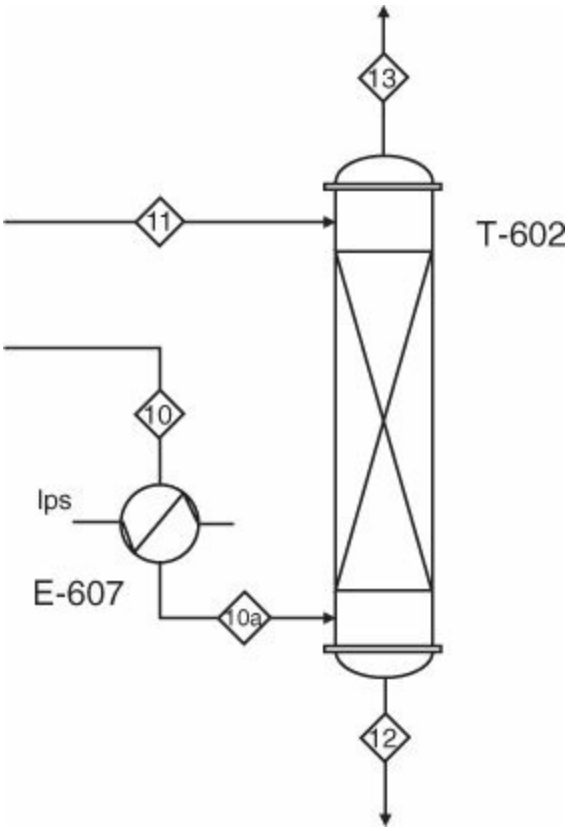


Figure E13.1. HCl Absorber in Allyl Chloride Separation Section (Unit 600), Appendix C

Table E13.1 shows the results for the two outlet streams from the absorber—Streams 12 and 13—for two simulations, each using a different thermodynamic model for the vapor-liquid equilibrium calculations. The second and third columns in the table show the results using the SRK (Soave [7], Redlich and Kwong [8]) model, which is the preferred model for many common components. The fourth and fifth columns show the results using a model that is specially designed to deal with ionic type compounds (HCl) that dissolve in water and then dissociate. The difference in results is remarkable. The HCl-water system is highly nonideal, and, even though the absorption of an acid gas into aqueous solutions is quite common, the SRK model is not capable of correctly modeling the phase behavior of this system. With the SRK model, virtually all the HCl leaves the absorber as a gas. Clearly, if the simulation were done using only the SRK model, the results would be drastically in error. This result is especially disturbing because SRK is the default thermodynamics package in many simulators.

Table E13.1. Results of Simulation of HCl Absorption Using Two Different Physical Property Models

Phase Component Flows (kmol/h)	Using SRK Model		Using PPAQ* Model	
	Stream 12 Liquid	Stream 13 Vapor	Stream 12 Liquid	Stream 13 Vapor
Propylene	0.05	57.48	—	57.53
Allyl chloride	0.01	—	0.01	—
Hydrogen chloride	0.91	18.78	19.11	0.58
Water	81.37	0.63	81.88	0.12
Total	82.34	76.89	101.00	58.23

*This is a model used in the CHEMCAD simulator especially for HCl-water and similar systems.

More details of model selection are given in Section 13.4.

The importance of thermodynamic model selection and its impact on the validity of the results of a simulation are discussed at length by Horwitz and Nocera [9], who warn

> **"You absolutely must have confidence in the thermodynamics that you have chosen to represent your chemicals and unit operations. This is your responsibility, not that of the software simulation package. If you relinquish your responsibility to the simulation package, be prepared for dire consequences."**

13.2.3. Selection and Input of Flowsheet Topology

The most reliable way to input the topology of the process flow diagram is to make a sketch on paper and have this in front of you when you construct the flowsheet on the simulator. Contrary to the rules given in Chapter 1 on the construction of PFDs, every time a stream splits or several streams combine, a simulator equipment module (splitter or mixer) must be included. These "phantom" units were introduced in Chapter 5 and are useful in tracing streams in a PFD as well as being required for the simulator. Most simulators allow the flowsheet topology to be input both graphically and by keyboard. Certain conventions in the numbering of equipment and streams are used by the simulator to keep track of the topology and connectivity of the streams. When using the graphical interface, the streams and equipment are usually numbered sequentially in the order they are added. These can be altered by the user if required. Care must be taken when connecting batch and continuous unit operations, because it is often assumed that "continuous" units approach equilibrium instantaneously.

13.2.4. Selection of Feed Stream Properties

As discussed in Section 13.1, the sequential modular approach to simulation requires that all feed streams be specified (composition, flowrate, vapor fraction, temperature, and pressure). In addition, estimates of recycle streams should also be made. Although feed properties are usually well defined, some confusion may exist regarding the number and type of variables that must be specified to define the feed stream completely. In general, feed streams will contain n components and consist of one or two phases. For such feeds, a total of $n + 2$ specifications completely defines the stream. This is a consequence of the phase rule. Giving the flowrate (kmol/h, kg/s, etc.) of each component in the feed stream takes care of n of these specifications. The remaining two specifications should also be independent. For example, if the stream is one phase, then giving the temperature and pressure of the

stream completely defines the feed. Temperature and pressure also completely define a multicomponent stream having two phases. However, if the feed is a single component and contains two phases, then temperature and pressure are not independent. In this case, the vapor fraction and either the temperature or the pressure must be specified. Vapor fraction can also be used to specify a two-phase multicomponent system, but if used, only temperature or pressure can be used to specify the feed completely. To avoid confusion, it is recommended that vapor fraction (υf) be specified only for saturated vapor ($\upsilon f = 1$), saturated liquid ($\upsilon f = 0$), and two-phase, single-component ($0 < \upsilon f < 1$) streams. All other streams should be specified using the temperature and pressure.

Use the vapor fraction (vf) to define feed streams only for saturated vapor ($vf = 1$), saturated liquid ($vf = 0$), and two-phase, single-component ($0 < vf < 1$) streams.

By giving the temperature, pressure, and vapor fraction for a feed, the stream is overspecified and errors will result.

13.2.5. Selection of Equipment Parameters

It is worth pointing out that process simulators, with a few exceptions, are structured to solve process material and energy balances, reaction kinetics, reaction equilibrium relationships, phase-equilibrium relationships, and equipment performance relationships for equipment in which sufficient process design variables and batch operations scheduling have been specified. For example, consider the design of a liquid-liquid extractor to remove 98% of a component in a feed stream using a given solvent. In general, a process simulator will not be able to solve this design problem directly; that is, it cannot determine the number of equilibrium stages required for this separation. However, if the problem is made into a simulation problem, then it can be solved by a trial-and-error technique. Thus, by specifying the number of stages in the extractor, case studies in which the number of stages are varied can be performed, and this information can be used to determine the correct number of stages required to obtain the desired recovery of 98%. In other cases, such as a plug flow reactor module, the simulator can solve the design problem directly—that is, calculate the amount of catalyst required to carry out the desired reaction. Therefore, before starting a process simulation, it is important to know what equipment parameters must be specified in order for the process to be simulated.

There are essentially two levels at which a process simulation can be carried out. The first level, Level 1, is one in which the minimum data are supplied in order for the material and energy balances to be obtained. The second level, Level 2, is one in which the simulator is used to do as many of the design calculations as possible. The second level requires more input data than the first. An example of the differences between the two levels is illustrated in Figure 13.4, which shows a heat exchanger in which a process stream is being cooled using cooling water. At the first level, Figure 13.4(a), the only information that is specified is the desired outlet condition of the process stream—for example, pressure and temperature or vapor fraction—if the stream is to leave the exchanger as a two-phase mixture. However, this is enough information for the simulator to calculate the duty of the exchanger and the properties of the process stream leaving the equipment. At the second level, Figure 13.4(b), additional data are provided: the inlet and desired outlet temperature for the utility stream, the fact that the utility stream is water, the overall heat transfer coefficient, and the heat-exchanger configuration or effectiveness factor, F. Using this information, the simulator calculates the heat-exchanger duty, the required cooling water flowrate, and the required heat transfer area.

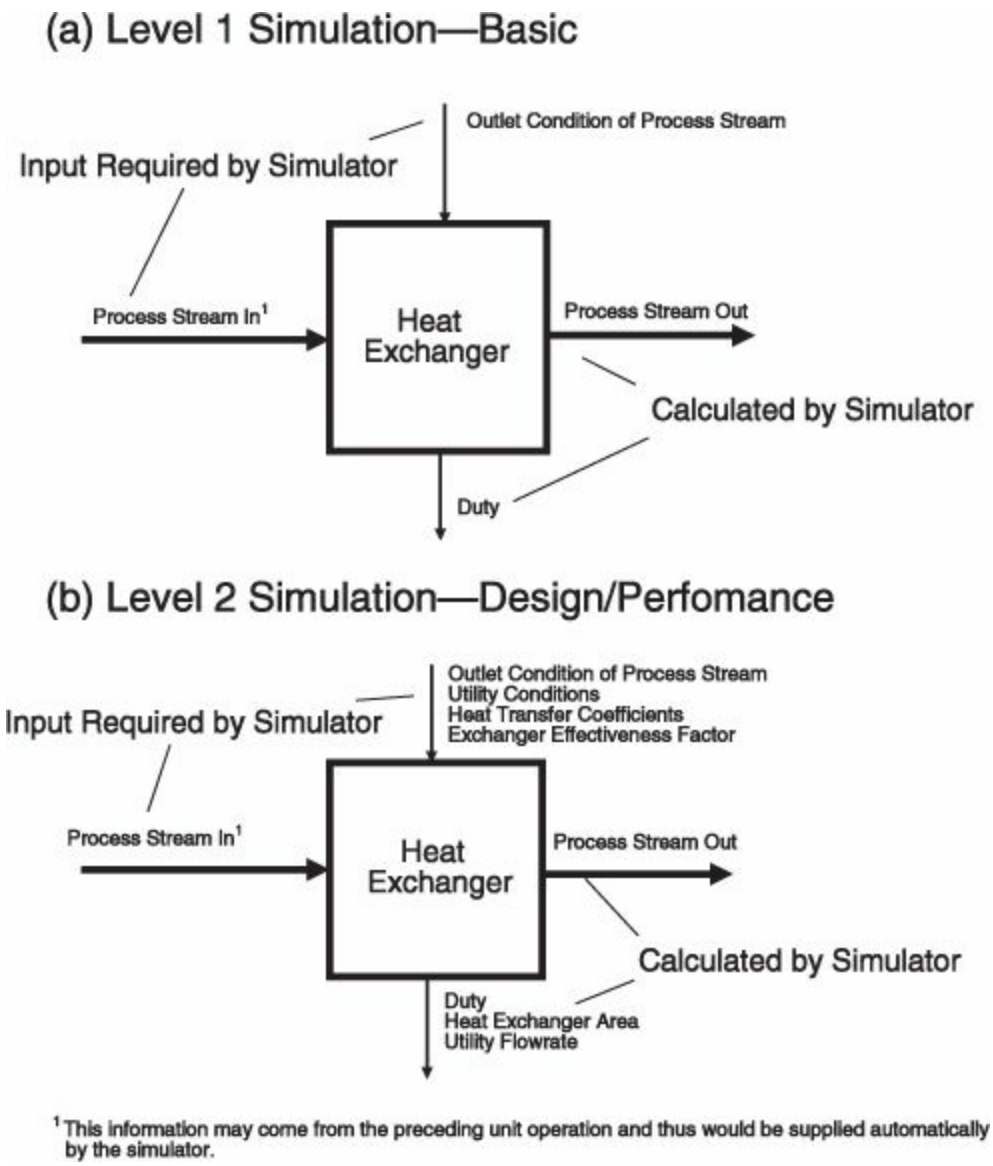


Figure 13.4. Information Required for Different Levels of Simulation

When attempting to do a simulation on a process for the first time, it is recommended that you provide the minimum data required for a Level 1 simulation. When you have obtained a satisfactory, converged solution, you can go back and provide more data to obtain desired design parameters, that is, a Level 2 solution.

When first simulating a process, input only the data required to perform the material and energy balances for the process.

The structure of the process simulator will determine the exact requirements for the input data, and such information will be available in the user manual for the software or on help screens. However, for Level 1 simulations, a brief list of typical information is presented below that may help a novice user prepare the input data for a process simulation.

Pumps, Compressors, and Power Recovery Turbines (Expanders). For pumps, the desired pressure of the fluid leaving the pump *or* the desired pressure increase of the fluid as it flows through the pump is all that is required.

For compressors and turbines, the desired pressure of the fluid leaving the device *or* the desired pressure increase of the fluid as it flows through the equipment is required. In addition, the mode of

compression or expansion—adiabatic, isothermal, or polytropic—is required.

Heat Exchangers. For exchangers with a single process stream exchanging energy with a utility stream, all that is required is the condition of the exit process stream. This can be the exit pressure and temperature (single-phase exit condition) or the exit pressure and vapor fraction (two-phase exit condition).

For exchangers with two or more process streams exchanging energy (as might be the case when heat integration is being considered), the exit conditions (pressure and temperature or vapor fraction) for both streams are required. The user must be aware of the possibility of temperature crosses in heat-exchange equipment. The simulator may or may not warn the user that a temperature cross has occurred but will continue to simulate the rest of the process. The results from such a simulation will not be valid, and the temperature cross must be remedied before a correct solution can be obtained. Therefore, it is recommended that the user check the temperature profiles for all heat exchangers after the simulation.

Fired Heaters (Furnaces). The same requirements for heat exchangers with a single process fluid apply to fired heaters.

Mixers and Splitters. Mixers and splitters used in process simulators are usually no more than simple tees in pipes. Unless special units must be provided—for example, when the fluids to be mixed are very viscous and in-line mixers might be used—the capital investment of these units can be assumed to be zero.

Mixers represent points where two or more process streams come together. The only required information is an outlet pressure or pressure drop at the mixing point. Usually, the pressure drop associated with the mixing of streams is small, and the pressure drop can be assumed to be equal to zero with little error. If feed streams enter the mixer at different pressures, then the outlet stream is assumed to be at the lowest pressure of the feed streams. This assumption causes little error in the material and energy balance. However, the correct analysis of the pressure profiles in a system where several streams mix is given in Section 22.4.

Splitters represent points at which a process stream splits into two or more streams with different flowrates but identical compositions. The required information is the outlet pressure or pressure drop across the device and the relative flows of the output streams. Usually, there is little pressure drop across a splitter, and all streams leaving the unit are at the same pressure as the single feed stream. In a batch operation, the splitter can be assigned on and off times to divert the inlet flow to various other units on a schedule.

Valves. Either the outlet pressure or pressure drop is required.

Reactors. The way in which reactors are specified depends on a combination of the input information required and the reactor category. Generally there are four categories of reactor: stoichiometric reactor, kinetic (plug flow or CSTR) reactor, equilibrium reactor, and batch reactor. All these reactor configurations require input concerning the thermal mode of operation: adiabatic, isothermal, amount of heat removed or added. Additional information is also required. Each reactor type is considered separately below.

Stoichiometric Reactor: This is the simplest reactor type that can be simulated. The required input data are the number and stoichiometry of the reactions, the temperature and pressure, and the conversion of the limiting reactant. Reactor configuration (plug flow, CSTR) is not required because no estimate of reactor volume is made. Only basic material and energy balances are performed.

Kinetic (Plug Flow and CSTR) Reactor: This reactor type is used to simulate reactions for which kinetics expressions are known. The number and stoichiometry of the reactions are required input data. Kinetics constants (Arrhenius rate constants and Langmuir-Hinshelwood constants, if used) and the form of the rate equation (simple first-order, second-order, Langmuir-Hinshelwood kinetics, etc.) are also required. Reactor configuration (plug flow, CSTR) is required. Options may be available to simulate cooling or heating of reactants in shell-and-tube reactor configurations in order to generate temperature profiles in the reactor.

Equilibrium Reactor: As the name implies, this reactor type is used to simulate reactions that obtain or approach equilibrium conversion. The number and stoichiometry of the reactions and the fractional approach to equilibrium are the required input data. In addition, equilibrium constants as a function of temperature may be required for each reaction or may be calculated directly from information in the database. In this mode, the user has control over which reactions should be considered in the analysis.

Minimum Gibbs Free Energy Reactor: This is another common form of the equilibrium reactor. In the Gibbs reactor, the outlet stream composition is calculated by a free energy minimization technique. Usually data are available from the simulator's databank to do these calculations. The only input data required are the list of components that one anticipates in the output from the reactor. In this mode the equilibrium conversion that would occur for an infinite residence time is calculated.

Batch Reactor: This reactor type is similar to the kinetic reactor (and requires the same kinetics input), except that it is batch. The volume of the reactor is specified. The feeds, outlets flows, and reactor temperature (or heat duty) are scheduled (i.e., they are specified as time series).

As a general rule, the least complicated reactor module that will allow the heat and material balance to be established should be used. The reactor module can always be substituted later with a more sophisticated one that allows the desired design calculations to be performed. It should also be noted that a common error made in setting up a reactor module is the use of the wrong component as the limiting reactant when a desired conversion is specified. This is especially true when several simultaneous reactions occur and the limiting component may not be obvious solely from the amounts of components in the feed.

Flash Units. In simulators, the term *flash* refers to the module that performs a single-stage vapor-liquid equilibrium calculation. Material, energy, and phase-equilibrium equations are solved for a variety of input parameter specifications. In order to specify completely the condition of the two output streams (liquid and vapor), two parameters must be input. Many combinations are possible—for example, temperature and pressure, temperature and heat load, or pressure and mole ratio of vapor to liquid in exit streams. Often, the flash module is a combination of two pieces of physical equipment, that is, a phase separator and a heat exchanger. These should appear as separate equipment on the PFD. Note that a flash unit can also be specified for batch operation, in which case

the unit can serve as a surge or storage vessel.

Distillation Columns. Usually, both rigorous methods (plate-by-plate calculations) and shortcut methods (Fenske and Underwood relationships using key components) are available. In preliminary simulations, it is advisable to use shortcut methods. The advantage of the shortcut methods is that they allow a design calculation (which estimates the number of theoretical plates required for the separation) to be performed. For preliminary design calculations, this is a very useful option and can be used as a starting point for using the more rigorous algorithms, which require that the number of theoretical plates be specified. It should be noted that, in both methods, the calculations for the duties of the reboiler and condenser are carried out in the column modules and are presented in the output for the column. Detailed design of these heat exchangers (area calculations) often cannot be carried out during the column simulation.

Shortcut Module: The required input for the design mode consists of identification of the key components to be separated, specification of the fractional recoveries of each key component in the overhead product, the column pressure and pressure drop, and the ratio of actual to minimum reflux ratio to be used in the column. The simulator will estimate the number of theoretical plates required, the exit stream conditions (bottom and overhead products), optimum feed location, and the reboiler and condenser duties.

If the shortcut method is used in the performance mode, the number of plates must also be specified, but the R/R_{min} is calculated.

Rigorous Module: The number of theoretical plates must be specified, along with the condenser and reboiler type, column pressure and pressure drop, feed tray locations, and side product locations (if side stream products are desired). In addition, the total number of specifications given must be equal to the number of products (top, bottom, and side streams) produced. These product specifications are often a source of problems, and this is illustrated in Example 13.2.

Several rigorous modules may be available in a given simulator. Differences between the modules are the different solution algorithms used and the size and complexity of the problems that can be handled. Tray-to-tray calculations can be handled for several hundred stages in most simulators. In addition, these modules can be used to simulate accurately other equilibrium staged devices, for example, absorbers and strippers.

Batch Distillation: This module is similar to the rigorous module, except that feeds and product draws are on a schedule (not continuous). Therefore, the start and stop times of the feeds and products must be specified, and a time series of tray concentrations and temperatures is generated by the simulator.

Example 13.2.

Consider the benzene recovery column in the toluene hydrodealkylation process shown in Figure 1.5. This column is redrawn in Figure E13.2. The purpose of the column is to separate the benzene product from unreacted toluene, which is recycled to the front end of the process. The desired purity of the benzene product is 99.6 mol%. The feed and the top and bottoms product streams are presented in Table E13.2, which is taken from Table 1.5.

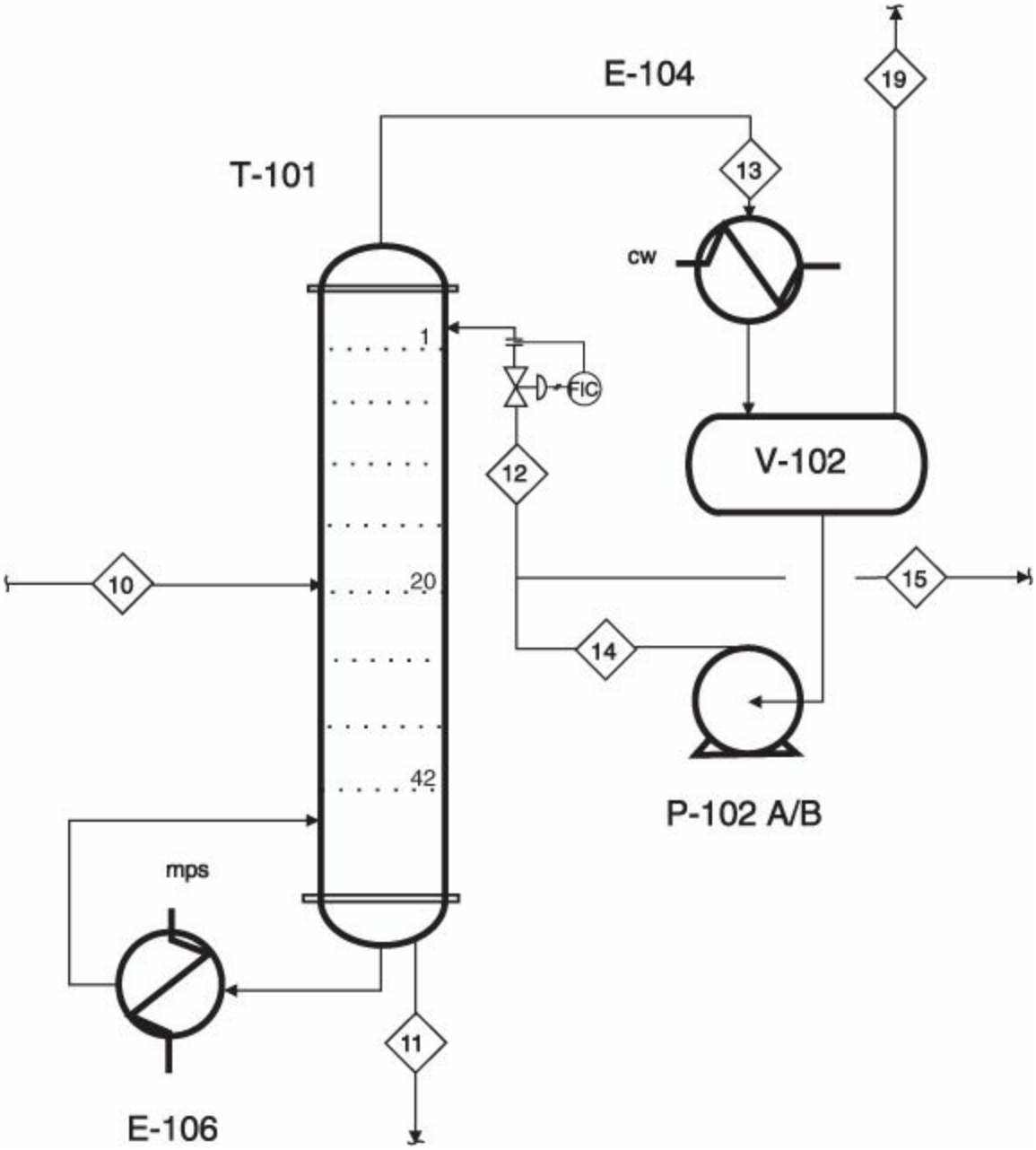


Figure E13.2. Benzene Column in Toluene Hydrodealkylation Process (from Figure 1.5)

Table E13.2. Stream Table for Figure E13.2

Component	Stream 10	Stream 15	Stream 19	Stream 11
Hydrogen	0.02	—	0.02	—
Methane	0.88	—	0.88	—
Benzene	106.3	105.2	—	1.1
Toluene	35.0	0.4	—	34.6

There are many ways to specify the parameters needed by the rigorous column algorithm used to simulate this tower.

Two examples are given:

1. The key components for the main separation are identified as benzene and toluene. The composition of the top product is specified to be 99.6 mol% benzene, and the recovery of toluene in the bottoms product is 0.98.
2. The top composition is specified to be 99.6 mol% benzene, and that of the recovery of benzene

in the bottoms product is 0.01.

The first specification violates the material balance, whereas the second specification does not. Looking at the first specification, if 98% of the toluene in the feed is recovered in the bottoms product, then 2% or 0.7 kmol/h must leave with the top product. Even if the recovery of benzene in the top product were 100%, this would yield a top composition of 106.3 kmol/h benzene and 0.7 kmol/h toluene. This corresponds to a mole fraction of 0.993. Therefore, the desired mole fraction of 0.996 can never be reached. Thus, by specifying the recovery of toluene in the bottoms product, the specification for the benzene purity is automatically violated.

The second specification shows that both specifications can be achieved without violating the material balance. The top product contains 99% of the feed benzene (105.2 kmol/h) and 0.4 kmol/h toluene, which gives a top composition of 99.6 mol% benzene. The bottoms product contains 1.0% of the feed benzene (1.1 kmol/h) and 34.6 kmol/h of toluene.

When giving the top and bottom specifications for a distillation column, make sure that the specifications do not violate the material balance.

If problems continue to exist, one way to ensure that the simulation will run is to specify the top reflux rate and the boil-up rate (reboiler duty). Although this strategy will not guarantee the desired purities, it will allow a base case to be established. With subsequent manipulation of the reflux and boil-up rates, the desired purities can be obtained.

Absorbers and Strippers. Usually these units are simulated using the rigorous distillation module given above. The main differences in simulating these types of equipment are that condensers and reboilers are not normally used. In addition, there are two feeds to the unit; one feed enters at the top and the other at the bottom.

Liquid-Liquid Extractors. A rigorous tray-by-tray module is used to simulate this multistaged equipment. It is imperative that the thermodynamic model for this unit be capable of predicting the presence of two liquid phases, each with appropriate liquid-phase activity coefficients.

13.2.6. Selection of Output Display Options

Several options will be available to display the results of a simulation. Often, a report file can be generated and customized to include a wide variety of stream and equipment information. In addition, a simulation flowsheet (not a PFD), *T-Q* diagrams for heat exchangers, vapor and liquid flows, temperature and composition profiles (tray-by-tray) for multistaged equipment, scheduling charts for batch operations, environmental parameters for exit streams, and a wide variety of phase diagrams for streams can be generated. The user manual should be consulted for the specific options available for the simulator you use.

13.2.7. Selection of Convergence Criteria and Running a Simulation

For equipment requiring iterative solutions, there will be user-selectable convergence and tolerance criteria in the equipment module. There will also be convergence criteria for the whole flowsheet simulation, which can be adjusted by the user.

The two most important criteria are number of iterations and tolerance. These criteria will often have

default values set in the simulator. Unless specific problems arise, these default values should be used in your simulations.

If the simulation has not converged, the results do not represent a valid solution and should not be used.

When convergence is not achieved, three common causes are as follows:

1. The problem has been ill posed. This normally means that an equipment specification has been given incorrectly. For example, see the first specification in Example 13.2 for the rigorous column module.
2. The tolerance for the solution has been set too tightly, and convergence cannot be obtained to the desired accuracy no matter how many solution iterations are performed.
3. The number of iterations is not sufficient for convergence. This occurs most often when the flowsheet has many recycle streams. Rerunning the flowsheet simulation with the results from the preceding run may give a converged solution. If convergence is still not obtained, then one way to address this problem is to remove as many recycle streams as possible. The simulation is then run, and the recycle streams are added back, one by one, using the results from the preceding simulation as the starting point for the new one. This method is discussed in more detail in Section 13.3.

Of the three reasons, the first one is by far the most common.

The most common reason for the failure of a simulation to converge is the use of incorrect or impossible equipment specifications.

13.3. Handling Recycle Streams

Recycle streams are very important and common in process flowsheets. Computationally, they can be difficult to handle and are often the cause for unconverged flowsheet simulations. There are ways in which the problems caused by recycle streams can be minimized. When a flowsheet is simulated for the first time, it is wise to consider carefully any simplifications that may help the convergence of the simulation. Consider the simulation of the DME flowsheet illustrated in Figure B.1.1, Appendix B. This flowsheet is shown schematically in Figure 13.5(a). The DME process is simple, no by-products are formed, the separations are relatively easy, and the methanol can be purified easily prior to being returned to the front end of the process. In attempting to simulate this process for the first time, it is evident that two recycle streams are present. The first is the unreacted methanol that is recycled to the front of the process, upstream of the reactor. The second recycle loop is due to the heat integration scheme used to preheat the reactor feed using the reactor effluent stream. The best way to simulate this flowsheet is to eliminate the recycle streams as shown in Figure 13.5(b). In this figure, two separate heat exchangers have been substituted for the heat integration scheme. These exchangers allow the streams to achieve the same changes in temperature while eliminating the interaction between the two streams. The methanol recycle is eliminated in Figure 13.5(b) by producing a methanol pseudo-output stream. The simulation of the flowsheet given in Figure 13.5(b) is straightforward; it contains no recycle streams and will converge in a single flowsheet iteration. Troubleshooting of the simulation, if input errors are present, is very easy because the flowsheet

converges very quickly. Once a converged solution has been obtained, the recycle streams can be added back. For example, the methanol recycle stream would be introduced back into the simulation. The composition of this stream is known from the preceding simulation, and this will be a very good estimate for the recycle stream composition. Once the simulation has been run successfully with the methanol recycle stream, the heat integration around the reactor can be added back and the simulation run again. Although this method may seem unwieldy, it does provide a reliable method for obtaining a converged simulation.

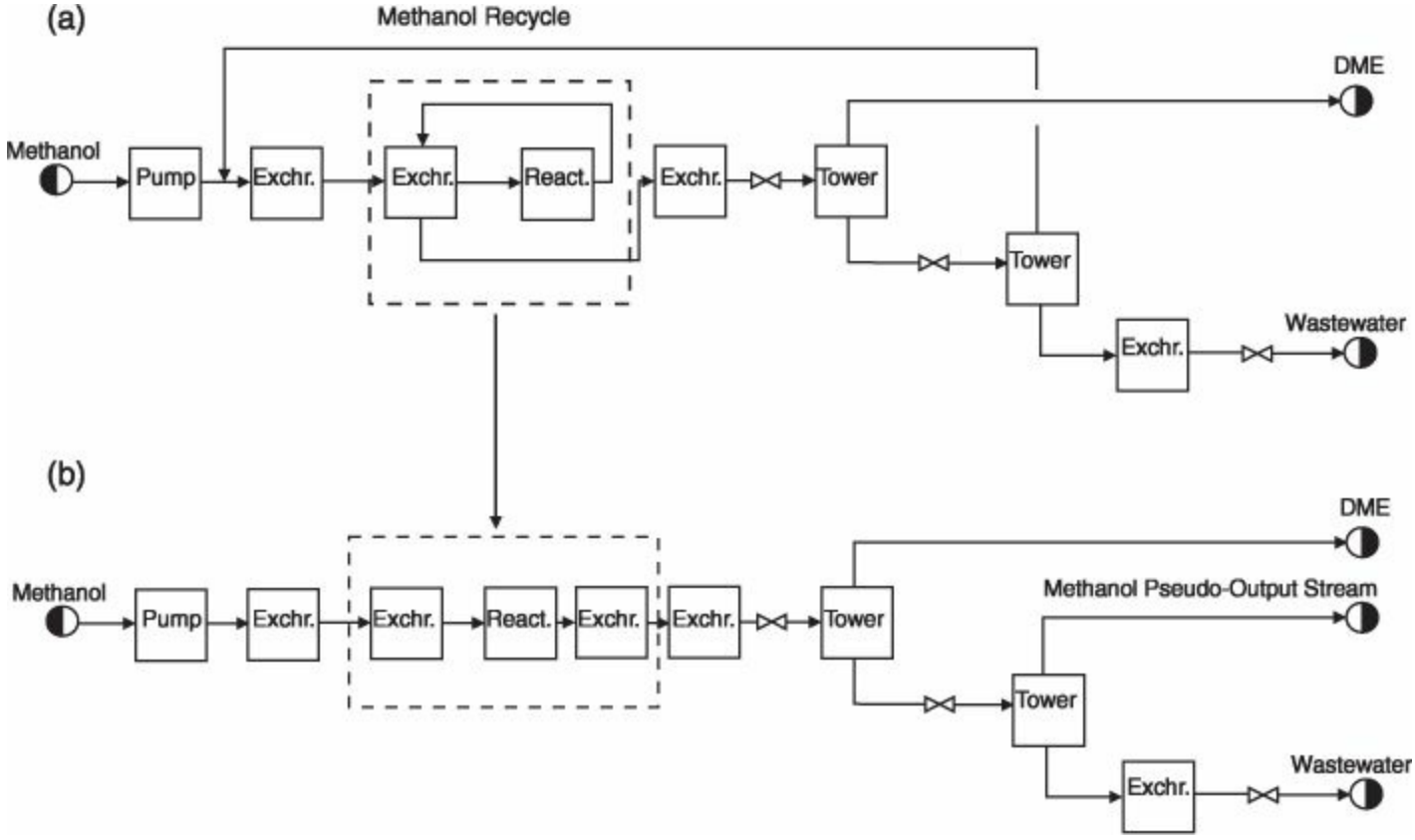


Figure 13.5. Block Flow Diagram for DME Process Showing (a) Recycle Structure and (b) Elimination of Recycles

For the DME flowsheet in Figure 13.5, the unreacted methanol that was recycled was almost pure feed material. This means that the estimate of the recycle stream composition, obtained from the once-through simulation using Figure 13.5(b), was very good. When the recycle stream contains significant amounts of by-products, as is the case with the hydrogen recycle stream in Figure 1.5 (Streams 5 and 7), the estimate of the composition using a once-through simulation will be significantly different from the actual recycle stream composition. For such cases, when purification of the recycle stream does not occur, it is best to keep this recycle stream in the flowsheet and eliminate all other recycle streams for the first simulation. Once a converged solution is reached, the other recycle streams can be added back one at a time.

Often, a series of case studies will need to be run using a base-case simulation as a starting point. This is especially true when performing a parametric optimization on the process (see Chapter 14). When performing such case studies, it is wise to make small changes in input parameters in order to obtain a converged simulation. For example, assume that a converged simulation for a reactor module at 350°C has been obtained, and a case study needs to be run at 400°C. When the equipment temperature in the reactor module is changed and the simulation is rerun, it may be found that the simulation does not converge. If this is the case, then, for example, go back to the base-case run, change the reactor temperature by 25°C, and see whether it converges. If it does, then the input can be

changed by another 25°C to give the desired conditions, and so on. The use of small increments or steps when simulating changes in flowsheets often produces a converged simulation when a single large change in input will not.

Often when simulating a process, it is the flowrate of products (not feeds) that is known—for example, production of 60,000 tonne/y of chemical X, with a purity of 99.9 wt%. Assume that a converged solution has been found in which all the product specifications have been met except that the flowrate of primary product is not at the desired value. For this case, it is a simple matter to multiply all the feeds to the process by a factor to obtain the desired flowrate of the product; that is, just scale the solution up or down by a constant factor and rerun the simulation to get the correct equipment specifications.

For more advanced simulation applications, such as optimizing or simulating existing plants, it may be necessary or useful to use controller modules in the simulation to obtain a desired result. For example, in a recycle loop it might be required that the ratio of two components entering a reactor be set at some fixed value. A controller module could be used to adjust the purge flowrate from the recycle stream to obtain this ratio. The use of controller modules introduces additional recycle loops. The way in which specifications for controllers are given can cause additional convergence problems, and this topic is covered in detail by Schad [10].

13.4. Choosing Thermodynamic Models

The results of any process simulation are never better than the input data, especially the thermodynamic data.

Everything from the energy balance to the volumetric flowrates to the separation in the equilibrium-stage units depends on accurate thermodynamic data.

If reaction kinetics information is missing, the simulator cannot calculate the conversion from a given reactor volume. Because such a calculation is not possible, only equilibrium reactor modules and those with specified conversions can be used.

Unfortunately, process simulators have default thermodynamics packages, which will —without warning—blindly miscalculate the entire flowsheet.

Only a few, readily available data are required to estimate the parameters in simple thermodynamic models. If the critical temperature and critical pressure are known for each pure component, the parameters for simple, cubic equations of state can be estimated. Even if these critical properties are unknown, they in turn can be estimated from one vapor pressure and one liquid density. Group-contribution models require even less information: merely the chemical structure of the molecule. However, these estimations can never be as accurate as experimental data. In thermodynamics, as elsewhere, *you get only what you pay for—or less!*

Compounding this problem is the development and implementation of expert systems to help choose the thermodynamic model. To date, these features merely offer false hope. Human thermodynamics experts do not recommend them.

A safe choice of thermodynamic model requires knowledge of the system, the calculation options of

the simulator, and the margin of error. In this section, guidance on choosing and using a thermodynamic model is given. In an academic setting, the choice of thermodynamic model affects the answers but not the ability of the student to learn how to use a process simulator—a key aspect of this book. Therefore, the examples throughout this book use simplistic thermodynamic models to allow easy simulation. In any real problem, where the simulation will be used to design or troubleshoot a process, the proper choice of thermodynamic model is essential. This section focuses on the key issues in making that choice, in using experimental data, and in determining when additional data are needed.

It has been assumed that the reader understands the basics of chemical engineering thermodynamics as covered in standard textbooks [4, 5, 6]. As pointed out before, it is extremely important that the chemical engineer performing a process simulation understand the thermodynamics being used. In a course, the instructor can often provide guidance. The help facility of the process simulator provides a refresher on details of the model choices; however, these descriptions do not include the thermodynamics foundation required for complete understanding. If the descriptions in the help facility are more than a refresher, the standard thermodynamics textbooks should be consulted.

If the thermodynamic option used by the process simulator is a mystery, the meaning of the results obtained from the simulation will be equally mysterious.

13.4.1. Pure-Component Properties

Physical properties such as density, viscosity, thermal conductivity, and heat capacity are generally not a serious problem in simulation. The group-contribution methods are reasonably good, and simulator databanks include experimental heat capacity data for more than a thousand substances. Although these correlations have random and systematic errors of several percent, this is close enough for most purposes. (However, they are not sufficient when you are paying for a fluid crossing a boundary based on volumetric flowrate.) As noted in Section 13.2.2, one should always be aware of which properties are estimated and which are from experimental measurements.

13.4.2. Enthalpy

Although the pure-component heat capacities are calculated with acceptable accuracy, the enthalpies of phase changes often are not. Care should be taken in choosing the enthalpy model for a simulation. If the enthalpy of vaporization is an important part of a calculation, simple equations of state should not be used. In fact, the “latent heat” or “ideal” options would be better. If the substance is above or near its critical temperature, equations of state must be used, but the user must beware, especially if polar substances such as water are present, as shown in Example 13.3.

Example 13.3.

A gas stream at 3000°F of the following concentration is to be cooled by evaporation of 500 kg/h of water entering at 70°F. Assume atmospheric pressure.

H_2	22.72 kg/h
N_2	272.24
CO	268.40
HCl	26.84

Perform a simulation to determine the final temperature of the cooled gas stream with the default

thermodynamic model and with the ideal model.

The default on most process simulators is an equation of state, either PR (Peng-Robinson) or SRK (Soave-Redlich-Kwong). These models give an outlet temperature of 480°F. The ideal model gives an outlet temperature of 348°F. The value calculated by the ideal model is closer to reality in this case because the equations of state do a poor job of estimating the enthalpy of vaporization of water, which is the most important property for the energy balance. The ideal model uses the experimentally determined value of this enthalpy of vaporization (from the databank).

13.4.3. Phase Equilibria

Extreme care must be exercised in choosing a model for phase equilibria (sometimes called the fugacity coefficient, *K*-factor, or fluid model). Whenever possible, phase-equilibrium data for the system should be used to regress the parameters in the model, and the deviation between the model predictions and the experimental data should be studied.

There are two general types of fugacity models: equations of state and liquid-state activity-coefficient models. An equation of state is an algebraic equation for the pressure of a mixture as a function of the composition, volume, and temperature. Through standard thermodynamic relationships, the fugacity, enthalpy, and so on for the mixture can be determined. These properties can be calculated for any density; therefore, both liquid and vapor properties, as well as supercritical phenomena, can be determined.

Activity-coefficient models, however, can only be used to calculate liquid-state fugacities and enthalpies of mixing. These models provide algebraic equations for the activity coefficient (γ_i) as a function of composition and temperature. Because the activity coefficient is merely a correction factor for the ideal-solution model (essentially Raoult's Law), it cannot be used for supercritical or "noncondensable" components. (Modifications of these models for these types of systems have been developed, but they are not recommended for the process simulator user without consultation with a thermodynamics expert.)

Equations of state are recommended for simple systems (nonpolar, small molecules) and in regions (especially supercritical conditions for any component in a mixture) where activity-coefficient models are inappropriate. For complex liquid mixtures, activity-coefficient models are preferred, but only if *all* of the binary interaction parameters (BIPs) are available.

Equations of State. The default fugacity model is normally either the SRK (Soave-Redlich-Kwong) or the PR (Peng-Robinson) equation. They (like most popular equations of state) normally use three pure-component parameters per substance and one binary-interaction parameter per binary pair. Although they give qualitatively correct results even in the supercritical region, they are known to be poor predictors of enthalpy changes, and (except for light hydrocarbons) they are not quantitatively accurate for phase equilibria.

The predicted phase equilibrium is a strong function of the binary interaction parameters (BIPs). Process simulators have regression options to determine these parameters from experimental phase-equilibrium data. The fit gives a first-order approximation for the accuracy of the equation of state. This information should always be considered in estimating the accuracy of the simulation. Additional simulations should be run with perturbed model parameters to get a feel for the uncertainty, and the user should realize that even this approach gives an optimistic approximation of

the error introduced by the model. If BIPs are provided in the simulator and the user has no evidence that one equation of state is better than another, then a separate, complete simulation should be performed for each of these equations of state. The difference between the simulations is a crude measure of the uncertainty introduced into the simulation by the uncertainty in the models. Again, the inferred uncertainty will be on the low side.

Monte-Carlo simulations (see Section 10.7) can be done with the results of the regression; however, present process simulators are not equipped to perform these directly. A simpler approach is to perform the simulation with a few different values of the BIPs for the equation of state. These values are typically 0.01 to 0.10. Larger values are rare, except in highly asymmetric systems. However, the difference between results calculated with values of, say, 0.01 and 0.02 can be large.

If BIPs are available for only a subset of the binary pairs, caution should be exercised. Assuming the unknown BIPs to be zero can be dangerous. Group-contribution models for estimating BIPs for equations of state can be used with caution.

There are usually six to ten equation-of-state choices, and a few mixing-rule choices. For polar or associating components or for heavy petroleum cuts, the help facility of the simulator should be consulted. Because different choices are available on the different simulators, they will not be covered here.

For most systems containing hydrocarbons and light gases, an equation of state is the best choice. One should initially choose the Peng-Robinson or Soave-Redlich-Kwong equation. (Note that neither the van der Waals nor Redlich-Kwong equation is a standard choice in simulators. These two equations of state were tremendous breakthroughs in fluid property models, but they were long ago supplanted by other models that give better quantitative results.) VLE (vapor-liquid equilibrium) data for each binary system can then be used with the regression utility to calculate the BIPs for the binary pairs and to plot the resulting model predictions against the experimental data. This regression is done separately for each equation of state. The equation that gives a better fit in the (*PTxy*) region of operation of the unit operation of interest is then used. If phase-equilibrium data are available at different temperatures, the temperature-dependent BIP feature of the simulator can be used. In the simulator databank, many BIPs are already regressed and available.

If neither simple equation of state adequately reproduces the experimental data, one of the other equations of state or other mixing rules, or a temperature-dependent BIP, may be needed. These often work better for polar-nonpolar systems. However, running the simulation more than once with different BIPs and with different thermodynamic models to judge the uncertainty of the result is recommended, as shown in Example 13.4. If the difference between the simulations seriously affects the viability of the process, a detailed uncertainty analysis is essential [11]. This is beyond the scope of this book.

Example 13.4.

Use both the Peng-Robinson and the Soave-Redlich-Kwong equations of state to calculate the methane vapor molar flowrate from a flash at the following conditions:

Temperature:	225 K
Pressure:	60.78 bar
Feed flowrates:	
Carbon dioxide	6 kmol/h
Hydrogen sulfide	24 kmol/h
Methane	66 kmol/h
Ethane	3 kmol/h
Propane	1 kmol/h

Compare the results for BIPs from the process simulator databank and with the BIPs set to zero.

The following results were obtained using CHEMCAD:

	Databank BIPs	Zero BIPs
Peng-Robinson	52.0 kmol/h	32.5 kmol/h
Soave-Redlich-Kwong	60.1 kmol/h	50.5 kmol/h

The two equations of state give different results, and the effect of setting the BIPs to zero is very significant.

For most chemical systems below the critical region, a liquid-state activity-coefficient model is the better choice.

Liquid-State Activity-Coefficient Models. If the conditions of the unit operation are far from the critical region of the mixture or that of the major component, and if experimental data are available for the phase equilibrium of interest (VLE or LLE), then a liquid-state activity-coefficient model is a reasonable choice. Activity coefficients (γ_i) correct for deviations of the liquid phase from ideal solution behavior, as shown in Equation (13.1).

$$\hat{\phi}_i^v \, y_i P = P_i^* x_i \gamma_i \phi_i^* \exp\left(\frac{1}{RT}\int_{P_i^*}^{P} v_i^l \, dP\right) \qquad (13.1)$$

where $\hat{\phi}_i^v$ is the fugacity coefficient of component i in the vapor-phase mixture at system temperature T and pressure P, y_i is the vapor mole fraction of i, P_i^* is the vapor pressure of pure i at T, x_i is the liquid mole fraction of i, ϕ_i^* is the fugacity coefficient of pure i at its vapor pressure at T, and v_i^l is the molar volume of pure liquid i at T.

The roles of the terms in Equation (13.1) are discussed in detail in standard thermodynamics texts. Here, it is sufficient to point out that the two terms closest to the equal sign (on either side of the equal sign) give Raoult's Law and that the most important of the remaining correction terms is usually γ_i, the activity coefficient. Thus, use of an activity-coefficient model requires values for the pure-component vapor pressures at the temperature of the system. There are several important considerations in using activity-coefficient models:

- If no BIPs are available for a given binary system, an activity-coefficient model will give results similar to but not necessarily the same as those for an ideal solution.
- The standard version of the Wilson equation cannot predict liquid-liquid immiscibility.

- The BIPs for various activity-coefficient models can be estimated by UNIFAC. However, caution must be exercised because increased uncertainty is inserted into the model with such estimation.
- Some BIP estimation may be done automatically by the simulator.
- There are no reliable rules for choosing an activity-coefficient model *a priori*. The standard procedure is to check the correlation of experimental data by several such models and then choose the model that gives the best correlation.
- Parameters regressed from VLE data are often unreliable when used for LLE prediction (and vice versa). Therefore, some process simulators provide a choice between two sets of parameter sets.
- Often ternary (and higher) data are not well predicted by activity-coefficient models and BIPs.
- The BIPs are typically highly correlated. This and the empirical nature of these models lead to similar fits to experimental data with very different values of the BIPs.

Some of these considerations are demonstrated in Examples 13.5 and 13.6.

Example 13.5.

Use the simulator databank BIPs for NRTL to calculate the vapor-liquid equilibrium for ethanol/water at 1 atm. Compare the results for BIPs set to zero. Regress experimental VLE data [12] to determine NRTL BIPs.

Figure E13.5(a) shows the *Txy* diagrams using the NRTL BIPs from the CHEMCAD databank and for these BIPs set to zero. Note that the latter case results in an ideal solution; thus, the azeotrope is missed. Regressing the experimental data for this system with the simulator regression tool gives the results shown in Figure E13.5(b). Although the BIPs in the databank (–55.1581, 670.441, 0.3031) and those regressed from the data (–104.31, 807.10, 0.28675) are quite different, the VLE calculated is very similar and is close to the experimental data.

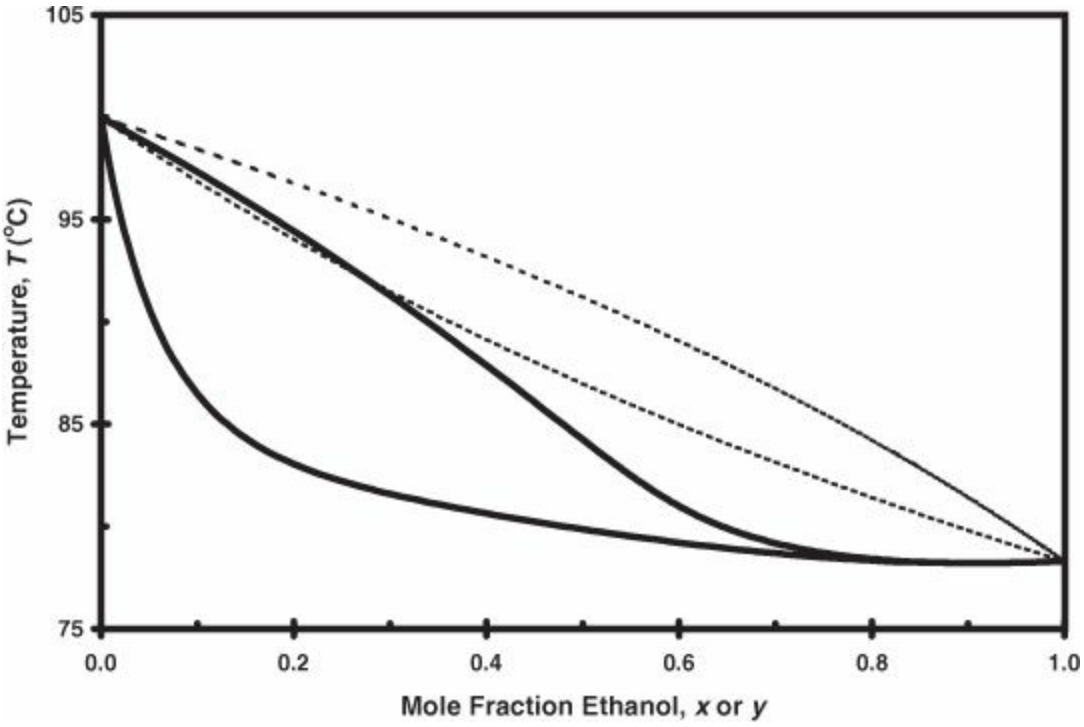


Figure E13.5(a). Vapor-Liquid Equilibrium for Ethanol/Water at 1 atm (*Solid curves are for CHEMCAD databank BIPs for NRTL. Dotted curves are for NRTL BIPs set to zero.*)

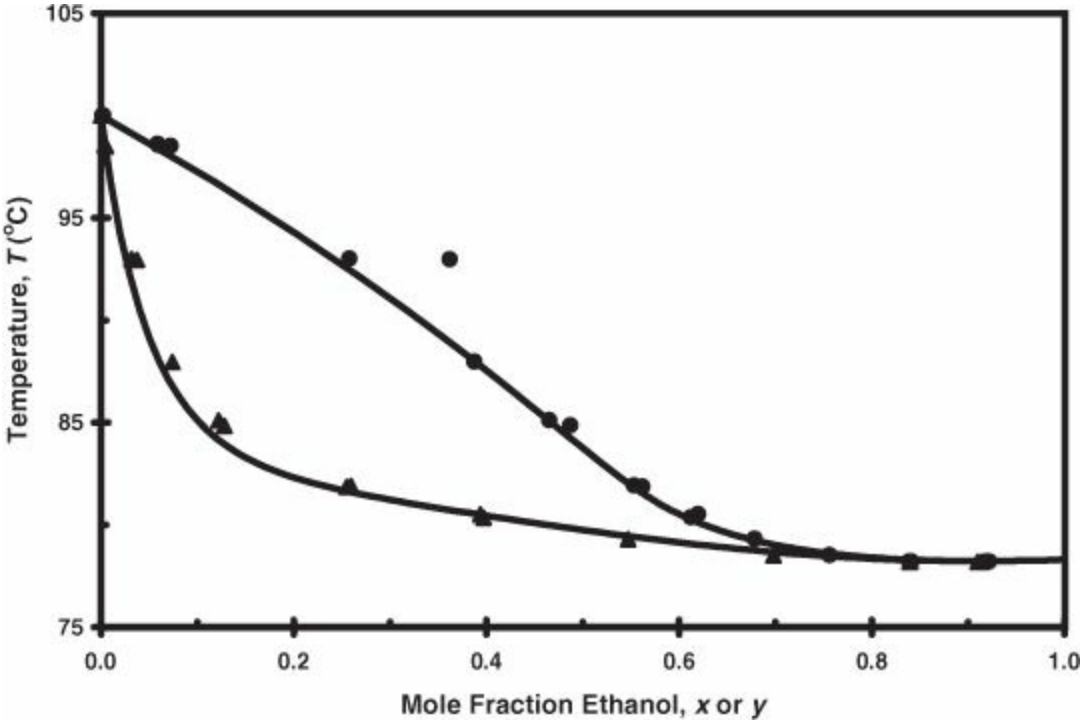


Figure E13.5(b). Vapor-Liquid Equilibrium for Ethanol/Water at 1 atm (*Solid curves are for NRTL BIPs regressed from data points shown.*)

Example 13.6.

Calculate the LLE for the ternary di-isopropyl-ether/acetic-acid/water using NRTL and the BIPs available for the three binary pairs in the simulator databank. Compare the prediction with ternary LLE data for this system at 24.6°C [13].

See Figure E13.6. The experimental phase envelope (dotted lines) is twice the size of the predicted one (solid lines). This would lead to gross error in extraction calculations. Note that if all the BIPs are set to zero, there is no liquid-liquid immiscibility region. However, if the ternary LLE data were used to regress all of the BIPs simultaneously, the fit would be quite good.

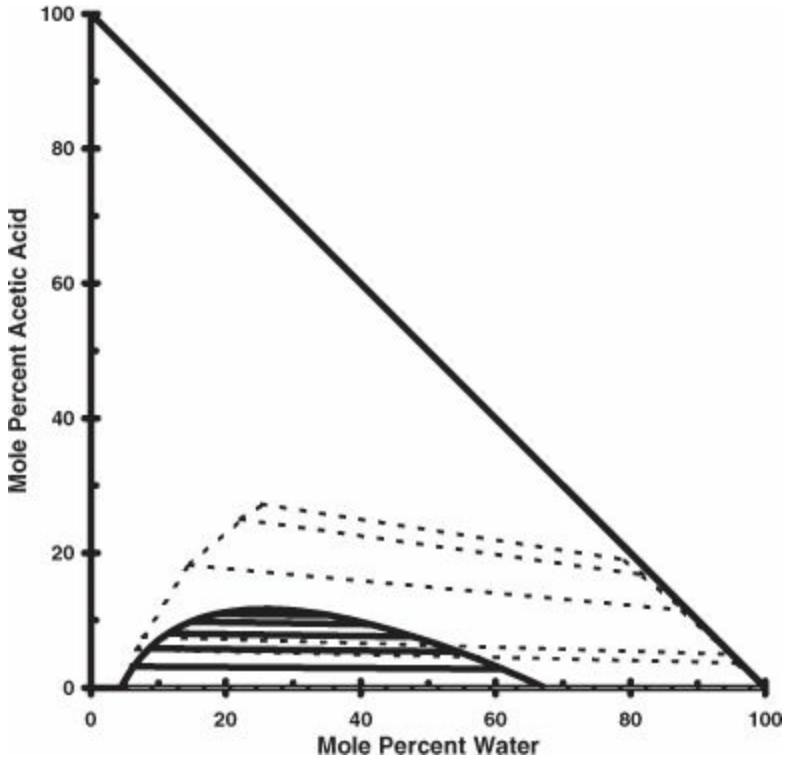


Figure E13.6. Liquid-Liquid Equilibrium for Di-isopropyl-Ether/Acetic-Acid/Water at 24.6°C

The recommended strategy for choosing a liquid-state, activity-coefficient model is as follows:

1. The simulator databank is checked for BIPs for all the binary pairs in the system. If these are available, they are most often from the DECHEMA Data Series [12, 13], but sometimes they are from different sources. Some simulators provide the literature citation; others do not. Each of the three most common models (Wilson, NRTL, UNIQUAC) has different values for BIPs, and they are not correlated from one model to another. Although BIPs for Wilson may not be available for partially immiscible systems (see above), if a binary pair has BIPs for NRTL or for UNIQUAC, the BIPs for that pair should be available for both models. If they are not, the original data are found and the BIPs are fit for the other model.
2. If phase-equilibrium data can be found for the binary pairs with missing BIPs, a regression is done with the simulator to find the missing BIPs.
3. For binary pairs that have no measured phase equilibria (there are many!), the UNIFAC estimation option of the simulator is used to estimate the BIPs. There are two UNIFAC methods: one for VLE and one for LLE. The choice depends on the type of equilibrium for the unit operation of interest.
4. If the unit operation of interest is an extraction or other operation involving LLE or VLLE and ternary data are available, the predictions of the three activity-coefficient models are checked for the ternary LLE.
5. One of the three methods usually shows a significantly better fit than the others. This method, *and the second-best method*, are used for the simulation. Comparing the two results provides a rough sense of the uncertainty of the calculation. Note that the "true" result is certainly not guaranteed to be between the two results. It is possible that this strategy will give a false sense of low uncertainty if the two methods give similar predictions that are far from the experimental data. This uncertainty strategy is used in the same way as is any heuristic from Chapter 11. Although this strategy is an analogue of a long-practiced experimental strategy and the basis for numerical analysis error estimation, it does take considerable engineering judgment. Good judgment comes from experience.
6. If the predictions from the activity-coefficient model chosen do not fit the measured data, a more detailed uncertainty analysis is needed. Although the details of such an analysis are outside the scope of this book, the most important decision is that one is warranted. Calibration of the uncertainty of simulation results is obtained from simulations run with different estimates (high and low, when possible).

The UNIFAC model is never used if experimental data are available for the binary system. UNIFAC is a group-contribution model for determining the BIPs for the UNIQUAC model (and by extension for the NRTL and Wilson models and for equations of state). Only chemical structure data are needed, but the calculations are not very accurate. When determining the numbers of groups within a molecule, one should always start with the largest group. This strategy minimizes the assumptions (and therefore the errors) in the model. Group-contribution models should be used with caution.

For many systems, a model such as UNIFAC may be the only option. If so, even a very crude uncertainty estimate can be difficult. If only one phase-equilibrium datum for the system can be found, its deviation from the model prediction is at least some estimate of the uncertainty (as long as that

datum was not used to regress parameters).

Using Scarce Data to Calibrate a Thermodynamic Model. Any experimental data on phase equilibria can be used to perform a crude calibration or verification of the model. It need not be the type of data that would be taken in the lab. If the recovery in a column for one set of conditions is known, for example, and if only one BIP is unknown, then the only value of the BIP that will reproduce that datum can be found. Such data are sometimes found in patents.

More Difficult Systems. The above discussions pertain to "easy" systems: (1) small, nonpolar or slightly polar molecules for equations of state and (2) nonelectrolyte, nonpolymeric substances considerably below their critical temperatures for liquid-state activity-coefficient models. Most simulators have some models for electrolytes and for polymers, but these are likely to be even more uncertain than for the easy systems. Again, the key is to find some data, even plant operating data, to verify and to calibrate the models. If the overall recovery from a multistage separation is known, for example, one can simulate the column, using the best-known thermodynamic model, and the deviation between the plant datum and the simulator result is a crude (optimistic) estimate of the uncertainty.

Because most thermodynamic options are semitheoretical models for small, nonpolar molecules, the more difficult systems require another degree of freedom in the model. The most common such modification is to make the parameters temperature dependent. This requires additional data, but there is some theoretical justification for using effective model parameters that vary with temperature.

Hybrid Systems. Often a process includes components as wide ranging as solids at room temperature to supercritical gases. They can include water, strong acids, hydrocarbons, and polymers. Often, no single thermodynamic model can be used reliably to predict the fugacities of such a wide range of components. For these cases, simulators allow for hybrid thermodynamic models. The breadth of hybridization varies from one simulator to another, but all at least allow for some components to be considered immiscible with respect to others. For example, the NRTL model may be used for binary pairs for which both compounds are subcritical, while Henry's Law is used for supercritical (so-called noncondensable) components. Each simulator allows for immiscibility of water and hydrocarbon liquid phases, with the compositions of hydrocarbons in the aqueous phase estimated with Henry's Law and the liquid-liquid equilibrium for water calculated based on ideal solution in the aqueous phase and some chosen model in the hydrocarbon-rich phase. The user should check each of these options, so that it is clear what the simulator is doing. Although Henry's Law does not necessarily mean that the phase is aqueous, the Henry's Law model in a process simulator may be developed only for aqueous systems.

Another kind of hybridization is the choice of auxiliary models for liquid-state activity-coefficient models. The model to use for the vapor phase can be specified and whether to make the Poynting correction. The best choice is to use an equation of state (PR or SRK) for the vapor-phase correction and to use the Poynting correction. Both corrections go smoothly to zero in the low-pressure limit, and neither should add greatly to the computational time for most flowsheets.

The final type of hybridization is the use of different models for different unit operations. Although this appears to be inconsistent at first, it is reality that thermodynamic models are not perfect and that some work much better for LLE than for VLE, some work better for low pressures and others for high pressures, and some work for hydrocarbons but not for aqueous phases. Furthermore, simulators

perform calculations for individual units and then pass only component flowrates, temperature, and pressure to the next unit. Thus, consistency is not a problem. Therefore, one should always consider the possibility of using different models for different unit operations. All the simulators allow this, and it is essential for a complex flowsheet. An activity-coefficient model can be used for the liquid-liquid extractor and an equation of state for the flash unit. This hybridization can be extremely important when, for example, some units contain mainly complex organics and other units contain light hydrocarbons and nitrogen.

Other Models. Different simulators have a variety of additional models beyond those mentioned above. For example, some have nonideal electrolyte thermodynamic models that calculate species equilibria, some have polymer thermodynamic packages, and some allow petroleum cuts to be represented automatically by pseudocomponents. Presently, these packages are less consistent across simulators and are not discussed here. However, the user should always investigate the range of models available for the simulator being used.

13.4.4. Using Thermodynamic Models

In summary, the assumed best thermodynamic model should be used, based on the rough guidelines above. However, a process should always be resimulated either with another model assumed to be equally good or with different model parameters (see Example 13.7). The appropriate perturbation to apply to the parameters is available from the experimental data regression or from comparison of calculated results with experimental or plant data. Such data should always be sought for the conditions closest to those in the simulation. If the application is liquid-liquid extraction, for example, liquid-liquid equilibrium data (rather than vapor-liquid equilibrium data) should be used in the parameter regression, even though the same activity-coefficient models are used for both liquid-liquid and vapor-liquid equilibria.

> **The availability of BIPs in the databank of a process simulator must never be interpreted as an indication that the model is of acceptable accuracy.**

These parameter values are merely the “best” for some specific objective function, for some specific set of data. The model may not be able to correlate even these data very well with this optimum parameter set. And one should treat a decision to use a BIP equal to zero as equivalent to using an arbitrary value of the BIP. The decision to use zero is, in fact, a decision to use a specific value based on little or no data.

Example 13.7.

Consider the DME Tower, T-201, in the DME process in Appendix B. Simulate this unit using a shortcut model with different liquid-state activity-coefficient models to determine the required number of stages for the reflux ratio and the recoveries shown in Appendix B. Include no corrections for heat of mixing. Then perform a rigorous column simulation to check the distillate purity. Compare the results.

The base case uses the UNIFAC model with vapor-phase fugacity correction. The specifications are as follows:

- Column pressures: top, 10.3 bar; bottom, 10.5 bar

- Key components: light, DME; heavy, methanol
- Light key recovery in distillate: 98.93%
- Heavy key recovery in bottoms: 99.08%
- Reflux ratio: 0.3631
- 70% plate efficiency

An initial CHEMCAD simulation confirms the value given in Appendix B of 22 actual stages.

Table E13.7 shows the results obtained from six simulations, all with the same input specifications but with different thermodynamic options. The number of actual stages calculated ranges from 15 to 22; however, the results for two of the simulations (denoted n/a in the table) indicated that the minimum reflux ratio was greater than that specified. Without further information about the ability of the various models to correlate experimental vapor-liquid equilibrium data, a precise solution to the problem is not possible. However, the differences in the results obtained indicate that the choice of thermodynamic model is a crucial one. Of special concern here is the choice of correction of fugacities (denoted w/correction). These corrections are the first and last terms in Equation (13.1). Note that these results were obtained using the CHEMCAD databank BIP values for the NRTL and UNIQUAC models. Different BIP values will yield different results.

Table E13.7. Comparison of Simulations for DME Column, T-201, for Various Thermodynamic Options

Thermodynamic Option	Number of Actual Stages Obtained from Shortcut Method	Distillate Purity Obtained with 22 Stages, Specified Reflux Ratio, and Shortcut Reboiler Duty	Required Reflux Ratio to Obtain DME Purity and Recovery with 22 stages
	Shortcut Method	Rigorous Simulation	Rigorous Simulation
UNIFAC w/correction	22	97.3 wt%	0.52
UNIFAC	15	95.0	0.47
NRTL w/correction	n/a	96.6	0.77
NRTL	21	97.6	0.49
UNIQUAC w/correction	n/a	97.1	0.58
UNIQUAC	18	97.6	0.48

To determine which model is best, data on the various binary pairs in the mixture are found. These data consist of measurements of temperature, pressure, and composition of a liquid in equilibrium with its vapor. Sometimes, the concentration of the vapor is also measured. From the temperature and the liquid-phase composition, the pressure and vapor-phase compositions are calculated with the thermodynamic model. The sum of the squared deviations between the experimental and the calculated pressure and between the experimental and the calculated vapor compositions is the objective function. The decision variables are the adjustable parameters in the thermodynamic model. Through the procedures of Chapter 14, the objective function is minimized and the optimum set of parameters is found. The standard process simulators incorporate a tool to do these regressions.

Of great concern is the purity of the overhead product. This stream is the DME product stream from the process, and the specification is 99.5 wt%. The third column in Table E13.7 shows the purity

obtained by rigorous, tray-by-tray simulations of this column. In each case, the number of stages, feed location, column pressures, reflux ratio, and reboiler duty were set at those shown in Appendix B. Again, only the thermodynamic option was varied. In the shortcut calculation, many assumptions are made, including the constancy of relative volatilities. For the rigorous calculation, the full power of the thermodynamic package is used in the phase-equilibrium and energy-balance calculations. In this example, the distillate purity specification would be very far off from that calculated with the shortcut method. As expected, the shortcut results are only preliminary to the rigorous column simulation.

The fourth column of Table E13.7 gives the reflux ratio required to meet both the DME purity and recovery specifications. The variation of this ratio from 0.47 to 0.77 is significant, because it is directly related to the required condenser and reboiler duties. If the NRTL w/correction calculation is closest to the truth, the reboiler duty required is 80% greater than that obtained in the baseline shortcut simulation. Ironically, this is the thermodynamics option suggested by the CHEMCAD expert system.

13.5. Case Study: Toluene Hydrodealkylation Process

The purpose of this section is to present the input information necessary to make a basic simulation of the toluene hydrodealkylation process presented in Chapter 1. The required input data necessary to obtain a Level 1 simulation are presented in Table 13.1. The corresponding simulator flowsheet is given in Figure 13.6. In Table 13.1, the equipment numbers given in the third column correspond to those used in Figure 13.6. In the first column, the equipment numbers on the toluene hydrodealkylation PFD (Figure 1.5) are given. It should be noted that there is not a one-to-one correspondence between the actual equipment and the simulation modules. For example, three splitters and six mixers are required in the simulation, but these are not identified in the PFD. In addition, several pieces of equipment associated with the benzene purification tower are simulated by a single simulation unit. The numbering of the streams in Figure 13.6 corresponds to that given in Figure 1.5, except when additional stream numbers are required for the simulation. In order to avoid confusion, these extra streams are assigned numbers greater than 90.

Table 13.1. Required Input Data for a Level 1 Simulation of Toluene Hydrodealkylation Process

Equipment Number	Simulator Equipment	Simulator Equip. No.	Input Streams		Output Streams		Required Input
TK-101	Mixer	m-1	1	11	90	—	Pressure drop = 0 bar
P-101	Pump	p-1	90	—	2	—	Outlet pressure = 27.0 bar
E-101	Hexch	e-1	92	—	4	—	Outlet stream vapor fraction = 1.0
H-101	Heater	h-1	4	—	6	—	Outlet temperature = 600°C
R-101	Stoic react	r-1	93	—	9	—	Conversion of toluene = 0.75
E-102	Flash	f-1	9	—	8	94	Temperature = 38°C Pressure = 23.9 bar
V-101	Flash	f-1	9	—	8	94	No input required because vessel is associated with flash operation
V-103	Flash	f-2	94	—	17	18	Temperature = 38°C Pressure = 2.8
E-103	Hexch	e-2	18	—	10	—	Outlet temperature = 90°C
T-101	Shortcut tower	t-1	10	—	19	11	Recovery of benzene in top product = 0.99 Recovery of toluene in top product = 0.01 R/R_{min} = 1.5 Column pressure drop = 0.3 bar
E-104	Shortcut tower	t-1	10	—	19	11	Included in tower simulation
E-106	Shortcut tower	t-1	10	—	19	11	Included in tower simulation
V-102	Shortcut tower	t-1	10	—	19	11	Not required in simulation
P-102	Shortcut tower	t-1	10	—	19	11	Not required in simulation
E-105	Hexch	e-3	95	—	15	—	Outlet temperature = 38°C
C-101	Compr	c-1	97	—	98	—	Outlet pressure = 25.5 bar
	Mixer	m-2	3	5	91	—	Pressure drop = 0 bar
	Mixer	m-3	2	91	92	—	Pressure drop = 0 bar
	Mixer	m-4	6	7	93	—	Pressure drop = 0 bar
	Mixer	m-5	17	96	99	—	Pressure drop = 0 bar
	Mixer	m-6	99	100	16	—	Pressure drop = 0 bar
	Splitter	s-1	8	—	97	96	Pressure drop = 0 bar
	Splitter	s-2	98	—	5	7	Pressure drop = 0 bar
	Splitter	s-3	19	—	100	95	Pressure drop = 0 bar

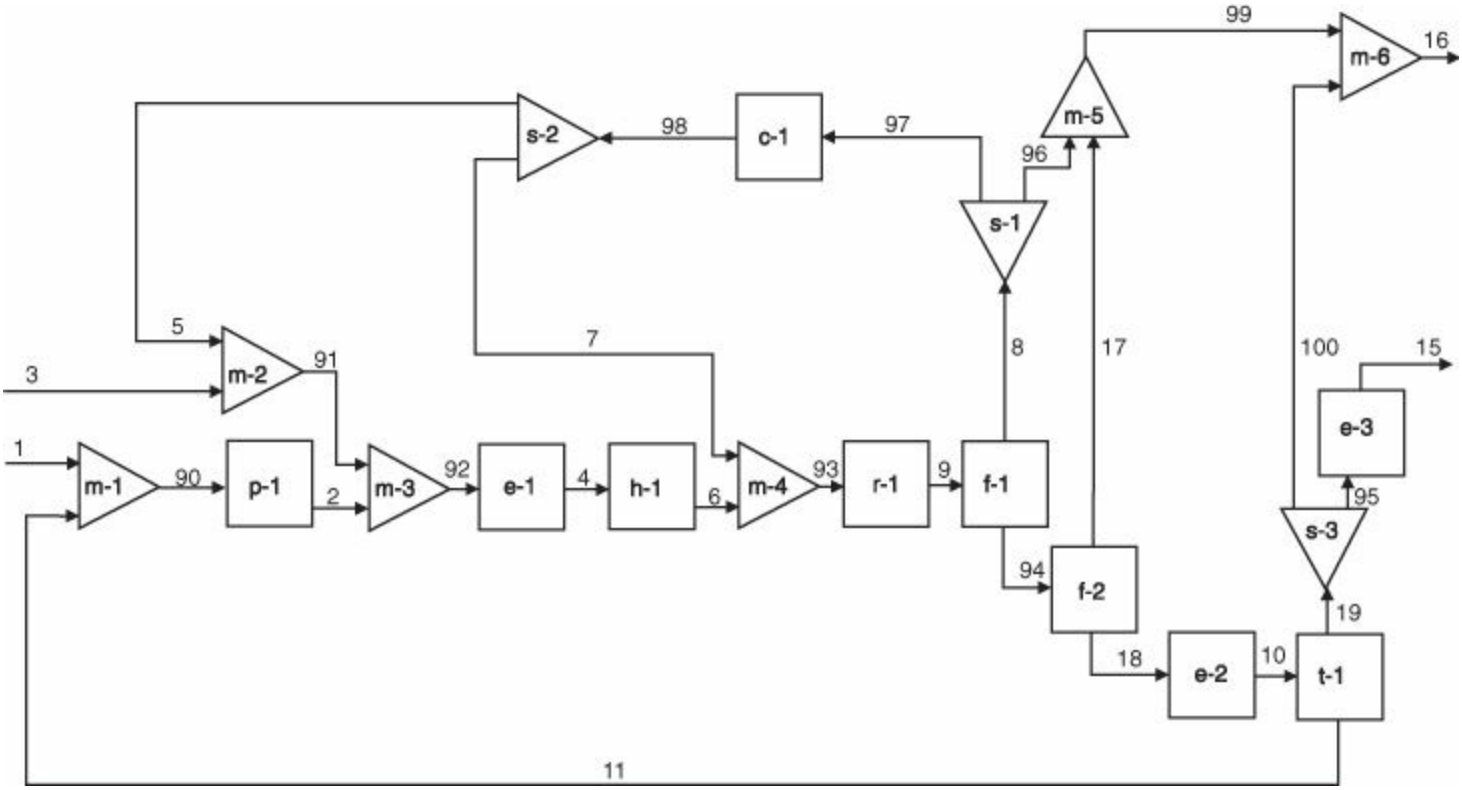


Figure 13.6. Flowsheet Structure Used in the Simulation of the Toluene Hydrodealkylation Process

In Table 13.2, the specifications for the feed streams are given. For this process, there are only two feed streams—Streams 1 and 3—corresponding to toluene and hydrogen, respectively. In addition, estimates of all the recycle streams should be given prior to beginning the simulation, and these are given in Table 13.2. However, these estimates need not be very accurate. Usually, any estimate is better than no estimate at all.

Table 13.2. Feed Stream Properties and Estimates of Recycle Streams

	Stream 1	Stream 3	Stream 11	Stream 5	Stream 7
Temperature (°C)	25.0	25.0	150.0	50.0	50.0
Pressure (bar)	1.9	25.5	2.8	25.5	25.5
Hydrogen (kmol/h)	—	286.0	—	200.0	20.0
Methane (kmol/h)	—	15.0	—	200.0	20.0
Benzene (kmol/h)	—	—	—	—	—
Toluene (kmol/h)	108.7	—	30.0	—	—

The data given in Tables 13.1 and 13.2 are sufficient to reproduce the material and energy balances for the toluene hydrodealkylation process. The use of these data to reproduce the flow table in Table 1.5 is left as an example problem at the end of the chapter. As mentioned in Section 13.3, some difficulty may arise when trying to simulate this flowsheet because of the three recycle streams. If you encounter problems in obtaining a converged solution, you should try to eliminate as many recycle streams as possible, run the simulation, and then add the recycle streams back into the problem one at

a time. The thermodynamic models for this simulation should be chosen using the guidelines in Section 13.4 or using the expert system in the simulator that you use. The results given in Chapter 1 for this process were obtained using the SRK models for enthalpy and phase equilibria.

13.6. Electrolyte Systems Modeling

A number of important chemical engineering applications involve electrolytes. Examples of such processes include the following:

- **Gas-treatment processes.** The most common examples are the use of alkanolamines and alkaline-salt solutions for acid-gas removal.
- **Wastewater treatment** for removal of undesired species and for neutralization before disposal. The most common example is the sour-water stripping (SWS) process used primarily for removing NH_3 and H_2S.
- **Electrochemical processes.** The most common examples include various types of fuel cells, batteries, electrolysis, and corrosion modeling.
- **Separation processes** such as extractive distillation, seawater desalination, and solution crystallization.

Even though it is possible to simulate these systems by writing user-supplied equations, the effort involved to obtain a reasonably accurate model can be significant. With recent advances in process simulators, there are a large number of available models within the simulator that can be customized, and the parameters can be modified to obtain reasonable accuracy. A cursory understanding of the theory of electrolyte systems is necessary for simulating these processes. Therefore, the theory of electrolyte systems will be discussed first along with a discussion of the various available models. These models differ widely in their levels of complexity. After that, the problem of how to set up these models will be discussed through an example. At the end of the chapter, more discussion on electrolyte systems modeling is included for the advanced user.

13.6.1. Fundamentals of Modeling Electrolyte Systems

In chemical processes, electrolyte systems with liquid and vapor phases are very common. These electrolyte models can be readily extended to systems involving solids (such as salts) with suitable modifications. Based on the type of the system, either liquid/liquid equilibrium or solid/liquid equilibrium (such as salt precipitation) must be considered. In an electrolyte system, simultaneous phase and chemical equilibrium calculations are performed.

A strong electrolyte completely dissociates into its constituent ions, whereas a weak electrolyte only partially dissociates. Therefore, a significant amount of the weak electrolyte can remain as molecular species in the solution. There can be one or more solvents in the electrolyte system. Salt precipitation can also occur in such systems. The presence of ions causes highly nonideal behavior in the liquid phase. This impacts both the physical properties as well as the phase and reaction equilibria. Therefore, representative modeling of the chemical and phase equilibria is very important for such systems. Interactions between molecule-molecule, molecule-ion, and ion-ion exist and should be captured in the model. These systems may vary widely because of their chemical compositions (aqueous or mixed solvent, dilute, or concentrated solutions). Their conditions may vary widely, ranging from ambient temperature and pressure to supercritical conditions. While choosing the thermodynamic and transport models, the user must be sure about the applicability of the available

models in the process simulator for the particular electrolyte systems being considered. The key considerations are:

1. Is the system aqueous?
2. Is it a strong electrolyte system?
3. Is it a mixed-solvent system?
4. What is the solute concentration?
5. What is the expected maximum temperature of the system?

In the following discussion, the impact of these questions on the model selection will be covered. The answer to the last question is, of course, the highest temperature in the system, which may occur in a column reboiler or in a fired heater.

There are a number of thermodynamic and transport models available in the open literature. Only some of them are available in process simulators. Most process simulators mention the limitations and applicability of the models in the online documentation. If not, this information can be obtained from the open literature.

The important task of modeling electrolyte systems, as in many other systems, is the calculation of the VLE. Even though the ions do not directly participate in the vapor/liquid equilibrium, they affect the solution properties and the fugacities of the species participating in the equilibrium. For the species in both the phases, the condition for equilibrium is

$$\hat{f}_i^v = \hat{f}_i^l \tag{13.2}$$

where $\hat{f}_i^v$ and $\hat{f}_i^l$ are the fugacity of species i in the vapor and liquid phases, respectively. Because of significant nonideality in the electrolyte systems, an activity-coefficient model is most often used for the liquid phase. The equilibrium condition can be written as

$$\hat{\phi}_i^v y_i P = x_i \gamma_i f_i^l \tag{13.3}$$

where $\hat{\phi}_i^v$, γ_i, f_i^l are the fugacity coefficient of species i in the vapor phase, the activity coefficient, and the fugacity of pure species i in the liquid phase, respectively. In terms of a Poynting correction factor formulation,

$$f_i^l = \phi_i^* P_i^* \exp \frac{v_i^l (P - P_i^*)}{RT} \tag{13.4}$$

where ϕ_i^*, P_i^*, v_i^l are the fugacity coefficient of saturated vapor, the saturation pressure, and the molar volume of the saturated liquid for the pure species i, respectively. $\hat{\phi}_i^v$ and ϕ_i^* can be readily calculated from an equation-of-state (EOS) model, and γ_i is calculated from the activity-coefficient model suitable for electrolyte systems and will be further discussed in detail. Quite often in chemical engineering applications, such as in sour-water stripping and acid-gas removal, the operating temperature is greater than the critical temperature of the species. For example, the critical temperatures of CO, CO_2, and CH_4 are –140°C, 31°C, and –82°C, respectively. Therefore, since Equation (13.4) requires a value for P_i^*, this equation cannot be applied. Usually, such systems are modeled with Henry's Law. Applying Henry's Law, the equilibrium condition can be written as

$$y_i \hat{\phi}_i P = x_i \gamma_i \frac{H_i}{\gamma_i^\infty} \tag{13.5}$$

where γ_i^∞ is the activity coefficient of species i in the mixture at infinite dilution evaluated at the

temperature (T) and pressure (P) of the mixture, and H_i is the Henry's Law constant of the species i.

For electrolyte systems, evaluation of the activity coefficients in the liquid phase is probably the most important calculation. The activity coefficient is often calculated from the Gibbs free energy. Once a suitable equation for the Gibbs free energy is obtained, other important thermodynamic properties such as enthalpy, entropy, heat capacity, and volume can be readily calculated from available thermodynamic relations. A discussion of calculation of excess Gibbs energy for electrolyte systems can be found in Appendix 13.1.

A number of thermodynamic models are available in the process simulator environment for calculating Gibbs free energy. Table 13.3 provides a quick guideline for the applicability of some of these models, which include models due to Pitzer [14, 15, 16], modified Pitzer for systems containing weak electrolytes and molecular nonelectrolytes [17], Bromley-Pitzer [18, 19], electrolyte NRTL (unsymmetric) [20], electrolyte NRTL (symmetric) [21], eNRTL-SAC (unsymmetric) [22], and eNRTL-SAC (symmetric) [23]. The eNRTL-SAC models are particularly applicable to pharmaceutical systems consisting of large, complex molecules along with electrolytes. For sour-water and amine systems, two special thermodynamic models are available in most process simulators. The model for the sour-water system is based on an American Petroleum Institute (API) publication [24]. The model for the amine system, popularly known as "AMINE" or "AMINES," is mainly based on the Kent-Eisenberg model [25]. This model is used for systems involving amines (mainly monoethanolamine, diethanolamine, diisopropanolamine, diglycolamine) and acid gases (mainly CO_2 and H_2S). However, some process simulators have extended this model to other amines and other species, along with extensions to a wider operating range. Most process simulators clearly mention the range of operating conditions, such as temperature, pressure, maximum acid-gas loading, and amine concentration, over which the model is expected to be reasonably accurate. For a detailed discussion and additional guidance about using the thermodynamic models mentioned previously, the simulator user manual and the published literature should be consulted. It should be noted that the simulator vendors keep adding new models and updating the parameters for greater accuracy and to enhance the applicability of their model. The discussion above and the data in Table 13.3 are based on currently available capabilities. The simulator documentation is a very good source for these updates. More discussion of the calculation of excess Gibbs energy for electrolyte systems using some of these models can be found in Appendix 13.1.

Table 13.3. Applicability of Some Thermodynamic Models for Calculating Gibbs Free Energy/Activity Coefficient for Electrolyte Systems

Model Name	Nonaqueous System	Mixed-Solvent System	Presence of Molecular Solutes	Ionic Concentration
Pitzer	No	No	No	< 6 molal
Modified Pitzer	No	No	Yes	< 6 molal
Bromley-Pitzer	No	No	No	< 6 molal
Electrolyte NRTL (Unsymmetric)	Yes (but cumbersome and can be inaccurate)	Yes	Yes	Wide range
Electrolyte NRTL (Symmetric)	Yes	Yes	Yes	Wide range
eNRTL-SAC (Unsymmetric)	Yes (but cumbersome and can be inaccurate)	Yes	Yes	< 6 molal
eNRTL-SAC (symmetric)	Yes	Yes	Yes	< 6 molal

The activity coefficients of the ions can be calculated from the excess Gibbs energy. In the molality scale, this is given by

$$\ln \gamma_{m,i} = \left(\frac{\partial (G^E/RT)}{\partial n_i} \right)_{P,T,n_j} \tag{13.6}$$

The activity coefficient is then converted to the mole-fraction scale for the VLE calculation. Other thermodynamic properties can be calculated from the excess Gibbs free energy using consistent thermodynamic relationships such as

$$S^E = -\left(\frac{\partial G^E}{\partial T} \right)_{P,x} \tag{13.7}$$

$$H^E = G^E + TS^E = -RT^2 \left(\frac{\partial (G^E/RT)}{\partial T} \right)_{P,x} \tag{13.8}$$

$$C_p^E = \left(\frac{\partial H^E}{\partial T} \right)_{P,x} = -T \left(\frac{\partial^2 G^E}{\partial T^2} \right)_{P,x} \tag{13.9}$$

$$v^E = \left(\frac{\partial G^E}{\partial P} \right)_{T,x} \tag{13.10}$$

Thermodynamic relationships similar to Equations (13.7) through (13.10) also hold true for the standard-state properties. Using these relationships, if one of the standard-state thermodynamic properties among heat capacity, enthalpy, entropy, Gibbs energy, and molar volume is known, other properties can be calculated.

Heat Capacity. One common approach in process simulators is to use the standard-state heat capacity to derive the other standard-state properties. The standard-state heat capacities can simply be expressed by a polynomial. If the parameters for such a polynomial are not available for some ionic species, their standard-state heat capacities can be calculated from correlations such as that of Criss and Cobble [26]. According to this correlation, which is based on the "correspondence" principle, partial molal heat capacity of an ionic species is given by

$$\overline{C}^0_{p_i}(T) \approx A_i(T) + B_i(T)\overline{S}^0_{i,25} \qquad (13.11)$$

where the parameters $A_i(T)$ and $B_i(T)$ depend upon the ion types and $\overline{S}^0_{i,25}$ is the standard-state ionic entropy at 25°C using an "absolute" scale. Note that $\overline{S}^0_{i,25}$ values are available for a number of ionic species in the open literature or can be calculated from a change in the enthalpy and Gibbs free energy data.

Molar Volume. Even though the molar volume/density can be calculated by thermodynamic relations such as Equation (13.10), this often results in a poor estimate. This information is particularly crucial for plant design and equipment sizing. For estimating the molar volume of an electrolyte system, Equation (13.12) can be written

$$v = x_w v_w + x_s v_s + x_{el} v_{el} \qquad (13.12)$$

In Equation (13.12), x_w, x_s, and x_{el} denote the mole fraction of water, all non-water solvents, and the electrolyte(s), respectively. In addition, υ_w denotes the molar volume of water that can be obtained from the steam tables. υ_s denotes the molar volume of the mixture of all non-water solvents. The molar volume of non-water solvents can be found using correlations such as the simple Rackett equation [27], the DIPPR equation [28], or the model of Campbell-Thodos [29]. In Equation (13.12), υ_{el} denotes the molar volume of the electrolyte that is usually calculated on the basis of the standard state as defined before. One very common correlation used in process simulators is due to Redlich and Meyer [30]:

$$v_{el} = v^{\infty}_{el} + A_1\sqrt{x_{el}} + A_2 x_{el} \qquad (13.13)$$

In Equation (13.13), V^{∞}_{el} is the true partial molar volume of the electrolyte at infinite dilution in water. A_1 and A_2 are constants that depend on the temperature of the system and the particular electrolyte. The molar volume of the ionic species can also be calculated from the Debye-Hückel limiting law.

Chemical Equilibrium. As the ionic reactions are generally fast, the reactions in an electrolyte system are often treated as equilibrium reactions. However, before performing the chemical equilibrium calculations, all possible reactions in the solutions must be identified. These reactions can be identified from the existing literature or by performing laboratory experiments. Identification of an appropriate reaction set is very important for the electrolyte systems, because the species compositions in the phases depend on both physical and chemical equilibrium. For liquid-phase reactions, the equilibrium constant can be written as

$$\prod_i (x_i\gamma_i)^{v_i} = K_{eq} = \exp\left(\frac{-\Delta G^0}{RT}\right) \qquad (13.14)$$

where v_i is the stoichiometric coefficient of species i in a reaction, and K_{eq} is the equilibrium constant. Equation (13.14) should be written for all the liquid-phase equilibrium reactions.

In modeling electrolyte systems, transport of reacting species to the reacting interface and transport of heat should also be precisely captured. So, the transport models should be selected carefully. The key transport properties are viscosity, thermal conductivity, diffusivity, and surface tension.

Viscosity. For calculating the viscosity of electrolyte systems, the simplest equation is [31]

$$\mu = \mu_0(1 + A\sqrt{c}) \qquad (13.15)$$

where μ and μ_0 are the viscosities of the electrolyte solution and the pure solvent, respectively, and c

is the concentration of electrolyte using a molarity scale. For the case of a mixed-solvent system, μ_0 can be calculated by an appropriate model such as the Andrade model [32] or by an appropriate mixing rule. The second term captures the change in the viscosity due to the presence of electrolytes. The coefficient A considers ion-ion interactions and can be calculated by the method of Falkenhagen and Dole [31] based on Debye-Hückel theory. The coefficient A is a function of solvent properties, ionic charges, mobilities, and temperature. Unfortunately, this equation is applicable only to very dilute systems, up to about 0.01 mol/L. A more widely used equation, which is applicable to solutions with concentrations up to about 0.1 mol/L, is due to Jones and Dole [33]:

$$\mu = \mu_0(1 + A\sqrt{c} + Bc) \tag{13.16}$$

The third term on the right-hand side is included to account for the interactions between the solvent and the ions. It should be noted that the solvent-solute interaction can affect the viscosity of the solution. For this reason, the B-coefficient has been studied widely. For more concentrated solutions, a quadratic term was added to Equation (13.16) by Kaminsky [34]. A generic framework that considers similar terms as before was proposed by Lencka et al. [35]. In this speciation-based model, three contributions are considered: a long-range electrostatic term based on the Onsager-Fuoss theory [36], contribution of individual ions, and contribution of interactions between all species (ions and neutral species). This model has proved to be very accurate up to a concentration of 30 mol/kg and up to a temperature of 300°C. Temperature dependence of the parameters used in the viscosity models should also be considered for better accuracy.

Thermal Conductivity. One of the widely used empirical correlations for calculating thermal conductivity of electrolyte solutions is the Riedel equation [37],

$$k = k_0 + \sum_i \alpha_i c_i \tag{13.17}$$

where k and k_0 are the thermal conductivities of the electrolyte solution and the solvent(s), respectively. α_i is the Riedel coefficient for ion i, and k_0 is calculated by some appropriate correlation or mixing rule for mixed-solvent systems. This equation is accurate for multicomponent systems up to medium concentrations. The Riedel correlation also fails to address the electrolyte systems that exhibit more complicated behavior than the simple linear expression considered in Equation (13.17). A generalized corresponding-states correlation for aqueous binary systems has been proposed by Qureshi et al. [38] using two system-dependent parameters for each binary solution and ten universal parameters. This model is very accurate over a wide range of concentration, pressure, and temperature. Like viscosity models, interactions between solvent-solvent and ion pair–solvent are considered for a mixed-solvent system. One of the key differences with the viscosity model is that the long-range electrostatic interaction term considered in the viscosity model does not have much contribution as derived from the Debye-Hückel-Onsager-Falkenhagen model.

Diffusion Coefficient. Multicomponent diffusion in electrolyte systems plays a key role not only in chemical process technologies but also in a large number of geological systems. For an electrolyte system, diffusivities of both the ions and molecular species need to be calculated. The diffusivities of the molecular species are usually calculated by an appropriate correlation such as that due to Wilke-Chang [39]. If the infinite dilution diffusivity is given by D_0, then considering the relaxation effect in an electrolyte solution, the Nernst-Hartley [40] model gives

$$D = D_0\left[1 + c\frac{d\ln\gamma_\pm}{dc}\right] \tag{13.18}$$

In Equation (13.18), $\gamma_\pm$ is the mean ionic activity coefficient and c is the molar concentration. D_0 can be calculated from the Nernst equation [41],

$$D_0 = \frac{RT}{F^2}\frac{z_+ + z_-}{z_+z_-}\frac{\lambda_+^0\lambda_-^0}{\lambda_+^0 + \lambda_-^0} \tag{13.19}$$

where F is Faraday's constant, z_+ and z_- are the valences of the ions, and λ_+^0 and λ_-^0 are the limiting equivalent conductivity of the cations and anions, respectively. It should be noted that this law is applicable only to simple binary electrolytes in very dilute solutions.

In Equation (13.19), a suitable model is required for calculating $\gamma_\pm$. If the Debye-Hückel model [42] is used, then

$$c\frac{d\ln\gamma_\pm}{dc} = -\frac{z_+z_-e^2\kappa}{16\pi\epsilon_s k_B T(1 + \kappa a)^2} \tag{13.20}$$

where K_B is the Boltzmann constant, a is the mean ionic diameter of the electrolyte, ϵ_s is the permittivity of the solvent, e is the elementary charge, and $1/\kappa$ is the Debye-Hückel length.

$$\kappa = \left(\frac{2Ne^2I}{\epsilon_s k_B T}\right)^{0.5} \tag{13.21}$$

where N is Avogadro's number and I is the ionic strength of the solution. Unfortunately, this formula is inaccurate even at concentrations as low as 0.01 N. In concentrated solutions, an additional term has been proposed by Onsager and Fuoss [36] to account for the electrophoretic effect. This effect occurs when the anions and cations migrating in the same direction face the same frictional resistance per ion. At higher concentration, a multiplicative term is introduced that captures the effect of the change in the viscosity in the ionic mobilities at finite concentration. Using the Stefan-Maxwell equation, this approach is found to be valid up to 4 M concentration [43]. The previous discussion again reiterates that a careful selection of the model for calculating diffusivity is required by considering the concentration of the electrolyte system and the number of solvents.

Surface Tension. For calculating surface tension, Onsager and Samaras [44] derived a limiting law neglecting the contribution from the activity coefficient. Considering one solute, the limiting law can be written as

$$\sigma = \sigma_0 - \frac{Ne^2c_{cc}}{2\epsilon_r}\left[\ln\left(\frac{\kappa e^2}{2\epsilon_r k_B T}\right) - 0.34557\right] \tag{13.22}$$

where σ_0 is the surface tension of the solvent mixture, ϵ_r is the relative permittivity of the solvent, and c_{cc} is the concentration of the solute in mole/cm^3. σ_0 can be calculated using appropriate correlations such as the DIPPR equation [28], an NIST polynomial [45], or by using some mixing rule. For univalent electrolytes, the appropriate relationship can be written as

$$\sigma = \sigma_0 + \frac{79.517c_L}{\epsilon_r}\log_{10}\left(\frac{1.143\times10^{-13}(\epsilon_r T)^3}{c_L}\right) \tag{13.23}$$

where c_L is the concentration of the solute in mole/L.

Although Equation (13.23), the grand-canonical Onsager-Samaras law based on the Gibbs adsorption

isotherm, is very accurate at low concentration (up to about 0.1 M), it underestimates the value of surface tension at higher concentrations. For concentrated solutions, the calculation of surface tension is mainly based on a canonical formalism where the Helmholtz free energy is directly related to the surface tension. For an air-water system, the expression for surface tension takes the following form [46]:

$$\sigma = \sigma_0 + k_B T[\delta \sum n_i + (\sum \vartheta_i^2 n_i)\lambda_B(.0483 + f(\kappa\delta, \epsilon_{rat}))] \qquad (13.24)$$

where δ is the thickness of the ion-free layer below the Gibbs dividing surface, and ϑ_i and n_i are the valence and number density of species i, respectively. λ_B is the Bjerrum length and is given by $\lambda_B = \frac{e^2}{4\pi\epsilon_{wat} k_B T'}$, and $\epsilon_{rat} = \epsilon_{air}/\epsilon_{wat}$, and

$$f(\kappa\delta, \epsilon_{rat}) = \int_0^\infty \ln\left[1 + \left(\frac{1 - \epsilon_{rat}}{1 + \epsilon_{rat}}\right)(\sqrt{1 + t^2} - t)^2 \exp(-2\kappa\delta t)\right] t dt \qquad (13.25)$$

Here ϵ_{air} and ϵ_{wat} are the permittivities of air and water, respectively. This formulation shows that the excess surface tension contains a contribution from the ion-free layer, as shown by the second term in Equation (13.24); the image interaction between the electrolyte ions and the ion-free layer, as shown by the third term; and the image interaction between the electrolyte ions and air, as shown by the fourth term. This model is difficult to implement in a process simulator environment without reasonable approximations. To the best of the authors' knowledge, this formulation is not implemented in any of the leading process simulators. However, it can be implemented in a process simulator as a user model. Discussions of user-added models can be found in Chapter 16, Section 16.2.

13.6.2. Steps Needed to Build the Model of an Aqueous Electrolyte System and the Estimation of Parameters

Multicomponent distillation involving electrolytes is one of the important operations in the chemical process industries. Examples include sour-water strippers, various types of amine-based systems, and alkaline-salt solutions for acid-gas removal. The following discussion concentrates on the simulation of distillation columns involving electrolyte systems. For modeling these systems, not only are the methods and models for the thermodynamic and transport properties important, but also the appropriate unit operation model should be implemented. To obtain a holistic idea of modeling such unit operations, an example of a distillation column will be given and explained. In the example, these property models are used in the overall modeling, and the system of equations that are solved in such systems will be considered. This example will clarify why the thermodynamic and transport models play key roles in the accuracy of the simulation results.

First, a brief review of equilibrium-stage modeling will be given. The equations to be solved are known as the MESH equations [47]. The **M**aterial balance equations are written for the n species that are present in the system. Appropriate aqueous-phase ionic reactions are considered as part of this material balance model. The phase-**E**quilibrium equations depend upon the particular thermodynamic model chosen, as mentioned earlier, and are written for the molecular species. The **S**ummation equations ensure that the mole fractions sum to unity and are written for the liquid and vapor phases. Finally, one ent**H**alpy balance equation is written. It should be noted that if the previous equations are satisfied and the ionic reactions are written properly, the charge balance will be satisfied automatically. Sometimes, for electrolyte systems, an additional constraint due to the charge balance

is imposed. Additionally, pressure drop equations may be considered.

In a nonequilibrium-stage modeling problem, the MERSHQ equations are written [47]. In a nonequilibrium-stage model, the mass transfer through the interface plays a key role. For simplicity, consider a film model for mass transfer. Here, separate **M**aterial balance equations are written for the liquid phase, vapor phase, liquid film, and vapor film. The ionic reactions take place in the liquid phase and usually have very fast kinetics; the reaction terms are usually considered in both the liquid film and the bulk liquid. If additional reactions take place in the vapor phase, those reactions must also be considered. The **E**nergy balance equations are written for the liquid phase, vapor phase, liquid film, and vapor film. At the interface, mass and energy fluxes are considered to be continuous. The transfer **R**ate equations are written for both mass and energy transfer rates. As before, the **S**ummation equations are written to ensure that the mole fractions sum to unity. The **H**ydraulic equations are written for calculating the pressure drop across each stage. The interface e**Q**uilibrium equations are written as the phase equilibrium is shown to exist only at the interface. Readers interested in the modeling and theory of multicomponent distillation columns are referred to the text by Taylor and Krishna [47]. Example 13.8 outlines the procedure involved in simulating a multicomponent distillation column. The problem considers the construction of a distillation column model for an electrolyte system in a process simulator using a rate-based simulation with a film model for mass transfer. Some of the steps are also applicable when simulating other unit operations. A detailed generic discussion of these steps, the parameters required at each stage, and possible sources of these parameters are provided in Appendix 13.2 at the end of this chapter.

Example 13.8.

Develop the model of a sour-water stripper (SWS) as shown in Figure E13.8(a). Consider the following ionic reactions:

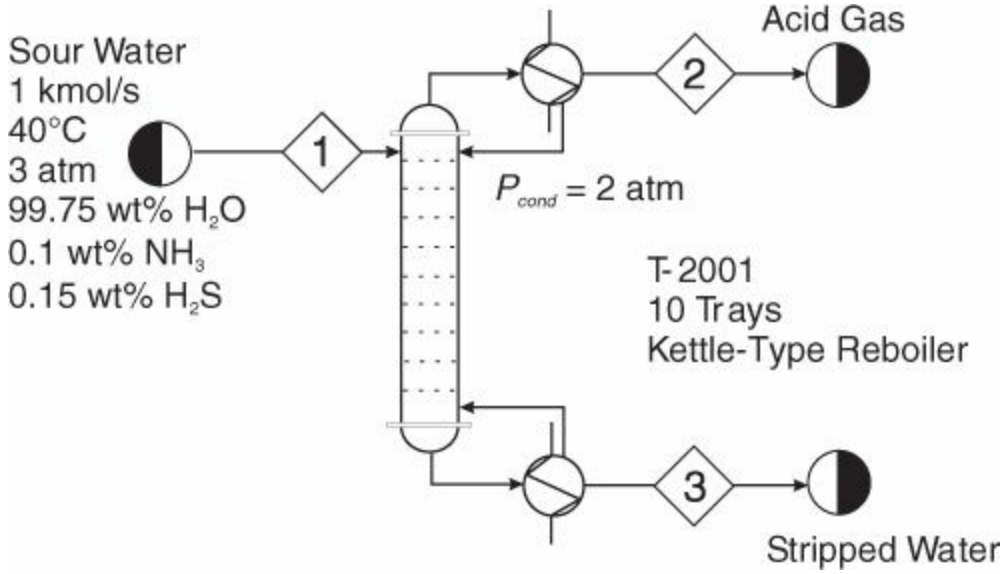


Figure E13.8(a). Schematic of the Sour-Water Stripper (SWS) Column

$$H_2O = H^+ + OH^-$$
$$H_2S = H^+ + HS^-$$
$$HS^- = H^+ + S^{-2}$$
$$NH_3 + H_2O = NH_4^+ + OH^-$$

For this system do the following:

1. Simulate both an equilibrium-stage and a nonequilibrium-stage model and compare the key results such as reflux ratio (RR), reboiler duty, and so on.
2. For comparison, also simulate an equilibrium-stage and a nonequilibrium-stage model without considering the electrolyte chemistry, that is, without the ionic reactions.
3. Develop another nonequilibrium-stage model without considering the fourth reaction.

The desired specification for the separation is that the bottom product should not have more than 30 ppmw NH_3 and 10 ppmw H_2S and the top product should have 25% (mole basis) acid gases (H_2S and CO_2).

Solution

Step 1: Generate the set of linearly independent ionic reactions.

The simulation is set up in Aspen Plus V7.2. It can also be set up in other compatible software platforms. In Aspen Plus V7.2, the "Electrolyte Wizard" can be used to generate a set of possible ionic reactions automatically. The reaction set and the linear independence of the reactions must be checked. In this case, the following equilibrium reactions are generated, the equilibrium constants are estimated by Aspen Plus V7.2, and these are in agreement with the existing literature:

$$H_2O = H^+ + OH^- \quad \ln K_{eq} = 132.89888 - \frac{13{,}445.9}{T} - 22.4773 \ln T$$

$$H_2S = H^+ + HS^- \quad \ln K_{eq} = 214.582443 - \frac{12{,}995.4}{T} - 33.5471 \ln T$$

$$HS^- = H^+ + S^{-2} \quad \ln K_{eq} = -9.741963 - \frac{8585.47}{T}$$

$$NH_3 + H_2O = NH_4^+ + OH^- \quad \ln K_{eq} = -1.256563 - \frac{3335.7}{T} + 1.4971 \ln T - 0.0370566T$$

Here T is in K, the concentration basis is mole fraction, and the reference state for the activity coefficients of ions is chosen to be the aqueous phase at infinite dilution, as mentioned previously. The equilibrium constants are automatically calculated by Aspen Plus V7.2 by using reference-state Gibbs free energies of the reactants and products in a particular reaction. In Aspen Plus, the electrolyte calculations can be done with a "true component" or an "apparent component" approach. In this example, the apparent components are H_2O, NH_3, and H_2S. The true components are H_2O, H^+, OH^-, H_2S, HS^-, S^{-2}, NH_3, and NH_4^+. In this simulation, the "true component approach" is followed by checking the corresponding box under "electrolyte calculation options" available under Data|Setup|Properties|Global. In Aspen Plus V7.2, this option is available in one of the setup steps in the electrolyte wizard.

Step 2: Select the appropriate thermodynamic models and check their parameters.

The electrolyte NRTL ("ElecNRTL" in Aspen Plus V7.2) thermodynamic model is used with a "true component" approach. Note that NH_3 and H_2S are considered to be Henry's Law species. To check the correctness of the thermodynamic model and its parameters, VLE results from the model are compared with the experimental data from Rumpf et al. [48] in Table E13.8(a).

Table E13.8(a). Comparison of the VLE Results from the Simulation with the Experimental Data [48]

Temperature (°C)	Molality		p_{NH_3} (MPa)			p_{H_2S} (MPa)		
	NH_3	H_2S	Exp	Model	% Error (abs)	Exp	Model	% Error (abs)
80	6.004	2.084	0.0619	0.0669	8.08	0.0372	0.0360	3.22
80	6.033	4.647	0.0204	0.0250	22.55	0.4231	0.4460	5.41
120	5.813	2.167	0.1660	0.1890	13.90	0.2362	0.2709	14.70
120	3.210	1.056	0.0984	0.1023	3.96	0.1186	0.1270	7.08

Since NH_3 and H_2S are declared as Henry's Law species, from Equation (13.13) it can be seen that the VLE calculation depends not only upon the activity coefficients calculated by the electrolyte NRTL model but also on the Henry's Law constants of the species NH_3 and H_2S. In Table E13.8(a), it is observed that the VLE results from the simulation are reasonable when compared to the experimental data. Therefore, the default parameters in Aspen Plus for the electrolyte NRTL model and Henry's Law constants are acceptable and need not be modified. The standard-state heat capacity parameters and the density parameters are not modified since the electrolyte solution is very dilute and it is a weak electrolyte system. So, the standard-state heat capacity and density are not expected to be much different from those of pure water.

Step 3: Select the appropriate transport models and check the parameters.

The default transport models for viscosity, surface tension, thermal conductivity, and diffusivity for the chosen property method are the Jones-Dole model (Equation [13.16]), Onsager-Samaras model (modified Equation [13.22]), Riedel model (Equation [13.17]), and Nernst-Hartley model (Equation [13.18]), respectively. These models with their default settings (option codes in Aspen Plus) and parameters are used because the electrolyte system considered here is very dilute, and these properties are not expected to differ much from those of pure water. For comparison, the surface tension of Stream 1 is compared with the surface tension of pure water and the literature data [49] in Figure E13.8(b).

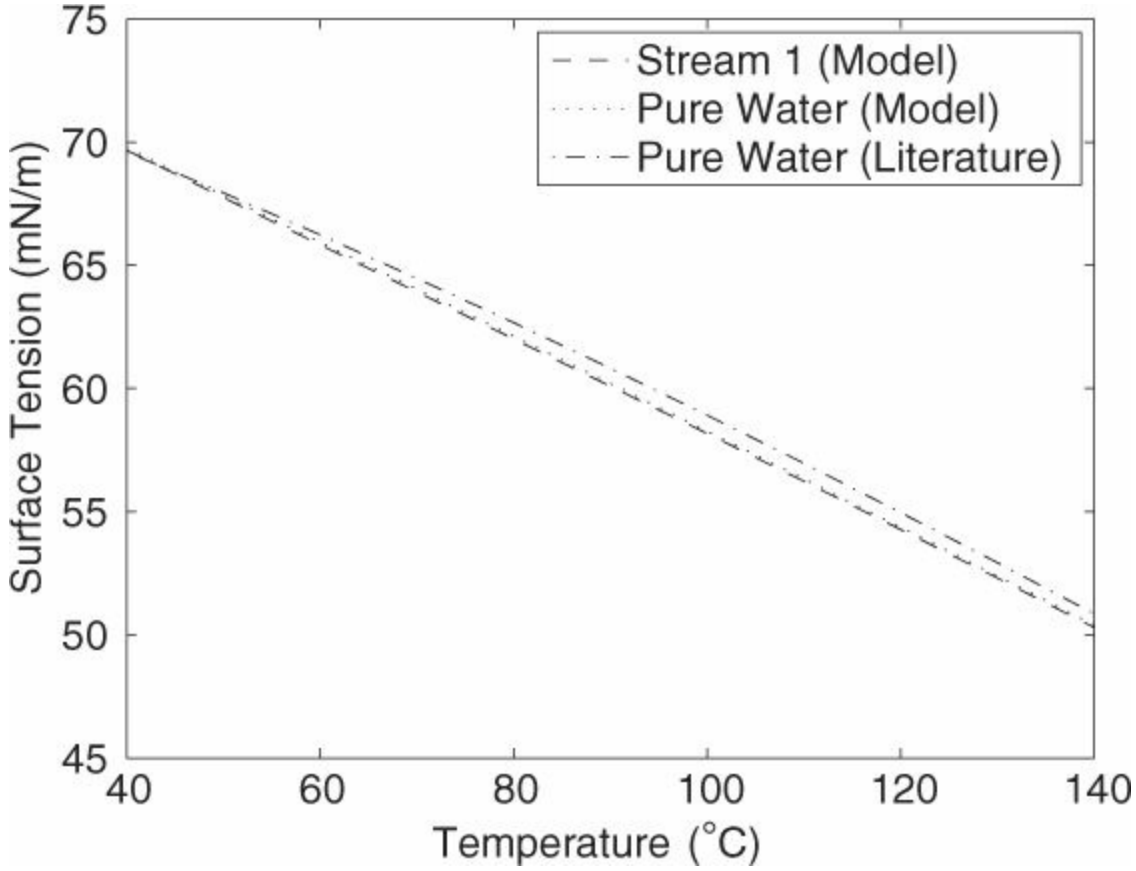


Figure E13.8(b). Surface Tension of Stream 1 and Pure Water from the Aspen Plus Model and Surface Tension of Pure Water from the Literature [49]

Step 4: Set up the distillation column.

First, the equilibrium-stage model is set up by using a "RadFrac" block in Aspen Plus V7.2. The column has 12 stages (including the reboiler and the condenser), the condenser is "partial-vapor," and the reboiler is "kettle" type. The column condenser pressure is 2 atm (abs), and the pressure drop per stage is 0.007 bar. Stream 1 is specified as given in the problem data and connected to stage 2. Streams 2 and 3 are connected to the condenser and bottom outlets, respectively. Tray sizing is done using single-pass Glitsch ballast-type trays, with the fractional approach to flooding being 0.8. First, a solution is obtained considering a reflux ratio of 2 (mole basis) and bottoms-to-feed ratio (mole basis) of 0.95. At this step, the product specifications are not satisfied, but this step is crucial to take care of any convergence problems and for generating the initial guess for subsequent solutions. The convergence is obtained by using the default "standard" algorithm (an inside-out algorithm) in Aspen Plus. As the H_2S specification in the bottom stream can be easily satisfied when the NH_3 specification is satisfied, two design specifications are now written to satisfy the product specifications. For maintaining the NH_3 specification in Stream 2, its value should be available in the stream results. However, this specification is on an apparent component basis, but this simulation is carried out with the "true component" approach. To calculate the apparent NH_3 composition (mass basis) in Stream 2, a user "property set" is set up under Data|Set up|Properties|Prop-Sets. The property name in Aspen Plus is "WXAPP" and is to be calculated for the component NH_3. Two "design specs" are written. The first one is to maintain the H_2O content in Stream 2 at 75% (mole). The second one is to maintain the NH_3 specification in Stream 3. For this, the "design specification type" under "specifications" is selected as "property value," and under the "property set," the user property set is selected. Two "vary" blocks are created. The "adjusted variables" are "bottoms to

feed ratio" and "reflux ratio." The results are shown in Table E13.8(b).

Table E13.8(b). Comparison of the Key Results from the Equilibrium-Stage Models (with and without Reactions) and the Nonequilibrium-Stage Models

	Equilibrium-Stage Model		Nonequilibrium-Stage Model		
	No Reaction	With Reaction	No Reaction	Fourth Reaction Off	With Reaction
RR (Mole)	0.52	1.60	3.94	3.94	6.82
Reboiler Duty (GJ/h)	23.77	25.01	27.50	27.50	30.65
Condenser Duty (GJ/h)	0.55	1.7	4.17	4.17	7.23
Tray Diameter (m)	1.36	1.39	1.44	1.44	1.51
Bottom Temp (°C)	121.83	121.83	122.21	122.21	122.21
Bottom Pressure (atma)	2.07	2.07	2.10	2.10	2.10
H_2S in Bottom (ppmw)	0	1	Trace	Trace	1.80

In the next step, the equilibrium model without the electrolyte chemistry is considered. Note that under this condition, only physical equilibrium is considered. The same thermodynamic model "ElecNRTL" is used, but the electrolyte NRTL model becomes the well-known NRTL model in the absence of ions. The key results are shown in Table E13.8(b).

The nonequilibrium-stage model with the electrolyte chemistry can simply be generated by copying the equilibrium-stage model with the electrolyte chemistry and then modifying it. Under "setup" options in the "configuration" menu, the "calculation type" is specified as "rate-based."

Here, the condenser pressure is specified, but the pressure drop per tray is removed since it will be calculated. Under "reactions," the electrolyte chemistry is considered in all the stages. Tray specifications are provided under "tray rating." The following specifications are used: Glitsch ballast tray with weir height of 46.55 mm; the number of valves per unit of active area is set to 139.92/m^2. Under "design/Pdrop" in the "setup" menu, the box for "update section pressure profile" is checked and the option for "fix pressure at" is selected as "top." The box for "rate-based calculations" is checked under "rate-based." Diffusion resistance in both the liquid and vapor films is considered. Because of the rapid ionic reactions, the reactions are also considered in the liquid film. The film is discretized by selecting the option "discrxn" under Tray Rating|Rate-based|Rate based|Film resistance|Liquid phase. For determination of mass transfer coefficients, heat transfer coefficients, and interfacial area, the correlations by Gerster et al. [50], Chilton and Colburn [51], and Scheffe and Weiland [52], respectively, are selected under Tray Rating|Rate-based|Correlations. The box for "design mode to calculate column diameter" under Tray Rating|Rate-based|Design is checked. The remaining settings are the default values in Aspen Plus V7.2. Again, the design specifications are written after an initial solution is obtained. The differences in the specifications/results are shown in Table E13.8(b). In addition, two other simulations are considered, both using the nonequilibrium-stage model. In the first example, all the reactions are turned off. In the second, only the fourth

reaction is turned off. The solution is obtained using the default settings for the solver. Aspen Plus V7.2 solves the rate-based distillation problem using Newton's method with the solution from the equilibrium-based mode as the initial guess.

In Table E13.8(b), it can be seen that considerable differences exist between the reflux ratios (RR) and condenser duties for all three models. If the nonequilibrium-stage model with all the reactions is considered to be a correct model for the system, then its condenser duty is 4.3 and 13.3 times greater than the equilibrium-stage model with and without reactions, respectively. On the other hand, the results from all three nonequilibrium models show that if the fourth reaction is not considered, the results are similar to the no-reaction case. Even though the electrolyte chemistry is automatically generated in many process simulators when a particular thermodynamic model is chosen, this example demonstrates that the user needs to be vigilant to ensure that all the important reactions are considered. It can be seen in Table E13.8(b) that the H_2S concentration in the column bottom stream is well below the required limit of 10 ppmw for all the simulations.

In Example 13.8, the default parameters for the thermodynamic and transport models were used. Because the sour-water system has been well studied for many years and the system is very dilute, the default parameters from Aspen Plus V7.2 are representative. However, for electrolyte systems, where the simulator databank parameters are not available or not representative, the parameters must be regressed, as shown in Example 13.5. More discussion on parameter estimation can be found in Chapter 16, Section 16.5.

13.7. Solids Modeling

Solids handling is abundant in the process industries. Starting from the fluidized catalytic cracking (FCC) unit in a petroleum refinery to the modern power plant using coal, various unit operations involve the handling of solids. Solids may significantly affect mass, momentum, and energy balances in a chemical system even if the solid is inert. In addition, the particle-size distribution of the solid can affect the operation of solid handling equipment such as cyclone separators, crushers and grinders, and crystallizers. Hence, for simulating these processes accurately, the fundamentals of solids modeling must be understood.

13.7.1. Physical Properties

Sections 13.2 and 13.4 provided a detailed account of the importance of selecting the appropriate physical property methods and models. Solids modeling is no exception to this approach. The systems involving solids can be composed of various well-defined solids (such as SiO_2, Fe_2O_3, etc.) or solids that themselves are heterogeneous mixtures of complex materials (such as coal or biomass). In addition, various polymorphs may be present. Polymorphs are different crystalline or amorphous forms of the same solid in which molecules have different arrangements and/or different molecular conformation. The polymorphs usually differ in their dissolution rate, melting temperature, reactivity, sublimation temperature, and other attributes. The properties of the solids depend not only upon their composition but also on their structure which is almost impossible to characterize in a process simulator. Therefore, many solids that are frequently encountered in the process industries are not available in simulator databanks. Quite often, the user has to declare the solids as a user-defined species, where the needed physical property data are provided. In addition, the thermodynamic and transport calculations that are important for modeling a particular system must be identified. The

following discussion considers only systems consisting of nonelectrolyte solids. Systems consisting of electrolyte solids (salts) should be treated as mentioned in Section 13.6.

There are some process operations (such as crystallization) and many metallurgical processes where solid-liquid equilibrium (SLE) is important. In many process simulators, no models exist for calculating SLE. However, in some process simulators, an empirical or semi-empirical approach is available for calculating the SLE. The condition for SLE is

$$\hat{f}_i^l = \hat{f}_i^s \tag{13.26}$$

where $\hat{f}_i^l$ and $\hat{f}_i^s$ are the fugacity of component i in the liquid and solid phases, respectively.

In terms of activity coefficients, Equation 13.26 can be written as

$$x_i \gamma_i^l = z_i \gamma_i^s \psi_i \tag{13.27}$$

where $\ln \psi_i = \int_{T_{m_i}}^{T} \frac{H_i^l - H_i^s}{RT^2} dT$, z_i is the solid mole fraction, and T_{mi} is the melting temperature of pure species i. Further simplification of the fugacity-coefficient integral can be made in terms of heat of fusion and heat-capacity change of melting.

For calculating γ_i^l, a suitable activity-coefficient model is used for the liquid phase. For calculating γ_i^s, a correlation (such as the Margules equation, Redlich/Kister expansion, Wilson equation, van't Hoff equation, etc.) or some polynomial equation for the activity-coefficient model is used. It should be noted that the van't Hoff equation is usually applied to systems where the solid- and liquid-phase species are chemically and structurally similar and, therefore, can be considered to have formed a near-ideal solid solution.

For a multicomponent system, the Margules equation is given by [53]

$$\ln \gamma_i^s = \sum_{k \neq i} z_k [A_{ki} + B_{ki}(z_k - 2z_i)] - \sum_{k<j} \sum z_k z_j [A_{kj} + 2B_{kj}(x_k - x_j)] \tag{13.28}$$

However, when strong specific interactions such as hydrogen bonding, dimerization, or association exist among some of the constituent molecules, the Margules equation often fails.

There are also a number of systems where solid-vapor equilibrium (SVE) or solid-liquid-vapor equilibrium is important. A sublimation curve may be constructed that represents the SVE on a P-T diagram for pure species. One of the important examples of SVE, being widely studied now, is the formation of gas hydrates or clathrate hydrates. For SVE,

$$\hat{f}_i^v = \hat{f}_i^s \tag{13.29}$$

In terms of activity coefficients,

$$y_i \hat{\phi}_i^v P = z_i \gamma_i^s f_i^s \tag{13.30}$$

In terms of the Poynting correction factor,

$$f_i^s = \phi_i^* P_i^* \exp \frac{v_i^s (P - P_i^*)}{RT} \tag{13.31}$$

where v_i^s is the molar volume of the solid for the pure species i. v_i^s is usually calculated by a polynomial function of temperature, ϕ_i^* and ϕ_i^* can be readily calculated from an equation-of-state model, γ_i^s and is calculated as before. Once γ_i^s is calculated, the excess Gibbs energy for the solid phase can be calculated by

$$\frac{G^{E,s}}{RT} = \sum_i z_i \ln \gamma_i^s \qquad (13.32)$$

This expression can then be used for methods that use Gibbs energy minimization techniques for equilibrium calculations. Other excess terms can then be calculated using Equations (13.7) through (13.10), as shown in the previous section. For certain chemical processes, the calculation of excess enthalpy is very important and should be checked by regressing with published data.

Similar to electrolyte systems, the standard-state properties can also be calculated by a similar approach. For example, if the standard-state heat capacity ($\overline{C}_p^0$) is known, the standard-state enthalpy, entropy, Gibbs energy, and molar volume can be calculated from similar equations as before.

The standard-state heat capacities can be simply expressed by a polynomial. Pure-component solid heat capacities can be expressed by the suitable DIPPR equations [28], by some polynomial function of temperature, or other standard sources for thermodynamic models and their parameters for pure species [45, 54].

There are some important process applications involving solids that are difficult to characterize in terms of their constituent species. Examples include various types of coal, pet cokes, biomass, and other naturally occurring materials. Common processes that involve these solids include combustion, gasification, and reactions involving metal oxides (such as in many chemical looping processes and ore-smelting processes). For such processes, the calculation of enthalpy and density (molar volume) plays a key role. These are usually calculated either from correlations or polynomials. Such formulations are heavily parameterized, and a reasonable estimate of these parameters is needed. Substantial information exists in the open literature that can be used to determine these parameters. The applicability of the form of the model for the solids involved must be checked, and then an estimate of the parameters must be made using regression tools, which are usually available in the process simulator. Parameter estimation using regression tools in a process simulator is discussed in Chapter 16, Section 16.5.

Diffusion in solids systems cannot be modeled in most commercial process simulators. Thermal conductivity of pure solids is often modeled with a polynomial in temperature or using some other correlation. The mixture thermal conductivity is modeled with a mole- or mass-weighted average or by using a simple mixing rule.

13.7.2. Parameter Requirements for Solids Model

Parameter requirements depend largely upon the system that is being modeled. For example, for a solids combustion system, the enthalpy calculation and the associated parameters must be correct. On the other hand, if a crystallization system is being modeled, the parameter requirements for the SLE calculation must be evaluated carefully. A set of guidelines for choosing the appropriate models and parameters for solids modeling is given:

1. If the Margules equation is used for calculating the activity coefficients of the species in the solid phase, the A and B parameters are required. These parameters are not composition or pressure dependent, but they are dependent on temperature. Experimental SLE data at different temperatures are needed to determine their temperature dependency. Quite often, these parameters vary with $1/T$.
2. For calculating the fugacity coefficient in the gas phase, interaction parameters may be needed based on the EOS used. Even though these parameters are available in process simulator

databanks for a large number of gaseous species, they may not be available for many species that are solid at room temperature. The presence of heterogeneous solids with complex structures will further complicate the situation. These parameters must be determined by regression of experimental data.

3. As mentioned before, most of the thermodynamic and transport models are empirical for solids systems. The applicability of a model for a particular system should be verified. This can be done by reviewing the existing literature and comparing the model predictions with experimental data in the operating region of interest. If the model parameters are already available in the databank, then the requirement of additional parameters should be checked along with any required modification to the existing parameters. The parameter requirements will depend on the model chosen. The polynomial models, frequently used in solids modeling, are usually linear-in-parameter (LIP) models. Therefore, a least-squares estimate can be obtained easily, even without using the process simulator.

Example 13.9.

p-Xylene is commercially separated from a mixture of xylenes in a crystallizer, because its freezing point is much higher than that of its other isomers [55]. The feed is first cooled and then sent to a scraped-surface heat exchanger. Since the wall of this heat exchanger is at a very low temperature, the crystals are formed on the wall. These crystals are then removed by scraping with a spring-loaded blade. Two stages are used to increase the product purity. For modeling purposes, only one stage of this process will be considered in this example. This first stage will be modeled as a chiller, E-2001, followed by a crystallizer, CR-2001, as shown in Figure E13.9(a).

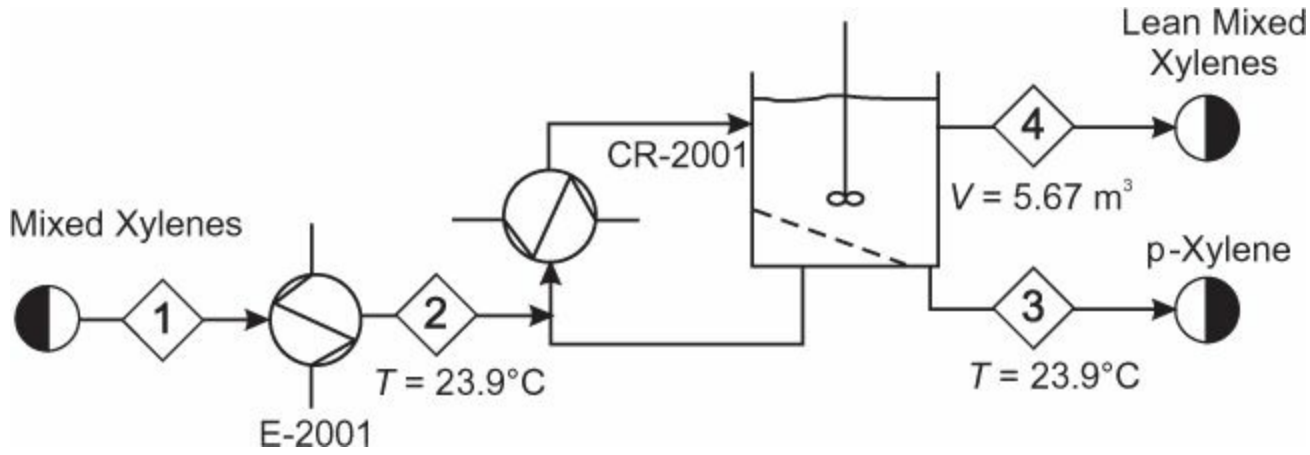


Figure E13.9(a). Flowsheet of the p-Xylene Crystallizer

Conditions of Stream 1 in Figure E13.9(a) are as follows:

Temperature (°C)	23.9
Pressure (bar)	1.38
Flowrate (m^3/h)	16.99
Composition (wt%)	
p-Xylene	15.8
m-Xylene	39.6
o-Xylene	20.0
Ethylbenzene	18.6
Toluene	6.0

For simplicity, consider that no recirculation occurs in the crystallizer. The crystal growth rate is given by

$$R_{CG} = 3.05 \times 10^{-8}\, S^{0.2} \text{ m/s}$$

where

$$S = \text{Supersaturation Ratio} = \frac{X_S - X_{S,eq}}{X_{S,eq}}$$

X_s is the mole fraction of solute in the liquid, and $X_{s,eq}$ is the mole fraction of solute in the liquid at crystallization temperature. The nucleation rate is given by

$$R_N = 8 \times 10^{13}\, S \text{ number of crystals nucleated/hr/ft}^3$$

Simulate this system and find out the mole fraction of p-xylene in the solvent in Stream 4, the flowrate of solid p-xylene leaving the crystallizer (flowrate of Stream 3), and the supersaturation ratio of Stream 4.

Solution

This system is simulated in PRO/II 8.3. All the species are selected from the SIMSCI databank. For the SLE, the van't Hoff equation is used. The melting temperature of the species present and the heat of fusion required for the van't Hoff equation are used from the SIMSCI databank. The solubility of p-xylene calculated by PRO/II matches very well with the experimental data [55], as shown in Figure E13.9(b). Therefore, no changes to the existing PRO/II parameters are necessary for the SLE calculation.

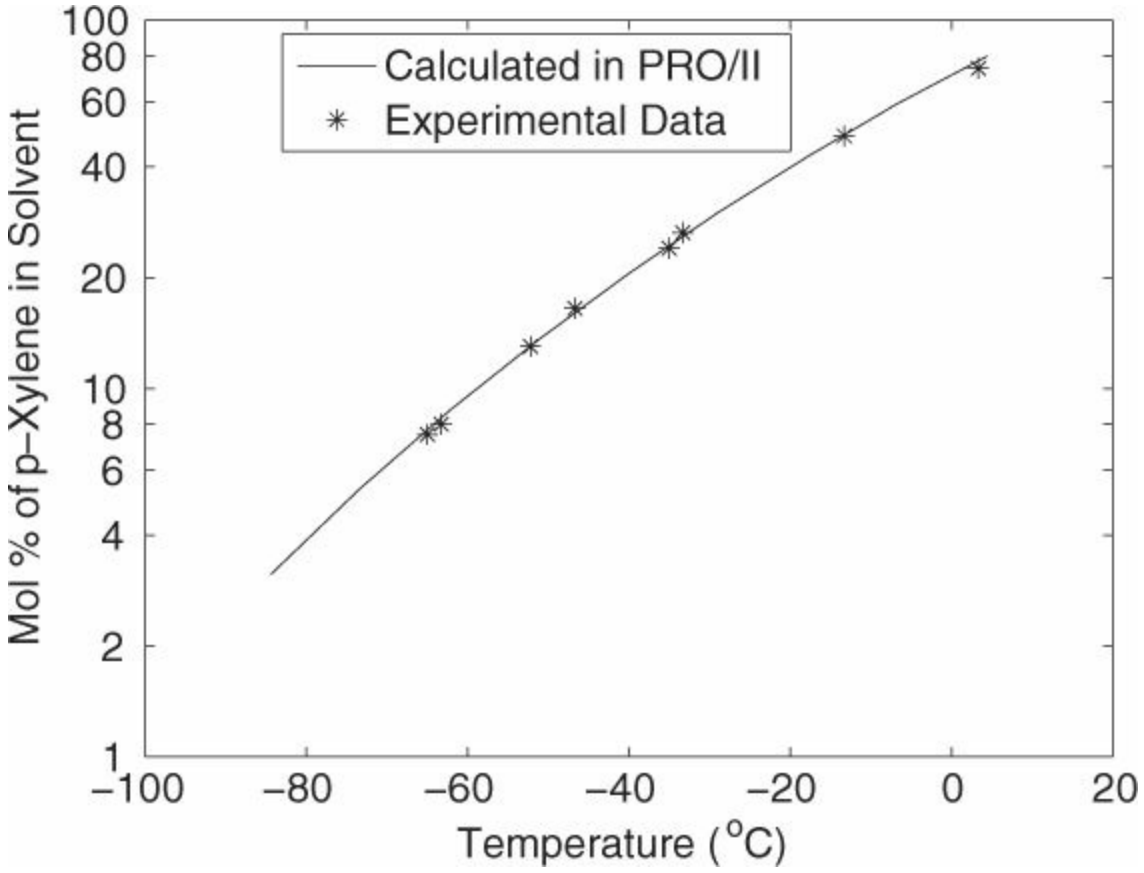


Figure E13.9(b). Comparison of p-Xylene Solubility between Experimental Data [56] and Calculated in PRO/II

Due to the very low temperature of operation and the species in the feed, no vapor phase exists. Therefore, the selection of thermodynamic model for VLE is immaterial. The enthalpy and density calculations are based on generalized correlations available under "library" methods in PRO/II, where the pure species properties are retrieved from the SIMSCI databank. The mole fraction of p-

xylene in the solvent in Stream 4 is 0.0607, the flowrate of p-xylene from the crystallizer (flowrate of Stream 3) is 14.37 kmol/h, and the supersaturation ratio of Stream 4 is 5.98×10^{-3}.

What You Should Have Learned

- The typical order for developing a process simulation is as follows:
  - Select a system of units (such as SI).
  - Choose the components.
  - Choose a thermodynamics package.
    - This must be done carefully.
    - The best package is the one that is confirmed experimentally.
    - A thermodynamics package cannot be chosen just because it gives the desired results or simplifies the simulation.
  - Construct the process by connecting unit operations.
  - Input the feed stream parameters.
  - Input the unit operation specifications.
  - Run the simulation.
- For choosing appropriate thermodynamic and transport models for electrolyte systems, the key considerations are the type of system (aqueous versus nonaqueous), what solvents and solutes are present and at what concentration, and the operating temperature.
- Quite often, the user has to provide the appropriate physical properties data for solids modeling in the commercial simulators.
- Requirement of parameters for solids modeling largely depends upon the system that is being modeled.

Appendix 13.1. Calculation of Excess Gibbs Energy for Electrolyte Systems

Before discussing the equations for calculating Gibbs free energy, it should be noted that any partial molar property can be written as a departure of that property from the standard state

$$\overline{M} = \overline{M}^0 + \overline{M}^E \qquad (13.33)$$

where $\overline{M}^0$ and $\overline{M}^E$ represent the standard-state and excess properties, respectively. Even though the standard state can be considered to be any defined state, usually a 1 M solution of the species extrapolated to infinite dilution is considered to be the standard state for aqueous electrolyte systems. Therefore, this state is usually called an infinite dilution state. For convenience, the aqueous activity coefficient of a dissolved species is usually defined with an asymmetric convention. With this convention, the activity coefficient approaches unity as the concentration approaches zero.

The molar Gibbs free energy of an electrolyte system can be expressed as

$$G_{mix} = x_w \mu_{c,w} + \sum_i x_i \mu_{c,i}^{\infty} + RT \sum_j x_j \ln x_j + RT \sum_k x_k \ln \gamma_k \qquad (13.34)$$

In Equation (13.34), the last term represents the excess Gibbs free energy, $\mu_{c,\omega}$ is the chemical potential of pure water, $\mu_{c,i}^{\infty}$ is the aqueous infinite dilution chemical potential, and the third term on the right-hand side captures the behavior of the species j in an ideal solution. It should be noted that

$\mu_{c,i}^{\infty}$ naturally appears because of the choice of the standard state. Additional terms must be added to the equation if nonaqueous solvents are also present.

If the excess Gibbs energy is represented in terms of activity coefficients, as in Equation (13.34), the nonideal contribution becomes a strong function of the model that is chosen for the activity coefficients. The activity coefficients for the electrolyte systems are expressed as a combination of long-range and short-range contribution terms. The long-range contribution represents the interaction in a dilute solution where the solutes are far apart. This term is usually represented by a Debye-Hückel term or a modified Debye-Hückel term. The short-range term is usually represented by summing up the interactions mainly between ion-ion, ion-molecule, and molecule-molecule pairs in a concentrated solution where the solute species are close to each other. Even though a number of formulations are available for calculating the activity coefficients, it is not possible to provide a detailed account of all the models here because of space limitations. However, based on popularity and implementation in commercial process simulators, the work of Pitzer and Chen will be presented here [14, 17, 20]. In most of these models, the excess Gibbs energy is written as

$$G^{ex} = G_{LF}^{ex} + G_{SF}^{ex} \tag{13.35}$$

where G_{LF}^{ex} and G_{SF}^{ex} represent the contribution due to the long-range and short-range forces, respectively. Various expressions are available for capturing the contributions of these forces. The models usually vary because of the different expressions used for capturing these forces. The activity coefficient can be obtained from the excess Gibbs energy from the chosen thermodynamic model. The modified Pitzer equation for excess Gibbs energy of strong aqueous electrolyte system is [17]

$$\frac{G^{ex}}{n_w RT} = f + \sum_c \sum_{c'} m_c m_{c'} \left(\theta_{cc'} + \sum_a m_a \psi_{cc'a} \right) + \sum_a \sum_{a'} m_a m_{a'} \left(\theta_{aa'} + \sum_c m_c \psi_{aa'c} \right) + 2 \sum_c \sum_a m_c m_a \left[B_{ca} + \frac{\sum_c m_c Z_c}{\sqrt{Z_c Z_a}} C_{ca} \right] \tag{13.36}$$

The first term captures the effect of the long-range Coulomb forces. The remaining terms are used to capture the effect of the short-range forces. In Equation (13.36), subscripts c and c', a and a' stand for cations and anions, respectively. Z is the absolute value of the ionic charge, n_ω is the mass of solvent water in kg, and m_j represents molality of any solute j. B and θ are binary-interaction terms, and C and ψ represent ternary-interaction terms. The cation-anion interaction parameters B and C are characteristic of single aqueous electrolyte systems, with parameter C being important only at high concentrations. The parameters θ and ψ account for the difference of interaction of the unlike ions of the same sign from the average of the like ions and are characteristics of each aqueous mixed-electrolyte system. f is considered to be a function of the ionic strength. Following Debye-Hückel [42],

$$f = -A_\phi (4I_x/b) \ln(1 + b\sqrt{I_x}) \tag{13.37}$$

where b is a parameter, the optimal value of which is found to be 1.2, and I_x is the ionic strength on a mole fraction basis, where

$$I_x = \frac{1}{2} \sum_i m_i z_i^2 \tag{13.38}$$

A_ϕ is the Debye-Hückel constant and is given by

$$A_\phi = \frac{1}{3}\left(\frac{2\pi N d_s}{1000}\right)^{0.5} \frac{e^3}{(\epsilon_r k_B T)^{1.5}} \tag{13.39}$$

where d_s is average solvent density.

As such, the modified Pitzer model does not consider the contribution of the molecular solutes, which is typical for many industrial processes where molecular nonelectrolytes and weak electrolytes are present. These limitations are addressed in the electrolyte-NRTL model [17, 20]. This model captures the short-range interactions similar to the NRTL (nonrandom two-liquid) model. The long-range, ion-ion contributions are captured by the Pitzer-Debye-Hückel model in much the same way as is done in the modified Pitzer equation. This model considers additional terms due to molecule-ion and molecule-molecule interactions and is, therefore, appropriate for weak electrolyte systems. For a multicomponent system, the contribution of the short-range forces due to the excess Gibbs energy is given by the electrolyte-NRTL model as

$$\frac{G^{ex}_{SF}}{RT} = \sum_m X_m \frac{\sum_j X_j G_{jm}\tau_{jm}}{\sum_k X_k G_{km}} + \sum_c X_c \sum_{a'} \frac{X_{a'}}{\sum_{a''} X_{a''}} \frac{\sum_j X_j G_{jc,a'c}\tau_{jc,a'c}}{\sum_k X_k G_{kc,a'c}} + \sum_a X_a \sum_{c'} \frac{X_{c'}}{\sum_{c'} X_{c'}} \frac{\sum_j X_j G_{ja,c'a}\tau_{ja,c'a}}{\sum_k X_k G_{ka,c'a}} \tag{13.40}$$

where subscripts *m, c* and *c′*, and *a* and *a′* stand for molecular species, cations, and anions, respectively. Subscripts *j* and *k* denote any species.

In Equation (13.40),

$X_j = x_j L_j$ where $L_j = Z_j$ for ions and unity for molecular species

$G_{ji} = \exp(-\alpha_{ji}\tau_{ji})$

$G_{ji,ki} = \exp(-\alpha_{ji,ki}\tau_{ji,ki})$

α and τ are NRTL nonrandomness and binary-interaction energy parameters, respectively, and *x* denotes the true liquid-phase mole fraction considering all species. This model is used for both aqueous and mixed-solvent multicomponent electrolyte systems over a wide range of concentrations and temperatures.

Appendix 13.2. Steps to Build a Model of a Distillation Column for an Electrolyte System Using a Rate-Based Simulation with a Film Model for Mass Transfer, the Parameters Required at Each Stage, and Possible Sources of These Parameters

Step 1: Generate the set of linearly independent ionic reactions.

The usual steps for the initial simulator setup for the operating conditions, units of measurement (UOM), and so on, are completed for all the molecular species in the system. In the initial step, it is crucial that all possible ionic reactions be considered. For many process simulators, these reactions are automatically generated. If not, the usual source for obtaining such a reaction set is research

literature. Even though a reaction set is automatically generated by the process simulator, it is a good idea to review it and modify it, if needed, based on previous studies reported in the literature.

The equilibrium constants for the ionic reactions are now considered. Usually these constants are automatically calculated by the simulator based on Gibbs energy change or are obtained from some existing databank. If needed, these values may be changed, based on results in the existing research literature. For the kinetic reactions, usually the pre-exponential factor, activation energy, and exponents on reactions and products must be provided.

At the end of this step, all the species present in the system are generated. If some of the ionic species and their required pure-component properties are not available in the existing simulator databank, then these species must be created and the required pure-component data provided. As discussed in the following paragraphs, the requirement of the pure-component-properties data depends upon the choice of the thermodynamic and transport property models.

Step 2: Select the appropriate thermodynamic models and verify their parameters.

The second important step is the selection of the thermodynamic models. The models should be appropriate for the type of system being modeled. As mentioned, the key property to calculate is the Gibbs free energy of the electrolyte system. Once the model is chosen, the required parameters can be determined by using the data regression system usually available in most process simulators. For example, in the electrolyte NRTL model, the model binary parameters are the nonrandomness factors $\alpha_{ca,m}$, $\alpha_{ca,ca'}$, $\alpha_{ca,c'a}$, and $\alpha_{mm'}$ and the energy parameters $\tau_{ca,m}$, $\tau_{m,ca}$, $\tau_{ca,ca'}$, $\tau_{ca',\ ca}$, $\tau_{ca,c'\ a}$, $\tau_{c'\ a,ca}$, $\tau_{mm'}$, and $\tau_{m'\ m}$. Applying this model to a propanol-water-NaCl system, the binary parameters are $\alpha_{water\text{-}propanol}$, $\alpha_{NaCl\text{-}water}$, $\alpha_{NaCl\text{-}propanol}$, $\tau_{NaCl\text{-}water}$, $\tau_{water\text{-}NaCl}$, $\tau_{NaCl\text{-}propanol}$, $\tau_{propanol\text{-}NaCl}$, $\tau_{water\text{-}propanol}$, and $\tau_{propanol\text{-}water}$. For the system mentioned above, the parameters $\alpha_{water\text{-}propanol}$, $\tau_{water\text{-}propanol}$, and $\tau_{propanol\text{-}water}$ can be regressed with LLE data for the propanol-water system. Since data for this aqueous electrolyte systems are abundant, the parameters $\alpha_{NaCl\text{-}water}$, $\tau_{NaCl\text{-}water}$, and $\tau_{water\text{-}NaCl}$ can be regressed with data from the NaCl-water system. The remaining three parameters can be found by regression using the mixed-solvent system. Use of the data regression tool in a process simulator environment was discussed earlier in this chapter and will be later in Chapter 16, Section 16.5. Quite often, only the excess properties are calculated from the excess Gibbs energy, while the standard-state properties are calculated from other thermodynamic properties, such as standard-state heat capacities.

For species that are only slightly soluble, Henry's Law is often used. The Henry's constant for at least the key components and solvents must be specified. For a mixed-solvent system, Henry's Law data are needed for each solvent-species pair. For example, if a system contains two solvents X and Y and two Henry species CO_2 and H_2S, Henry's parameter should be supplied for X-CO_2, X-H_2S, Y-CO_2, and Y-H_2S. These parameters can be readily calculated from the experimental binary VLE data of the corresponding systems or obtained from handbooks, such as Perry's handbook [57].

As mentioned before, the standard-state heat capacity may be used for calculating other standard-state properties. If it is calculated from heat capacity polynomials, then the coefficients for such polynomials must be available for all the solvents, the molecular solutes, and the ionic species. In a process simulator, these data are usually available for a large number of molecular solutes and solvents. If the heat capacity is missing for some ionic species, it can be calculated using the Criss-

Cobble [26] correlation, as mentioned previously. Next the values for $A_i(T)$, $B_i(T)$, and $\overline{S}^0_{i,25}$ are needed. A large database for heat capacity polynomials or for the Criss-Cobble parameters is available in the open literature [26, 58]. These parameters are usually determined from calorimetric data by considering heats of solution. Data are available for temperatures up to 200°C. Criss and Cobble suggested a simple extrapolation of the entropy parameters beyond 200°C. The validity of such extrapolation needs to be checked on an individual basis. The good news is that most of the common chemical engineering applications with electrolyte systems have operating temperatures below 200°C.

For calculating the molar volume/density, the required parameters should be available and must be appropriate. For example, if the Redlich-Meyer correlation is used for molar volume of the electrolytes, then the values for V^{∞}_{el}, A_1, and A_2 are required for all the electrolytes present in the system along with the parameters required for calculating molar volume of water and all other solvents. These parameters can be determined by experimental density data of the appropriate systems. For a mixed-solvent system, appropriate parameters are needed for the correlation/mixing law used to calculate the value of υ_s in Equation (13.12).

Step 3: Select appropriate transport models and verify their parameters.

For some unit operation and equipment models, the transport model may not play any role at all. Usually, this is the result of a simplified model or a simplifying assumption about the transport of the species. For example, if an equilibrium-stage model is developed and the pressure drop is provided by the user, the transport model is probably not used. Sometimes the transport properties are calculated by the simulator for use in the sizing routines.

The viscosity model should be chosen based on the process application. In most viscosity models, in the absence of electrolytes, the viscosity of the pure-solvent/mixed-solvent, μ_0, is calculated by an appropriate model. There can be parameter requirements for this model. In addition, model parameters are needed for the correction term. For example, if the Jones-Dole model is chosen for the propanol-water-NaCl system discussed before, the Jones-Dole parameters A and B are needed for the electrolyte NaCl in this mixed-solvent system. Quite often, the coefficients A and B are expressed by some other correlation. In that case, the corresponding parameters are needed. These parameters are usually determined by regressing with experimental viscosity data of binary/ternary systems.

For calculation of the surface tension, if the Onsager-Samaras law is applicable, model parameters will be needed for the appropriate model for calculating σ_0 of the pure solvent/solvent mixture. Equation (13.22) is written for a single solute, and for a multicomponent system, an appropriate mixing law can be used. The dielectric constant of the solvent mixture should be calculated with an appropriate law. The correlation for the dielectric constant can have parameters for its temperature dependency. These parameters can be found from experimental data of the solvent mixture and its dielectric properties.

For thermal conductivity, an appropriate model is selected based on the concentration and the particular system being modeled. If the Riedel correlation is used, the Riedel coefficient α_i should be known at least for the major species in the solution. These coefficients can be found by regressing with experimental thermal conductivity data.

For calculating diffusivity, an appropriate model should be chosen considering the concentration of the electrolyte system and the number of solvents as mentioned before. If the Nernst-Hartley model is

used, parameter a is needed. Usually, the parameters for diffusivity models are regressed with tracer diffusion data.

Step 4: Set up the distillation column simulation.

The appropriate distillation column block is inserted in the simulator, the number of trays is specified (which can be optimized later), the feed(s) is connected, and the feed composition(s) is provided. The feed location(s) is specified, and other column specifications such as pressure, existence of reboiler/condenser, and so forth, are provided. The decision about the appropriate operating pressure is included in the standard textbooks on distillation column design and will not be discussed here. However, the bubble point and dew point calculations required for this purpose can be performed easily in the process simulator. The feed location is evident for some applications. For example, while simulating an absorber, the solvent is fed on the top tray and the feed gas is fed on the bottom tray. In cases where the feed location is not clear, it can be optimized along with the number of trays by using tools readily available in many simulators (such as using the design mode for the shortcut column option). The number of feed trays should be decided considering both the capital and operating costs. For further information, see Chapter 14 on optimization.

The stages on which the ionic reactions take place must be specified. Usually, for an electrolyte system, all the stages including the reboiler and condenser are considered. For very fast reactions using a rate-based distillation column, as would be the case for most ionic reactions, the reactions should be considered to take place in the liquid film as well. The holdup volume of the films is needed to find the reaction rate. For calculating the holdup volume, a correlation is used for a particular type of tray/packing and the tray/packing design details are needed. Many simulators ignore the holdup volume in the downcomers. A simple solution is to use an appropriate scaling factor. Again, if thermodynamic equilibrium is assumed, then the holdup is not important.

For the film model, tray/packing design details are required for calculating mass transfer coefficients and heat transfer coefficients that are used in the mass, equilibrium, rate, and enthalpy equations. One issue is with the determination of the film thickness. For low flux, it can be shown that the film thickness is given by [47]

$$l = \frac{\overline{D}}{\overline{k}_m} \tag{13.41}$$

where $\overline{D}$ and $\overline{k}_m$ are average diffusivity and mass transfer coefficient, respectively. For calculating the total mass and heat transfer rates in the interface for use in the material (M) balance and energy (E) balance equations for the film region, it is necessary to estimate the interfacial area. For tray columns, the net interfacial area is [47]

$$a = a' h_f A_b \tag{13.42}$$

where a' is the interfacial area per unit volume of froth, h_f is the froth height, and A_b is the bubbling area. For the packed columns, the net interfacial area is [47]

$$a = a' h A_c \tag{13.43}$$

where a' is the interfacial area per unit volume, h is the height of a section of packing, and A_c is the cross-sectional area of the column. Appropriate correlations are used for determining a'. In the process simulators, various correlations are available that usually provide the value of the net interfacial area directly for a type of tray/packing. The profile of the calculated interface area can be available depending on the simulator of choice. In Aspen Plus V7.2, the interface profiles are

reported under "interface profile" when the desired "property options" are selected under "rate-based report."

For rate-based distillation, the system of equations is usually solved by Newton's method, by homotopy continuation, or by a combination of both. If the default settings fail to converge, intervention may be required. With Newton's method, the initial guess plays a strong role in aiding convergence. Process simulators have their own default techniques to generate initial guesses, but these techniques may fail, particularly for electrolyte systems. An estimate of one or more variables, such as pressure, temperature, or compositions, can help convergence. Usually, it is not a good idea to consider some strict design specifications during the first attempt to solve the system. Not only can such design specifications be infeasible due to the current column specification, but they can fail to be realized due to a poor initial guess. Temperature profiles of distillation columns for a number of electrolyte systems are usually available in the open literature and can be used as an initial estimate. Another approach is to solve an equilibrium-stage model first and then use the solution as the initial guess for the nonequilibrium model. The first objective is to get a converged model. Newton's method requires the calculation of a Jacobian. The partial derivatives of thermodynamic properties are not only very difficult to obtain for the complicated thermodynamic models for electrolytes but are also computationally intensive. More information about the calculation of Jacobians and other related issues can be found in Chapter 16, Section 16.3. Even though the discussion in Section 16.3 concentrates on the solution of the entire flowsheet and in this section the focus is on the solution of a distillation column model for electrolyte systems, many of the issues are similar if Newton's method or a quasi-Newton method is used.

13.8. Summary

In this chapter, the general components of a process simulator and the seven types of input required to simulate a process successfully were reviewed. Each of the seven required inputs was covered in detail: selection of chemical components, selection of thermodynamic models, selection of process topology, selection of feed stream properties, selection of equipment parameters, selection of output options, and selection of convergence criteria.

Special attention was paid to the role of recycle streams in obtaining converged solutions, and methods to help convergence were discussed. The selection of thermodynamic models and their importance were discussed in depth. A case study for the toluene hydrodealkylation process given in Chapter 1 was given and the required data to complete a process simulation were presented.

Fundamental concepts on electrolyte systems modeling were presented, along with a discussion of the available thermodynamic and transport models in the current process simulators. Further details on the calculation of the Gibbs free energy/activity coefficient were provided in Appendix 13.1. An example was provided to show the steps involved in developing a model of a multicomponent distillation column involving electrolytes. Further discussion of the steps was provided in Appendix 13.2. In Section 13.7, the essentials of solids modeling were discussed. A short discussion on the parameter requirements for solids modeling was provided followed by an example. Overall, this chapter has laid the foundation for developing steady-state simulation using commercial process simulators.

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Short Answer Questions

1. In the activity-coefficient model of an electrolyte system, how is the effect of the long-range forces included?
2. Even though the ions do not directly participate in the VLE of an electrolyte system, why does their presence affect the VLE of an electrolyte system?
3. The reboiler temperature of an electrolyte process is known to be 150°C–200°C. One of the species present in this system is H_2S. How would you model the fugacity of H_2S in the liquid phase?
4. An electrolyte NRTL model is used for VLE calculation of a strong electrolyte system consisting of four species. How many binary interaction parameters are needed? What are they?
5. You are developing an equilibrium-stage model of a distillation column with fixed pressure drop in an electrolyte system. Is the model for surface tension important? Explain.
6. A model of biomass combustion in an industrial furnace is to be developed. Calculation of which thermodynamic property is the most important?

Problems

7. For the toluene HDA process, using the data given in Tables 13.1 and 13.2, simulate the process and compare the results with those given in Chapter 1, Table 1.5. Remember that the number of actual plates is given in Table 1.7, and an efficiency of 0.6 was assumed.
8. For the DME flowsheet given in Appendix B, Figure B.1.1, list the minimum input information required to obtain mass and energy balances for this process. Using the process simulator available to you, simulate the DME process and compare your results to those given in Table B.1.1.
9. For the isopropyl alcohol to acetone process flowsheet given in Appendix B, Figure B.10.1, list the minimum input information required to obtain mass and energy balances for this process. Using the process simulator available to you, simulate the isopropyl alcohol to acetone process, and compare your results to those given in Table B.10.1.
10. Using the results from Problem 13.7 and Tables 1.5 and 1.7, compare the results for the simulation of the benzene recovery column, T-101, using a shortcut method and a rigorous method. One way to do this comparison is to use the number of theoretical plates from the shortcut method as an input to the rigorous method. The rigorous method is used to simulate the same separation as the shortcut method, that is, the same overhead purity and recovery. The difference in the methods is then reflected by the difference between the reflux required for both methods. Comment on the difference for this nearly ideal system. Remember that there is no need to simulate the whole flowsheet for this problem; just use the input to the column from Table 1.5.

11. In Problem 13.7, you should have simulated the reactor as a stoichiometric reactor with 75% per pass conversion. In order to estimate the volume of the reactor, it is necessary to have kinetics expressions. For the catalytic hydrodealkylation of toluene, assume that the reaction is kinetically controlled with the following kinetics:

$$-r_{tol} = kc_{tol}c_{hyd}^{0.5} \quad \frac{\text{kmol}}{\text{m}^3_{\text{reactor}}\text{s}}$$

where

$$k = 2.833 \times 10^7 e^{-\frac{17814}{T(K)}} \quad \frac{\text{m}^{1.5}}{\text{kmol}^{0.5}\text{s}}$$

With these kinetics, simulate the reactor in Figure 1.5 as a two-stage packed-bed adiabatic reactor with a "cold shot" (Stream 7) injected at the inlet to the second bed. The maximum temperature in the reactor should not exceed 655°C, and this will occur at the exit of both beds; that is, design the system for this maximum outlet temperature for both packed beds. Compare your results with the total volume of the catalyst given in Table 1.7.

12. As noted in Section 13.5, the results provided for the toluene hydrodealkylation process are based on the SRK model for both enthalpy and phase equilibria. Determine the BIPs for this model used by the simulator available to you. If you have access to more than one simulator, compare the BIPs from each. Simulate the benzene column (T-101) using the shortcut simulation module and the specifications given in Table 13.1 and the conditions of feed stream (10) given in Example 13.2. Rerun the simulation with all the BIPs set to zero. Compare the results.
13. Determine what thermodynamic models were used for each of the processes in Appendix B. Explain why each was chosen, and give at least one other thermodynamic model that is reasonable and should be tried for each process.
14. For the system DME/methanol/water, determine the BIPs used in the simulator available to you for each of these thermodynamic models: NRTL, Wilson, and UNIQUAC. Simulate T-202 using a shortcut module for each of these models, and compare the number of theoretical stages required for the specified recoveries and $R/R_{min} = 1.5$.
15. Find VLE data in the literature for the system methanol/water. Regress these data to determine the BIPs for the UNIQUAC model. Compare the results of these with the results obtained using the BIPs available in the simulator databank and with the results obtained using the UNIFAC model.
16. Using the Henry's Law model in the simulator available to you, determine the concentration of oxygen (ppm by mass) in water at 25°C and at 35°C if the water is in equilibrium with air. Compare the results obtained to those calculated using the PR model with the BIPs available in the simulator databank.
17. Using the help facility of the simulator available to you, determine how the simulator handles VLE calculations with supercritical components when an activity-coefficient model is specified. (Note that P_i^* in Equation 13.1 is undefined for these components.)
18. For the ethylbenzene flowsheet given in Appendix B, Figure B.2.1, list the minimum input information required to obtain mass and energy balances for this process. Using the process simulator available to you, simulate the ethylbenzene process and compare your results to those given in Table B.2.1.

19. For the styrene flowsheet given in Appendix B, Figure B.3.1, list the minimum input information required to obtain mass and energy balances for this process. Using the process simulator available to you, simulate the styrene process and compare your results to those given in Table B.3.1.
20. For the maleic anhydride flowsheet given in Appendix B, Figure B.5.1, list the minimum input information required to obtain mass and energy balances for this process. Using the process simulator available to you, simulate the maleic anhydride process and compare your results to those given in Table B.5.1.
21. For the ethylene oxide flowsheet given in Appendix B, Figure B.6.1, list the minimum input information required to obtain mass and energy balances for this process. Using the process simulator available to you, simulate the ethylene oxide process and compare your results to those given in Table B.6.1.
22. For the formalin flowsheet given in Appendix B, Figure B.7.1, list the minimum input information required to obtain mass and energy balances for this process. Using the process simulator available to you, simulate the formalin process and compare your results to those given in Table B.7.1.
23. Investigate the batch aspects of the simulator available to you. Remember that these could include reactor, separation, and scheduling modules as well as others.
24. Determine which thermodynamic models were used for each of the processes in Appendix B. Explain why each was chosen, and give at least one other thermodynamic model that is reasonable and should be tried for each process.
25. Using the Henry's Law model in the simulator available to you, determine the concentration of oxygen (ppm by mass) in water at 10°C and 27°C if the water is in equilibrium with air. Compare the results obtained to those calculated using the SRK model with the BIPs available in the simulator databank.
26. As noted in Section 13.5, the results provided for the toluene hydrodealkylation process are based on the SRK model for both enthalpy and phase equilibria. Simulate the benzene column (T-101) with the PR model instead, using the shortcut simulation module and the specifications given in Table 13.1 and the conditions of feed stream (10) given in Example 13.2. Determine the BIPs for the PR model used by the simulator. Rerun the simulation with all the BIPs set to zero. Compare the results.
27. Figure P13.27 is the absorber in an acid-gas removal (AGR) plant.

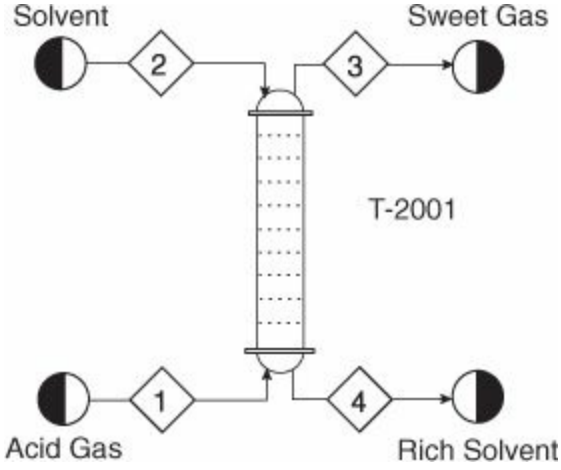


Figure P13.27. Schematic of the Absorber of an AGR Plant Using MDEA as the Solvent

The solvent, Stream 2, in this plant is a chemical solvent, methyl diethanolamine (MDEA). It is fed to the top of the column. The acid gas, Stream 1, is fed to the bottom of the column. The conditions of Streams 1 and 2 are given in Table P13.27. The column has 20 theoretical stages. Simulate an equilibrium-stage model of this column considering the important ionic reactions and a suitable thermodynamic model for this electrolyte system. The column top pressure is 1.6 atm. Consider the following reactions [59, 60]:

$$R'R''R''N + CO_2 + H_2O = R'R''R''NH^+ + HCO_3^-$$
$$CO_2 + OH^- = HCO_3^-$$
$$H_2O = H^+ + OH^-$$
$$H^+ + CO_3^{2-} = HCO_3^-$$
$$H_2S = H^+ + HS^-$$
$$HS^- = H^+ + S^{2-}$$

Table P13.27. Feed Stream Data for Problem 13.27

	Stream 1	Stream 2
Temperature (°C)	38.0	38.0
Pressure (atm)	1.8	1.6
Total Flow(kmol/h)	47.33	61.19
Composition (mol%)		
H_2O	4.2	84.7
CO_2	10.5	0.022
H_2S	1.7	6.0×10^{-5}
CH_4	2.5	—
N_2	49.5	—
O_2	0.1	—
CO	18.9	—
H_2	12.6	—
MDEA	—	15.3

What are the compositions and temperatures of Stream 3 and Stream 4?

28. Consider the same problem as Problem 13.27, but now develop a nonequilibrium-stage model with 20 theoretical stages. The first two reactions shown in Problem 13.27, even though reversible, are kinetically limited, while the rest of the reactions can be considered to be fast and at equilibrium. Consider using single-pass valve trays with the appropriate diameter (which can be calculated by the process simulator—assume 80% of flooding) and 152 valves/m^2 of active area. Consider a tray spacing of 0.6096 m and a weir height of 46.55 mm. Fix the top pressure at 1.6 atm and calculate the pressure drop through the entire column. Depending on the process simulator available to you, consider appropriate transport models and account for the mass transfer resistance in both the liquid and vapor films. Since the related ionic reactions are very fast, consider that the ionic reactions also take place in the liquid film. Compare the results for Streams 3 and 4 with the results from Problem 13.27.
29. Consider Problem 13.28. The solvent MDEA becomes rich in acid gases. To recycle this

solvent, it is first heated to 90°C in exchanger E-2001 and then sent to the top stage of the stripper T-2002 as shown in Figure P13.29. Develop a nonequilibrium-stage model of the stripper with 20 theoretical stages, a partial-vapor condenser, and a kettle-type reboiler. Reflux ratio (mole basis) = 0.7 and bottoms/feed ratio (mole basis) = 0.97. The pressure in the condenser is 1.4 atm, and the pressure drop through the entire column should be calculated. Consider the ionic reactions in all the stages, including the condenser and reboiler. It can be assumed that all ionic reactions reach equilibrium in the condenser and reboiler because of the longer residence times. Assume that the tray hardware is similar to the absorber. The mass transfer and the ionic reactions in the liquid and vapor films can be modeled similarly to Problem 13.28. For this problem determine the following:

a. What are the duties of the stripper and reboiler?

b. What are the compositions of Streams 6 and 7?

c. What operating condition(s) of the stripper would you change if you wanted to increase the purity of Stream 7?

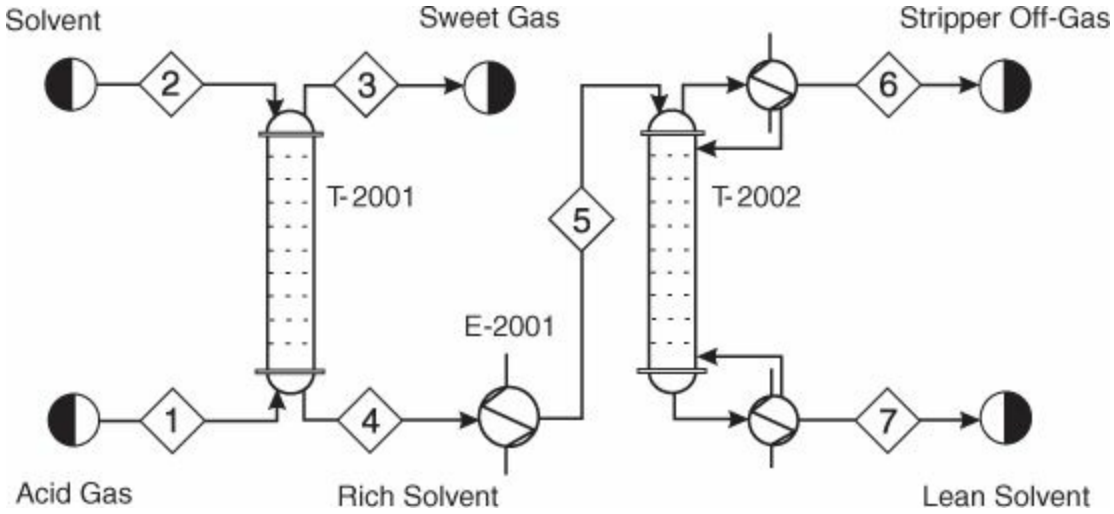


Figure P13.29. Schematic of the Absorber and Stripper of an AGR Plant Using MDEA as the Solvent

30. Develop a model of a coal combustor fed with Illinois no. 6 coal, a bituminous coal, at 2 atm pressure. The atmospheric air for combustion is available at a temperature of 150°C. The flow of combustion air is 10% more than the stoichiometric requirement. The coal is also available at 150°C. The composition for Illinois no. 6 coal is

Proximate Analysis (wt%)	
Moisture	11.12
Ash	9.70
Volatile Matter	34.99
Fixed Carbon	44.19
Ultimate Analysis (wt%)	
Moisture	11.12
Carbon	63.75
Hydrogen	4.50
Nitrogen	1.25
Chlorine	0.29
Sulfur	2.51
Ash	9.70
Oxygen	6.88

The combustor is adiabatic. Assume the carbon conversion to be 100%. The high heating value (HHV) of the coal is reported to be 27,113 kJ/kg. Compare the heating value estimated by the process simulator with this reported value. As mentioned before, most of the models for heterogeneous solids are empirical. Modify the parameters of the enthalpy model to match the reported heating value. What is the composition at the outlet of the combustor?

31. A biomass stream, Stream 1 in Figure P13.31, is being dried in a direct dryer, V-2001, by a stream of hot N_2. Develop a model for this dryer. The composition of Stream 1 (wt%) is

Cellulose	55.0
Hemicellulose	15.0
Lignin	12.5
Moisture	15.0
Ash	2.5

The ash can be considered to be pure calcium oxide (CaO). The flowrate of biomass is 500 kg/min. Assume adiabatic operation in V-2001 with a pressure drop of 0.1 bar. What models would be appropriate for the solids density and enthalpy calculations? If the model parameters are not available for the biomass components in the simulator of your choice, use values from the open literature. The desired moisture content of Stream 4 is 1% (wt). As many commercial process simulators do not have the capability to model the SVE for such processes, assume that the desired moisture content is achieved at 110°C. What is the required flowrate of N_2?

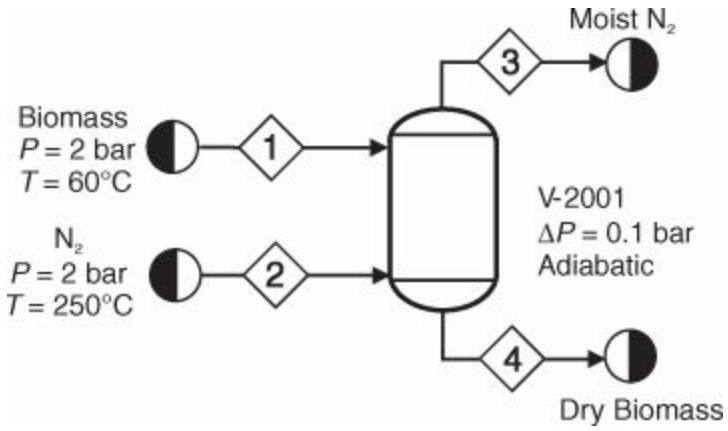


Figure P13.31. Flowsheet of a Biomass Dryer

32. Wood pellets, Stream 1 in Figure P13.32, are first dried by indirect heating with the flue gas and

then combusted. Model this system using a heat exchanger, E-2001, followed by a flash separator, V-2001. The dried wood pellets are combusted in an adiabatic combustor, R-2001, where combustion air is supplied in 15% excess of the stoichiometric requirement. The hot flue gas is used for raising steam in a boiler. The boiler can be simply modeled as a heat exchanger where the flue gas is cooled to 300°C. The flue gas then exchanges heat in E-2001 before being vented through the stack. For simplicity consider the pressure drop through each piece of equipment to be 0.1 bar. The composition of wood pellets is

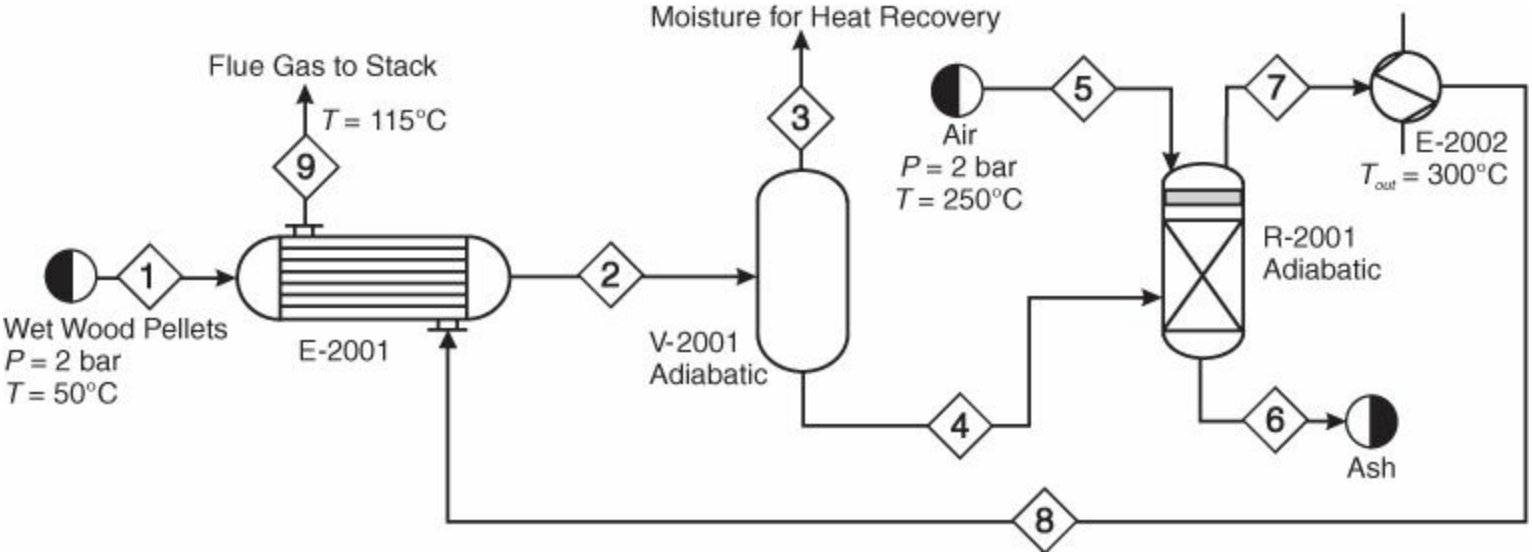


Figure P13.32. Simple Flowsheet of a Wood Combustion System

Proximate Analysis (wt%)	
Moisture	8.80
Ash	2.40
Volatile Matter	73.00
Fixed Carbon	15.80
Ultimate Analysis (wt%)	
Moisture	8.80
Carbon	47.00
Hydrogen	5.00
Nitrogen	0.49
Sulfur	0.08
Ash	2.40
Oxygen	36.23

The HHV of the wood pellets is 18,969 kJ/kg. Feel free to include additional blocks in the process simulator that you need to use to model the combustor operations appropriately. Assume the conversion of carbon to be 100%. As many commercial process simulators do not have the capability to model the SVE for such processes, assume that 90% of the moisture in the feed is separated in the dryer (i.e., leaves in Stream 3).

a. What are the temperatures of Streams 2, 4, and 7?

b. What is the composition of Stream 7?

c. Perform an overall energy analysis of this system and compare with the reported HHV. Modify the parameters of the enthalpy model to match the HHV.

Chapter 14. Process Optimization

What You Will Learn

- Optimization is not an obscure, esoteric concept.
- The terms *objective function* and *decision variable* will be defined.
- The concepts of topological and parametric optimization will be defined and the procedures for using them will be covered.
- The approach for single-variable, two-variable, and multivariable optimization will be covered.
- The approach to optimizing batch processes will be covered.

Optimization is the process of improving an existing situation, device, or system such as a chemical process. This chapter presents techniques and strategies to

- Set up an optimization problem
- Quantify the value of a potential improvement
- Identify quickly the potential for improvement
- Identify the constraints, barriers, and bottlenecks to improvement
- Choose an appropriate procedure to find the best change
- Evaluate the result of the optimization

This chapter will start with some basic definitions of terms and then investigate several techniques and strategies to perform the optimization of a process.

14.1. Background Information on Optimization

In optimization, various terms are used to simplify discussions and explanations. These are defined below.

Decision variables are those independent variables over which the engineer has some control. These can be continuous variables such as temperature, or discrete (integer) variables such as number of stages in a column. Decision variables are also called **design variables**.

An **objective function** is a mathematical function that, for the best values of the decision variables, reaches a minimum (or a maximum). Thus, the objective function is the measure of value or goodness for the optimization problem. If it is a profit, one searches for its maximum. If it is a cost, one searches for its minimum. There may be more than one objective function for a given optimization problem.

Constraints are limitations on the values of decision variables. These may be linear or nonlinear, and they may involve more than one decision variable. When a constraint is written as an equality involving two or more decision variables, it is called an **equality constraint**. For example, a reaction may require a specific oxygen concentration in the combined feed to the reactor. The mole balance on the oxygen in the reactor feed is an equality constraint. When a constraint is written as an inequality involving one or more decision variables, it is called an **inequality constraint**. For example, the catalyst may operate effectively only below 400°C, or below 20 MPa. An equality constraint

effectively reduces the **dimensionality** (the number of truly independent decision variables) of the optimization problem. Inequality constraints reduce (and often bound) the search space of the decision variables.

A **global optimum** is a point at which the objective function is the best for all allowable values of the decision variables. There is no better acceptable solution. A **local optimum** is a point from which no small, allowable change in decision variables in any direction will improve the objective function.

Certain classes of optimization problems are given names. If the objective function is linear in all decision variables and all constraints are linear, the optimization method is called **linear programming**. Linear programming problems are inherently easier than other problems and are generally solved with specialized algorithms. All other optimization problems are called **nonlinear programming**. If the objective function is second order in the decision variables and the constraints are linear, the nonlinear optimization method is called **quadratic programming**. For optimization problems involving both discrete and continuous decision variables, the adjective **mixed-integer** is used. Although these designations are used in the optimization literature, this chapter mainly deals with the general class of problems known as MINLP, **mixed-integer nonlinear programming**.

The use of linear and quadratic programming is limited to a relatively small class of problems. Some examples in which these methods are used include the optimal blending of gasoline and diesel products and the optimal use of manufacturing machinery. Unfortunately, many of the constraints in chemical processes are not linear, and the variables are often a mixture of continuous and integer. A simple example of a chemical engineering problem is the evaluation of the optimal heat exchanger to use in order to heat a stream from 30°C to 160°C. This simple problem includes continuous variables, such as the area of the heat exchanger and the temperature of the process stream, and integer variables, such as whether to use low-, medium-, or high-pressure steam as the heating medium. Moreover, there are constraints such as the materials of construction that depend, nonlinearly, on factors such as the pressure, temperature, and composition of the process and utility streams. Clearly, most chemical process problems are quite involved, and care must be taken to consider all the constraints when evaluating them.

14.1.1. Common Misconceptions

A common misconception is that optimization is a complex, esoteric, mathematical exercise. In fact, optimization is usually a dynamic, creative activity involving brainstorming, exploring alternatives, and asking, "What if . . .?"

Although some problems are simple enough to be posed in closed form and to be solved analytically, most real problems are more interesting.

For example, Figure 14.1(a) shows a classical curve of annualized pumping cost versus pipe diameter. The annualized pumping cost includes annualized equipment (pump plus pipe) cost and power (operating) cost. These two components of cost have been calculated based on smooth cost functions and are shown as separate curves on Figure 14.1(a). The combined curve represents the total annualized cost. Using these results, one can analytically determine the pipe diameter at which the slope of the combined cost curve is zero and the second derivative is positive. It is important to note that, even with all the assumptions used in this analysis, the minimum annualized cost does not occur at the pipe diameter where the two component curves cross.

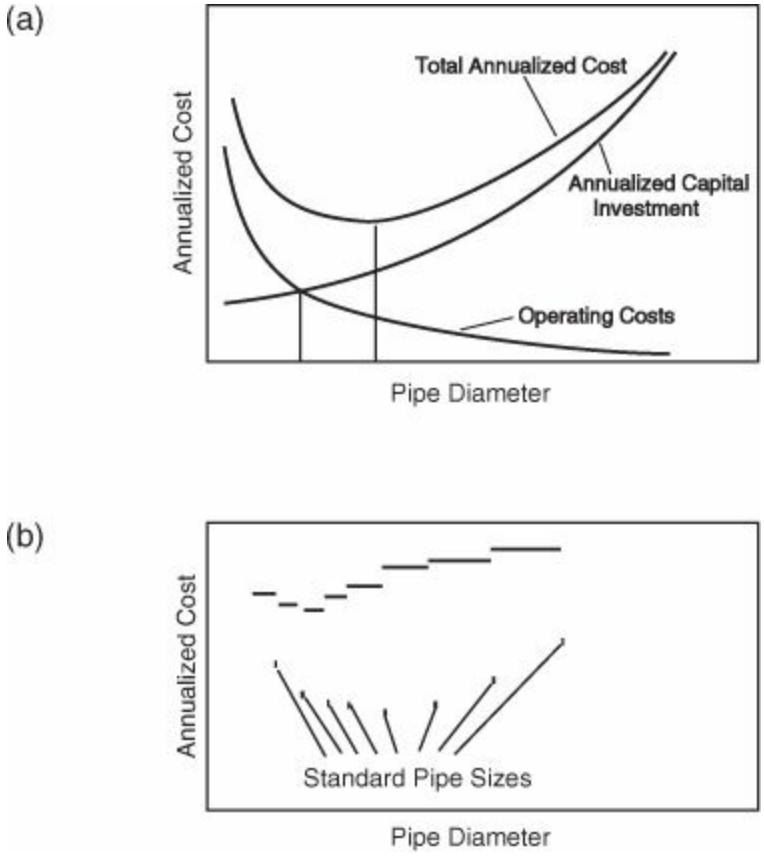


Figure 14.1. Optimization Using Continuous and Discrete Functions of Pipe Diameter

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The point of intersection of the curves of annual operating cost and of annualized capital cost is not the optimum.

In reality, the cost function (if one were to calculate it) would look something like Figure 14.1(b), because only certain pipe diameters and pump sizes are standard equipment. Other sizes could be produced, but only at much higher costs. Thus, only a few cost evaluations are needed—those at the standard pipe sizes.

Another common misconception is that the optimum will usually be found at a point where the first derivatives of the cost function are zero. Even when the cost function is continuous and smooth, this is seldom the case and should never be assumed. Nearly all problems of any reasonable complexity have optima along at least one constraint. Figure 14.2 shows such a case. Again, both annualized capital costs and operating costs are included. Although there is a point of zero slope (point "A"), the best design (minimum annual cost) shown is at point "B."

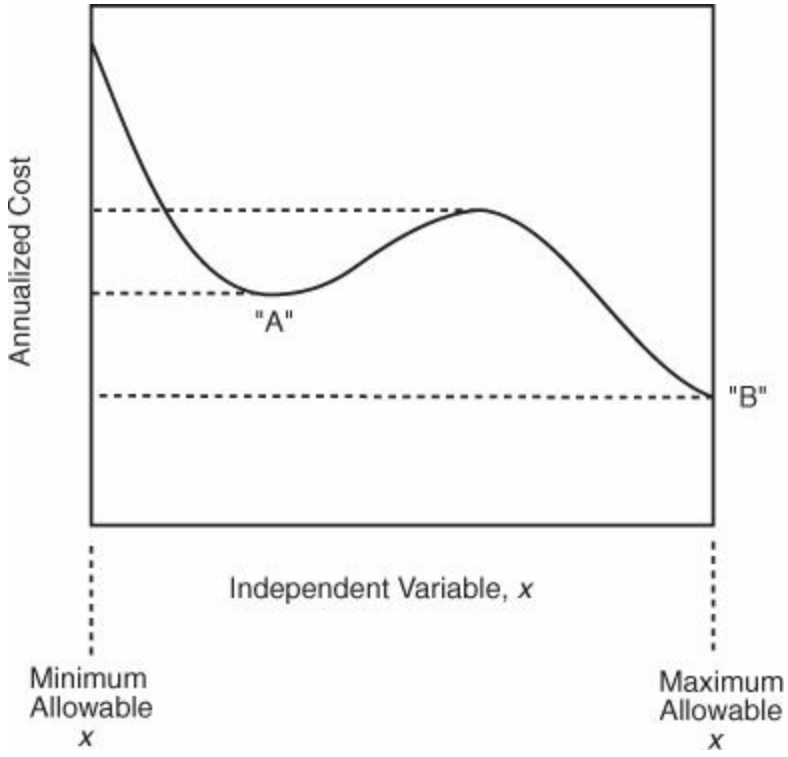


Figure 14.2. Location of the Optimum Value of a Variable

One must not assume that the best solution has been found when it merely has been bracketed. Such an assumption not only leads to a false conclusion but also ignores useful information for estimating the true optimum solution. For example, Figure 14.3(a) shows three points that have been calculated for the optimization of the temperature of a flash unit. If the objective function is continuous and smooth, and if there is indeed only one minimum, then the optimum lies between points "A" and "C." However, there is no reason to believe that point "B" is the optimum, and there are insufficient data to determine whether the optimum lies to the left or to the right of point "B." However, by approximating the objective function simply by a quadratic, for the three points bracketing the optimum, the optimum can be estimated, as shown on the left-hand side of Figure 14.3(b). However, the true curve may look like the right-hand side of Figure 14.3(b). To be certain that the optimum has been located correctly, more points should be evaluated between "A" and "C," using successive quadratic approximations based on the best point achieved plus the closest point on either side of it.

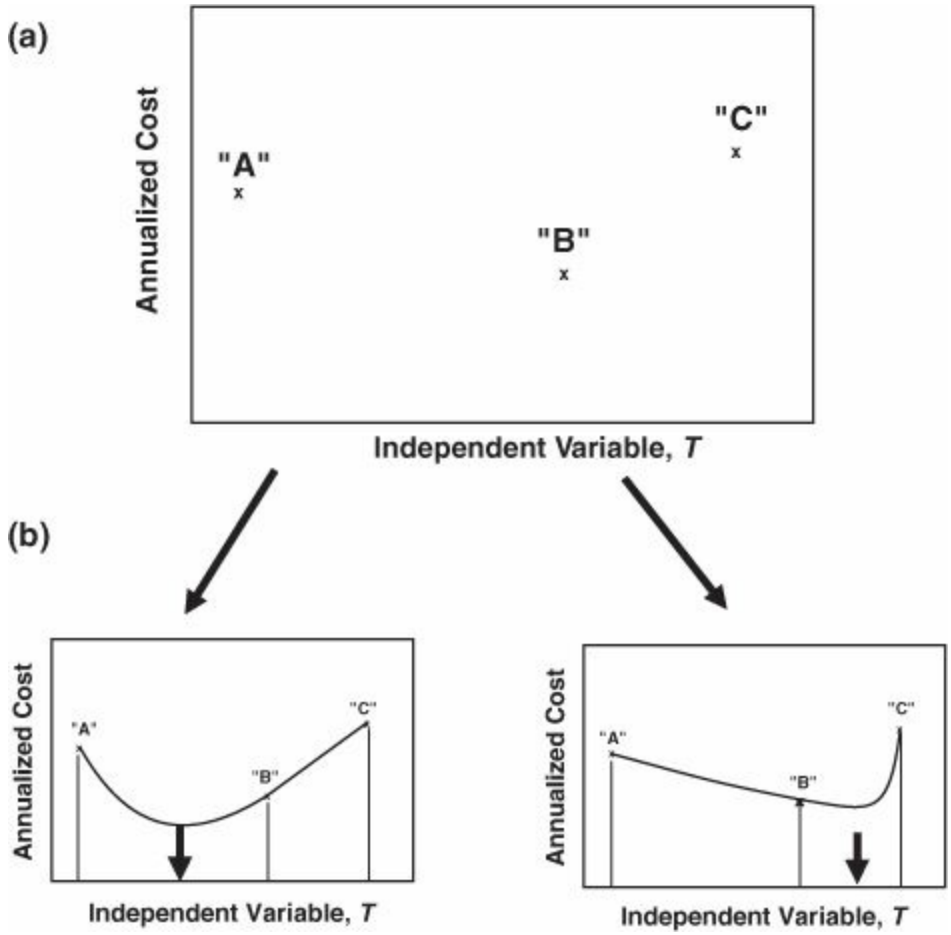


Figure 14.3. Different Locations of Optimum Using Identical Data

14.1.2. Estimating Problem Difficulty

A key step in any problem-solving strategy is to estimate the effort required to reach the solution. Not only can this estimate provide motivation, but it can also help to redirect resources if the effort (time, money, personnel) required for a "complete" solution is more than the effort available. The first step is to decide whether the problem at hand is an "easy" problem or a "difficult" problem. Table 14.1 lists some characteristics of inherently easy and inherently difficult problems.

Table 14.1. Characteristics of Easy and Difficult Optimization Problems

Easy Problems	Difficult Problems
Few decision variables	Many decision variables
Independent (uncorrelated) decision variables	Correlated decision variables
Discrete decision variables	Mixed discrete and continuous decision variables
Topological optimization first	Parametric optimization first
Single process units	Multiple, interrelated process units
Separate constraints for each decision variable	Constraints involving several decision variables
Constraints are obvious	Constraints are not obvious or become obvious only after the optimization has begun
Single objective	Multiple objectives
Objective function easy to quantify	Objective function difficult to quantify
Linear objective function	Highly nonlinear objective function
Smooth objective function	Kinked objective function
No local optima	Many deep, local optima

For a typical flowsheet, such as the DME (dimethyl ether) PFD in Figure B.1.1 (Appendix B), there are many decision variables. The temperature and pressure of each unit can be varied. The size of each piece of equipment involves decision variables (usually several per unit). The reflux in tower T-201 and the purity of the distillate from T-202 are decision variables. There are many more. Clearly, the simultaneous optimization of all of these decision variables is a difficult problem. However, some subproblems are relatively easy. If Stream 4 (the exit from the methanol preheater) must be at 154°C, for example, the choice of which heat source to use (lps, mps, or hps) is easy. There is only a single decision variable, there are only three discrete choices, and the choice has no direct impact on the rest of the process. The problem becomes more difficult if the temperature of Stream 4 is not constrained.

14.1.3. Top-Down and Bottom-Up Strategies

For any real process of any complexity, the true "global" optimum (at which any change in any decision variable would degrade the system) will not be found. If it could be found with an acceptable level of effort, one would concentrate on minute changes in decision variables. Rather than become bogged down in such details, experts at optimization tend to look alternately at the big picture and at the details. The overview encourages one to make bold changes in process configuration or variable values, but the closer study is needed to confirm whether the changes are true improvements.

The strategy of looking at the big picture first, followed by the detailed study, is called **top-down**. Looking at the DME flowsheet, such a strategy might lead to one questioning the need for E-201 (Methanol Preheater) and E-203 (DME Cooler). A detailed study of the flowsheet would confirm whether these two units should be eliminated in favor of a larger E-202 (Reactor Cooler). On the other hand, a detailed study of incremental changes in the heat duties of these two heat exchangers would have led to the same solution. Such a strategy is called **bottom-up**. Before investing too much time in detailed calculations, check the big picture. When the big picture is not clear or leads to conflicting alternatives, run the detailed calculations. The key is flexibility.

Details of the top-down and bottom-up approaches are covered in Sections 14.3 and 14.4 under topological and parametric optimization.

14.1.4. Communication of Optimization Results

As will be discussed in Chapter 29 (on the CD), the best strategy for obtaining results is not the best strategy for presenting those results to others. Although the goal of optimization is to find the best solution (and the sensitivity of that solution, as explained in Section 14.6) efficiently, the goal of the presentation is to convince the audience clearly that the solution is the best. Thus, one must explain the ranges of decision variables that were searched, show that the solution is (most likely) not merely a local minimum, and show the degradation in the objective function from moving away from the solution. For example, as discussed in Section 14.4, it is more efficient to change more than one decision variable at a time when searching for the optimum; however, it is better to communicate the validity of the optimum by using families of curves in which any single curve involves the variation of only one decision variable (see Figure 14.6).

14.2. Strategies

In this section, the DME process from Appendix B is used as an example. Stream and unit numbers refer to those in Figure B.1.1.

14.2.1. Base Case

A **base case** is the starting point for optimization. It may be a very simple conceptual flowsheet, it may be a detailed design, or it may be an actual plant whose operation one wishes to improve.

Because the goal of optimization is to *improve* the process, it is essential that one start from a defined process, that is, a base case.

The choice of a base case is straightforward: Choose the best available case. For example, if one has already determined (through prior analysis) that heat integration greatly improves the process, the base case should include the heat integration. The level of detail of the base case is also a crucial decision. At a minimum, the analysis must be detailed enough to provide the calculation of the objective function. If the objective function includes both capital costs and operating costs, the base-case analysis must include sizing and costing of equipment, as well as the material and energy balances and utility costs. The analysis must be detailed enough to show the effect of all important decision variables on the objective function. In the DME example, because the temperature of R-201 affects unit E-202, the base-case analysis must include this effect.

Although the ability to calculate the objective function and how it changes with variations in all decision variables is essential, the base case certainly need not be a completed design. For example, details of T-201 such as tray spacing, weir height, and so on are not important at this point in the problem, and a shortcut rather than a rigorous tower simulation will suffice.

However, it is essential to include enough detail in the base case. Capital costs for individual major pieces of equipment are needed, as are utility costs broken down by type and unit. Creating a calculational model that lumps all costs together (even if correctly annualized by the methods shown in Chapter 10) is not very helpful, because specific modifications to the flowsheet are masked. For example, a lumped EAOC (equivalent annual operating cost) would not show whether the cost for the

reactor, R-201, was relatively small (leading to a conclusion to increase its size) or the steam costs for E-201 were especially high (leading to a search for an alternative heat source).

Table 14.2. Data Required for Base Case (in Addition to PFD and Flow Tables)

Capital	Operating	Material
Installed cost, each equipment	Utility flowrates (each type)	Total cost for each raw material
Installed cost, each category	Utility targets (Section 15.2)	Value of purged or wasted material
Estimated credit for equipment used elsewhere in plant (for existing processes)	Utility costs on $/GJ basis	Total product value
	Estimated uncertainties	Estimated uncertainties
Estimated uncertainties	Other operating costs	

Table 14.2 provides a list of useful information that should be available for the base case. If the optimization problem is for an existing plant, the original capital cost is not relevant. However, methods for the estimation of capital costs for new equipment should be available, as should some estimate of the value that any removed equipment has when used in other parts of the total plant.

The scope of the base case (and therefore of the optimization) must be chosen. Usually, the battery limits for the analysis are defined by functional groupings, company organization, location of large surge or storage facilities, or convenience. However, if the scope is too small, important effects will be missed. For example, if the scope of optimization is R-201, the effect of reactor product composition on tower T-201 is missed. On the other hand, if the scope is too broad, one can become overwhelmed by the interactions. One could include, for example, the effect on the internal cost of medium-pressure steam of changes in steam usage. Such an expansion of scope clearly would not be warranted. Typically, column reflux ratio can be optimized separately, but reactor conditions (T, P, conversion), recycle rates, and separator recoveries should be optimized together.

14.2.2. Objective Functions

The optimization can begin only after the objective function is selected. It must be chosen so that the extreme maximum (or minimum) is the most desired condition. For example, minimizing the EAOC is typically considered (rather than the installed capital cost) or maximizing net profit (rather than gross sales). If the objective function is poorly chosen or imprecise, the solution will be worthless.

The most common objective functions have units of dollars. The recurring costs can be discounted to obtain a net present value (NPV), or the capital costs can be annualized to obtain an EAOC, as discussed in Chapter 10. Usually, this value is for the process unit. However, if a smaller scope is defined for part of the optimization (e.g., T-201 reflux), then the EAOC or NPV used should not include capital and recurring cost contributions that do not change significantly over the ranges of the varied decision variables. For example, optimization of the reflux for T-201 does not significantly affect the costs for the rest of the flowsheet (other than the ancillary units E-204, E-205, V-201, and P-202). Thus, the raw material costs, reactor costs, and other capital and utility costs should not be included. If they were, the total variation in the objective function might be in the fourth or fifth digit. The total EAOC or NPV is not accurate to this level, but the changes caused by the tower optimization are.

This focus on the changes to the costs (or savings) rather than on the total costs is called **incremental analysis**. Modification of the design or operation of the plant continues as long as the improvement

gained (the **return**) for an incremental investment is greater than the **benchmark** (or hurdle) rate. In Chapter 10, the details of this form of investment analysis are covered. In optimization, the implementation of incremental analysis requires careful choice of the objective function, as described above.

Some objective functions are not directly based on economics. For example, one may be asked to maximize the production of DME from an existing plant or to minimize the contaminant concentration in the wastewater stream. However, the objective function should be quantitative. Furthermore, a rational basis for any objective function (monetary or nonmonetary) should be developed. For example, if the goal is to maximize profit (rather than revenues), then maximizing the production of DME may not be desirable. Similarly, if the goal is to cause the least harm to the environment, then minimization of the contaminant concentration (rather than the total contaminant flowrate) may not be the best approach.

14.2.3. Analysis of the Base Costs

The first analysis of the base costs should be to determine targets of an idealized process. The value for the objective function should be determined based on the assumption of equilibrium conversion, no equipment or utility costs, and perfect separations. The profit for such a case is called the **gross profit margin**, or simply the **margin** (see Chapter 10).

Next, a form of Pareto [1] analysis should be used. This analysis is based on the observation that, for most problems, a large fraction of the objective function (e.g., 80%) is due to a small fraction of the contributing factors (e.g., 20%). For example, Table 14.3 shows the contribution to the EAOC for the different types of equipment and for the operating costs and raw materials for the DME process given in Appendix B. Only a few of these categories account for the bulk of the total cost. For this case, as with many chemical processes, the raw material costs swamp all other costs and are treated separately. In this case, the overriding goal is to convert as much of the raw materials into product as possible. From this standpoint, the waste of methanol is very low and the net savings that can be made from better use of the methanol amounts to only $30,300/y. The calculations for this analysis are covered in the next section. However, assuming that methanol is already being purchased from the cheapest source, the focus should not be on reducing the cost of raw materials, because this will not have a significant effect on reducing the cost of producing DME. The single largest operating cost is the medium-pressure steam. A greater improvement in the objective function can be made by lowering steam costs than can be obtained by lowering any other cost category.

Table 14.3. Ranking of Contributions to the *EAOC* for DME Process

Category	Contribution to *EAOC* ($/y)
Raw materials	11,215,000
Raw material (at 100% conversion) = $11,185,000	
Target savings = $30,300	
Medium-pressure steam	695,000
Towers and vessels	210,000
Heat exchangers	170,000
Pumps (including electricity)	160,000
Reactor	70,000
Cooling water	31,000
Wastewater treatment	1000
Total	**12,552,000**

All figures are for 1996 prices.

Basically, this first analysis of the base case provides a target for optimization and a road map to proceed to the solution. It should be noted that all cost figures for this chapter are based on 1996 prices from the first edition of this text. These numbers will change with time, but the basic approach to the products and main conclusions will remain the same.

14.2.4. Identifying and Prioritizing Key Decision Variables

Based on the Pareto ranking of effects on the objective function, the key decision variables are chosen. For the DME process, the methanol cost is high, but there are assumed to be no by-product reactions. The product DME is assumed to be at its purity specification. The only methanol loss is in the wastewater; thus, the purity of the bottoms product of T-202 could be a decision variable. At present, approximately 0.27% of the methanol feed leaves in the wastewater. Thus, the target savings attainable can be calculated as $30,300/y.

Medium-pressure steam is used in three units: E-201, E-204, E-206. The first of these is used to vaporize the reactor feed at 154°C, which is lower than the temperature of low-pressure steam. Because low-pressure steam is less expensive than medium-pressure steam, changing this heat source should be considered. Similarly, the duty of E-204 (a tower reboiler) does not necessarily require medium-pressure steam.

The base-case single-pass conversion is 80%. If this can be increased, the costs (capital plus operating) of all units in the recycle loop will be decreased. This includes all the equipment in the flowsheet except P-201 and E-208. The conversion is set by the reactor inlet temperature (T_5) and pressure (P_5) and the volume of the reactor.

Thus, the single-pass conversion has been identified as an important dependent decision variable. With the techniques presented in Section 14.4, the optimum can be determined. The conversion is a secondary (decision) variable. There are an infinite number of temperature, pressure, and reactor-volume combinations for a given conversion. Prioritizing these three primary decision variables requires knowledge of the sensitivity of the objective function to changes in these variables. Although there are elegant mathematical techniques for estimating these sensitivities, the most efficient technique is often to evaluate the objective function at the limits of the variables. This is a standard

experimental design technique (two-level factorial design) that is of great help in choosing key decision variables. If the cost changes little when the reactor pressure changes from its upper limit to its lower limit, then another variable (such as temperature) should be chosen.

Another strategy to determine decision variables is to consider how the process is controlled. Any variable that must be controlled is a decision variable. There are alternative control strategies for equipment and for processes, but a well-designed control system reduces the degrees of freedom to zero without overconstraining the process. The controlled variable is a secondary decision variable; the variable manipulated by the final control element is the primary decision variable.

Considering the DME process in Figure B.1.1, the flowrate of methanol is a decision variable, as are the temperature of Stream 4 (controlled by steam pressure in E-201), the temperature of Stream 8 (controlled by the cooling water rate to E-203), the pressure of the reactor (controlled by the valve between Streams 8 and 9), and so on. The two columns have their own control systems, which show that the reflux to the column and the heat input to the reboiler are decision variables. Note that simple (two-product) distillation columns have two decision variables (in addition to the column pressure), but many different combinations are possible. Because the number of decision variables is equal to the number of controlled variables, which is equal to the number of operational specifications, one can look at any process simulator setup for a column and see the myriad choices.

The other type of decision variable is an equipment characteristic. The reactor volume and the number of stages are examples. Each specification that must be made before ordering a piece of equipment is a decision variable. Thus, the area of a heat exchanger and the aspect ratio of a packed-bed reactor are decision variables.

Once the decision variables have been identified and prioritized, the techniques of topological optimization (Section 14.3) and parametric optimization (Section 14.4) can be applied.

14.3. Topological Optimization

As previously discussed in Sections 14.1 and 14.2, there are essentially two types of optimization that a chemical engineer needs to consider. The first is termed topological optimization and deals with the topology or arrangement of process equipment. The second type is parametric optimization, and it is concerned with the operating variables, such as temperature, pressure, and concentration of streams, for a given piece of equipment or process. In this section, topological optimization is discussed. Parametric optimization is addressed in Section 14.4.

14.3.1. Introduction

During the design of a new process unit or the upgrading of an existing unit, topological optimization should, in general, be considered first. The reasons for this are twofold. First, topological changes usually have a large impact on the overall profitability of the plant. Second, parametric optimization is easiest to interpret when the topology of the flowsheet is fixed. It should be noted that combinations of both types of optimization strategies may have to be employed simultaneously, but the major topological changes are still best handled early on in the optimization process.

The questions that a process engineer needs to answer when considering the topology of a process include the following:

1. Can unwanted by-products be eliminated?
2. Can equipment be eliminated or rearranged?

3. Can alternative separation methods or reactor configurations be employed?
4. To what extent can heat integration be improved?

The ordering of these questions corresponds approximately to the order in which they should be addressed when considering a new process. In this section, these questions are answered and examples of processes are given in which such topological rearrangements may be beneficial.

14.3.2. Elimination of Unwanted Nonhazardous By-products or Hazardous Waste Streams

This is clearly a very important issue and should be addressed early on in the design process. The benefit of obtaining 100% conversion of reactants with a 100% selectivity to the desired product should be clear. Although this goal is never reached in practice, it can be approached through suitable choices of reaction mechanisms, reactor operation, and catalyst. A chemical engineer may not be directly involved in the choice of reaction paths. However, one may be asked to evaluate and optimize designs for using alternative reactions in order to evaluate the optimum scheme.

In many cases, due to side reactions that are suppressed but not eliminated by suitable choices of catalyst and operating conditions, unwanted by-products or waste streams may be produced. The term *unwanted by-product* refers to a stream that cannot be sold for an overall profit. An example of such a by-product would be the production of a fuel stream. In this case, some partial economic credit is obtained from the by-product, but in virtually all cases, this represents an overall loss when compared with the price of the raw materials used to produce it. An example illustrating the cost of purifying a by-product for sale is given in Example 14.1.

Example 14.1.

Consider the process given in Figure C.8 in Appendix C (on the CD), for the production of cumene. In this process, benzene and propylene react in a gas-phase catalytic reaction to form cumene, and the cumene reacts further to form p-diisopropyl benzene (DIPB), a by-product sold for its fuel value.

$$C_6H_6 + C_3H_6 \rightarrow \underset{\text{cumene}}{C_9H_{12}}$$

$$C_9H_{12} + C_3H_6 \rightarrow \underset{\text{p-diisopropyl benzene}}{C_{12}H_{18}}$$

From the information given in Table C.14, estimate the yearly cost of producing this waste, Stream 14. Assume that the costs of benzene, propylene, and fuel credit are \$0.27/kg, \$0.28/kg, and \$2.5/GJ, respectively.

From Table C.14, the composition of the DIPB waste stream is 2.76 kmol/h DIPB and 0.92 kmol/h cumene. The standard heats of combustion for DIPB and cumene are given below:

Cumene –5.00 GJ/kmol

DIPB –6.82 GJ/kmol

Revenue for sale as fuel = [(2.76) (6.82) + (0.92) (5.00)](8000)(2.5) = \$468,000/y Cost of equivalent raw materials:

Benzene = (2.76 + 0.92) (78) (8000) (0.27) = \$620,000/y

Propylene = (2.76(2) + 0.92) (42) (8000) (0.28) = \$606,000/y

Net cost of producing DIPB stream = $(620 + 606 - 468) \times 10^3$ = \$758,000/y

---

From Example 14.1, it is clear that the production of DIPB is very costly and impacts negatively the overall profitability of the process. Improved separation of cumene would improve the economics, but even if all the cumene could be recovered, the DIPB would still cost an estimated $608,000/y to produce. A better option would be to find ways of minimizing DIPB production. This is investigated further in Example 14.2.

Example 14.2.

What process changes could be made to eliminate the production of the DIPB waste stream in Figure C.8 (on the CD)?

There are several possible solutions to eliminate the DIPB stream:

1. Reduce the per-pass conversion of propylene in the reactor. This has the effect of suppressing the DIPB reaction by reducing the cumene concentration in the reactor.
2. Increase the ratio of benzene to propylene in the feed to the reactor. This reduces the propylene concentration in the reactor and hence tends to suppress the DIPB reaction.
3. Obtain a new catalyst for which the DIPB reaction is not favored as much as with the current catalyst.

Each of these remedies has an effect on the process as a whole, and all these effects must be taken into account in order to evaluate correctly the best (most profitable) process. Some of these effects will be discussed in the following sections.

Alternatively, a hazardous waste stream may be produced. In such cases additional costly treatment steps (either on-site or off-site) would be required in order to render the material benign to the environment. The economic penalties for these treatment steps—incineration, neutralization, and so on—are often great and may severely impact the overall economic picture for the process. In addition to the economic penalties that the production of waste streams cause, there are political ramifications that may overshadow the economic considerations. For many companies, the production of hazardous wastes is no longer an acceptable process choice, and alternative reaction routes, which eliminate such waste streams, are aggressively pursued.

14.3.3. Elimination and Rearrangement of Equipment

Both the elimination and rearrangement of equipment can lead to significant improvements in the process economics. Algorithms for these topological changes are under development. However, the approach used here is one based on intuitive reasoning and illustrated by process examples. Both topics are considered separately below. The rearrangement of heat transfer equipment is considered as a separate topic in Chapter 15.

Elimination of Equipment. It is assumed that the starting point for this discussion is a PFD in which all process equipment serves a valid function: that is, the process does not contain any redundant equipment that can be eliminated immediately.

The elimination of a piece of equipment is often the result of a change in operating conditions and can thus be considered the end product of a series of parametric changes. In Example 14.3 the first alternative in Example 14.2 is considered.

Example 14.3.

Evaluate the topological changes in the cumene PFD, Figure C.8, which can be made by reducing the per-pass conversion of propylene in the reactor.

As the single-pass conversion of propylene (the limiting reactant) in the reactor is reduced, the DIPB production decreases due to the lowering of the cumene concentration in the reactor. At some point, the second distillation column and the associated equipment can be removed, because all the DIPB produced can leave the process in the cumene product, Stream 13.

Although the second distillation column (T-802), associated equipment (E-805, E-806, V-804, and P-805 A/B), and utility costs may be eliminated, this may not be the most economical alternative. The increase in the size of other equipment in the front end of the process, due to an increase in the recycle flows and the accompanying increase in utility costs, may overwhelm the savings from the elimination of the second tower and associated equipment. However, one should be aware of the consequences of reducing the DIPB production, because the elimination of the tower represents a step change in the profitability function that might otherwise be overlooked. This step change in the objective function is illustrated in Figure 14.4.

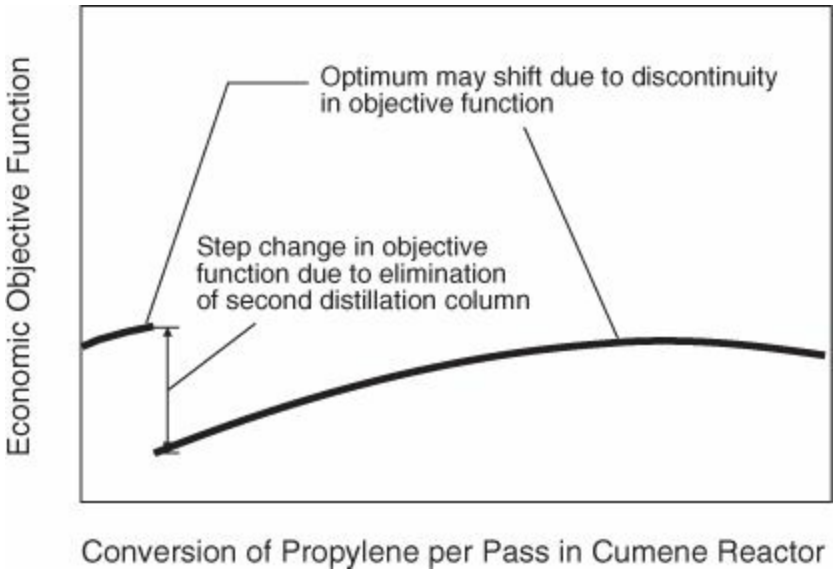


Figure 14.4. The Effect of a Topological Change on a Parametric Optimization

Rearrangement of Equipment. There are certain guidelines that should be followed when the sequence of equipment is considered. Some are obvious. For example, one should try to pump a liquid rather than compress a gas; thus, it will always be better to place a pump before a vaporizer rather than a compressor after it. However, other topological changes are somewhat more subtle. The most common examples of equipment rearrangement are associated with the separation section of a process and the integration of heat transfer equipment. In this section the sequencing of separation equipment is the focus, and heat integration is covered in Chapter 15. The separation sequence for the DME process is considered in Example 14.4.

Example 14.4.

Consider the dimethyl ether (DME) process shown in Figure B.1.1 (Unit 200) and Tables B.1.1 and B.1.2. The process is quite straightforward and consists of a gas-phase catalytic reaction in which methanol is dehydrated to give DME with no appreciable side reactions.

$$2CH_3OH \rightarrow (CH_3)_2O + H_2O$$

$$DME$$

The reactor effluent stream is cooled and sent to two distillation columns. The first column separates DME product from the water and unreacted methanol. The second column separates the methanol, which is recycled, from the water, which is then sent to a wastewater treatment facility to remove trace organic compounds.

Is there any economic advantage gained by changing the order of the distillation so that the water is removed first and the DME and methanol are separated in the second column?

There is no simple way to determine whether the separation sequence given in Example 14.4 should be changed. In order to evaluate which alternative is better, a rigorous parametric optimization for both topologies should be made and the configuration with the best economics should be chosen. Although it may not always be possible to determine which sequence is best by inspection only, there are some guidelines that may help determine which sequences are worthy of further consideration. The following guidelines are presented in Tables 11.13 and 12.2:

1. Perform the easiest separation first—that is, the one least demanding of trays and reflux—and leave the most difficult to the last.
2. When neither relative volatility nor feed composition varies widely, remove components one by one as overhead products.
3. When the adjacent ordered components in the feed vary widely in relative volatility, sequence the splits in order of decreasing volatility.
4. When the concentrations in the feed vary widely but the relative volatilities do not, remove the components in order of decreasing concentration.

Example 14.5 applies these guidelines to the DME problem.

Example 14.5.

Apply the guidelines for column sequencing to the DME process using the information given in Table B.1.1 and Figure B.1.1.

From Table B.1.1, the composition of the stream leaving the reactor and entering the separation section is as follows:

	Flowrate (kmol/h)	Mole Fraction	Relative Volatility (P = 10.4 bar)
DME	130.5	0.398	49.4
MeOH	64.9	0.197	2.2
Water	132.9	0.405	1.0

The relative volatilities for the components are taken from a simulation of the process, using CHEMCAD, with a UNIQUAC/UNIFAC estimation for the vapor-liquid equilibrium (VLE). By applying the guidelines given above, it would appear that the easier separation is the removal of DME, and, according to Rule 1, this should be removed first, which is what is done currently. The other guidelines do not add any additional guidance, and it may be concluded that the current sequence is probably the best. However, no mention is given in the guidelines of special

considerations for water. Because water has a very high latent heat of vaporization, the duties of the condensers and reboilers in the columns will be higher than for similar flows of organic materials. By removing the DME first, water must be reboiled in both columns. This suggests that there may be some advantage to removing the water first and then separating the DME and methanol. This case is considered in Problem 14.16 at the end of this chapter. Therefore, this example illustrates a new guideline that should be added to those in Chapters 11 and 12.

Special consideration is necessary when dealing with mixtures of polar compounds or other components that can form azeotropes or give rise to more than one liquid phase. As components are separated from a stream, the remaining mixture of components may fall into regions where two or more liquid phases are present or in which pairs of compounds form azeotropes. This can greatly increase the complexity of a separation and may strongly influence the sequence in which components or products are separated. This topic is considered in Chapter 12, and the reader is referred to this material for a more complete explanation and methods for evaluating azeotropic systems.

14.3.4. Alternative Separation Schemes and Reactor Configurations

Early in the design process, it is important to consider the use of alternative technologies to separate products from unused reactants and waste streams and to evaluate alternative reactor configurations. The topic of alternative reactor configurations is considered in Chapter 23, and only alternative separation technologies are considered here. If one picks up any textbook on mass transfer or unit operations, it is immediately apparent that there exist a myriad of different technologies to separate chemical components. Despite the wide range of separation technologies available to the process engineer, when considering liquid-gas processes, the vast majority of separations are composed of distillation, gas absorption and liquid stripping, and liquid-liquid extraction. According to Humphrey and Keller [2], 90% to 95% of all separations, product recoveries, and purifications in the chemical process industry consist of some form of distillation (including extractive and azeotropic distillation). The relative maturity of distillation technology coupled with its relatively inexpensive energy requirements make distillation the default option for process separations involving liquids and vapors. Many notable exceptions exist, and alternatives to distillation technology may have to be used. Two examples occur when the relative volatilities of two components are close to 1 (for example, less than 1.05) or if excessively high pressures or low temperatures are required to obtain a liquid-vapor mixture. A comprehensive list of alternative separation techniques is not offered in this text. The approach taken here is to emphasize the importance of recognizing when a nontraditional technology might be employed and how it may benefit the process. Further details of the choice of alternative separation techniques are given in Table 12.1. An example of using alternative separation schemes is given in Example 14.6.

Example 14.6.

In the toluene hydrodealkylation process shown in Figure E14.6 (taken from Figure 1.5), the fuel gas leaving the unit, Stream 16, contains a significant amount of hydrogen, a raw material for the process. Currently, there is no separation of Stream 8. The mixture of methane and hydrogen leaving V-102 is split in two, with one portion recycled and the other portion purged as fuel gas. What benefit would there be in separating the hydrogen from the methane in Stream 8 and recycling a hydrogen-rich stream to the reactor? What technology could be used to achieve this separation?

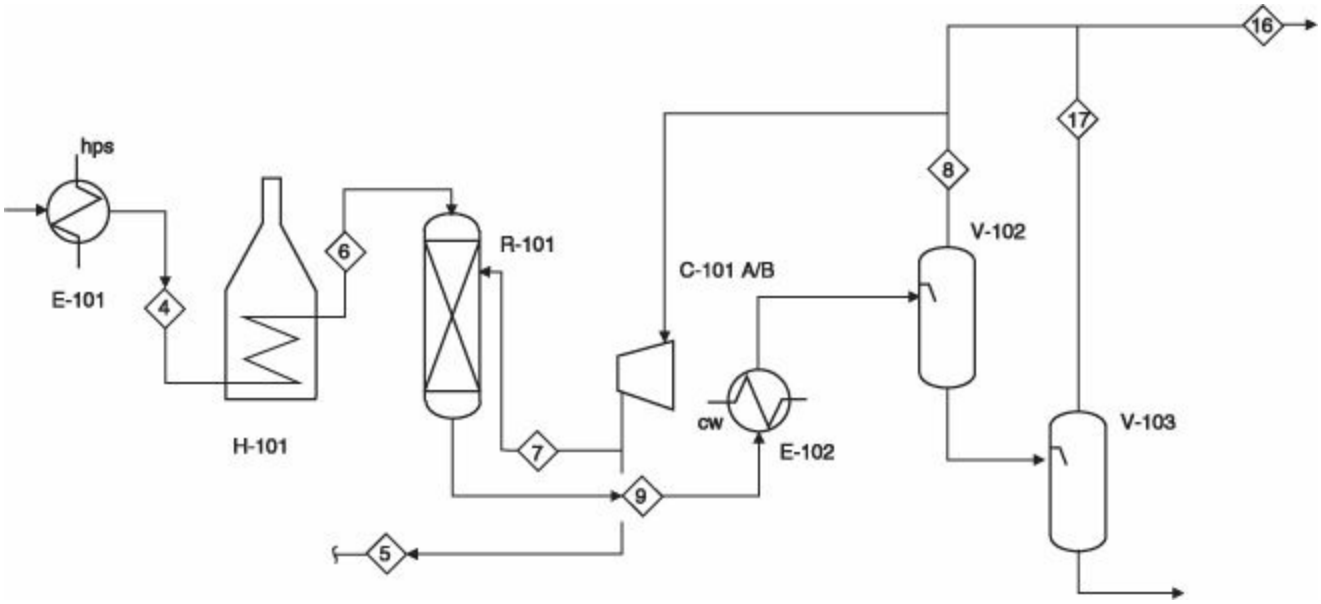


Figure E14.6. Toluene Hydrodealkylation Reactor and Hydrogen Recycle Loop

Significant benefits may be derived by sending a hydrogen-rich recycle stream back to the front end of the process. The methane that is currently recycled acts as a diluent in the reactor. By purifying the recycle stream, all the equipment in the reactor loop, E-101, H-101, R-101, E-102, and C-101, could be made smaller (because the amount of methane in the feed to each piece of equipment would be reduced), and the utility consumption for the heat-exchange equipment would also be reduced. In addition, the amount of hydrogen feed, Stream 3, would be reduced because far less hydrogen would leave in the fuel gas, Stream 16.

Several technologies exist to purify hydrogen from a stream of light hydrocarbons. It should be noted that distillation is not a viable option for this separation because the temperature at which methane begins to condense from Stream 8 is less than –130°C. The two most likely candidates for this separation are membrane separation, in which hydrogen would preferentially diffuse through a polymer membrane, and pressure swing adsorption, where methane would preferentially adsorb onto a bed of molecular sieve particles. In both of these cases, the potential gains outlined above are offset by the capital cost of the additional separation equipment and increased compression costs for the membrane case, where the permeate, high in hydrogen, would be obtained at a much lower pressure than the feed gas. In order to evaluate such process alternatives correctly, the economics associated with the new topology would have to be assessed, taking into account all the savings and costs outlined above. The case of implementing a membrane separator is considered in the problem report in Chapter 30 (on the CD).

14.4. Parametric Optimization

In optimizing a chemical process, the key decision variables must be identified early in the optimization procedure. This is necessary in order to reduce the computational effort and time and make the problem tractable. The choice of key decision variables is crucial to the efficiency of the optimization process. An exhaustive list of potential decision variables is not presented here. However, some important variables that should be considered for most processes are listed below.

1. Operating conditions for the reactor—for example, temperature, pressure, concentration of reactants. The temperature range may be restricted by catalyst properties; that is, catalyst may sinter at high temperatures or be inactive at low temperatures.

2. Single-pass conversion in the reactor. The selectivity will be determined by the conditions mentioned in (1) and the single-pass conversion.
3. Recovery of unused reactants.
4. Purge ratios for recycle streams containing inerts.
5. Purity of products (this is often set by external market forces).
6. Reflux ratio and component recovery in columns, and flow of mass separating agents to absorbers, strippers, extractors, and so on.
7. Operating pressure of separators.

Because most chemical processes utilize recycles to recover unused reactants, any changes in operating conditions that occur within a recycle loop will impact all the equipment in the loop. Consequently, the whole flowsheet may have to be resimulated and the economics reworked (capital investments and costs of manufacture) every time a new value of a variable is considered.

For variables that do not lie within a recycle loop, optimization may be simplified. An example is a distillation column in a separation sequence in which two products are purified and sent to storage. The operation of such a column does not impact any part of the process upstream and can therefore be considered independently after the upstream process has been optimized. First, single- and two-variable optimizations for single pieces or small groups of equipment are considered. Then overall process optimization strategies are studied.

14.4.1. Single-Variable Optimization: A Case Study on T-201, the DME Separation Column

When considering the optimization of a distillation column, the variables to be considered are reflux ratio, operating pressure, percent recovery of key components, and purity of the products. For our initial case study, consider that the column pressure and the feed to the column are fixed. Figure B.1.1 and Table B.1.1 present the following information:

Feed, Stream 9	
Temperature	89°C
Pressure	10.4 bar
Vapor fraction	0.148
Molar flows (kmol/h)	
Dimethyl ether	130.5 kmol/h
Methanol	64.9 kmol/h
Water	132.9 kmol/h
Total Flow	**328.3 kmol/h**

In addition, the product specification for the DME is that it be 99.5 wt% pure. Assume that 98.9% of the DME in the feed must be recovered in the final product. Note that for this column, the pressure, reflux ratio, and percent recovery of DME are all process variables that can be optimized. Focus first on the reflux ratio; later, relax the constraint on the operating pressure and carry out a two-variable optimization.

In order to proceed with the optimization, choose an objective function. For this example, considering the reflux ratio as the only decision or design variable, the only costs that will be affected by changes in reflux are the capital and operating costs associated with the column. In order to account correctly for both one-time costs and operating costs, an objective function that takes into account the time

value of money (see Chapter 10 for the different criteria used for assessing profitability) should be used. Use the before-tax NPV as the objective function:

$$OBJ = FCI_{TM} + COM_d(P/A, i, n)(P/F, i, n_{startup})$$
$$= FCI_{TM} + (0.18FCI_{TM} + 1.23C_{UT})(P/A, i, n)(P/F, i, n_{startup}) \quad (14.1)$$

It should be noted that the value of the cost of manufacturing term without depreciation, COM_d, in Equation (8.2) includes a term with the fixed capital investment based on the total module cost (FCI_{TM}) and the cost of utilities. The other terms are not relevant to the optimization because they do not change with reflux ratio. Using a plant life of ten years after start-up and a 10% internal rate of return and assuming a construction period of one year, Equation (14.1) reduces to

$$OBJ = FCI_{TM} + (0.18FCI_{TM} + 1.23C_{UT})(6.145)(0.909)$$
$$= 2.005FCI_{TM} + 6.871C_{UT} \quad (14.2)$$

The fixed capital investment term includes the total module costs for T-201, E-204, E-205, V-201, and P-202 A/B. The utility costs include the electricity for P-202 and the heating and cooling utilities for E-204 and E-205, respectively. A series of case studies were run (using the CHEMCAD process simulator) for different reflux ratios for this column, and the equipment costs (evaluated from CAPCOST using mid-1996 prices) and utility costs (also from 1996) are presented in Table 14.4 along with the objective function from Equation (14.2). A plot of the (R/R_{min}) versus the objective function is shown in Figure 14.5. The optimum value of R/R_{min} is seen to be close to 1.12. Moreover, for values greater than 1.1, the objective function changes slowly with R/R_{min}. It should be noted that the results of this univariate search technique are presented as a continuous function of R/R_{min}. However, in reality, the objective function exists only at a set of points on Figure 14.13 (shown by the data symbols on the dotted curve), each point representing a column with an integer number of plates.

Table 14.4. Data for DME Column Optimization, R/R_{min}, versus *OBJ*

R/R_{min}	*FCI* ($\$10^3$)	Steam Cost ($\$10^3$/y)	Cooling Water Cost ($\$10^3$/y)	Electrical Cost ($\$10^3$/y)	Total Utility Cost ($\$10^3$/y)	*OBJ* from Eq. (14.2) ($103)
1.01	684	72.50	4.04	0.48	77.02	−1911
1.02	509	72.72	4.05	0.48	77.24	−1551
1.03	441	72.96	4.06	0.48	77.50	−1417
1.04	411	73.15	4.07	0.48	77.70	−1358
1.11	354	74.68	4.13	0.49	79.31	−1255
1.27	342	78.16	4.28	0.51	82.95	−1256
1.60	322	85.04	4.54	0.55	90.17	−1265

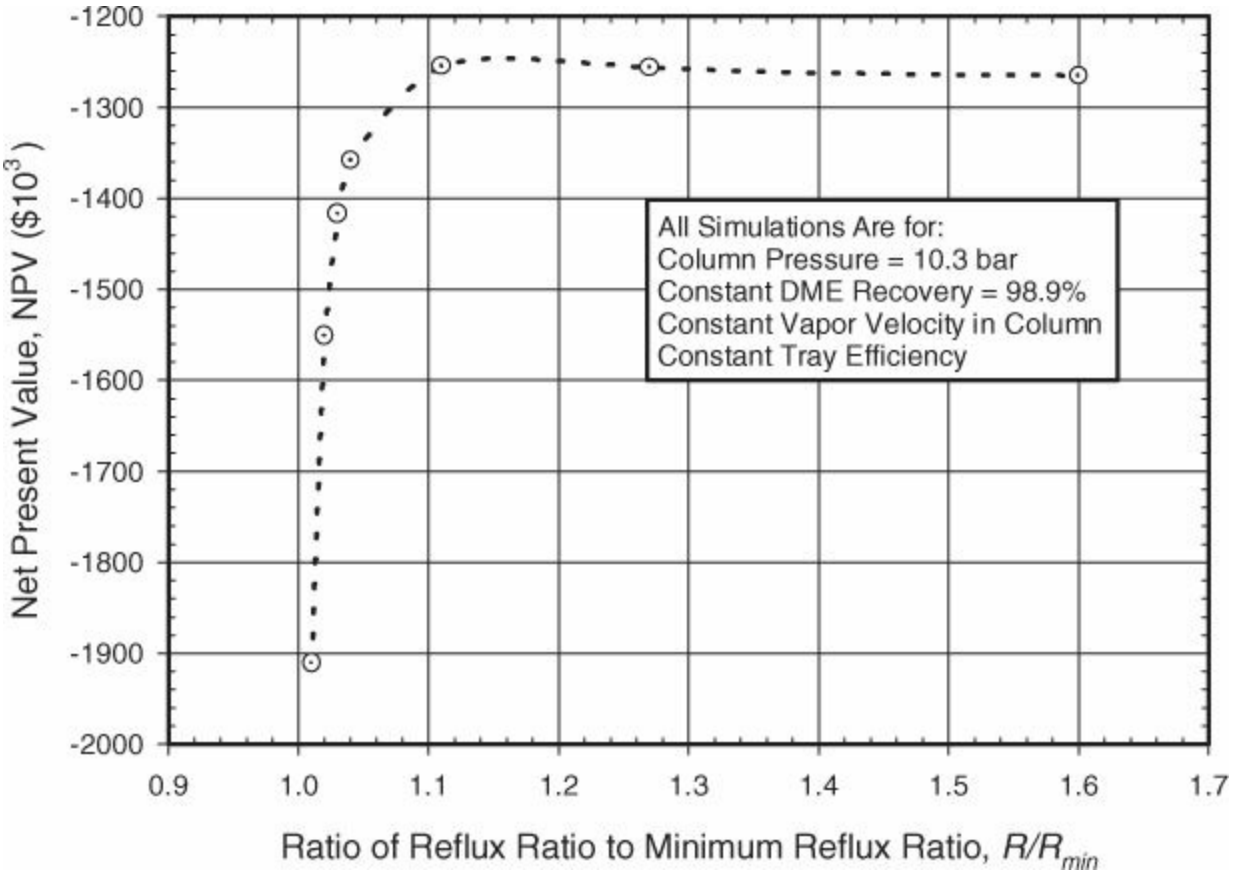


Figure 14.5. Single-Variable Optimization for DME Column, T-201. All figures based on 1996 prices/costs.

14.4.2. Two-Variable Optimization: The Effect of Pressure and Reflux Ratio on T-201, the DME Separation Column

The effect of pressure on the operation of T-201 is considered next. It may be tempting to take the result from Section 14.4.1 and, by holding the value of R/R_{min} constant at 1.12, carry out a univariate search on the pressure. However, the results from such a technique will not yield the optimum pressure or R/R_{min} values. This is because as pressure changes, the optimum reflux ratio also changes. In order to optimize this situation correctly, both the pressure and R/R_{min} must be varied and the best combination should be determined. This problem can be approached in many ways. In the following example, pick different pressures and repeat the procedure used in Section 14.4.1 for each pressure, and then plot the results. This is not a particularly efficient procedure, but it yields plots that are easy to interpret. This is an example of a bivariate search technique. The data for this problem are presented in Table 14.5 and plotted in Figure 14.6. From the results shown in Figure 14.6, it is clear that the relationship between pressure and NPV at the optimum R/R_{min} is highly nonlinear. In addition, the optimum value of R/R_{min} does not remain constant with pressure, as shown by the dotted line in Figure 14.6, although, for this example, $(R/R_{min})_{opt}$ does not change very much with pressure over the range considered here.

Table 14.5. Data for Two-Variable Optimization of DME Column, T-201

Pressure (Bar)	13.5	11.5	10.3	9.0[a]	9.0[b]	7.5
R/R_{min}	OBJ	OBJ	OBJ	OBJ	OBJ	OBJ
1.01	−2052	−1975	−1911	−1890	−1926	−5203
1.02	−1699	−1613	−1551	−1511	−1547	−4847
1.03	−1560	−1474	−1417	−1373	−1409	−4719
1.04	−1499	−1411	−1358	−1310	−1347	−4665
1.11	−1394	−1312	−1255	−1213	−1250	−4616
1.27	−1365	−1288	−1256	−1204	−1243	−4715
1.60	−1385	−1309	−1265	−1216	−1259	−4955

[a]Using lp steam.
[b]Using mp steam.
All costs in $1000 using data from 1996, first edition of text.

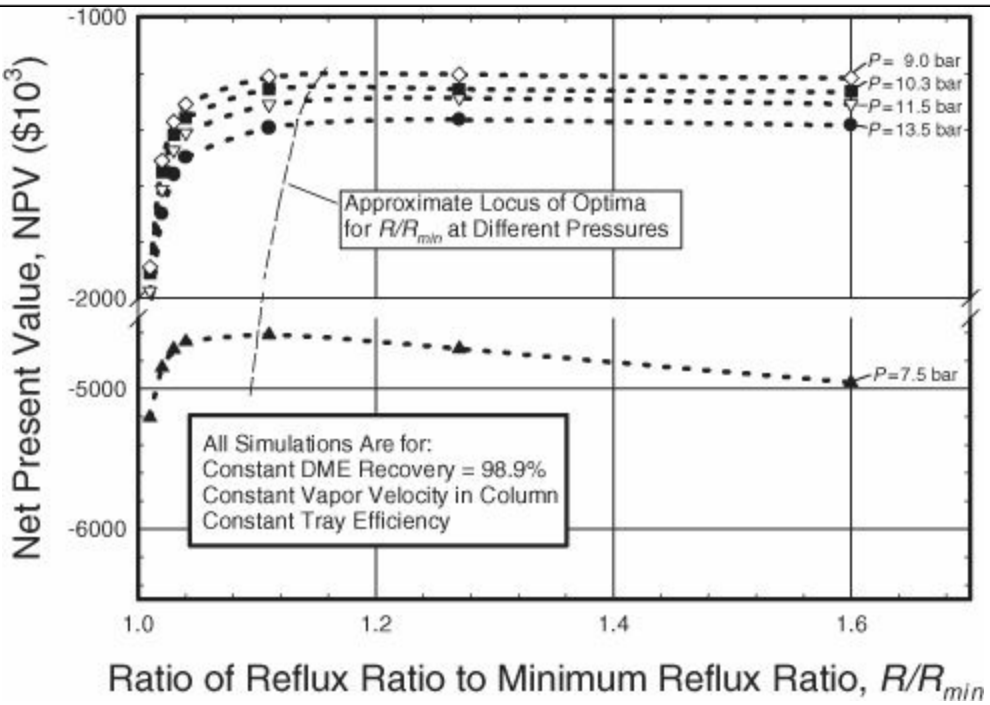


Figure 14.6. Optimization of DME Column, T-201, for Two Variables (Pressure and R/R_{min})

It was stated at the beginning of this section that the topology of the distillation column and associated equipment should remain fixed while carrying out the parametric optimization. This may unduly constrain the overall optimization of the process and, for this case, limits the range of pressures over which the optimization may be considered. Moreover, when carrying out this optimization, it was necessary to change some of the utilities used in the process, and this significantly impacted the results. Consider the information presented in Table 14.6, in which the utility and fixed capital investment (FCI) breakdown is given for the case of R/R_{min} = 1.27 (which is close to the optimum value for all the cases). It is clear that several changes in utilities were implemented. Some were required in order to obtain viable processes; others were changed in order to improve the economics. First, consider the switch from medium-pressure steam to low-pressure steam for a process pressure of 9.0 bar. The results are shown in Tables 14.5 and 14.6 and are plotted in Figure 14.7. It is clear that there is a small but significant increase in the NPV when low-pressure steam is substituted for medium-pressure steam. The reason for this increase is that the reduction in utility costs (due to less expensive low-pressure steam) outweighs the increase in equipment costs (due to a smaller

temperature driving force and higher operating pressure in E-204, the column reboiler). A switch to low-pressure steam is actually possible for all of the operating pressures shown, with the exception of 13.5 bar, because the reboiler temperature for these cases is less than 160°C, the temperature at which low-pressure steam condenses.

Table 14.6. Breakdown of Costs and Process Information for R/R_{min} = 1.27

Pressure (bar)	13.5	11.5	10.3	9.0	9.0	7.5
mp steam	89.79	82.44	78.16	—	72.26	—
lp steam	—	—	—	62.80	—	56.67
Cooling water	4.23[a]	4.26[a]	4.28[a]	8.61[b]	8.61[b]	—
Refrig. water	—	—	—	—	—	539.35[c]
Electricity	0.53	0.52	0.51	0.50	0.50	0.49
FCI	357	344	342	354	340	307
NPV	−1339	−1263	−1230	−1178	−1217	−4692
R_{min}	0.3528	0.3214	0.3024	0.2810	0.2810	0.2562
$T_{condenser}$ (°C)	57	50	46	40	40	34
$T_{reboiler}$ (°C)	164	157	153	147	147	140

[a] $\Delta T = 10°C$.
[b] $\Delta T = 5°C$.
[c] $\Delta T = 10°C$.
All costs in $1000 or $1000/y based on 1996 data.

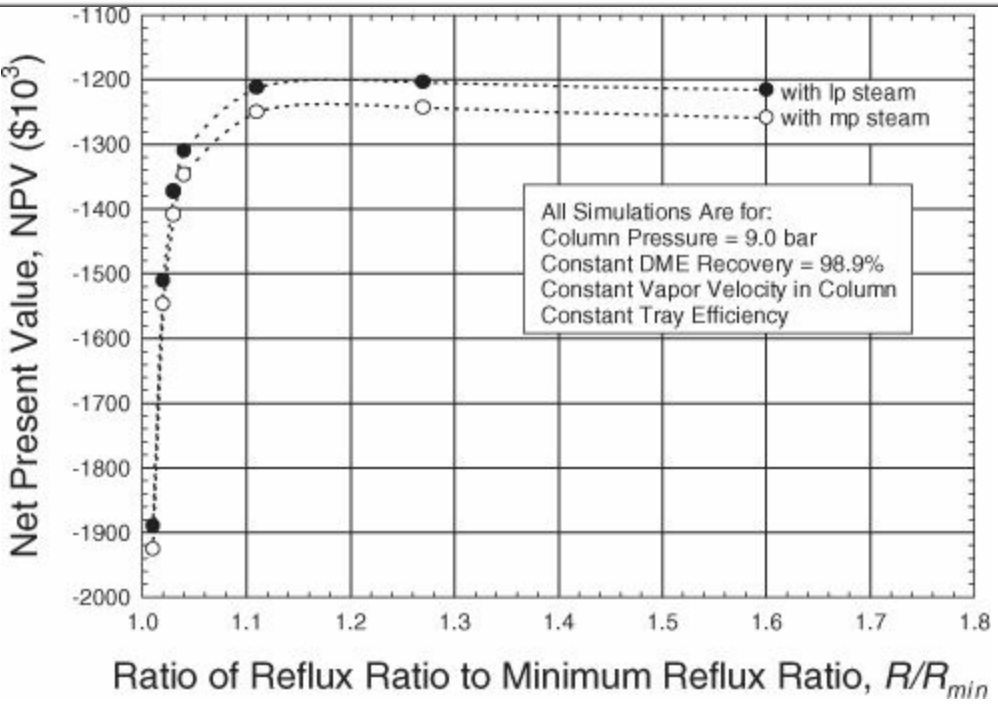


Figure 14.7. The Effect of Changing Utilities in the Reboiler for T-201 at a Column Pressure of 9.0 Bar

Next, consider a change in the cooling water utility. As the operating pressure of the column decreases, the bottom and top temperatures also decrease. One consequence is that low-pressure steam may be used in the reboiler, as considered above. In addition, as the top temperature in the column decreases, a point is reached where a temperature increase of 10°C for the cooling water can

no longer be used. This occurs at an operating pressure of 9.0 bar. Cooling water can be used to condense the overhead vapor from the column, but the temperature increase of the utility must be reduced. The results shown are for a change in cooling water temperature of 30°C (in) to 35°C (out). As the operating pressure is reduced still further to 7.5 bar, the column top temperature decreases to 34°C. At this point, the use of cooling water becomes almost impossible; that is, the flow of cooling water and the area of the exchanger would become extremely large, and any slight changes in cooling water temperature would have a large impact on the process. For this reason, refrigerated water is substituted as the cooling utility for this case. The result is a very large increase in the cost of the utilities and a resulting decrease in the objective function (NPV) as shown in Figure 14.8.

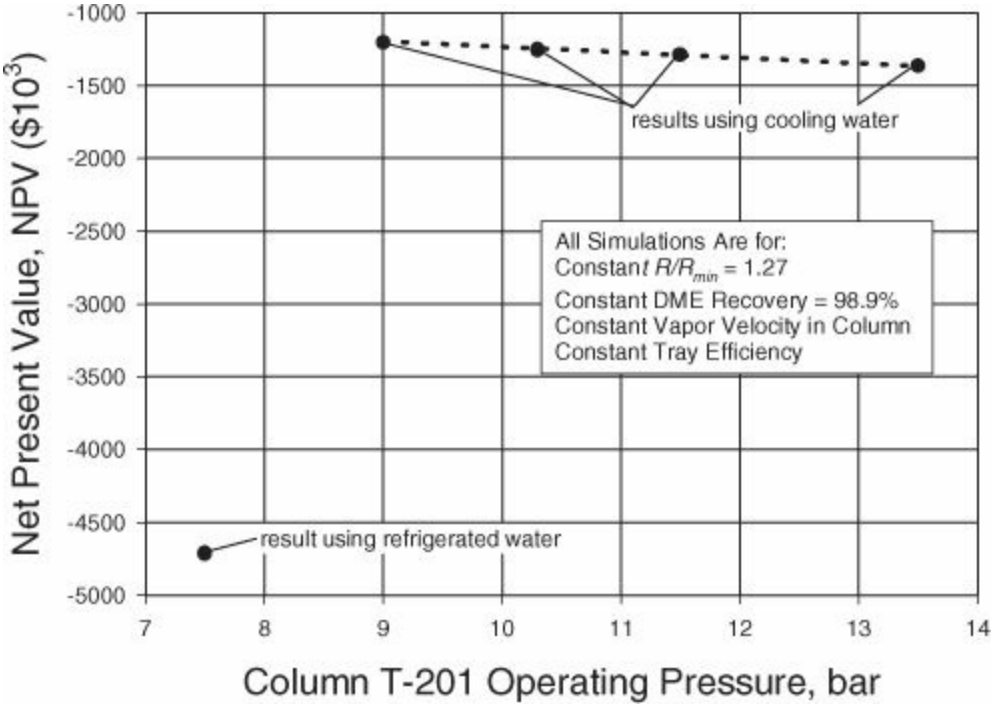


Figure 14.8. The Effect of the Operating Pressure of T-201 on the NPV (All Data for R/R_{min} = 1.27)

The example in this section clearly illustrates the need to consider changes in utilities when process conditions change.

During parametric optimization, changes in operating conditions may require corresponding changes in utilities.

14.4.3. Flowsheet Optimization Using Key Decision Variables

As stated previously, when the decision variables for an optimization lie within a recycle loop, then evaluation of the objective function becomes more complicated. As an example, consider the DME flowsheet given in Appendix B, Figure B.1.1. The possible decision variables, for even such a simple flowsheet as this, are numerous. In this example, consider three variables: single-pass conversion in the reactor (x), fractional recovery of the DME product in tower T-201 (f), and reactor pressure (p). Even with only three variables, it is not clear how many runs should be performed, nor is it clear over what range of the decision variables runs should be performed.

The first step, therefore, in doing such optimizations should be to choose the range over which the decision variables should be varied. The ranges chosen for this example are

$$0.7 < x < 0.9,\ 0.983 < f < 0.995,\ 12.70 \text{ bar} < p < 16.70 \text{ bar}$$

The choice of these ranges is somewhat arbitrary, although it is useful to include maximum and/or minimum constraints as end points for these ranges. For example, it has been found from research in the laboratory that, for the current catalyst, a maximum single-pass conversion of 90% and a maximum operating pressure of 16.70 bar should be used because of equilibrium constraints and to avoid undesirable side reactions. The upper limits for x and p represent upper constraints for these variables, which should not be exceeded. On the other hand, the lower limits for p and x are arbitrary and could be changed if the optimization results warrant looking at lower values. The choice of the range of f values is again arbitrary, although experience indicates that the fractional recovery of product (f) should be close to 1.

The next question to be answered is how many points should be chosen for each variable. If three values for each variable are used, then there would be a total of (3)(3)(3) = 27 simulations to run. A conservative estimate of the length of time to run a simulation, collect the results, evaluate the equipment parameters, price the equipment, estimate the utility costs, and finally evaluate the objective function is, for example, 2 hours per run. This would yield a total time investment of (2)(27) = 54 hours of work! This is a large time investment and would be much larger if, for example, five variables were considered, so it makes sense to minimize the number of simulations carried out. With this in mind, only the end points of the range for each variable are used; namely, (2)(2)(2) = 8 simulations will be run. This still represents a significant investment of time but is more reasonable than the previous estimate. Essentially what is proposed is to carry out a 2^k factorial experiment (Neter and Wasserman [3]), where k is the number of decision variables (three for this case). In essence, each evaluation of the objective function (dependent variable) can be considered the result of an experimental run in which the independent variables (x, f, and p) are varied. The test matrix used is given in Table 14.7. The low range for each variable is designated 0, and the high range is designated 1. Thus, the run named DME011 represents the process simulation when the conversion is 0.7 (x is at its low value), fractional recovery is 0.995 (f is at its high value), and the pressure is at 16.7 bar (p is at its high value). For each of the eight cases shown in Table 14.7, a simulation was carried out and all equipment and operating costs determined. The results for these cases and the base case are also presented in Table 14.7.

Table 14.7. Test Matrix and Results for Three Variable Optimizations of DME Process

Run Number	Variable 1 = x 0 = 0.7 1 = 0.9	Variable 2 = f 0 = 0.983 1 = 0.995	Variable 3 = p 0 = 12.7 bar 1 = 16.7 bar	*FCI* ($1000)	Utilities ($1000/y)	*OBJ* (NPV) ($1000)
Base Case	0.8	0.989	14.7	1297	732	−7630
DME000	0.7	0.983	12.7	1378	782	−8136
DME001	0.7	0.983	16.7	1381	872	−8760
DME010	0.7	0.995	12.7	1393	780	−8152
DME011	0.7	0.995	16.7	1440	868	−8851
DME100	0.9	0.983	12.7	1210	539	−6130
DME101	0.9	0.983	16.7	1261	634	−6885
DME110	0.9	0.995	12.7	1232	537	−6160
DME111	0.9	0.995	16.7	1299	634	−6961

All figures based on 1996 data.

Once the results have been obtained, interpretation and determination of the optimum operating conditions must be carried out. The results in Table 14.7 are shown graphically in Figure 14.9. In this figure, the region over which the optimization has been considered is represented by a cube or box with each corner representing one of the test runs. Thus, the bottom left-hand front corner represents DME000, the top right-hand rear corner represents DME111, and so on. The values of the objective function are shown at the appropriate corners of the box. Also shown is the base-case simulation (for the conditions in Table B.11.1), which lies at the middle of the box (this is due to choosing the ranges for each variable symmetrically about the base-case value). First, analyze these results in terms of general trends using a method known as the **analysis of means**. Then fit a model for the objective function in terms of the decision variables, and use this to estimate the optimum conditions or, more correctly, to give direction as to where the next test run should be performed. This approach is termed a **response surface analysis** and is a powerful method to interpret and correlate simulation results.

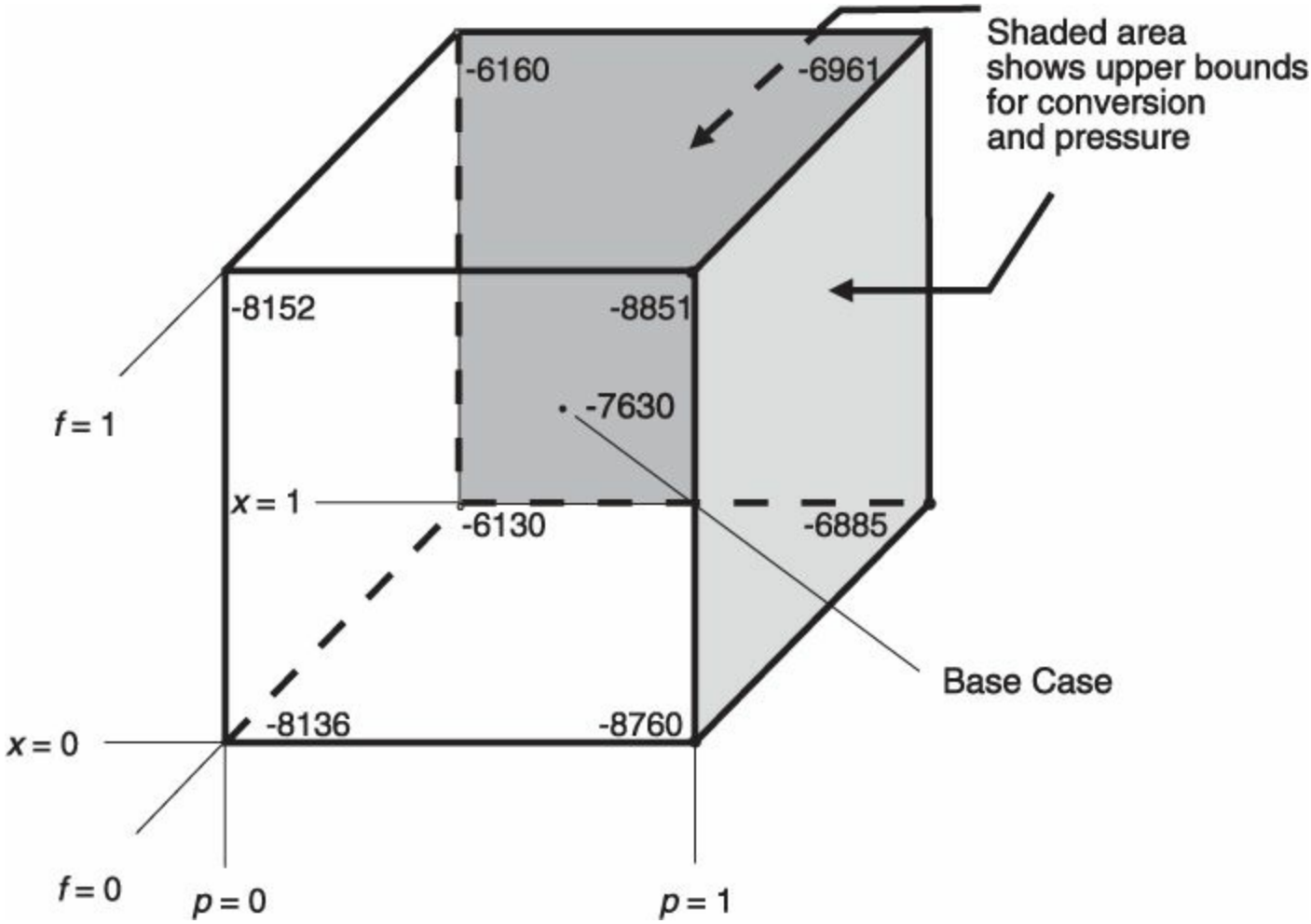


Figure 14.9. Results for Three-Variable Optimization on DME Process; Objective Function Values Are Shown at the Corners of the Test Cube

Sensitivity of Objective Function to Changes in Decision Variables: Analysis of Means. Using the data from Table 14.7 and Figure 14.9, estimate how a change in each variable affects the NPV. This is simply done by averaging all the results at a given value of one variable and comparing them with the average value at the other level of that variable. This yields the following results:

$$\text{Conversion, } x = 0.7,\ \text{NPV}_{avg,x=0} = (-8136 - 8760 - 8152 - 8851)/4 = -8475$$

$$\text{Conversion, } x = 0.9,\ \text{NPV}_{avg,x=1} = (-6130 - 6885 - 6160 - 6961)/4 = -6534$$

$$\text{Recovery, } f = 0.983,\ \text{NPV}_{avg,f=0} = (-8136 - 8760 - 6130 - 6885)/4 = -7478$$

$$\text{Recovery, } f = 0.995,\ \text{NPV}_{avg,f=1} = (-8152 - 8851 - 6160 - 6961)/4 = -7531$$

$$\text{Pressure, } p = 12.7 \text{ bar},\ \text{NPV}_{avg,p=0} = (-8136 - 8152 - 6130 - 6160)/4 = -7145$$

$$\text{Pressure, } p = 16.7 \text{ bar},\ \text{NPV}_{avg,p=1} = (-8760 - 8851 - 6885 - 6961)/4 = -7864$$

From these results, it can be concluded that the single-pass conversion has the greatest influence on the NPV, followed by the reactor pressure, with the recovery of DME having only a slight effect. Moreover, the results suggest that NPV will be maximized (least negative value) by using high conversion, low pressure, and low (within the range chosen) DME recovery. Although the maximum NPV that was obtained from these simulations was –$6,130,000 (DME100), it should not be assumed that this is the true maximum, or that the maximum lies within the range of decision variables considered thus far. In fact, the above analysis suggests a move to a new range for pressure and DME recovery.

In order to estimate the maximum for the objective function, further simulations at different conditions will need to be done. Use the results from Table 14.7 to choose the next values for the decision variables. From the results in Table 14.7 and Figure 14.9, it can be concluded that operating the reactor at the highest conversion allowable ($x = 0.9$) yields the optimum NPV and that reducing the reactor pressure also improves the NPV. Compared with these two effects, the recovery of DME is not very important, and it will be ignored for now. It should be noted that for the given topology of the flowsheet, all the DME produced in the reactor leaves as product, because the DME not recovered in T-201 simply gets recycled back to the reactor from the top of T-202. Thus, for this case, the DME recovery is not very important. However, this is usually not the case. By eliminating one decision variable from the search (f) and noting that another variable is constrained at its maximum value ($x = 0.9$), the problem has been reduced to a one-dimensional search (p). The question is, What should be the next value of p? Although p can be decreased by some arbitrary amount, it should be noted that there may be another constraint as p is lowered. In fact, in Section 14.4.2, a detrimental change in the NPV was identified when the pressure in T-201 became so low that refrigerated water was required as the utility for the overhead condenser. Noting the pressure drops through the system and control valves, the lowest pressure at which the reactor can be run and still operate T-201 at 9.0 bar, which is close to the lower limit for using cooling water, is $p = 10.7$ bar. Thus, the next simulation should be carried out at ($x = 0.9, f = 0.983, p = 10.7$).

Modeling the Objective Function in Terms of the Decision Variables. It is useful to be able to estimate NPV values for new conditions before actually running the simulations. This can be done by using the results from Table 14.7 to model the NPV as a function of x, f, and p. An infinite number of functional forms can be chosen for this model. However, the following form is chosen:

$$\text{NPV} = a_0 + a_1x + a_2f + a_3p + a_4xf + a_5xp + a_6fp + a_7xfp \qquad (14.3)$$

where $a_0, a_1, \ldots a_7$ are constants that are fit using the data from Table 14.7. This model uses eight arbitrary constants, which will allow the function to predict the NPV exactly at each corner point of the experimental design. In addition, this form of model is a simple multivariable polynomial, and the regression techniques to find $a_0, a_1, \ldots a_7$ are well established [3]. For these data, the following form for the objective function is obtained:

$$\text{NPV} = -63{,}254 + 55{,}556x + 49{,}448f + 3573p - 44{,}198xf - 3133xp - 3677fp + 3021xfp \qquad (14.4)$$

The accuracy of the model is tested by comparing the predictions of Equation (14.4) with all the data in Table 14.7. The results are shown in Table 14.8.

Table 14.8. Predictions of Model for *NPV* in Equation (14.4) with Data from Table 14.7

Test Run	Result from Table 14.7	Prediction from Equation (14.4)
Base Case	−7630	−7502
DME000	−8136	−8134
DME001	−8760	−8758
DME010	−8152	−8150
DME011	−8851	−8849
DME100	−6130	−6127
DME101	−6885	−6881
DME110	−6160	−6157
DME111	−6961	−6957

All figures are in $1000.

From the results in Table 14.8, it can be seen that the model predicts the eight test runs exactly (differences in the last significant figure are due to round-off errors in coefficients in Equation [14.4]) gives. The prediction for the base case is also good, although the model tends to underpredict the NPV a little. The expected value of NPV can also be predicted for the next simulation ($x = 0.9$, $f = 0.983$, $p = 10.7$), and Equation (14.4) gives NPV = –5750. The actual value for the NPV for this new simulation is –5947, which is higher than the predicted value by about 3%.

At this point, clearly the optimum is close. Whether further simulations are warranted depends on the accuracy of the estimate being used to obtain the costs and the extra effort that must be expended to analyze further simulations. If further refinement of the estimate of the optimum conditions is required, then the model, Equation (14.4), can be modified to include terms in p^2 and used to refine further the grid of decision variables. Alternative approaches for more comprehensive models are considered by Ludlow et al. [4].

One final point should be made. This problem is fairly typical of real design optimizations in that the optimum conditions lie on several of the constraints for the variables. Even though a simple polynomial model has been used to describe the NPV, Equation (14.4), which will tend to force the optimum to lie on the constraints, similar results would be obtained if nonlinear models had been used to describe the NPV.

14.5. Lattice Search Techniques versus Response Surface Techniques

For problems involving many decision variables, there are three types of parametric optimization techniques:

1. **Analytical Techniques Based on Finding the Location Where Gradients of the Objective Function Are Zero:** These are effective if the objective function is continuous, smooth, and has only a few local extrema. Sometimes the objective function can be approximated as a smooth function, and techniques exist to condition an objective function to reduce the number of extrema. However, for the common, complex problems encountered in flowsheet optimization, analytical techniques are usually ineffective.
2. **Response Surface Strategies Such as Those Discussed in Sections 14.2 and 14.4:** These can be used when the conditions required for analytical techniques are not met. However, one must

search the interior of the decision variable space extrema, which can be done by three-level (and higher-level) factorial designs [3, 4]. Fractional factorial designs are essential for higher-level and higher-dimensionality problems. As the dimensionality (number of decision variables) and the number of constraints increase, so does the probability that the optimum lies on the boundary of the allowable search space. This makes response surface techniques especially attractive.

3. **Pattern Search Techniques:** These are iterative techniques that are used to proceed from an initial guess toward the optimum, without evaluating derivatives or making assumptions about the shape of the objective function surface. From the initial guesses of the decision variables, a direction is chosen, a move is made, and the objective function is evaluated. If an improvement is detected, further moves are made in that direction. Otherwise, the search continues in a new direction. There are many strategies for choosing the search direction, deciding when to change direction, what direction to change to, and how far to move in each iteration. Crude methods of this type evaluate the objective function at each of the "nearest neighbor" points in each direction. The **Simplex-Nelder-Mead** [5] method uses $(n + 1)$ points when there are n decision variables to determine the next move. This is the smallest number of points that can give information about changes in the objective function in all directions. A related strategy is **simulated annealing** [6], in which all moves (good and bad) have nonzero probability of being accepted. Good moves are always accepted, and bad moves are accepted, but less frequently the larger the degradation in the objective function.

Both the pattern search and the response surface techniques allow the use of discrete decision variables. Topological changes can always be represented by changes in discrete decision variables (such as those defining the flowsheet topology), so these techniques can accommodate both parametric and topological optimization.

The response surface techniques are preferred during the early phases of design. They serve the multiple uses of prioritizing the decision variables, scoping the optimization problem to determine an estimate of the target improvement possible, and performing the parametric and topological optimizations.

14.6. Process Flexibility and the Sensitivity of the Optimum

Before any optimization result can be understood, one must consider the flexibility of the process and the (related) sensitivity of the result. A process must be able to operate with different feedstocks, under varying weather conditions (especially important for cooling utilities), over a range of catalyst activities, at different production rates, and so on. A process that is optimum for the "design" or "nameplate" conditions may be extremely inefficient for other operating conditions. The common analogy is a car that can operate at only one speed. Clearly, the design of the car could be optimized for this one condition, but the usefulness of such a car is very limited.

The **sensitivity of the optimum** refers to the rate at which the objective function changes with changes in one of the decision variables. Here, there is an apparent contradiction. Decision variables are chosen because the objective function is most sensitive to them, and therefore the process needs to be controlled very close to the optimum values of the decision variables to stay near the optimum. In fact, the objective function evaluations made during the optimization allow one to determine how precise the control must be and, most importantly, to determine the penalty for failure to control the decision variable to within prescribed limits. This is another of the interplays between optimization

and process control.

The effects of process sensitivity and flexibility can best be shown with a family of curves such as shown in Figure 14.6. Regardless of the techniques used to *find* the optimum, it is only through these visual representations that the results of optimization can be effectively conveyed to those who will use them. They are essentially performance curves for the process, where the performance is measured as the value of the objective function.

14.7. Optimization in Batch Systems

Unlike continuous systems, batch operations do not run under steady-state conditions, and their performance varies with time. As discussed in Chapter 3, the important issues with batch systems are the optimal scheduling of different equipment to produce a variety of products and the determination of optimal cycle times for batch processes. Therefore, the optimization of batch operations often involves determining the "best" processing time for a certain operation, the "best" time at which a certain action should take place, or the "best" distribution of actions over a period of time. The optimization of batch processes is, in itself, a very broad topic and certainly beyond the scope of this section of this chapter. Rather than try to address the many interesting problems in this field, the approach here is to illustrate several important concepts through the use of examples. The interested reader is encouraged to read further into this subject [7–10].

14.7.1. Problem of Scheduling Equipment

Consider a simple case of scheduling a set of equipment used to produce multiple products. For example, let us assume that there are three products of interest (A, B, C) manufactured from the same chemical feedstock F. The production of each of the three chemicals follows a different sequence and requires the use of different equipment (a reactor **R**, a separator **S**, and a precipitator **P**) for different periods of time. This information, along with relative feed and product prices, is shown in Table 14.9. The times shown in the table reflect the combined time required for filling, operating, emptying, and cleaning each piece of equipment for each product.

Table 14.9. Equipment Time Requirements for Products A, B, and C

Product	Time in Reactor (h)	Time in Separator (h)	Time in Precipitator (h)	Value of Product ($/kg Product)	Cost of Feed ($/kg Product)
A	7	4	0	0.75	0.25
B	15	3	3	1.12	0.27
C	25	4	2	1.41	0.23

The costs of the feeds are different for each product because of differences in process efficiencies. In general, the longer it takes to make a product, the more valuable the product. The question that must be answered is, How should the equipment be scheduled to maximize the revenue from the products?

Another complication in this type of scheduling problem is that the production steps are sequential: R→S→P. This means that when a reactor has finished producing a product, the separator should be available to carry out the next step in the process, and, similarly, the precipitator should be available when the separation has finished. This problem was chosen with the assumption that the separator and precipitator are always available to handle the products from the reactor, because the longest

processing time for a given piece of equipment is always shorter than the shortest time for the preceding operation (4 < 7, 3 < 4). For this case, the solution to the problem is simple because the only piece of equipment that must be considered is the reactor; the reaction step is the limiting step in each process.

Problem Formulation. Let the number of batches produced per year for Products A, B, and C be x_1, x_2, and x_3, respectively. Assuming the size of each batch is the same and equal to W kg, then the objective function for the optimization, which is the total profit, is

$$Maximize\ OF = Wx_1(0.75 - 0.25) + Wx_2(1.12 - 0.27) + Wx_3(1.41 - 0.23)$$

or

$$Maximize\ OF = 0.5\ Wx_1 + 0.85\ Wx_2 + 1.18\ Wx_3 \qquad (14.5)$$

The constraints for the problem relate to the total time for processing:

$$\left.\begin{array}{l} x_1 \geq 0 \\ x_2 \geq 0 \\ x_3 \geq 0 \end{array}\right\} \qquad (14.6)$$

$$7x_1 + 15x_2 + 25x_3 \leq (365)(24) = 8760 \qquad (14.7)$$

Equation (14.7) simply states that the equipment (reactor) is available 24 hours a day for the whole year. The solution of the problem is the maximization of Equation (14.5) subject to the constraints given in Equations (14.6) and (14.7). The solution is trivial, yielding that the optimum strategy is to make only chemical A with $x_1 = 1251$ batches per year and $OF = \$625.7W$.

Addition of Market Constraints. Now consider a slightly more realistic version of the problem. This time, consider the situation where market forces indicate that a maximum of 800 batches of A in a year can be sold and that to meet contractual obligations, at least 10 batches of B and 7 batches of C must be produced in a year. These additional constraints are given as

$$\left.\begin{array}{l} x_1 \leq 800 \\ x_2 \geq 10 \\ x_3 \geq 7 \end{array}\right\} \qquad (14.8)$$

The resulting solution is $x_1 = 800$, $x_2 = 199$, $x_3 = 7$, and $OF = \$577.4W$. Not surprisingly, the extra constraints have caused the OF to be reduced. This solution shows that after the contractual obligations have been fulfilled, and as much of Product A has been made as is allowed, as much of Product B as is allowed should be made. In other words, the order of profitable products is A > B > C.

Considering Other Equipment. Now look at the situation where the time taken to process the products through the other equipment becomes a limiting factor. To illustrate this type of problem, the basic problem is modified, as shown in Table 14.10.

Table 14.10. Equipment Time Requirements for Products A, B, and C for the Case When the Time for Separation and/or Precipitation Constrains the Solution

Product	Time in Reactor (h)	Time in Separator (h)	Time in Precipitator (h)	Value of Product ($/kg Product)	Cost of Feed ($/kg Product)
A	7	10	8	0.75	0.25
B	15	7	6	1.12	0.27
C	25	5	2	1.41	0.23

If the complication of sequencing of operations to allow a product to move through the system is ignored, for the moment, then the additional constraints imposed in Table 14.10 can be formulated as

Separator constraint $10x_1 + 7x_2 + 5x_3 \leq 8760$ (14.9)

Precipitator constraint $8x_1 + 6x_2 + 2x_3 \leq 8760$ (14.10)

Solving the problem including the market constraints given in Equation (14.8) results in $x_1 = 701$, $x_2 = 245$, $x_3 = 7$, and $OF = \$567.2W$. The results show that, with the inclusion of the constraints for the other equipment, it is no longer optimal to make as much of Product A as the market can handle, but, instead, making more of Product B is more profitable. If the values of x_1, x_2, and x_3 are substituted into the equipment time constraints (Equations [14.7], [14.9], and [14.10]), the result is

Reactor usage $7x_1 + 15x_2 + 25x_3 = 8757 \leq 8760$

Separator usage $10x_1 + 7x_2 + 5x_3 = 8760 \leq 8760$

Precipitator usage $8x_1 + 6x_2 + 2x_3 = 7092 \leq 8760$

It should be noted that the values for x_1, x_2, and x_3 have been rounded to the nearest integer, and, in fact, the total times for the reactors and separators are both 8760 hours. From these results, it is seen that the first two constraints meet the equality, but the constraint for the precipitator shows that this piece of equipment has spare capacity; it is not being used all the time. This spare capacity represents an inefficiency in equipment use and might be worth further investigation; however, some spare capacity is often desirable from an operability point of view. The fact that both the reactor and the separator are used all the time might create a scheduling problem when implementing the "optimal" mix of chemicals predicted by this latest solution. The reason for this is that, in general, when the times for different operations are not the same or not some simple multiple of each other and both pieces of equipment are used all the time, there will be periods of time when one or the other piece of equipment must sit idle. Hence, the true optimum would be less than that obtained by using this approach. This restriction could be eliminated by providing intermediate storage tanks between the different equipment that would allow each piece of equipment to operate all the time, as discussed in Chapter 3, Section 3.5.2. In this case, the optimum solution given for this problem can be realized, but there is an additional hidden cost of buying the intermediate storage tanks. Alternatively, by using multiple single-product campaigns, discussed in Chapter 3, this optimal solution might be obtainable. However, the implementation of single-product campaigns leads to the use of additional product storage and hence more capital investment.

The problem could have been formulated by specifying the constraints in terms of the total number of hours to produce a product. This would be given by

$$Maximize\ OF = 0.5\ Wx_1 + 0.85\ Wx_2 + 1.18\ Wx_3 \quad (14.11)$$

subject to the constraints in Equations (14.6) and (14.8), and

$$(7 + 10 + 8)x_1 + (15 + 7 + 6)x_2 + (25 + 5 + 2)x_3 \leq 8760 \quad (14.12)$$

or

$$25x_1 + 28x_2 + 32x_3 \leq 8760 \qquad (14.13)$$

The optimal solution to this problem is $x_1 = 0$, $x_2 = 10$, $x_3 = 265$, and $OF = \$321.2W$. The OF is considerably smaller than the previous solution. Moreover, if the total time that the reactor, separator, and precipitator are operating is evaluated, the following results are found:

Reactor usage $7x_1 + 15x_2 + 25x_3 = 6775 \leq 8760$

Separator usage $10x_1 + 7x_2 + 5x_3 = 1395 \leq 8760$

Precipitator usage $8x_1 + 6x_2 + 2x_3 = 590 \leq 8760$

Although this is certainly a valid solution, the separation and precipitation equipment sit idle most of the time. One possible way to sequence the operations for this solution is shown in Figures 14.10(a) and 14.10(b). The sequence for this solution would follow that shown in Figure 14.10(a) for (265)(32) = 8480 h, with the remaining period of (10)(28) = 280 h following the sequence shown in Figure 14.10(b). There are many ways to improve the profitability of the scheme shown in Figures 14.10(a) and 14.10(b). For example, it can be seen that a batch run for Product A could be squeezed into the schedule every time a batch of B or C is made. This is illustrated in Figures 14.10(c) and 14.10(d).

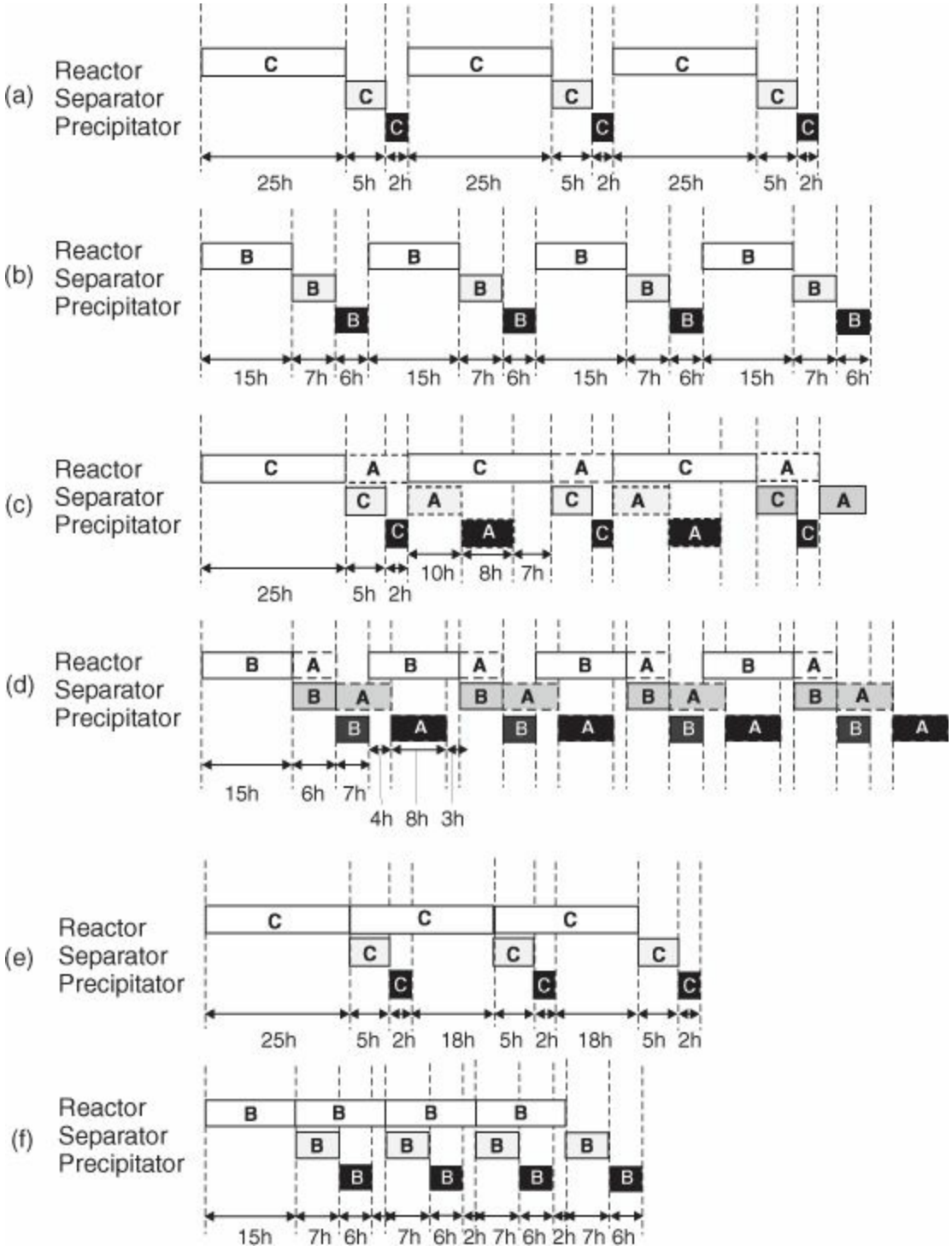


Figure 14.10. Different Configurations for Batch Scheduling Example

By making additional Product A, the value of OF increases from $\$321.4W$ to $321.4W + (265 + 10)(0.5)W = \$458.9W$. Moreover, the equipment usages increase to

Reactor usage $7(275) + 15(10) + 25(265) = 8700 \leq 8760$

Separator usage $10(275) + 7(10) + 5(265) = 4145 \leq 8760$

Precipitator usage $8(275) + 6(10) + 2(265) = 2790 \leq 8760$

An alternative change in the scheduling for this problem is illustrated in Figures 14.10(e) and 14.10(f). In this case, the idle time for the reactor is eliminated by implementing a batch of C or B as soon as the reactor becomes available. This essentially eliminates the reactor downtime. This saves 7 hours per batch of C and 13 hours per batch of B, leaving a period of (7)(265) + (13)(10) = 1985 hours of additional processing time during which more A, B, or C could be made. This same scheme could also be applied to Figure 14.10(d) by moving the sequence of events for producing Product B

to the left by 7 hours. This would again eliminate any downtime for the reactor and would free up another (7)(10) = 70 hours per year of time to make other products and additional profit.

Clearly, the possible sequences are numerous. In the above examples, reactor downtime could be eliminated, and a constraint was encountered. However, a different configuration could have been used as the starting point, such as producing only A and B, and a different constrained solution that might have been more profitable would have been reached. The optimum configuration is not intuitively obvious, nor is how to go about formulating and optimizing the problem. The problems in this section were all solved using the solver in Microsoft Excel that uses the generalized reduced gradient (GRG2) nonlinear optimization code. However, specialized software is available to help formulate and solve these types of batch scheduling problems. The software most often used in batch scheduling optimization solves mixed-integer, nonlinear programming (MINLP) problems [8]. The topic of batch scheduling has its roots in the field of operations research, which is a shared discipline of industrial and chemical engineers.

A final point of interest involves the degree of consolidation that is possible for batch scheduling problems and the degree that is desirable, which may be different from each other. For the simple example of three chemical products using three pieces of equipment, it was shown how to compress the scheduling so that the reactor is being used all the time. However, this puts an additional burden on the operators. For the cases shown in Figures 14.10(a) and 14.10(b), a single operator per shift might be able to cover all the operations (loading feed, monitoring, emptying product, cleaning equipment, etc.) required. However, as operations get squeezed together, more operators are needed, and errors, which are bound to happen on occasion, have a much greater effect on production. The trade-offs between efficient equipment usage and operability must be considered in order to develop robust and profitable operations.

14.7.2. Problem of Optimum Cycle Time

Another problem that arises in batch operations is the question, What is the optimal time to run a particular operation? For example, consider the simple case of a batch reactor producing a product via a first-order, irreversible reaction. The conversion of product follows a simple exponential relationship, as shown in Figure 14.11.

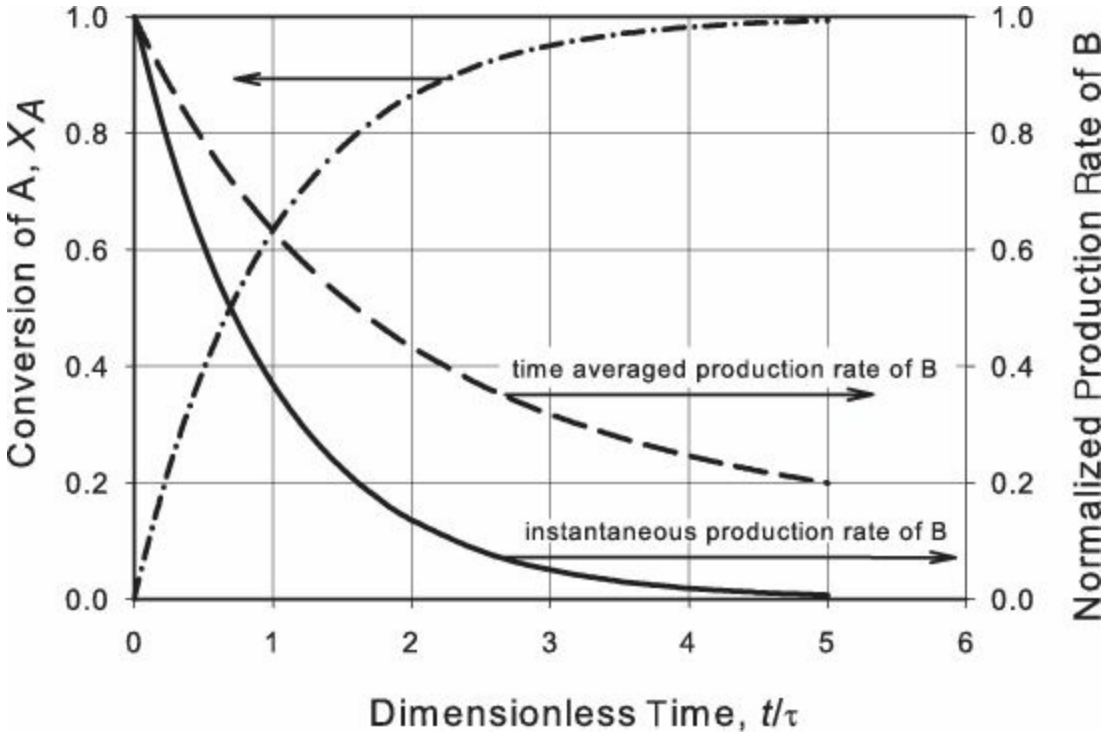


Figure 14.11. Conversion of A and Production of B for the Simple First-Order Reaction A→B as a Function of Dimensionless Time in a Batch Reactor

Therefore, the longer the material reacts, the more product is made. However, the rate at which product is formed slows with time, and the average production rate drops. These trends are shown by the curves plotted in Figure 14.11. Both the instantaneous and time-averaged production rate of Product B are seen to decrease with time. Because this is a batch operation, the optimal time to run the reaction must be determined. Because there are costs associated with cleaning and recharging feed to the equipment, these should be taken into account when determining the optimal cycle time for the batch.

Formulation of the Problem. Assume that the production of product in a liquid-phase batch reactor, in which A→B, follows a simple first-order, elementary reaction given by

$$N_B = VC_{A0}X_A = VC_{A0}\left[1 - \frac{C_A}{C_{A0}}\right] = VC_{A0}[1 - e^{-kt}] \qquad (14.14)$$

where N_B is the moles of Product B formed in the reactor after time = t, V is the volume of the batch reactor, C_{A0} is the concentration of reactant at time = 0, C_A is the concentration of reactant at time = t, and k is the reaction rate constant.

Let the value of the product be \$$x$/kmol, let the value of the reactant be \$$y$/kmol, and let the cost of cleaning and preparing the reactor for the next batch be \$$C_{clean}$. The time to clean and prepare the reactor for the next batch is t_{clean} and the reaction time is t_{react}. The cycle time, θ, is simply the sum of the cleaning and reaction time:

$$\theta = t_{clean} + t_{react} \qquad (14.15)$$

The objective function for this problem is the average "profit" over the cycle time, which is given by

$$OF = \frac{xN_B - y(VC_{A0} - N_B) - C_{clean}}{\theta} = \frac{N_B(x + y) - yVC_{A0} - C_{clean}}{t_{react} + t_{clean}} \qquad (14.16)$$

The numerator of Equation (14.16) is the profit from Product B minus the cost of unused reactant A

minus the cost of cleaning. The denominator is simply the total time for the cycle and thus averages the profit over the cycle time. This formulation of the *OF* assumes that the unused reactant is not recovered and recycled and that the cost of downstream processing (separation of B from A, and purification of B) is not affected by the extent of reaction. Both these assumptions should be relaxed if information about the downstream processes is available.

Substituting Equation (14.14) into Equation (14.16) and noting that $t = t_{react}$ yields

$$OF = \frac{(x + y)VC_{A0}[1 - e^{-kt}] - yVC_{A0} - C_{clean}}{t + t_{clean}} = \frac{A_1 - B_1 e^{-kt}}{C_1 + t} \qquad (14.17)$$

where

$$A_1 = (x + y)VC_{A0} - yVC_{A0} - C_{clean} = xVC_{A0} - C_{clean}$$

$$B_1 = (x + y)VC_{A0}$$

$$C_1 = t_{clean}$$

Differentiating the *OF* with respect to t and setting the derivative equal to 0 yields the following expression for $t_{opt} = t_{react,\ optimum}$:

$$(B_1 kC_1 + B_1 kt_{opt} + B_1)e^{-kt_{opt}} - A_1 = 0 \qquad (14.18)$$

The positive real root of this equation gives the optimum time to react the batch. An example to illustrate this optimization procedure is given in Example 14.7.

Example 14.7.

Determine the optimal batch reaction and cycle time for the first-order, irreversible reaction A→B using the following data and plot the *OF* [Equation (14.17)] as a function of θ.

$$V = 5\ \text{m}^3$$

$$C_{A0} = 2\ \text{kmol/m}^3$$

$$k = 0.3173\ \text{h}^{-1}$$

$$t_{clean} = 2\ \text{h}$$

$$x = \$700/\text{kmol}$$

$$y = \$400/\text{kmol}$$

$$C_{clean} = \$1200$$

$$A_1 = xVC_{A0} - C_{clean} = (700)(5)(2) - 1200 = 5800$$

$$B_1 = (\text{x} + \text{y})VC_{A0} = (400 + 700)(5)(2) = 11{,}000$$

$$C_1 = t_{clean} = 2$$

Substituting into Equation (14.18) yields

$$(B_1 kC_1 + B_1 kt_{opt} + B_1)_e^{-kt_{opt}} - A_1 =$$

$$[(11{,}000)(0.3173)(2) + (11{,}000)(0.3173)\text{t}_{opt} + 11{,}000]e^{-0.3173\text{t}_{opt}} - 5800 = 0$$

$$(6980 + 3490\text{t}_{opt} + 11{,}000)e^{-0.3173t_{opt}} - 5800 = 0$$

From this, t_{opt} = 6.0 h, t_{clean} = 2.0 h, and $\theta_{opt} = t_{clean} + t_{react} = 2.0 + 6.0 = 8.0$ h

A plot of the *OF* as a function of θ is shown in Figure E14.7.

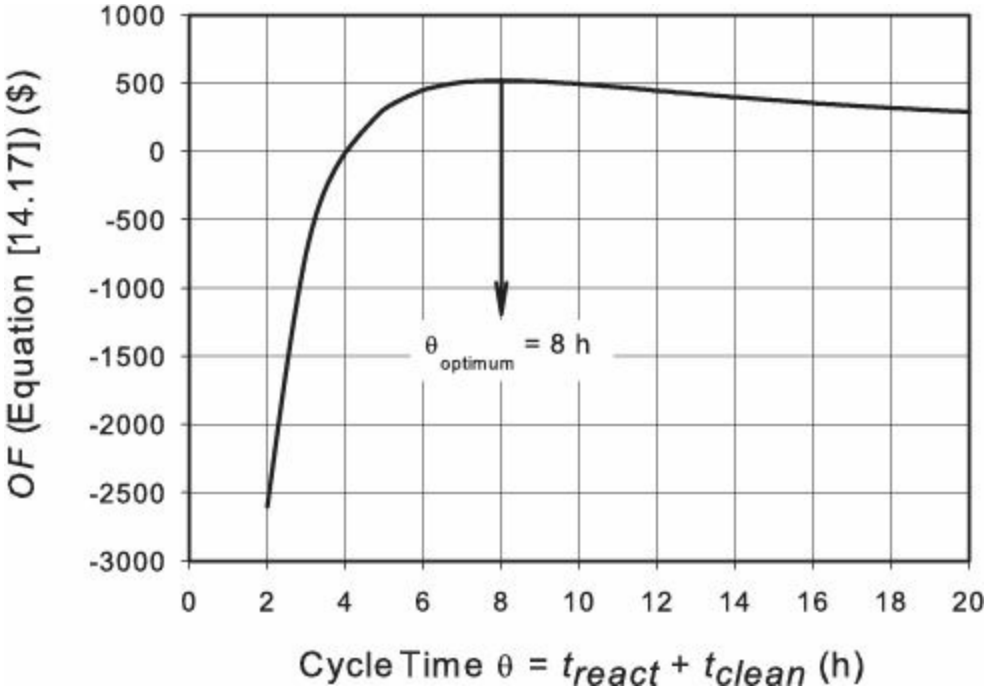


Figure E14.7. Results of Example 14.7 Showing the *OF* as a Function of Cycle Time

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Similar problems to the optimal cycle time for a batch reaction arise when considering the optimal cycle times for cleaning heat exchangers prone to excessive fouling or for cleaning filters.

14.8. Summary

In this chapter, several definitions commonly used in the area of optimization were introduced. In addition, the idea of applying a Pareto analysis to the base case was investigated. This type of analysis often reduces the number of decision variables that should be considered and the range over which the optimization should take place.

The differences between parametric and topological optimization were investigated, and strategies were suggested for each type of optimization.

The strategy for optimizing a process flowsheet using response surface concepts from the statistical design of experiments was introduced. The method was then illustrated using the DME flowsheet from Appendix B.

Finally, an introduction to the optimization of batch processes was given. Specifically, methods to determine the optimal mix of products in a multiproduct batch facility and the determination of optimum cycle time were covered.

What You Should Have Learned

- That anyone can perform optimization
- The definitions of *objective function* and *decision variable*
- That the general optimization procedure is base-case, topological, then parametric optimization
- The procedures for completing single-variable, two-variable, and multivariable optimization
- How optimization results should be represented

- How to approach the optimization of batch processes

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Short Answer Questions

1. Describe a Pareto analysis. When is it used?
2. What is the difference between parametric optimization and topological optimization? List one example of each.
3. What is an objective function? Give two examples of one.

Problems

4. In general, when using cooling water (cw) as a utility, the outlet temperature of the water leaving any process exchanger and returning to the cooling tower is limited to about 40°C to avoid excessive fouling in the process exchangers. In a series of laboratory experiments on fouling, the inlet cw temperature was fixed at 30°C, and the dimensionless fouling ratio was recorded for exit cooling water temperatures in the range of 36°C to 46°C.

Cooling Water Exit Temperature, °C	Dimensionless Fouling Ratio
36	1.11
38	1.05
40	1.00
42	0.86
44	0.74
46	0.64

The fouling ratio is simply the ratio of the time between scheduled cleanings of the exchanger tubes compared to the time required at 40°C. For example, if an exchanger with a cw exit temperature of 40°C requires cleaning once a year (12 months), then an exchanger with a cw exit temperature of 46°C requires cleaning every (0.64)(12) = 7.68 months. The advantage of using higher cw exit temperatures is that less cooling water flow is required; hence, the pumping costs for cw are lower. For a typical heat exchanger in a process with an exit cw temperature of 40°C, the yearly pumping and cleaning costs are $400/y and $2400/y, respectively. Using these costs and the information in the table above, determine the optimal cw exit temperature. Assume that the pumping costs are proportional to the flow of cooling water, that they include an amortized cost for the pump and the cost of electricity to run it, and that the cost of the heat exchanger is essentially unchanged for small differences in the cw exit temperature.

5. Consider the removal of condensable components from the reactor effluent stream of an acetone production process, shown in Figure P14.5. The removal process consists of a cooling water exchanger and a refrigerated water (rw) exchanger, as shown in the figure. For this problem, assume that a downstream acetone stripper will not be used, and all acetone and isopropyl alcohol (IPA) in Stream 5 will be lost and not recovered.

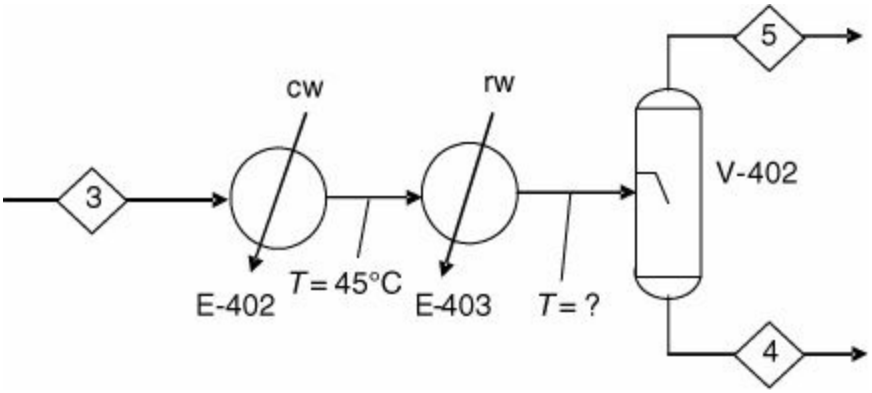


Figure P14.5. Recovery System for Problem 14.5

The composition and conditions of Stream 3 are givein the following table. The pressure drop through each exchanger is 0.14 bar. The purpose of the problem is to optimize the recovery of acetone and IPA in Stream 4 by determining the optimal size of heat exchanger E-403. The costs of E-402 and V-402 may be assumed to be fixed. Any acetone lost in Stream 5 should be valued at the equivalent cost of the IPA required to produce it, and the cost of IPA is given in Table 8.4.

Properties of Stream 3 in Problem 14.5	
Temperature (°C)	160
Pressure (bar)	1.91
Vapor fraction	1.0
Component mole flow (kmol/h)	
Hydrogen	34.78
Acetone	34.94
Isopropyl alcohol	3.86
Water	19.04

Determine the optimal recovery of IPA and acetone for this system using an objective function of the EAOC based on an 8000 h operating year. Any simulations should be carried out using a suitable process simulator using the UNIFAC *K*-value option and the latent heat enthalpy option. The overall heat transfer coefficient for E-403 may be taken as 200 W/m^{2}K. Utility costs should be obtained from Chapter 8, and the cost of E-403 is approximated by the following equation:

$$C_{TM}[\$] = 10{,}000\{A[m^2]\}^{0.6} \qquad \text{(P14.5)}$$

6. Consider the compression of feed air into a process that produces maleic anhydride, shown in Figure P14.6. The air enters the process at a rate of 10 kg/s at atmospheric pressure and 25°C. It is compressed to 3 atm in the first compressor. The compression is 65% efficient based on a reversible, adiabatic process. Prior to entering the second stage of compression (where the air is compressed to 9 atm at the same efficiency), the air flows through a water-cooled heat exchanger where the temperature is cooled to $T_{air,2}$.

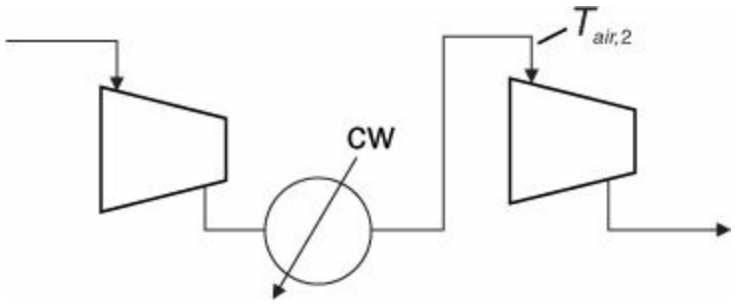


Figure P14.6. Two-Stage Compression for Problem 14.6

Assume that frictional pressure drops in the connecting pipes and in the exchangers are negligible. For the design of the exchanger, assume that

$$U = 42 \text{ W/m}^2\text{°C},\ T_{cw,in} = 30\text{°C}, \text{ and } T_{cw,out} = 40\text{°C}$$

For economic calculations, assume the following:

- The fixed capital investment is equal to the total module cost of the compressor (centrifugal), the compressor drive (electric), and heat exchanger (shell-and-tube, floating-head). The following equations should be used to evaluate these costs:

$$C_{TM,\,compr}[\$] = 12{,}500\{P[kW]\}^{0.68} \qquad \text{(P14.6.1)}$$

$$C_{TM,\,drive}[\$] = 600\{P[kW]\}^{0.9} \qquad \text{(P14.6.2)}$$

$$C_{TM,\,exch}[\$] = 2700\{A[m^2]\}^{0.82} \qquad \text{(P14.6.3)}$$

- Utility costs should be taken from Table 8.4, and use an electric drive efficiency of 95% and a

65% compressor efficiency.

- F factors should be calculated for the heat exchanger, and these will change as $T_{air,2}$ changes (see Chapter 15 for equations for F).
- Assume a hurdle rate of 8% and an equipment/project life of 5 years.

Using results from a simulator, determine the optimum size (area) of the heat exchanger and the corresponding value of $T_{air,2}$.

7. When pumping a liquid from one location to another, the diameter of the pipeline plays a critical role in determining the amount of power (electricity) required to pump the liquid. For a given flow of liquid, the amount of power required by the pump to move the liquid between locations decreases as the diameter of the pipe increases. However, the cost of the piping increases with diameter. Therefore, for a given flowrate of liquid and a given distance between locations, there exists an optimal pipe diameter that minimizes the cost of the system comprising the pump and pipe.

   It is required to find the optimal pipe diameter for a system through which 100,000 barrels per day of oil are pumped over a distance of 100 miles.

   The overall cost of the system includes the equipment costs (pump and piping), which are one-time purchases, and the operating cost (electricity for the pump), which occurs all the time. The time value of money must be taken into consideration when defining an objective function. For this project, it is desired to minimize the equivalent annual operating cost (EAOC) of the pump and piping system that is defined in Equation (P14.7.1):

$$EAOC[\$/y] = \sum_{i=1}^{2} PC_i[\$](A/P,i,n)[1/y] + UC[\$/y] \qquad \text{(P14.7.1)}$$

   where PC_i is the purchase cost of the pump and the pipe, and UC is the operating (utility) cost for the utilities (electricity to run the pump). Assume that the effective interest rate is 9% p.a. and that the length of the project, n, is 15 years.

   The relationships between the flowrate (Q) of oil, the pipe diameter (d_{pipe}), and the power required for the pump ($\dot{W}_{pump}$) are

$$\dot{W}_{pump} = \frac{32 f \rho Q^3 L_{pipe}}{\varepsilon_{pump} \pi^2 d_{pipe}^5} \qquad \text{(P14.7.2)}$$

   where ρ is the density of the fluid being pumped (930 kg/m^3), and ε_{pump} is the efficiency of the pump (assume this is 85%, or 0.85). Using SI units (m, s, kg), the units of power in Equation (P14.7.2) are Watts (W). Assume that the cost of electricity is \$0.05/kWh, where a kWh is the energy used in one hour by a device consuming 1 kW. Assume that the pump operates 24 h a day 365 days per year.

   In Equation (P14.7.2), the term f is the friction factor, which is a function of the flowrate and the pipe diameter and is given by Equation (P14.7.3):

$$\frac{1}{\sqrt{f}} = -4 \log\left[\frac{\varepsilon}{3.7 d_{pipe}} + \left\{\frac{6.81}{\mathrm{Re}}\right\}^{0.9}\right] \qquad \text{(P14.7.3)}$$

   where ε is the roughness of the pipe (assume a value of 0.045 mm),

$\text{Re} = \text{Reynolds number} = \dfrac{4Q\rho}{\pi d_{pipe}\mu}$, and μ is the viscosity of the oil (assume μ = 0.01 kg/ms).

The cost of the pump can be estimated using Equation (P14.7.4):

$$PC_{pump} = \$8000(\dot{W}_{pump}[\text{kW}])^{0.6} \qquad \text{(P14.7.4)}$$

The cost of piping is given by Equation (P14.7.5):

$$PC_{pipe}[\$/\text{ft of pipe}] = 10d_{pipe}[\text{inch}] + 2d_{pipe}^{1.4}[\text{inch}] \qquad \text{(P14.7.5)}$$

Present your final results as two plots. The first should show how each term in Equation (P14.7.1) changes with d_{pipe} (x-axis), and the second plot should show the EAOC (y-axis) as a function of d_{pipe} (x-axis). Explain the reason for the trends seen in each of these plots.

8. A liquid-phase biological reaction is used to produce an intermediate chemical for use in the pharmaceutical industry. The reaction occurs in a large, well-stirred bioreactor that is illustrated in Figure P14.8. Because this chemical is temperature sensitive, the maximum operating temperature in the reactor is limited to 65°C. The feed material is fed to the reactor through a heat exchanger that can increase the temperature of the reactants (contents of the reactor), which in turn increases the rate of the reaction. This is illustrated in Figure P14.8. The time spent in the bioreactor (space time) must be adjusted in order to obtain the desired conversion of reactant. As the temperature in the reactor increases, so does the reaction rate, and hence the size (and cost) of the reactor required to give the desired conversion decreases. It is desired to determine the optimal temperature at which to maintain the reactor (and to preheat the feed). The costs to be considered are the purchase cost of the reactor and heat exchanger and the operating cost for the energy to heat the feed.

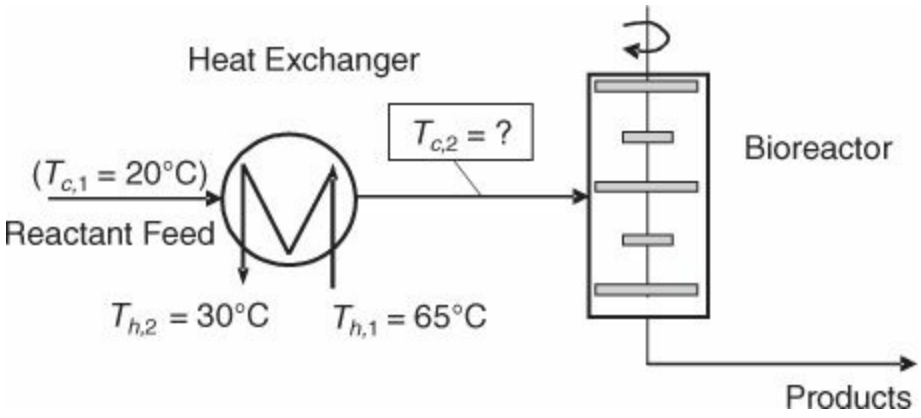


Figure P14.8. Process Flow Diagram of the Feed Preheater and Bioreactor

It is desired to optimize the preheat temperature for a flow of 5000 gal/h. The feed has the properties of water (ρ = 1000 kg/m^3, C_p = 4.18 kJ/kg°C) and enters the heat exchanger at a temperature of 20°C. Reactor feed is to be heated with a heating medium that is available at a temperature of 65°C and must leave the heat exchanger at 30°C. Therefore, the desired reactor inlet temperature is adjusted by changing the flowrate of the heating medium. The physical properties of the heating medium are ρ = 920 kg/m^3, and C_p = 2.2 kJ/kg°C.

The reaction rate for this reaction, $-r_A$, is given in terms of the concentration of reactant A (C_A) by the following equation:

$$-r_A = kC_A \qquad \text{(P14.8.1)}$$

where

$$k[s^{-1}] = 7\exp\left\{-\frac{3300}{T[K]}\right\} \qquad \text{(P14.8.2)}$$

The design equation for the reactor is given by

$$V = \frac{v_o X_A}{k(1 - X_A)} \qquad \text{(P14.8.3)}$$

where V is the reactor volume (m^3), υ_o is the volumetric flowrate of fluid into the reactor (m^3/s), and X_A is the conversion (assumed to be 80%, or 0.8, for this reaction).

The design equation for the heat exchanger is given by

$$Q = M_c C_{p,c}(T_{c,2} - T_{c,1}) = M_h C_{p,h}(T_{h,1} - T_{h,2}) = UAF\Delta T_{lm} \qquad \text{(P14.8.4)}$$

where

$$\Delta T_{lm} = \frac{(T_{h,2} - T_{c,1}) - (T_{h,1} - T_{c,2})}{\ln \dfrac{(T_{h,2} - T_{c,1})}{(T_{h,1} - T_{c,2})}} \qquad \text{(P14.8.5)}$$

and

$F = 0.8$ (assume that this is constant for all cases)

U = overall heat transfer coefficient = 400 W/m^2K

The optimal reactor inlet temperature is the one that minimizes the equivalent annual operating costs (EAOC) given by

$$EAOC[\$/y] = \sum_{i=1}^{2} PC_i[\$](A/P,i,n)[1/y] + UC[\$/y] \qquad \text{(P14.8.6)}$$

where PC_i is the purchase equipment cost for the heat exchanger and reactor and UC is the operating (utility) cost for the heating medium. For this problem use i = 7% p.a. and n = 12 years.

The purchase cost of the reactor is given by

$$PC_{reactor} = \$20{,}000V^{0.85} \qquad \text{(P14.8.7)}$$

where V is the volume of the reactor in m^3. The cost of the heat exchanger is

$$PC_{exchanger} = \$12{,}000\{A[m^2]\}^{0.57} \qquad \text{(P14.8.8)}$$

where A is the area of the heat exchanger in m^2. The cost of the heating medium is

$$UC[\$/h] = \$5\times10^{-6}Q[kJ/h] \qquad \text{(P14.8.9)}$$

Present your final results as two plots. The first should show how each term in Equation (P14.8.6) changes with $T_{c,2}$, and the second plot should show the EAOC (y-axis) as a function of $T_{c,2}$ (x-axis). Explain the reason for the trends seen in each of these plots.

9. A typical binary distillation column and related equipment are shown in Figure P14.9.

When designing distillation columns, it is common to optimize the column using the reflux ratio, R, as the decision variable. The overall cost of building the column and running it must be considered when optimizing the design. The capital investment (cost) for the equipment includes the cost of the column plus the costs of the reboiler, condenser, reflux drum, and reflux pump. For this project consider only the costs of the column and the two heat exchangers (reboiler and condenser). The operating costs include the cost of the cooling medium (water) for the condenser and the heating medium (steam) for

the reboiler. Because the equipment costs are one-time purchase costs and the operating costs (steam and water) occur all the time, the time value of money must be taken into consideration when defining an objective function. For this project it is desired to minimize the equivalent annual operating cost (EAOC) of the column that is defined in Equation (P14.9.1):

$$EAOC[\$/y] = \sum_{i=1}^{3} PC_i[\$](A/P,i,n)[1/y] + \sum_{i=1}^{2} UC_i[\$/y] \qquad \text{(P14.9.1)}$$

where PC_i is the purchase cost of the column and heat exchangers, and UC_i is the operating (utility) cost (cooling water and steam). Assume that the effective interest rate, i, is 8% p.a. and that the length of the project, n, is 10 years.

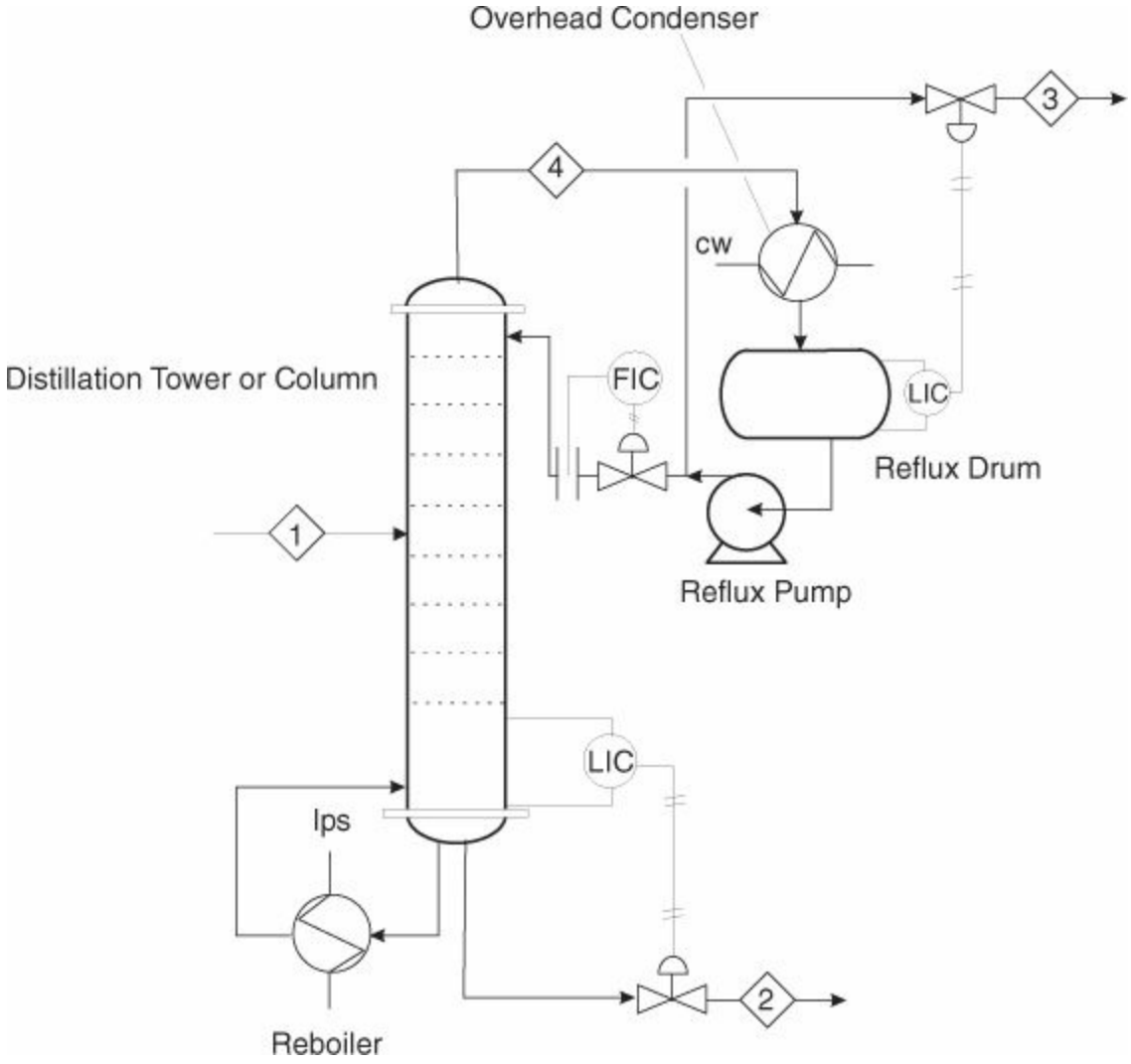


Figure P14.9. Illustration of the Main Pieces of Equipment Used in Distillation

It is desired to optimize a distillation column (calculate the value of R that minimizes the EAOC) to separate 1000 kmol/h of an equal molar feed of benzene and toluene into a top product containing 99.5 mol% benzene with a recovery of benzene of 98%. The recovery of benzene refers to the ratio of total amount (kmol) of benzene in the top product to that entering in the feed. The column is to operate at a pressure of 1 atm. y_i is defined as the mole fraction of benzene in the top stream, and x_i as the mole fraction of benzene in the bottom stream.

The relationship between the reflux ratio, R, and the number of stages or trays in the column, N, is given by the following relationships:

$$N_{min} \frac{\ln\left\{\frac{y_i}{x_i}\frac{1-x_i}{1-y_i}\right\}}{\ln \alpha} \quad \text{(P14.9.2)}$$

$$Y = \frac{N - N_{min}}{N + 1} \quad \text{(P14.9.3)}$$

$$R_{min} = \frac{2}{\alpha - 1} \quad \text{(P14.9.4)}$$

$$X = \frac{R - R_{min}}{R + 1} \quad \text{(P14.9.5)}$$

$$Y = 1 - \exp\left\{\left[\frac{1 + 54.4X}{11 + 117.2X}\right]\left[\frac{X - 1}{\sqrt{X}}\right]\right\} \quad \text{(P14.9.6)}$$

where α is the relative volatility of the benzene with respect to the toluene, which is equal to 2.3 for this system.

The costs of utilities for the overhead condenser (cooling water = cw) and reboiler (steam) are given by

$$UC_{cw}[\$/h] = \$3.54 \times 10^{-7} V \lambda_V \quad \text{(P14.9.7)}$$

$$UC_{steam}[\$/h] = 20 UC_{cw}[\$/h] \quad \text{(P14.9.8)}$$

where λ_V is the latent heat of vaporization (kJ/kmol) of benzene at its normal boiling point, and V (kmol/h) is the total vapor flow from the top of the column. The purchase cost of the column is given by

$$PC_{col} = \$10{,}000 V_{col}^{0.85} \quad \text{(P14.9.9)}$$

where $V_{col} = \pi D^2 L/4$ is the volume of the column in m^3 and D[m] and L[m] are the diameter and height of the column, respectively. The diameter and height of the column are given by

$$D[\text{m}] = 0.15(V[\text{kmol/h}])^{0.5} \quad \text{(P14.9.10)}$$

$$L[\text{m}] = N \quad \text{(P14.9.11)}$$

The purchase costs of the condenser and reboiler may be taken as 10% and 20% of the cost of the column, respectively.

Present your final results as two plots. The first should show how each term in Equation (P14.9.1) changes with R/R_{min}, and the second plot should show the EAOC (y-axis) as a function of R/R_{min} (x-axis). Explain the reason for the trends seen in each of these plots.

10. A chemical process recovers heat by transferring energy from a gas stream to a cold brine stream. During the heating of the brine, salts deposit on the heat-exchanger surfaces and cause significant fouling. The consequence of this fouling is that the heat transferred to the brine is reduced, causing additional heat, in the form of condensing steam, to be required later on in the process. A portion of a process flow diagram is shown in Figure P14.10.

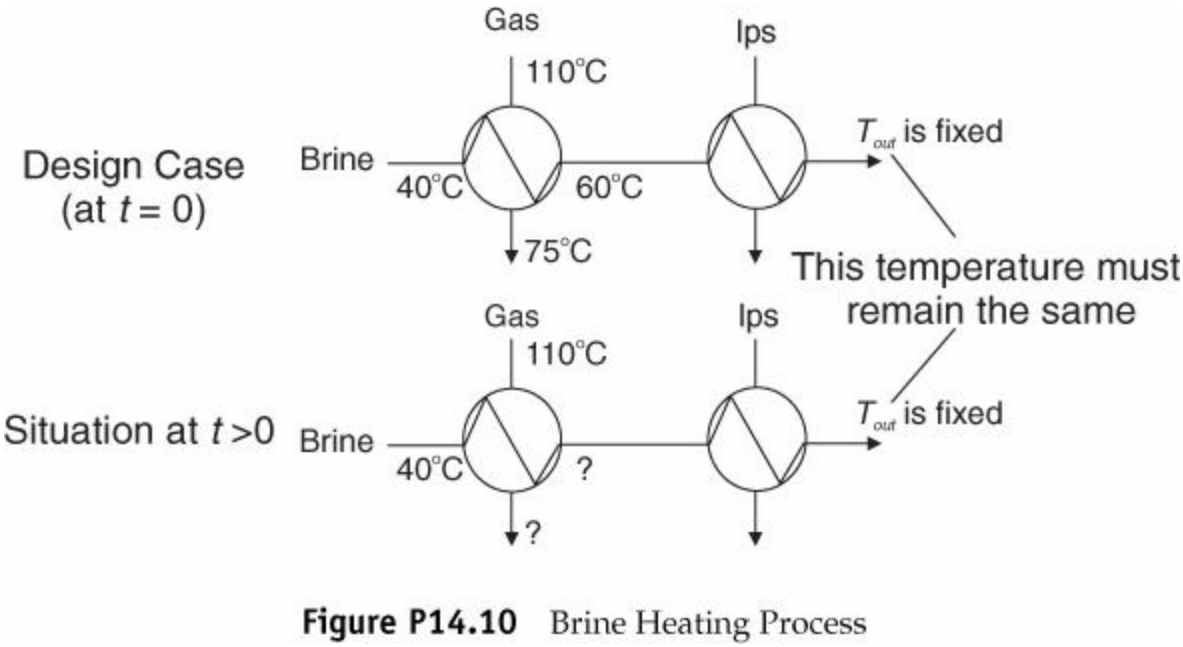


Figure P14.10 Brine Heating Process

It is known that the heat transfer coefficient for a brine/gas heat exchanger changes as the following function of time:

$$U = 75(1 - 0.12t) \text{ W/m}^2\text{°C}$$

where t is the time in months after cleaning the heat exchanger, and U is the overall heat transfer coefficient.

The cost of cleaning the exchanger is \$15,000, but there is no downtime for the process. At design conditions (unfouled exchanger surface), the flow of gas (c_p = 800 J/kg°C) is 40,000 kg/h, and the flow of brine (c_p = 4000 J/kg°C) is 14,000 kg/h. The gas enters the heat exchanger at a temperature of 110°C and leaves at 75°C. The brine enters the exchanger at 40°C and leaves at 60°C. The exchanger has an LMTD correction factor F = 0.9, which may be assumed not to change during the fouling process. If the flows and inlet temperatures of the streams remain constant, what is the optimal cycle time for cleaning the heat exchanger? Assume that as the brine outlet temperature drops from 60°C due to the fouling of the exchanger surface, additional low-pressure steam at a cost of \$8.00/GJ is used to heat the brine back to 60°C.

11. Consider the determination of the optimal cycle time for a batch reactor similar to that covered in Example 14.7. Repeat the analysis using the following parameters:

$$V = 7 \text{ m}^3$$

$$C_{A0} = 3 \text{ kmol/m}^3$$

$$k = 0.153 \text{ h}^{-1}$$

$$t_{clean} = 1.5 \text{ h}$$

$$x = \$350/\text{kmol}$$

$$y = \$200/\text{kmol}$$

$$C_{clean} = \$800$$

12. Consider the problem given in Example 14.7 for the case when the reaction is 2A→B and the reaction is second order with respect to A. Derive an expression, similar to Equations (14.19) and (14.20), for the optimal cycle time in terms of the relevant parameters.
13. Consider the following batch sequencing problem:

Two chemicals A and B are to be produced. Each chemical requires the use of a mixer/reactor and a separator unit. The amount of each product made in a batch is the same. The times required to make each chemical along with the value of each chemical are given in the table below.

Process Unit	Process to Make A	Process to Make B
Mixer/Reactor	6 h	8 h
Separator	7 h	6 h
Value of product	$2.3/kg	$4.0/kg
Cost of feed	$0.35/kg	$1.25/kg

Marketing predictions and forecasting suggest that any amount of A can be sold but that a maximum of 250 batches of B can be sold in a year.

a. Ignoring scheduling issues and assuming that both pieces of equipment can be run for all 8760 hours in a year, determine the optimal mix of Products A and B.

b. There is virtually no product storage available in the current plant, and once a batch is made it is sent directly to a tank car and shipped out. Can the answer from Part (a) be accommodated taking into account the scheduling of products without intermediate storage and without using single-product campaigns for A and B (see Chapter 3 for a discussion and an explanation of campaigns)? If the answer is no, then determine the optimum schedule and maximum profit.

c. Would your answers from Parts (a) and (b) change if there were no restriction on the amount of B that could be produced and sold?

14. Consider the problem described in the table below in which Products A, B, and C are made. The amount of each product made per batch is the same.

Product	Time in Reactor (h)	Time in Separator 1 (h)	Time in Separator 2 (h)	Value of Product ($/kg Product)	Cost of Feed ($/kg Product)
A	15	10	8	1.35	0.25
B	7	7	6	0.97	0.27
C	25	5	2	1.41	0.23

At least 50 batches of each product must be produced in a year, and each piece of equipment is available for the same 8000 hours a year.

a. Ignoring scheduling issues, determine the optimal mix of Products A, B, and C.

b. Can the answer from Part (a) be accommodated taking into account the scheduling of products without intermediate storage and without using single-product campaigns? (See Chapter 3 for a discussion and explanation of campaigns.)

15. Perform a parametric optimization for the second distillation column, T-202, in the DME process, Figure B.1.1, using reflux ratio and pressure as the independent variables and NPV as the objective function. You should follow the approach used in Section 14.4.2, which considered the first column, T-201, for this process.

16. For the DME process shown in Figure B.1.1, complete a parametric optimization for both columns when the order of separation is reversed. This means that the first column will remove water as a bottoms product and the second column will separate DME from methanol. The

approach used in Problem 14.15 should be followed here, with pressure and reflux ratio used as the independent variables and NPV as the objective function. Compare the results from Problem 14.15 with your results from this problem to determine which is the better separation sequence for the DME process.

17. For the DME column (T-201), find the operating pressure at which a switch from medium- to low-pressure steam (for use in the reboiler, E-204) yields an improvement in the NPV. Refer to Section 14.4.2 for a discussion of what costs to consider for this problem.

Chapter 15. Pinch Technology

What You Will Learn

- Pinch technology involves heat or mass integration.
- There are procedures for obtaining the "optimum" heat integration or mass integration network, and these methods are closely related.
- A method to design the minimum utility heat exchanger network using the minimumnumber of heat exchangers.

15.1. Introduction

Whenever the design of a system is considered, limits exist that constrain the design. These limits often manifest themselves as mechanical constraints. For example, a distillation of two components that requires 400 equilibrium stages and a tower with a diameter of 20 m would not be attempted, because the construction of such a tower would be virtually impossible with current manufacturing techniques. A combination of towers in series and parallel might be considered but would be very expensive. These mechanical limitations are often (but not always) a result of a constraint in the process design. The example of the distillation column given above is a result of the difficulty in separating two components with similar volatility. When designing heat exchangers and other unit operations, limitations imposed by the first and second laws of thermodynamics constrain what can be done with such equipment. For example, in a heat exchanger, a close approach between hot and cold streams requires a large heat transfer area. Likewise, in a distillation column, as the reflux ratio approaches the minimum value for a given separation, the number of equilibrium stages becomes very large. Whenever the driving forces for heat or mass exchange are small, the equipment needed for transfer becomes large and it is said that the design has a pinch. When considering systems of many heat- or mass-exchange devices (called **exchanger networks**), there will exist somewhere in the system a point where the driving force for energy or mass exchange is a minimum. This represents a pinch or pinch point. The successful design of these networks involves defining where the pinch exists and using the information at the pinch point to design the whole network. This design process is designed as pinch technology.

The concepts of pinch technology can be applied to a wide variety of problems in heat and mass transfer. As with other problems encountered in this text, both design and performance cases can be considered. The focus of this chapter is on the implementation of pinch technology to new processes for both heat-exchanger networks (HENs) and mass-exchanger networks (MENs). Retrofitting an existing process for heat or mass conservation is an important but more complicated problem. The optimization of such a retrofit must consider the reuse of existing equipment, and this involves extensive research into the conditions that exist within the process, the suitability of materials of construction to new services, and a host of other issues. By considering the design of a heat- (or mass-) exchange network for existing systems, the solution that minimizes the use of utility streams can be identified, and this can be used to guide the retrofit to this minimum utility usage goal.

The approach followed in the remainder of this chapter consists of establishing an algorithm for designing a heat- (mass-) exchanger network that consumes the **minimum** amount of **utilities** and

requires the **minimum number of exchangers (MUMNE)**. Although this network may not be optimal in an economic sense, it does represent a feasible solution and will often be close to the optimum.

15.2. Heat Integration and Network Design

Even in a preliminary design, some form of heat integration is usually employed. Heat integration has been around in one form or another ever since thermal engineering came into being. Its early use in the process industries was most apparent in the crude preheat trains used in oil refining. In refineries, the thermal energy contained in the various product streams is used to preheat the crude prior to final heating in the fired heater, upstream of the atmospheric column. Because refineries often process large quantities of oil, product streams are also large and contain huge amounts of thermal energy. Even when energy costs were very low, the integration of the energy contained in process streams made good economic sense and was therefore practiced routinely.

The growing importance of heat integration in the chemical process industries (CPI) can be traced to the large increase in the cost of fuel/energy starting in the early 1970s. The formalization of the theory of heat integration and pinch technology has been attributed to several researchers: Linnhoff and Flower [1], Hohmann [2], and Umeda et al. [3]. The approach used here follows that given by Douglas [4], and the interested student is encouraged to study this reference for additional insight into the broader concepts of energy integration.

It was shown in Chapter 2 that, as the PFD evolves, the need to heat and cool process streams becomes apparent. For example, feed usually enters a process from a storage vessel that is maintained at ambient temperature. If the feed is to be reacted at an elevated temperature, then it must be heated. Likewise, after the reaction has taken place, the reactor effluent stream must be purified, which usually requires cooling the stream, and possibly condensing it, prior to separating it. Thus, energy must first be added and then removed from the process. The concept of heat integration, in its simplest form, is to find matches between heat additions and heat removals within the process. In this way, the total utilities that are used to perform these energy transfers can be minimized, or rather optimized. Example 15.1 is presented to give the reader insight into the rationale for heat and energy integration.

Example 15.1.

Figure E15.1 shows two configurations for the DME reactor feed and effluent heat-exchange system. In both cases the feed enters from the left at 154°C; it is heated to 250°C prior to being fed into the adiabatic catalytic reactor, R-201. The same amount of reaction takes place in both configurations, and the reactor effluent is then cooled to 100°C prior to entering the separation section of the process. The only difference between the two systems is the way in which the heat exchange takes place. In Figure E15.1(a) the feed is heated with high-pressure steam and the effluent is cooled with cooling water. However, this does not make good economic sense. Because heat is generated in the reactor, it would make better sense to use this heat from the reaction to heat the reactor feed. This is what is done in Figure E15.1(b). The reactor effluent is partially cooled by exchanging heat with the cool, incoming feed. Compared with the configuration of Figure E15.1(a), the heat integration saves money in two ways: (1) The cooling water utility is reduced and the high-pressure steam is eliminated, and (2) heat exchanger E-203 is smaller because the duty is reduced, and E-202 is also smaller due to the fact that hps condenses at 254°C, which means the ΔT driving force in the exchanger is very small and the area is large. The economics for the two exchangers and utilities for both cases for a 10%

discount rate and a 10-year plant life are summarized in Table E15.1.

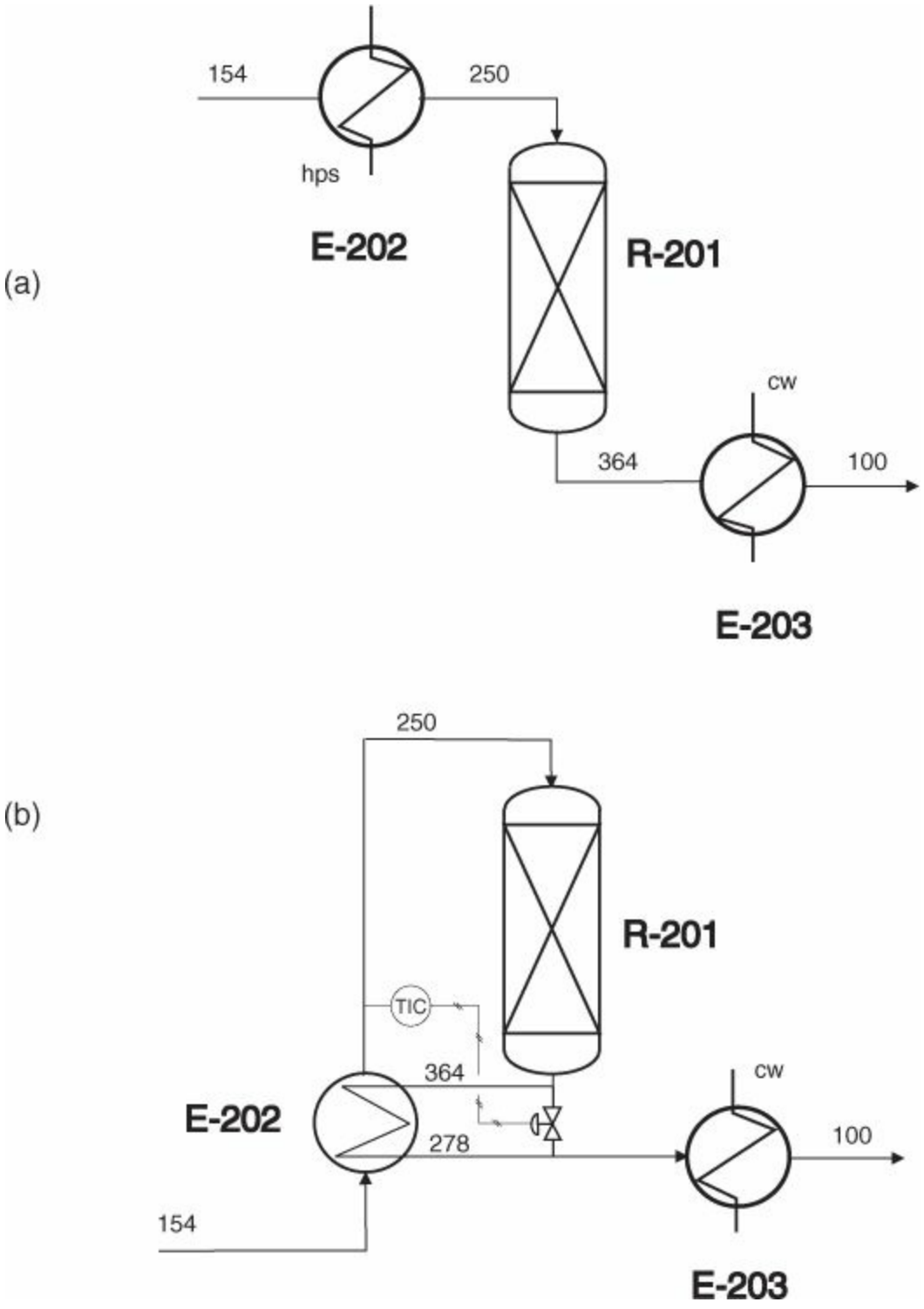


Figure E15.1. DME Reactor Feed and Effluent Heat-Exchange System (a) without Heat Integration and (b) with Heat Integration

Table E15.1. Cost Comparison for Example 15.1

	No Heat Integration	With Heat Integration
Fixed capital investment	$346,000	$244,600
Cost of utilities	–$210,000/y	–$36,820/y
Net present value	–$1,636,000	–$471,000

The savings received over the life of the plant by using heat integration are (–471,000 + 1,636,000) = $1,165,000!

From Example 15.1, it should be apparent that considerable savings are achieved by integrating heat within the process. Rather than try to implement this heat integration on an ad hoc basis, as in the example, a formal way of approaching these types of problems is presented.

The general algorithm is presented to give the minimum number of exchangers requiring the minimum utility requirements for a given minimum approach temperature. The algorithm to solve the minimum utility (MUMNE) problem consists of the following steps:

1. Choose a minimum approach temperature. This is part of a parametric optimization (see Chapter 14) because for every minimum approach temperature a different solution will be found.
2. Construct a temperature interval diagram.
3. Construct a cascade diagram, and determine the minimum utility requirements and the pinch temperatures.
4. Calculate the minimum number of heat exchangers above and below the pinch.
5. Construct the heat-exchanger network.

It is important to remember that the object of this exercise is to obtain a heat-exchanger network that exchanges the minimum amount of energy between the process streams and the utilities and uses the minimum number of heat exchangers to accomplish this. This network is almost never the optimum economic design. However, it does represent a good starting point for further study and optimization.

Each of the five steps given above is considered in detail as illustrated in Example 15.2.

Example 15.2.

In a process, there are a total of six process streams that require heating or cooling. These are listed below along with their thermal and flow data. A stream is referred to as "hot" if it requires cooling, and "cold" if it requires heating. The temperature of the stream is not used to define whether it is "hot" or "cold."

Stream No.	Condition	Flowrate, $\dot{m}$ (kg/s)	C_p (kJ/kg°C)	$\dot{m}C_p$ (kW/°C)	T_{in} (°C)	T_{out} (°C)	$Q_{available}$ (kW)
1	Hot	10.00	0.8	8.0	300	150	1200
2	Hot	2.50	0.8	2.0	150	50	200
3	Hot	3.00	1.0	3.0	200	50	450
4	Cold	6.25	0.8	5.0	190	290	–500
5	Cold	10.00	0.8	8.0	90	190	–800
6	Cold	4.00	1.0	4.0	40	190	–600
Total							–50

For this system, design the MUMNE network.

It should be noted that the overall heat balance for these streams yields a net enthalpy change of 50 kW. This does not mean that a heat-exchanger network can be designed to exchange heat between the hot and cold streams by receiving only 50 kW from a hot utility. This is because the analysis takes into account only the first law of thermodynamics, that is, an enthalpy balance. In order to design a

viable heat-exchanger network, it is also necessary to consider the second law of thermodynamics, which requires that thermal energy (heat) only flow from hot to cold bodies. As a consequence, the utility loads will, in general, be significantly higher than those predicted by a simple overall enthalpy balance.

Step 1: Choose a Minimum Approach Temperature. This represents the smallest temperature difference that two streams leaving or entering a heat exchanger can have. Typical values are from 5°C to 20°C. The value 10°C is chosen for this problem, noting that different results will be obtained by using different temperature approaches. The range of 5°C to 20°C is typical but not cast in concrete. Indeed, any value greater than zero will yield a viable heat-exchanger network. The effect of using different minimum approach temperatures on the economics of the process will be discussed in a later section. But the economic trade-offs are straightforward. As the minimum approach temperature increases, the heat transfer area for the process heat exchangers decreases, but the loads on the hot and cold utilities increase. Therefore, capital investment decreases but the operating costs increase. Methods for estimating the total surface area of the exchanger network and the equivalent annual operating cost of the network are discussed in a later section.

Step 2: Construct a Temperature Interval Diagram. In a temperature interval diagram, all process streams are represented by a vertical line, using the convention that hot streams that require cooling are drawn on the left-hand side and cool streams requiring heating are drawn on the right. The left- and right-hand axes are shifted by the minimum temperature difference chosen for the problem, with the right-hand side being shifted down compared with the left. The temperature interval diagram for Example 15.2 is shown in Figure 15.1. In this figure, each process stream is represented by a vertical line with an arrow at the end indicating the direction of temperature change. Horizontal lines are then drawn through the ends of the lines and divide the diagram into temperature intervals. For this problem, there are four temperature intervals. The net amount of available energy from all the streams in a given temperature interval is given in the right-hand column. The convention of (+) for excess energy and (–) for energy deficit is used. Thus, if the right-hand column contains a positive number for a given temperature interval, this implies that there is more than enough energy in the hot streams to heat the cold streams in that temperature interval. In addition, because the cold streams have been shifted down by the minimum approach temperature, energy can flow from left to right within a given temperature interval without violating the second law of thermodynamics. The summation of the numbers in the right-hand column is the net deficit or surplus enthalpy for all the streams, which for this example is –50 kW.

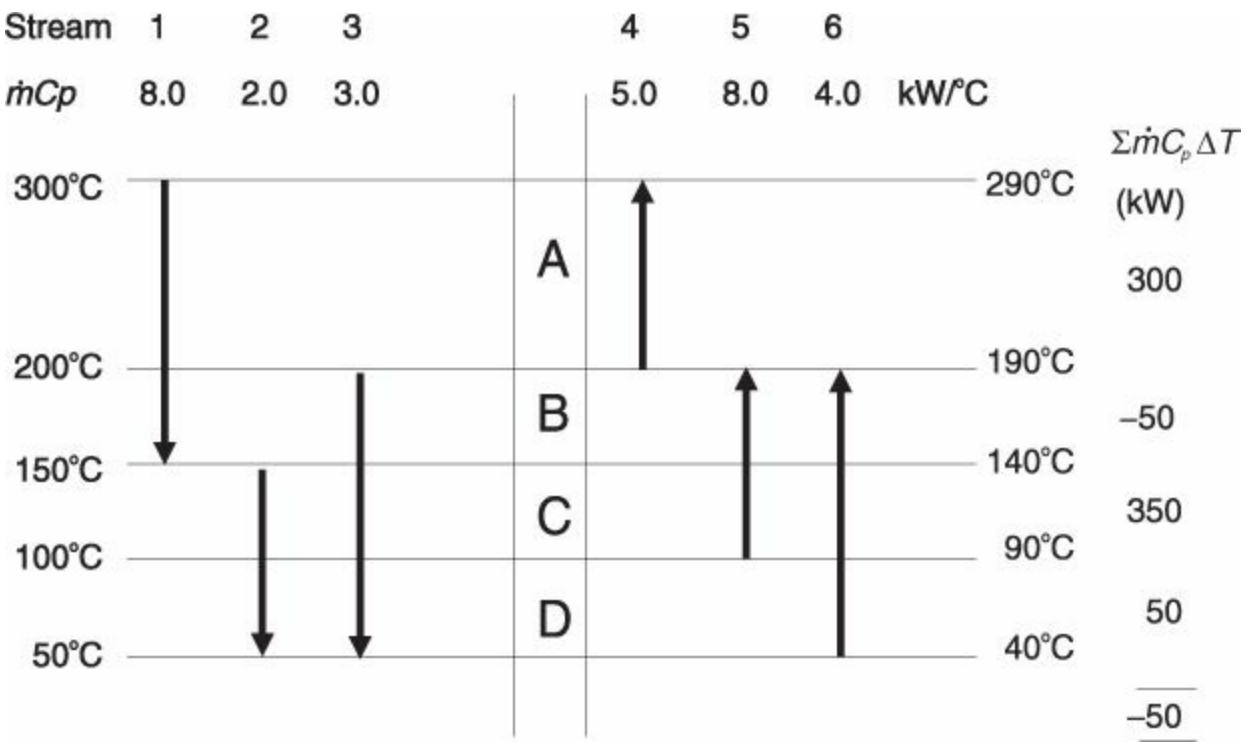


Figure 15.1. Temperature Interval Diagram for Example 15.2

Step 3: Construct a Cascade Diagram. The next step in the MUMNE algorithm involves constructing a cascade diagram like the one illustrated in Figure 15.2. The cascade diagram simply shows the net amount of energy in each temperature interval. Because energy can always be transferred down a temperature gradient, if there is excess energy in a given temperature interval, this energy can be **cascaded** down to the next temperature level. It should be noted that for systems in which only thermal energy is being transferred, excess energy cannot be transferred upward to a higher temperature interval. This is a result of the second law of thermodynamics—that transfer of energy up a temperature gradient is possible only if work is done on the system, for example, if a heat pump is used. Energy continues to be cascaded in this manner, and the result is shown in Figure 15.2. From the cascade diagram, it is evident that there is a point in the diagram at which no more energy can be cascaded down, and that energy most often must be supplied from the hot utility to the process. This point is represented by line a–b in the diagram. Below this line, the cascading process can continue; but, again, at some point, excess heat must be rejected from the process to the cold utility. The line a–b is termed the **pinch zone** or **pinch temperature**. By following the procedure described above, the minimum energy is transferred from the hot utility to the process and from the process to the cold utility. The proof of this is straightforward and is illustrated in Figure 15.3. Consider the situation in Figure 15.2 but now consider an additional transfer of energy, Q, from the hot utility to the process above the pinch. This energy must be cascaded down through the pinch and rejected from the process to the cold utility. This must be true, since a first-law balance on the system requires that the difference between the hot and cold utility demands be constant and equal to the difference in total enthalpies between the hot and cold streams (–50 kW for this example). Therefore, if heat is transferred across the pinch zone, the net result will be that more heat will have to be added from the hot utility and rejected to the cold utility. The criterion of not transferring energy across the pinch zone and cascading energy whenever possible guarantees that the energy requirements to and from the utilities will be minimized. From Figures 15.2 and 15.3, it can be concluded that the minimum utility requirements for this problem are 100 kW from the hot utility and 50 kW to the cold utility, with the net difference equal to –50 kW, which is consistent with the overall enthalpy balance. The pinch

temperatures are 100°C and 90°C for the hot and cold streams, respectively.

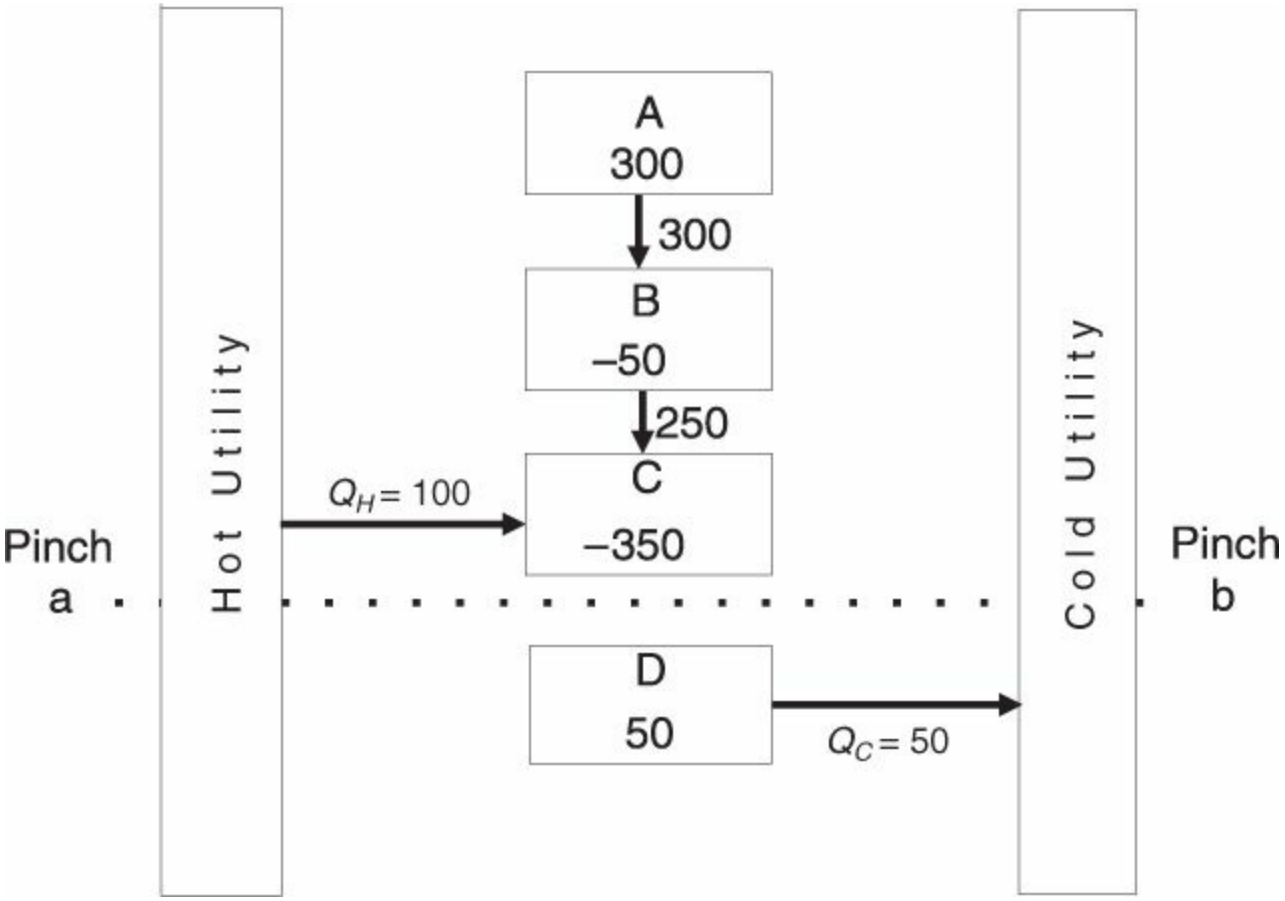


Figure 15.2. The Cascade Diagram for Example 15.2

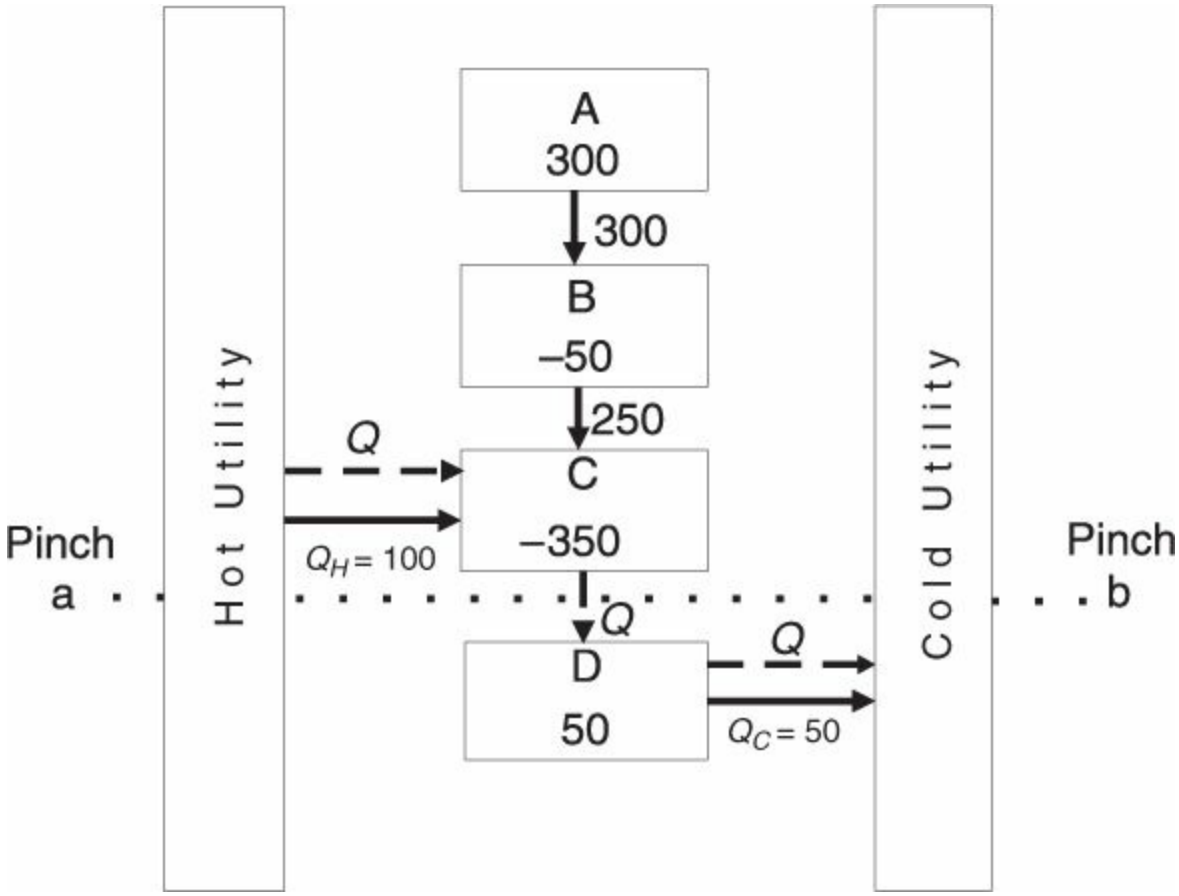


Figure 15.3. The Effect of Transferring Energy through the Pinch

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To minimize the hot and cold utility requirements, energy should not be transferred

across the pinch.

At this point, it is important to note that not all problems have a pinch condition. The cascade diagrams for two situations that do not have a pinch are illustrated in Figure 15.4. In Figure 15.4(a), heat is only cascaded downward or rejected to the cold utility. The conditions of the hot and cold streams are such that after cascading energy downward, either there is an excess of energy or the energy is exactly balanced in every temperature interval. In this situation, there is no need to supply energy from the hot utility to the process. In Figure 15.4(b), the opposite situation exists. In this case, heat is only cascaded downward or supplied from the hot utility. The conditions of the hot and cold streams are such that after cascading energy downward, either there is an energy deficit, or the energy is exactly balanced in every temperature interval. In this situation, there is no need to reject energy from the process to the cold utility. Although much of the remaining discussion focuses on processes that have a pinch, the approach for designing the MUMNE network remains essentially the same.

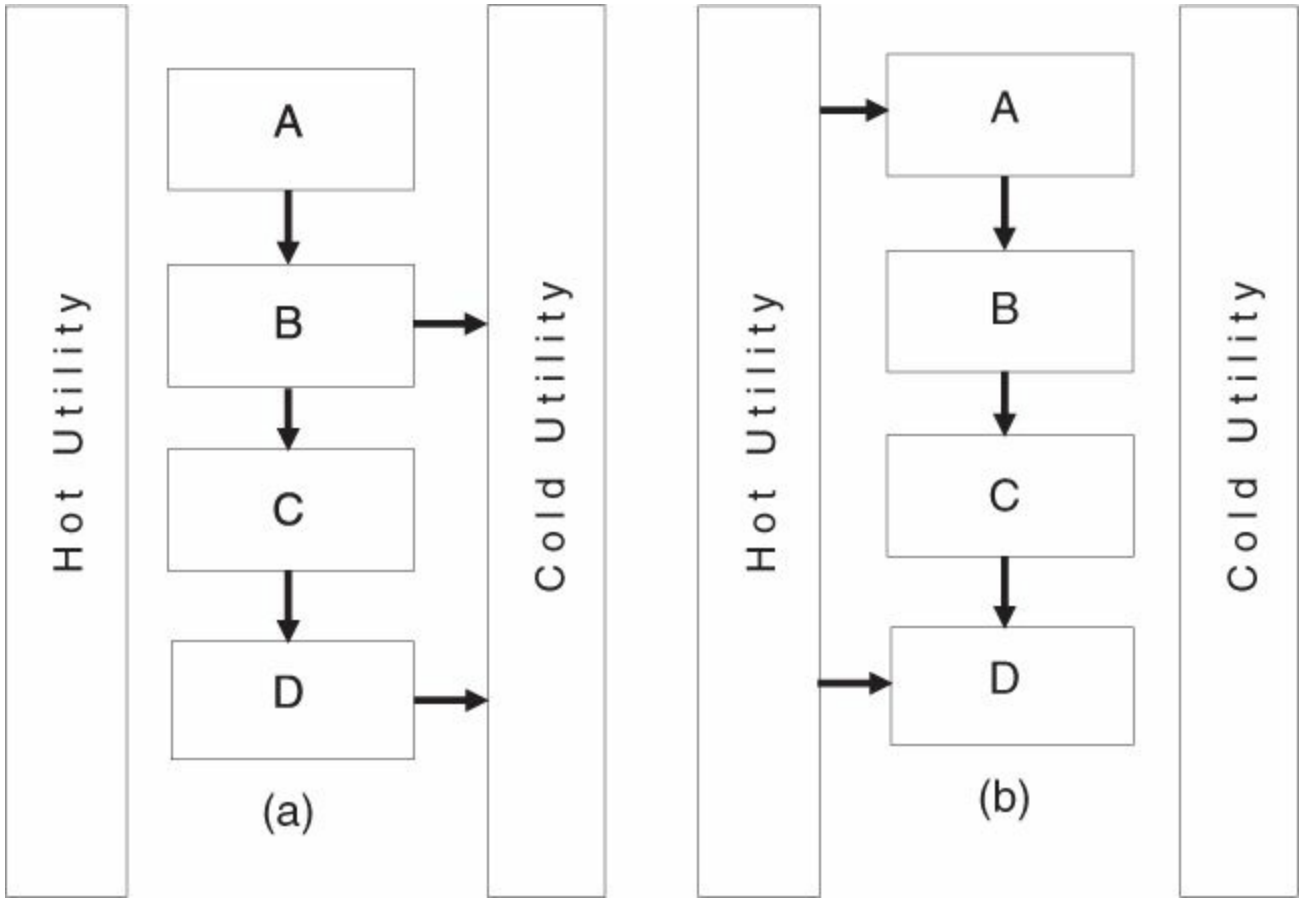


Figure 15.4. Examples of Cascade Diagrams for Problems without a Pinch

Step 4: Calculate the Minimum Number of Heat Exchangers. Once the pinch temperatures have been found from Step 3, it is necessary to find the minimum number of heat exchangers required to carry out the heat transfer for the minimum utility design. From this point on, the heat transfer problem will be split into two, and above and below the pinch will be considered as separate systems.

Above the Pinch. The easiest way to evaluate the minimum number of heat exchangers required is to draw boxes representing the energy in the hot and cold process streams and the hot utility as shown at the top of Figure 15.5. Energy is now transferred from the hot streams and hot utility to the cold streams. These energy transfers are indicated by lines, with the amount of energy transferred shown to the side of the lines. Clearly, all the energy in the hot streams and utilities must be transferred to the cold streams. For each line drawn, one heat exchanger is required; thus, by minimizing the number of

lines, the number of heat exchangers is minimized. It should be pointed out that although the number of heat exchangers equals the number of connecting lines, the lines drawn at this stage may not represent actual heat exchangers. The actual design of an exchanger network is covered in Step 5.

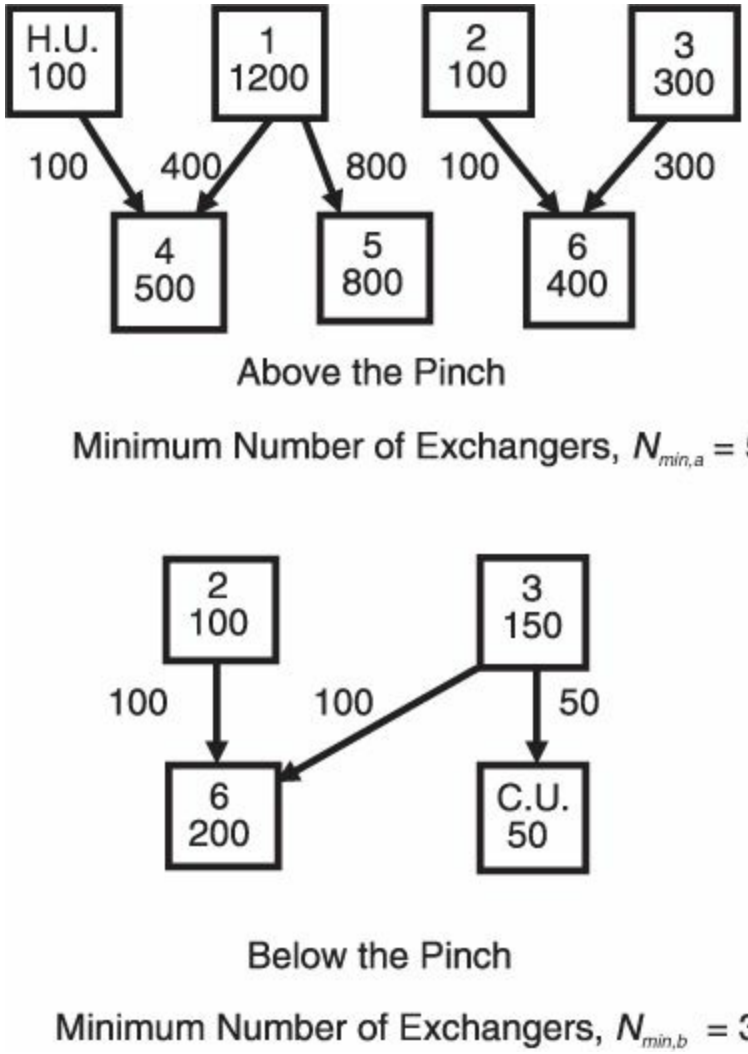


Figure 15.5. Calculation of Minimum Number of Exchangers for Example 15.2

Below the Pinch. The same method is used to calculate the minimum number of exchangers below the pinch. The diagrams for above and below the pinch are shown in Figure 15.5, and from this it can be seen that five exchangers are required above the pinch and three below the pinch, or a total of eight heat exchangers for the entire network.

From Figure 15.5, it can be seen that above the pinch, the problem is split into two subproblems. This split is possible because the energy in two of the hot streams (Streams 2 and 3) exactly matches the energy requirement of one of the cold streams (Stream 6). Below the pinch, such a partition of the problem is not possible. Such exact matches between groups of hot and cold streams are often not possible, and if such matches do not exist, then for a given problem, above or below the pinch, the following relationship can be written:

$$\text{Min. No. of exchangers} = \text{No. of hot streams} + \text{No. of cold streams} + \text{No. of Utilities} - 1 \quad (15.1)$$

The result in Equation 15.1 is consistent with the result in Figure 15.5 for below the pinch.

For systems without a pinch, the same approach for the minimum number of exchangers as described above can be used, but the problem no longer needs to be split into two parts. For the case considered here, assuming that the problem did not have a pinch (and hence only one utility is required) and that Equation 15.1 is applicable,

Minimum number of exchangers = 3 + 3 + 1 – 1 = 6

Step 5: Design the Heat-Exchanger Network. Again, the systems above and below the pinch are considered separately.

Design above the Pinch. To start, draw the temperature interval diagram above the pinch, Figure 15.6. The algorithm used to design the network starts by matching hot and cold streams at the pinch and then moving away from the pinch.

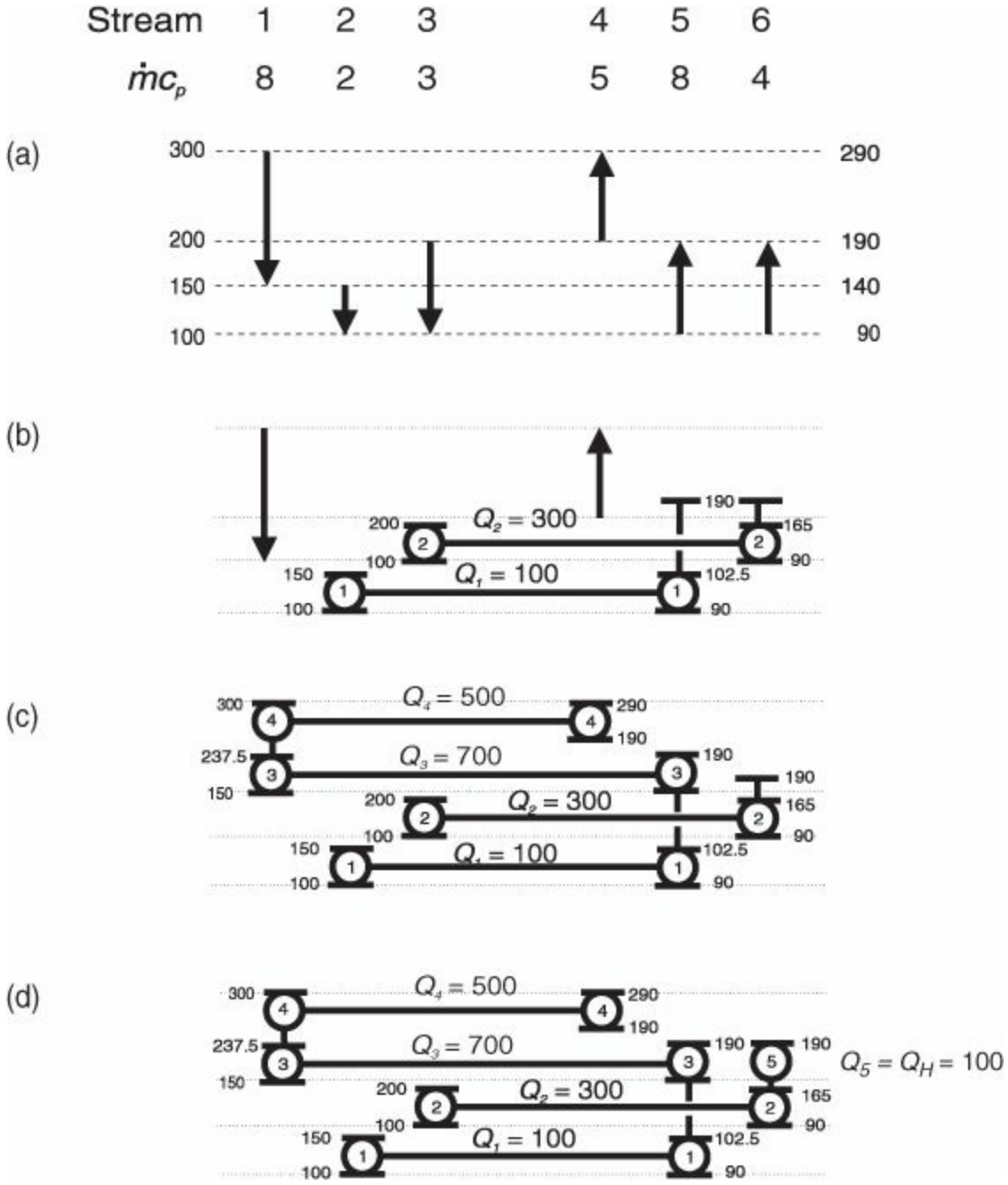


Figure 15.6. Design of Heat-Exchanger Network above the Pinch Zone for Example 15.2

Design at the Pinch. For streams at the pinch, match streams such that $\dot{m}c_{p,hot} \leq \dot{m}c_{p,cold}$. Using this criterion ensures that ΔT_{min} from Step 1 is not violated. Figure 15.6(a) shows that Stream 2 or 3 can be matched with Stream 5 or 6. Note that, for this step, only streams that are present at the pinch temperature are considered. The next step is to transfer heat from the hot streams to the cold streams by placing heat exchangers in the temperature diagram. This step is shown in Figure 15.6(b). There are two possibilities when matching streams at this point: Exchange heat between Streams 2 and 5

and between Streams 3 and 6, or exchange heat between Streams 2 and 6 and between Streams 3 and 5. Only the first combination is shown in Figure 15.6(b). A heat exchanger is represented by two circles connected by a solid line; each circle represents a side (shell or tube) of the exchanger. It is important to exchange as much heat between streams as possible. The temperatures of the streams entering and leaving the exchangers are calculated from an enthalpy balance. For example, consider the enthalpy change of Stream 5 as it passes through Exchanger 1. The total heat transferred is Q_1 = 100 kW and $\dot{m}c_{p,5} = 8$; therefore, the temperature change for Stream 5, $\Delta T_5 = 100/8 = 12.5°C$. Thus, the temperature change for Stream 5 through Exchanger 1 is 90°C to 102.5°C, as shown in Figure 15.6(b).

Design Away from the Pinch. The next step is to move away from the pinch and look at the remaining hot and cold streams. There are several ways in which heat may be exchanged from Stream 1 (the only remaining hot stream) and the three cold Streams 4, 5, and 6. The criterion for matching streams at the pinch does not necessarily hold away from the pinch; however, it is important to make sure that when the network is designed the following constraints are not violated:

1. A minimum approach temperature of 10°C, set in Step 1, is used throughout the design.
2. Only five exchangers are used for the design above the pinch, as calculated in Step 3.
3. Heat is added from the coolest possible source. (This is explained in more detail in the section on problems with multiple utilities.)

The matching of streams and the final design of the network are shown in Figures 15.6(c) and 15.6(d). From these figures, it is clear that there is a design with five heat exchangers, the minimum approach temperature is nowhere less than 10°C, and that heat is added to the process at the lowest temperature consistent with this system, that is, 190°C.

Design below the Pinch. The approach for the design below the pinch is similar to that described for above the pinch. Start at the pinch and match streams, and then move away from the pinch and match the remaining streams. The temperature interval diagram below the pinch is shown in Figure 15.7(a).

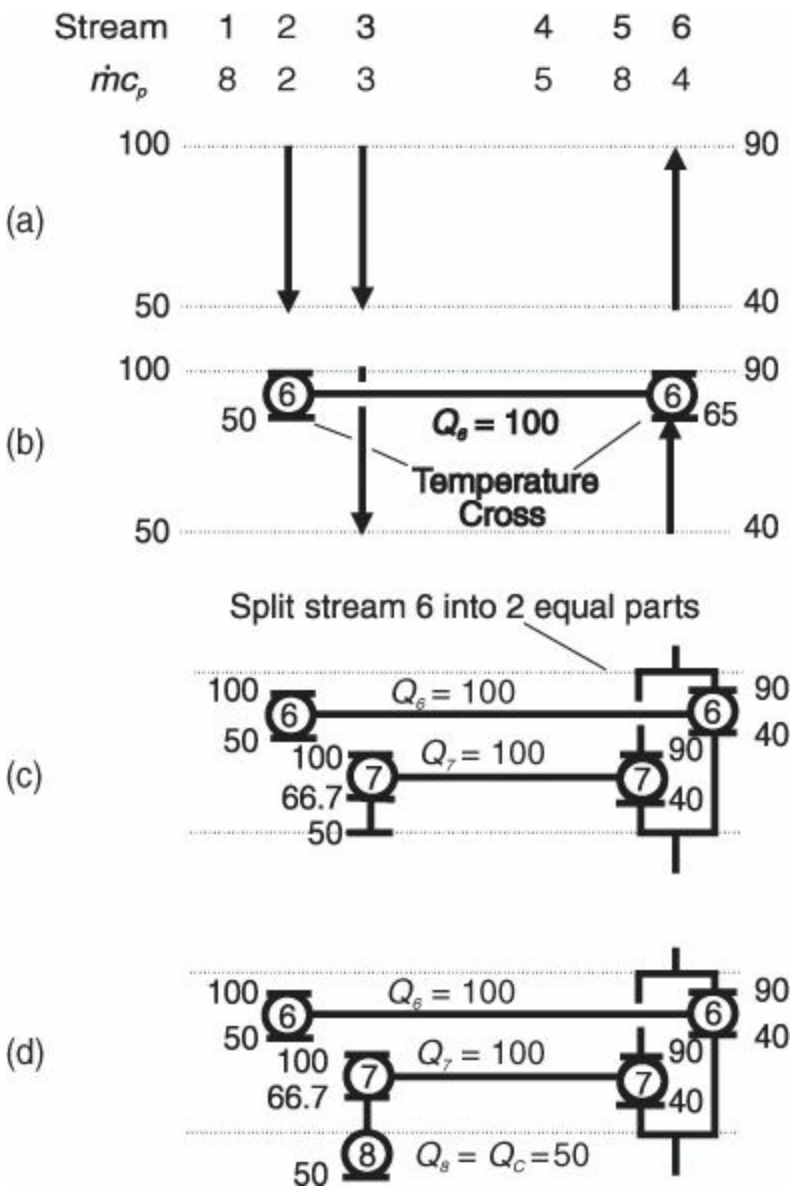


Figure 15.7. Design of Heat-Exchanger Network below the Pinch Zone for Example 15.2

Design at the Pinch. For streams at the pinch, match streams such that $\dot{m}cp,hot \geq \dot{m}c_{p,cold}$. Using this criterion ensures that ΔT_{min} from Step 1 is not violated. Figure 15.7(a) shows that for the three streams at the pinch this criterion cannot be met. This problem can be overcome by splitting the cold Stream 6 into two separate streams. However, before considering this, examine what happens by trying to match streams that violate the above condition. In Figure 15.7(b), Stream 2 is matched with Stream 6. The net result is impossible because it would cause a temperature cross in the exchanger, and that violates the second law of thermodynamics. To maintain the minimum temperature approach set in Step 1, Stream 6 is split into two equal streams, each having an $\dot{m}c_p = 2.0$. These split streams can now be matched with hot Streams 2 and 3 without violating the criterion above. The net result is shown in Figure 15.7(c), from which it can be seen that the minimum temperature difference is always greater than or equal to 10°C. It should be noted that Stream 6 could be split in a number of ways to yield a viable solution. For example, it could be split into streams with values of 3 and 1.

Design Away from the Pinch. The final step is shown in Figure 15.7(d), where the third exchanger is added to transfer the excess heat to the cold utility.

The final heat-exchanger network is shown in Figure 15.8. The exchangers are represented by single circles, with fluid flowing through both sides. This network has the minimum number of heat

exchangers, eight, for the minimum utility requirements, $Q_H = 100$ kW and $Q_C = 50$ kW, using a minimum approach temperature, $\Delta T = 10°C$. As mentioned earlier, different results will be obtained by using different minimum approach temperatures.

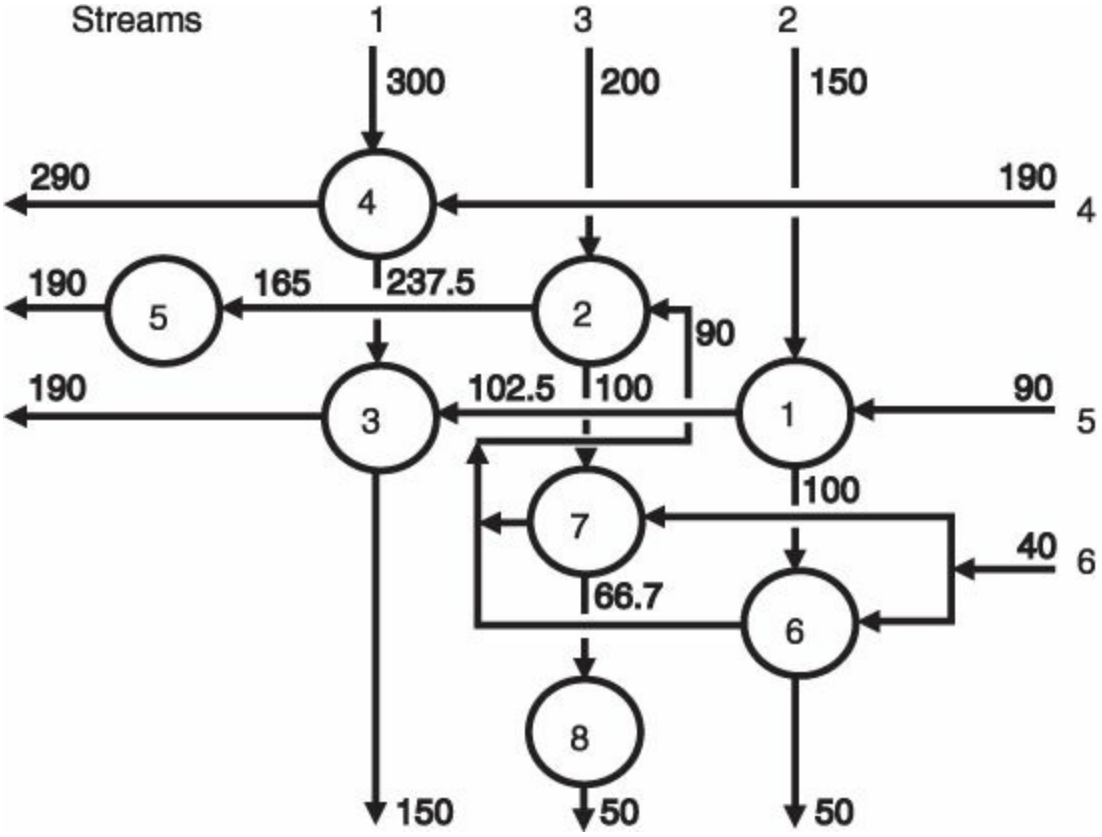


Figure 15.8. MUMNE Network for Example 15.2

To this point, the emphasis has been on the topology of the exchanger network, that is, the interaction between the different streams required to give the minimum utility case. In order to complete the design, it is necessary to estimate the heat transfer area of the exchanger network, which in turn allows a capital cost estimate to be made. If heat transfer coefficients for the heat exchangers in Figure 15.8, including appropriate fouling coefficients, are known, then the size of the exchangers can be calculated. Film heat transfer coefficients may be estimated using typical heat transfer coefficients from Table 11.11, previous data on similar streams, published data on similar streams, or values calculated from standard methods. For example, the Sieder-Tate equation [5] could be used for the tube side and the Donahue equation [6] for the shell side, along with the fluid properties and typical fluid velocities. The heat transfer areas calculated from such estimates will give a good indication of the heat transfer areas required for the overall exchanger network. Such data are suitable for cost estimates using the CAPCOST program. This procedure is illustrated in Examples 15.3 and 15.4.

Example 15.3.

An estimate of the individual film heat transfer coefficients for the hot and cold streams in Example 15.2 are given in Table E15.3. These film coefficients include appropriate fouling factors for the streams.

Table E15.3. Film Heat Transfer Coefficients for Streams in Example 15.2

Stream	Film Heat Transfer Coefficient, W/m²°C
1	400
2	270
3	530
4	100
5	250
6	80

Using the information in Table E15.3, calculate the heat transfer areas for the process-process heat exchangers given in the exchanger network shown in Figure 15.8.

Consider Exchanger 1 in Figure 15.6. The design equation is given as

$$A_1 = \frac{Q_1}{U_1 \Delta T_{lm,1} F_1}$$

where F_1 is the log-mean temperature correction factor for Exchanger 1. Assume a value of 0.8 for the calculations. A discussion of F factors follows in a later section. The data given in Figure 15.6 give

$$\Delta T_{lm,1} = \frac{(150 - 102.5) - (100 - 90)}{\ln \frac{150 - 102.5}{100 - 90}} = \frac{47.5 - 10}{\ln \frac{47.5}{10}} = 24.1°C$$

$$U_1 = \frac{1}{\frac{1}{270} + \frac{1}{250}} = 129.8 \text{ W/m}^2°C$$

Substituting this information in the design equation gives the following:

$$A_1 = \frac{100 \times 10^3}{(130)(24.1)(0.80)} = 40.0 \text{ m}^2$$

This procedure can be repeated for all the process heat exchangers in the network, for example, Exchangers 1, 2, 3, 4, 6, and 7. These results are summarized in the following table:

Exchanger	ΔT_{lm} (°C)	U (W/m²°C)	Q (kW)	F	A (m²)
1	24.1	129.8	100	0.8	40.0
2	20.0	69.5	300	0.8	270.3
3	47.5	153.8	700	0.8	119.7
4	24.1	80.0	500	0.8	324.6
6	10.0	61.7	100	0.8	202.5
7	17.0	69.5	100	0.8	105.8
Total					1063.0

Example 15.4.

For Example 15.3, estimate the heat-exchanger area needed for the utility exchangers, that is, Exchangers 5 and 8 in Figure 15.8.

Exchanger 5

For this exchanger, the temperature of the cold stream, Stream 6, must be increased from 165°C to 190°C. This requires a hot utility such as steam. Clearly, the correct pressure of steam to use is the lowest one available that gives a temperature driving force of at least 10°C (for this case). A review of Table 8.4 shows that only high-pressure steam is hot enough to heat Stream 6. Assume a film coefficient of 2000 W/m^2°C for condensing steam. In addition, assuming that no desuperheating or subcooling occurs, the steam condenses at a constant temperature, and therefore the F correction factor is equal to 1. Hence,

$$\Delta T_{lm,5} = \frac{(255 - 190) - (255 - 165)}{\ln\dfrac{(255 - 190)}{(255 - 165)}} = \frac{-25}{\ln\dfrac{65}{90}} = 76.8°C$$

$$U_5 = \frac{1}{\dfrac{1}{2000} + \dfrac{1}{80}} = 76.9 \text{ W/m}^2\text{°C}$$

$$A_5 = \frac{Q_5}{U_5 \Delta T_{lm,5} F_5} = \frac{100 \times 10^3}{(76.9)(76.8)(1.0)} = 16.9 \text{ m}^2$$

Exchanger 8

For this exchanger, the temperature of the hot stream must be decreased from 66.7°C to 50°C. This can be accomplished using cooling water. Assume that cooling water is available at 30°C and must be returned at 40°C, and a typical film heat transfer coefficient for cooling water (including a scaling or fouling factor) is assumed to be 1000 W/m^2°C. Therefore,

$$\Delta T_{lm,8} = \frac{(66.7 - 40) - (50 - 30)}{\ln\dfrac{66.7 - 40}{50 - 30}} = \frac{6.7}{\ln 1.335} = 23.2°C$$

$$U_8 = \frac{1}{\dfrac{1}{530} + \dfrac{1}{1000}} = 346 \text{ W/m}^2\text{°C}$$

$$A_8 = \frac{Q_8}{U_8 \Delta T_{lm,8} F_8} = \frac{50 \times 10^3}{(346)(23.2)(0.8)} = 7.8 \text{ m}^2$$

Total heat transfer area for the entire heat-exchanger network = 7.8 + 16.9 + 1063.0 = 1087.7 m^2.

At this stage, heat-exchanger areas for the network can be combined with the cost of purchasing utilities to give a reasonably complete economic analysis. However, if the effect of the minimum temperature approach is to be investigated, then the complete algorithm outlined in Steps 1–5 and Examples 15.2, 15.3, and 15.4 must be applied repeatedly for different minimum temperature approaches. It should be noted that Steps 1–4 can be readily programmed, but the algorithm for matching streams and exchanging energy outlined in Step 5 is not unique and is not easily computed. Rather than complete the design of the network as given in Step 5, it is possible to estimate approximately the heat transfer area for the network and therefore investigate the effect of changing temperature on the overall cost. The algorithm for estimating the heat transfer area is discussed in the next section.

15.3. Composite Temperature-Enthalpy Diagram

Physically, the pinch zone, previously mentioned, represents a point in the heat-exchanger network at which at least one heat exchanger, or two streams, will have the minimum approach temperature set in Step 1. This point is perhaps more clearly shown in a composite enthalpy-temperature diagram. This diagram is essentially the same as the combination of all the *T-Q* diagrams for all the exchangers in the network. Such a diagram for this example is shown in Figure 15.9 and is constructed by plotting the enthalpy of all the hot streams and all the cold streams as a function of temperature:

Hot Streams

Temperature Interval	Temperature (°C)	Enthalpy of Hot Streams in Temperature Interval (kW)	Cumulative Enthalpy of Hot Streams (kW)
	50	0	0
D	100	(2 + 3)(100 – 50) = 250	250
C	150	(2 + 3)(150 – 100) = 250	500
B	200	(8 + 3) (200 – 150) = 550	1050
A	300	(8) (300 – 200) = 800	1850

Cold Streams

Temperature Interval	Temperature (°C)	Enthalpy of Cold Streams in Temperature Interval (kW)	Cumulative Enthalpy of Cold Streams (kW)
	40	0	0
D	90	(4)(90 – 40) = 200	200
C	140	(8 + 4)(140 – 90) = 600	800
B	190	(8 + 4) (190 – 140) = 600	1400
A	290	(5) (290 – 190) = 500	1900

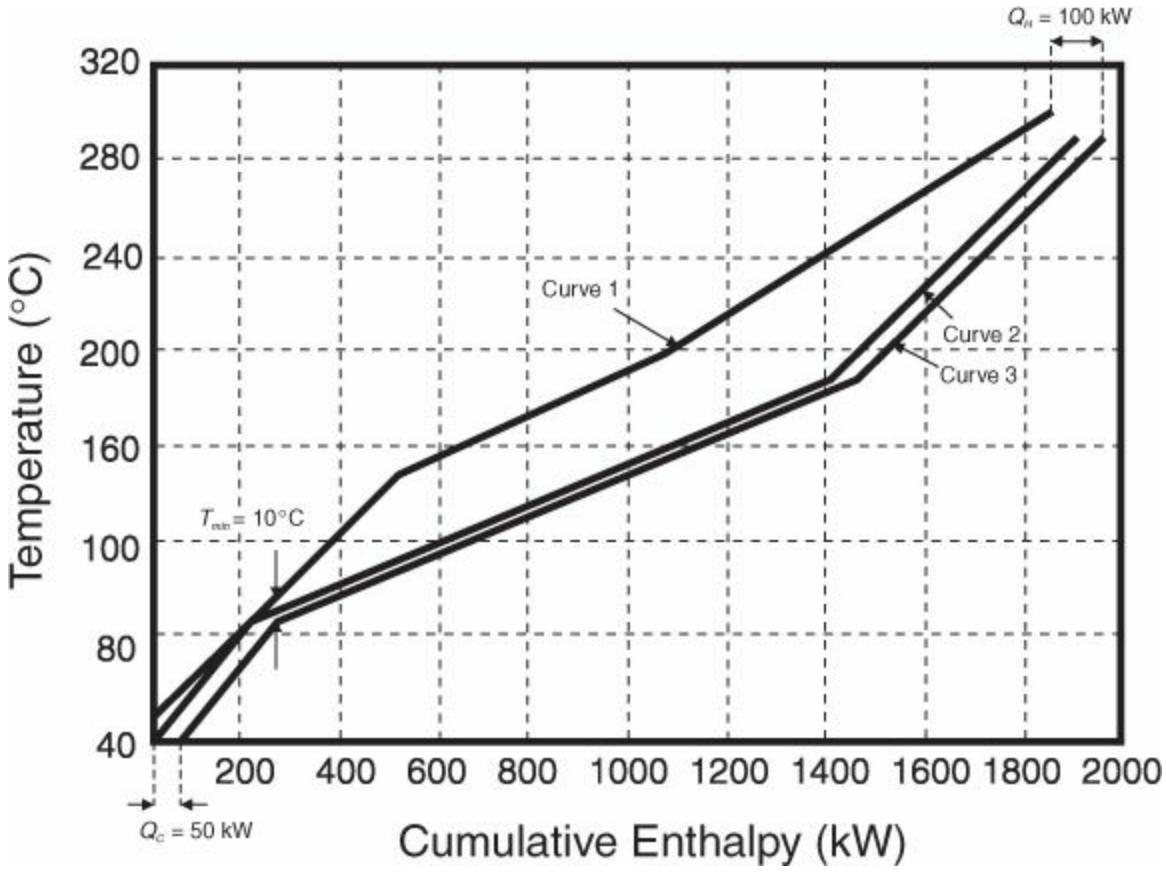


Figure 15.9. Composite Temperature-Enthalpy Diagram for Showing Effect of Changing Minimum Temperature Approach

These data are plotted in Figure 15.9 as Curves 1 and 2, respectively. From Figure 15.1, it can be seen that these two curves cross, which is physically impossible. This situation can be remedied by shifting the cold curve to the right. Curve 3 represents the case when the composite cold stream is shifted 50 kW to the right. For this case, it can seen that there exists a point at which the vertical distance between the hot and cold stream curves is at a minimum. This is the pinch zone. The case shown in Curves 1 and 3 corresponds to the situation when the minimum approach temperature between the streams is 10°C, the value chosen in Step 1. Comparing this curve (Curve 3) and the hot stream curve (Curve 1), it can be seen that the horizontal distances between the left- and right-hand ends of the curves represent the total duties from the cold and hot utilities, respectively, for the minimum utility case. Thus, the information shown in Figure 15.9 is consistent with the temperature interval diagram and the cascade diagram. In fact, it is exactly the same information but presented in a different way. From Figure 15.9, it should be clear that as the minimum approach temperature decreases, so do the minimum utility requirements. However, the temperature driving force within the heat-exchanger network will also decrease, and this will require larger, more expensive heat transfer equipment. Clearly, the optimum network must balance exchanger capital investment against operating (utility) costs.

15.4. Composite Enthalpy Curves for Systems without a Pinch

It was shown earlier that some problems do not possess a pinch condition. For these cases, only one utility (hot or cold) is required. This situation is illustrated on the temperature-enthalpy diagrams in Figure 15.10. In Figure 15.10(a), the typical heat-exchanger network problem containing a pinch is shown. If the minimum approach temperature is reduced, then the composite enthalpy curve for the cold streams (at the bottom) moves to the left and becomes closer to the hot stream composite enthalpy curve. For the problem shown in Figure 15.10(b), there exists a critical value for the

minimum temperature approach, $\Delta T_{min,crit}$, at which the hot utility requirement (Q_H) becomes zero and the cold utility requirement becomes a minimum, $Q_{C,min}$. If the minimum approach temperature is reduced below this critical value, as in Figure 15.10(c), the hot stream composite energy curve overlaps the cold stream curve at both ends. Heat must be rejected to the cold utility at the high temperature end (right-hand side of the figure), as well as at the low temperature end (left-hand side of the figure). However, the combined cold utility duty remains at $Q_{C,min}$. Therefore, below $\Delta T_{min,crit}$, the cold utility duty is constant and the hot utility duty is zero. Above $\Delta T_{min,crit}$, both the hot and cold utility duties increase with increasing ΔT_{min}.

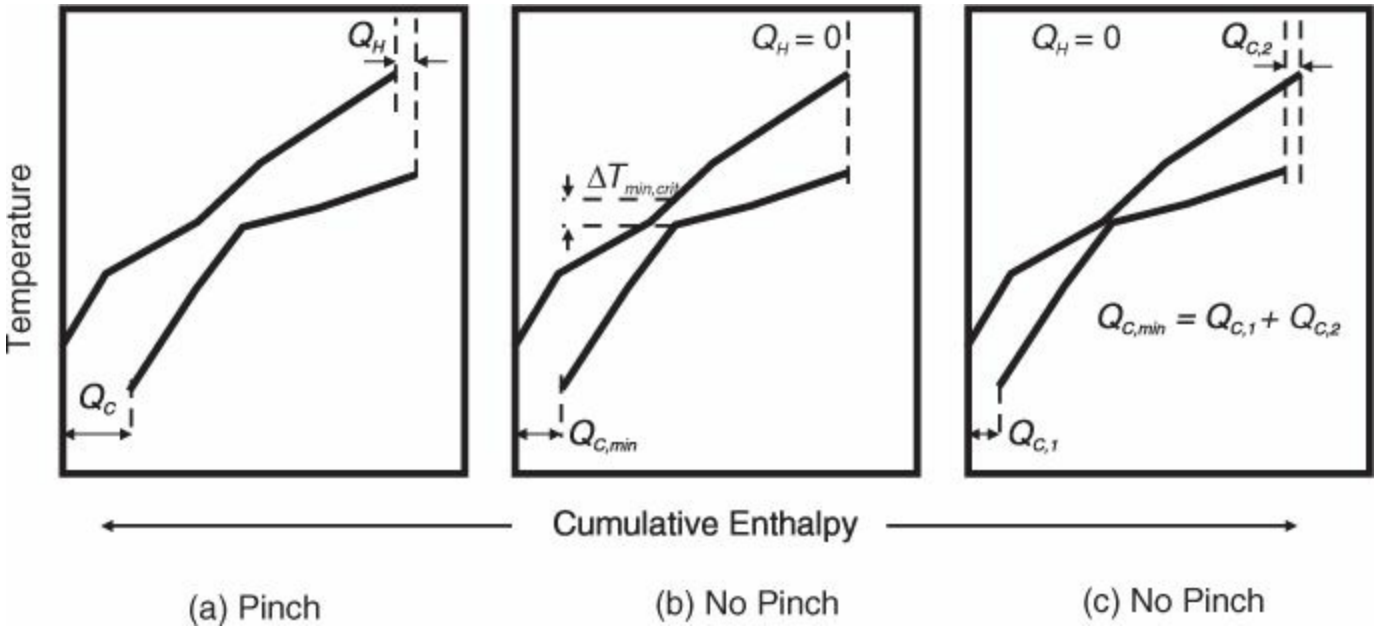


Figure 15.10. Composite Temperature-Enthalpy Diagram Showing a Problem without a Pinch Point

It can be seen that a case similar to that described above exists when the cold stream composite enthalpy curve can overlap the hot stream curve at both ends. For this case, a critical value of ΔT_{min} exists for which the cold utility duty is zero. Above this critical value, both utilities are required, but below it, no cold utility is needed, and the hot utility duty remains constant, but heat must be added to the system at both the hot and cold ends of the diagram.

15.5. Using the Composite Enthalpy Curve to Estimate Heat-Exchanger Surface Area

As stated earlier, the composite enthalpy curve can be used to estimate the heat-exchanger surface area of the network. For the case of a single heat exchanger, it is convenient to plot the enthalpy-temperature relationships on a diagram such as Figure 15.11(a). The basic rating equation used for preliminary heat-exchanger design is

$$Q = UA\Delta T_{lm}F$$

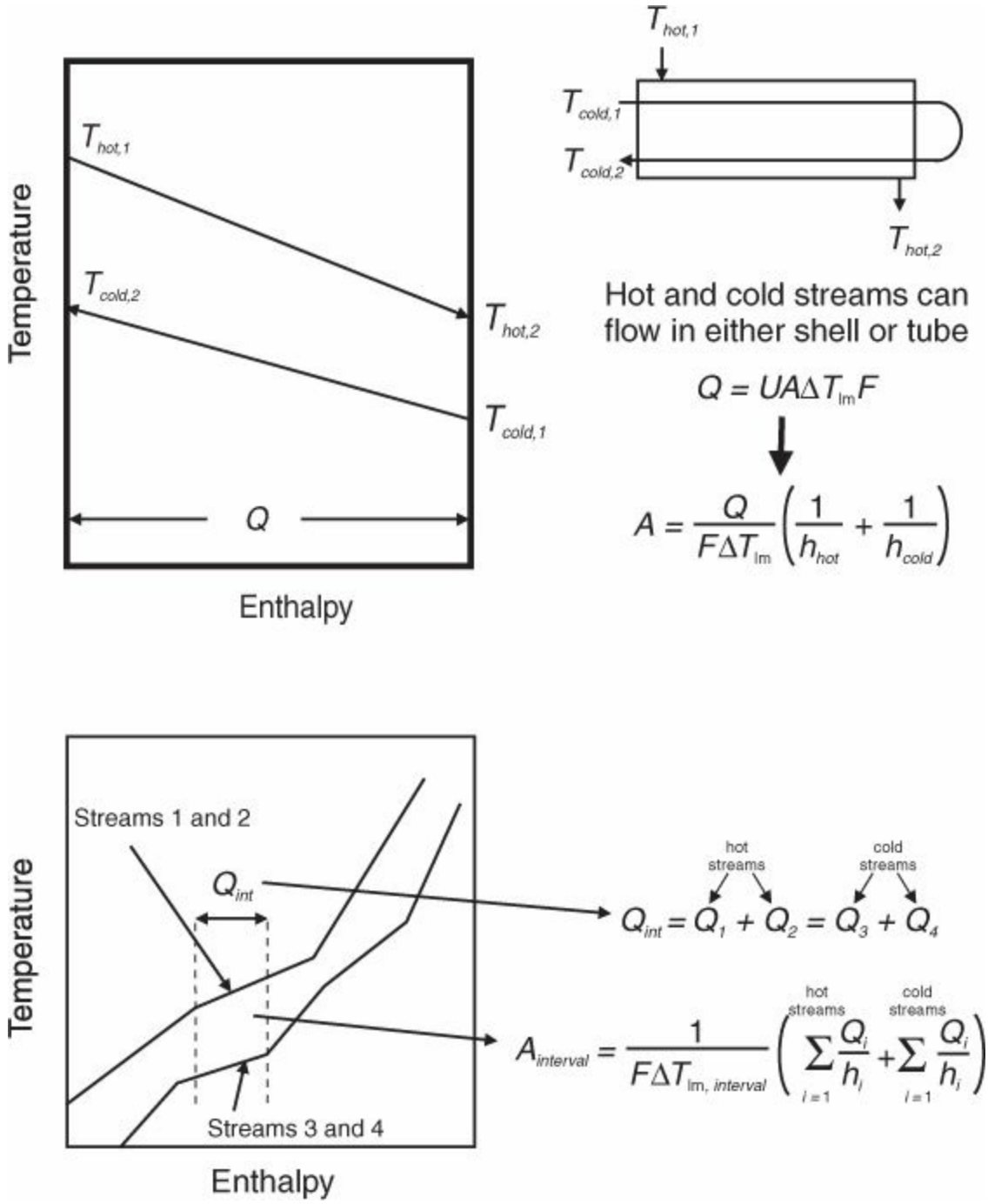


Figure 15.11. Composite Temperature-Enthalpy Diagram Showing a Problem without a Pinch Point

If the individual film heat transfer coefficients (including any appropriate fouling factors) for the hot and cold streams are known, then this equation can be rewritten as

$$A = \frac{1}{U}\frac{Q}{\Delta T_{lm}F} = \left[\frac{1}{h_{hot}} + \frac{1}{h_{cold}}\right]\frac{Q}{\Delta T_{lm}F} = \frac{1}{\Delta T_{lm}F}\left[\frac{Q}{h_{hot}} + \frac{Q}{h_{cold}}\right] \qquad (15.2)$$

The application of Equation (15.2) was demonstrated in Examples 15.3 and 15.4.

Consider now a portion of the composite enthalpy curve shown in Figure 15.11(b). This curve is made up of two hot streams (1 and 2) and two cold streams (3 and 4). Both the hot streams and both the cold streams have the same temperature change in the interval. However, in general, the enthalpy in either of the hot streams is not the same as the enthalpy in either of the cold streams. Instead, the sum of the enthalpies in the hot streams is equal to that in the two cold streams. This means that different streams cannot be matched in this temperature (enthalpy) interval, because the enthalpy of

individual hot and cold streams will be different. However, an estimate of the heat transfer area required to transfer all the energy in the temperature interval can be made by applying Equation 15.2 to both the hot and cold streams in the interval [2, 7]. This result may be generalized as follows:

$$A_{\text{interval}} = \frac{1}{\Delta T_{\text{lm,interval}} F}\left[\sum_{i=1}^{\text{hot streams}} \frac{Q_i}{h_i} + \sum_{i=1}^{\text{cold streams}} \frac{Q_i}{h_i}\right] \tag{15.3}$$

where the summation is made for all streams (hot and cold) contained in the interval, and Q_i is the enthalpy change of the stream in the interval.

Clearly, the composite enthalpy diagram can be divided into intervals in which the number of hot and cold streams is constant. The total heat transfer area for the network may be estimated by adding the areas for each interval obtained from Equation 15.3. Ahmad et al. [8] state that the result in Equation 15.3 should predict the minimum area required for a given minimum temperature approach to within about 10%, as long as the film heat transfer coefficients do not differ by a factor of 10 or more. This estimate of accuracy seems to be somewhat optimistic, and a more realistic number might be ±25%. Nevertheless, when looking for the optimum temperature approach, the method used above should give reasonable predictions. Example 15.5 illustrates the methodology to estimate heat transfer areas using this technique.

Example 15.5.

For the problem introduced in Example 15.1, and using the film heat transfer coefficients from Examples 15.3 and 15.4, estimate the heat transfer area for the proposed network. Compare the result to that obtained in Example 15.4.

The composite enthalpy diagram for this problem is shown in Figure E15.5. This is the same figure as Figure 15.9, except that temperatures and enthalpies for the different segments have been added. Within each segment, the composite enthalpy curves for the hot and cold streams are straight lines, which implies that the number of streams in each segment is constant because the slope of the line is $1/\sum \dot{m} c_p$. In order to generate this information, heat balances must be applied along with the information in the temperature interval diagram, Figure 15.1. For example, consider Segment 1 of Figure E15.5. The hot stream temperature at the border of Segments 1 and 2 must be computed (this is not shown on the original composite temperature-enthalpy diagram, Figure 15.9). Because Q_1 is the cold utility duty and is equal to 50 kW, the temperature for the composite hot stream is given by the following simple enthalpy balance:

$$\sum_{i=\text{hot streams}} (\dot{m} c_p)_{i,1} \, \Delta T_1 = Q_1$$

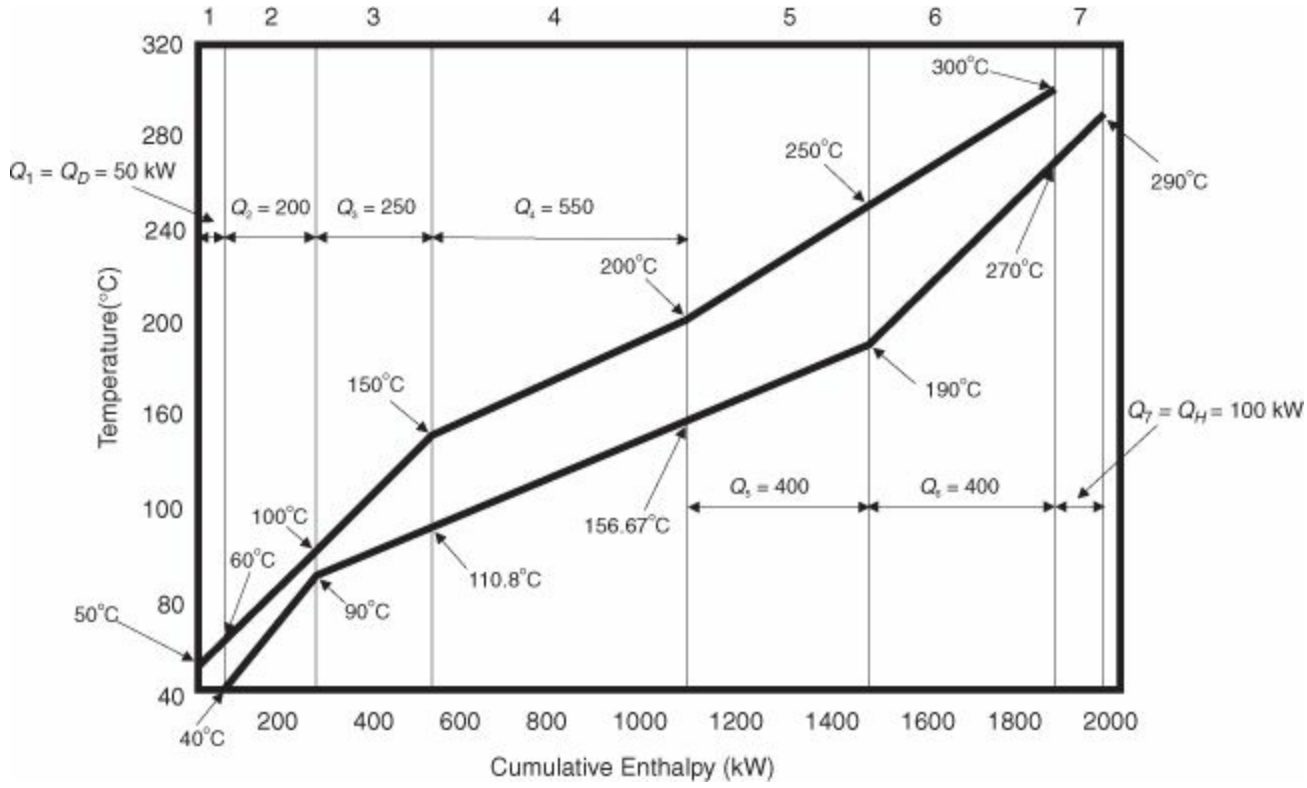


Figure E15.5. Composite Temperature-Enthalpy Diagram for Example 15.5 (Minimum Temperature Approach = 10°C and All Enthalpies Are Given in kW)

Figure 15.1 shows that Streams 2 and 3 lie in the temperature range of Segment 1 (>50°C and <100°C). Therefore,

$$\sum_{i=\text{hot streams}} (\dot{m}Cp)_{i,1}\Delta T_1 = (2000 + 3000)\Delta T_1 = Q_1 = 50{,}000 \text{ W}$$

$$\Delta T_1 = \frac{50{,}000}{5000} = 10°\text{C}$$

Thus, the composite hot stream temperature at the border of Segments 1 and 2, $T_{hot,1\text{-}2} = 50 + 10 = 60°\text{C}$.

In a similar way, the temperature of the composite cold streams between Segments 3 and 4 can be calculated as

$$\sum_{i=\text{cold streams}} (\dot{m}Cp)_{i,3}\,\Delta T_3 = Q_3$$

From Figure 15.1, Streams 5 and 6 lie in the temperature range (>90°C and <190°C). Therefore, the composite cold stream temperature at the border of Segments 3 and 4 is given by

$$\sum_{i=\text{cold streams}} (\dot{m}Cp)_{i,3}\Delta T_3 = (8000 + 4000)\Delta T_3 = Q_3 = 250{,}000 \text{ W}$$

$$\Delta T_3 \frac{250{,}000}{(8000 + 4000)} = 20.83°\text{C}$$

$$T_{cold,3-4} = 90 + 20.83 = 110.83°\text{C}$$

Similar calculations must be performed to establish the data given in Figure E15.5.

To estimate the area for each of the segments, Equation 15.3 is applied to each segment. The results of these calculations for the process-process heat exchangers (Segments 2–6) are given in Table E15.5. The total heat transfer area for the heat-exchanger network (ignoring the utility exchangers for now) is 788 m^2.

Table E15.5. Summary of Heat Transfer Area Calculations for Example 15.5

		Temperature Interval Shown in Figure E15.5						
	h kW/m²°C	1	2	3	4	5	6	7
$Q_{interval}$, kW		50[a]	200	250	550	400	400	100[b]
$Q_{stream,1}$, kW	0.40		0.0	0.0	400.0	400.0	400.0	
$Q_{stream,2}$, kW	0.27		80.0	100.0	0.0	0.0	0.0	
$Q_{stream,3}$, kW	0.53		120.0	150.0	150.0	0.0	0.0	
$Q_{stream,4}$, kW	0.10		0.0	0.0	0.0	0.0	400.0	
$Q_{stream,5}$, kW	0.25		0.0	166.7	366.7	266.7	0.0	
$Q_{stream,6}$, kW	0.08		200.0	83.3	183.3	133.3	0.0	
$T_{hot,1}$, °C			60	100	150	200	250	
$T_{hot,2}$, °C			100	150	200	250	300	
$T_{cold,1}$, °C			40	90	110.83	156.67	190	
$T_{cold,2}$, °C			90	110.83	156.67	190	270	
ΔT_{lm}, °C			14.43	21.37	41.2	51.22	43.28	
$\Sigma(Q_i/h_i)$			$\frac{80}{0.27}+\frac{120}{0.53}+\frac{200}{0.08}$ = 3022.7	$\frac{100}{0.27}+\frac{150}{0.53}+\frac{166.7}{0.25}+\frac{83.3}{0.08}$ = 2361.4	$\frac{400}{0.40}+\frac{150}{0.53}+\frac{166.7}{0.25}+\frac{83.3}{0.08}$ = 5041.1	$\frac{400}{0.40}+\frac{266.7}{0.25}+\frac{133.3}{0.08}$ = 3733.1	$\frac{400}{0.40}+\frac{400}{0.10}$ = 5000	
$A_{network}$			$\frac{3022.7}{(14.43)(0.8)}=261.9$	$\frac{2361.4}{(21.4)(0.8)}=138.2$	$\frac{5041.1}{(41.2)(0.8)}=152.9$	$\frac{3733.1}{(51.2)(0.8)}=91.1$	$\frac{5000}{(43.3)(0.8)}=144.4$	

[a]This is the duty of the cold utility exchanger.
[b]This is the duty of the hot utility exchanger.
Total Process-Process Exchanger Area for Network = 261.9 + 138.2 +152.9 + 91.1 + 144.4 = 788.5 m²

The area calculated following the five-step algorithm, and computed in Example 15.3, was 1063 m^2. For this case, the method of estimating the heat transfer area of the heat-exchanger network from the composite temperature-enthalpy diagram (Example 15.5) underestimates the area by 26%. Although this value would be unacceptable for final design purposes, this method can be easily programmed, and the effect on the total cost of the network of changing the minimum approach temperature or process changes can be computed easily. The final step in computing the fixed capital investment of the heat-exchanger network is to compute the area and configuration for each of the heat exchangers in the network.

15.6. Effectiveness Factor (F) and the Number of Shells

To this point, it has been assumed that the log-mean temperature correction factor, F, for all exchangers is the same and equal to 0.8. The reason that F is not assumed to be equal to unity is that, for heat exchangers in most practical applications, the flows of the hot and cold streams are never purely countercurrent. The most common type of heat exchanger in use in the chemical process industries is the shell-and-tube (S&T) type. These units are typically made as multiples of the basic 1-shell pass, 2-tube pass (1-2) design. When estimating the fixed capital investment associated with the purchase and installation of the heat-exchanger network, the number of 1-2 S&T exchangers is needed in addition to the total surface area of the network.

A schematic diagram of a 1-2 S&T exchanger is shown in Figure 15.12. It can be seen that the basic flow patterns of the shell and tube fluids are not countercurrent. Indeed, the flow patterns of the two fluids are very complicated. However, for 1-2 S&T exchangers a reasonable assumption is that the shell-side fluid flows cocurrently with the tube-side fluid in one direction and countercurrently in the other direction. Using this idealized model of the fluid flow, an analytical expression may be

computed for the F factor (Bowman et al. [9]). This expression is given as

$$F_{1-2,S\&T} = \frac{\sqrt{(R^2+1)}}{(R-1)} \frac{\ln\left[\frac{1-P}{1-RP}\right]}{\ln\left[\frac{2-P\left(R+1-\sqrt{(R^2+1)}\right)}{2-P\left(R+1+\sqrt{(R^2+1)}\right)}\right]} \tag{15.4}$$

where $R = (\dot{m}C_p)_{cold}/(\dot{m}C_p)_{hot}$ and $P = (t_{c,out} - t_{c,in})/(t_{h,in} - t_{c,in})$.

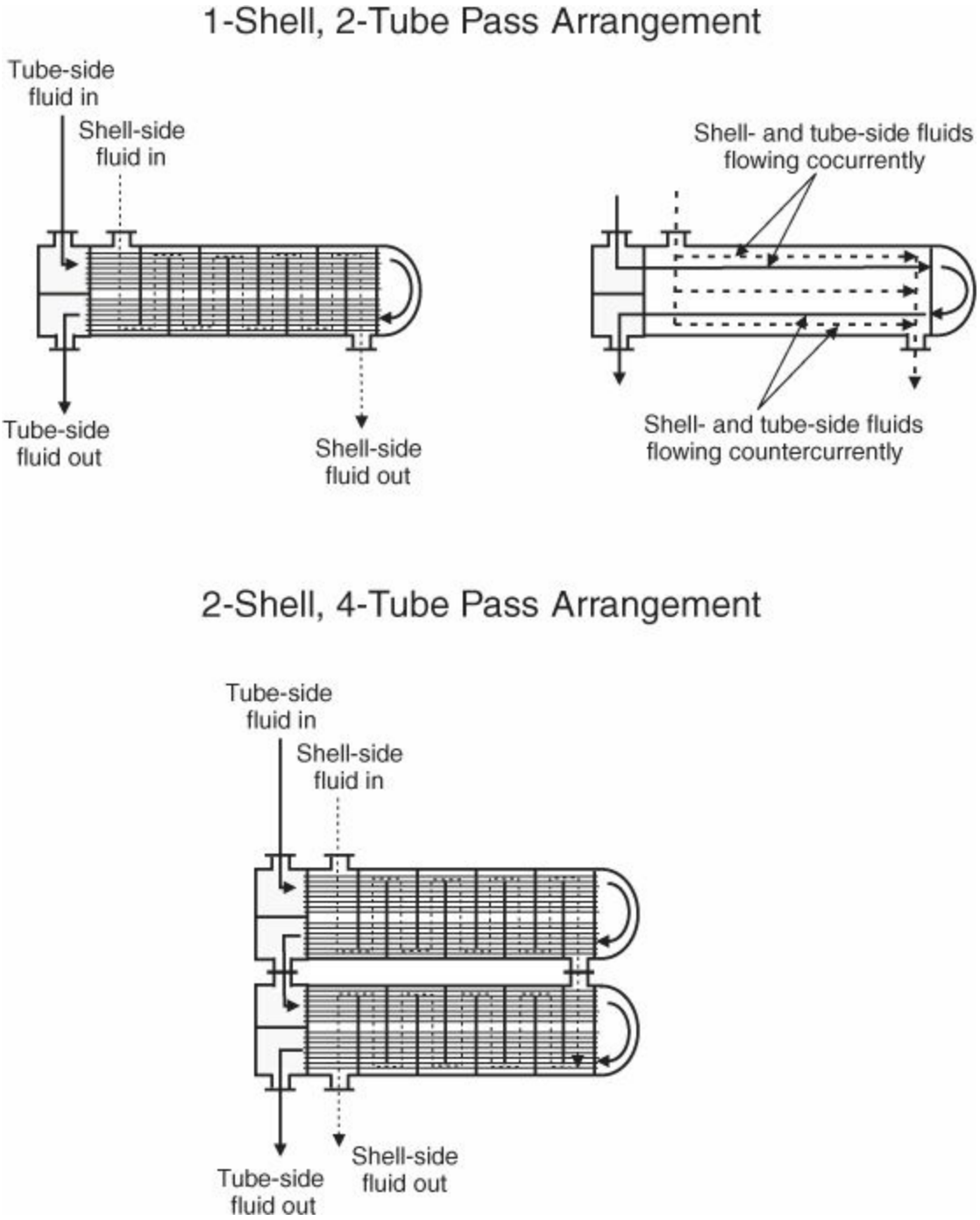


Figure 15.12. Flow Patterns in 1-2 and 2-4 Shell-and-Tube Heat Exchangers

For the case when $R = 1$, Equation (15.4) reduces to

$$F_{1-2,S\&T} = \frac{P\sqrt{2}}{(1-P)\ln\left[\frac{2-2P-P\sqrt{2}}{2-2P+P\sqrt{2}}\right]} \tag{15.5}$$

The relationship between $F_{1\text{-}2,S\&T}$ and P and R is illustrated in Figure 15.13. From this figure it is clear that for a given value of R, the temperature correction factor, F, drops off precipitously as a critical value of P is reached. In fact, for any given value of R, there exists a maximum value of P given by

$$P_{max} = \frac{2}{R + 1 + \sqrt{(R^2 + 1)}} \qquad (15.6)$$

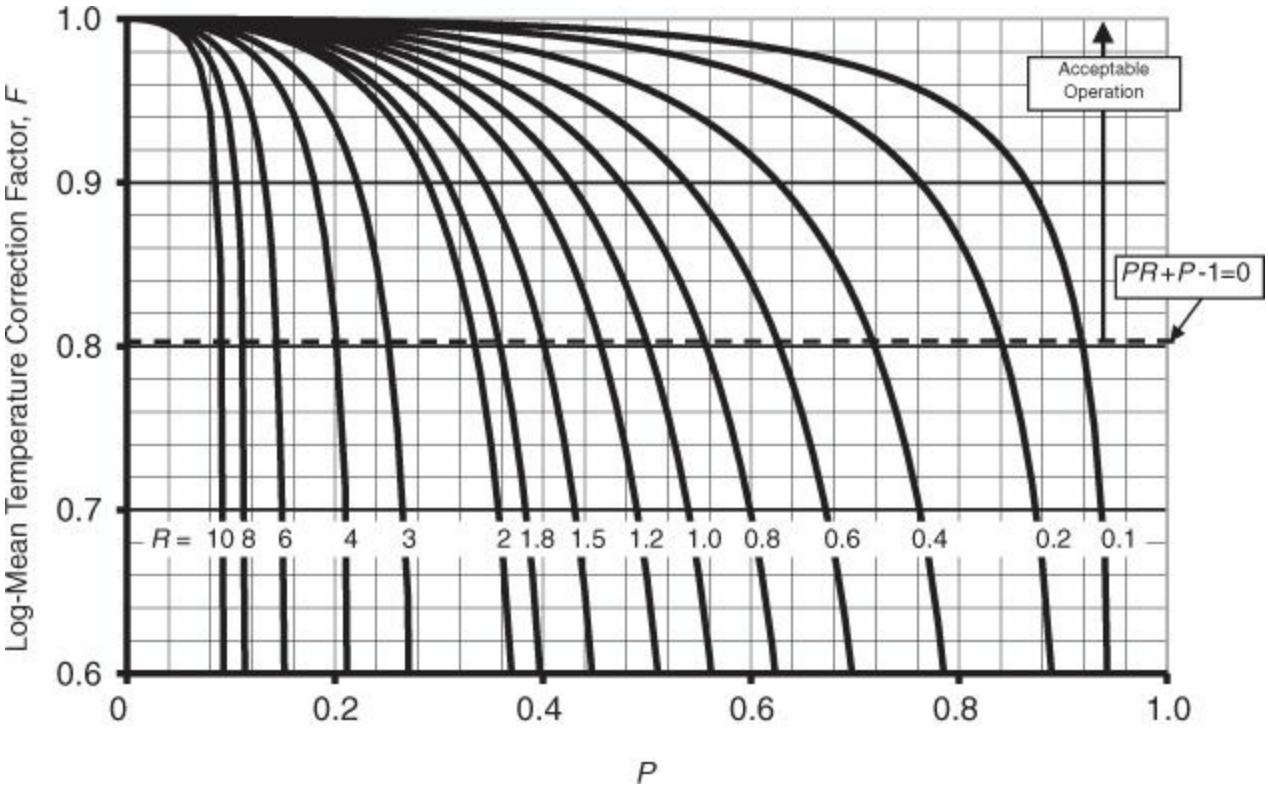


Figure 15.13. Logarithmic-Mean Temperature Correction Factor, *F*, for a 1-Shell, 2-Tube Pass Heat Exchanger

This phenomenon can be explained by the fact that as the temperature between the hot exit and cold entrance streams approaches zero, the efficiency of the 1-2 design is reduced. This effect is illustrated in Figure 15.14. For pure cocurrent flow, the highest temperature that the cold stream can be heated to is equal to the hot stream exit temperature. Because half of the flow in a 1-2 S&T exchanger is co-current, it is not surprising that the efficiency (temperature correction factor, F) of the heat exchanger starts to decrease rapidly when this condition is reached. For the condition $T_{h,2} = T_{c,2}$ the relationship between P and R is given in Equation (15.7):

$$P + PR - 1 = 0 \qquad (15.7)$$

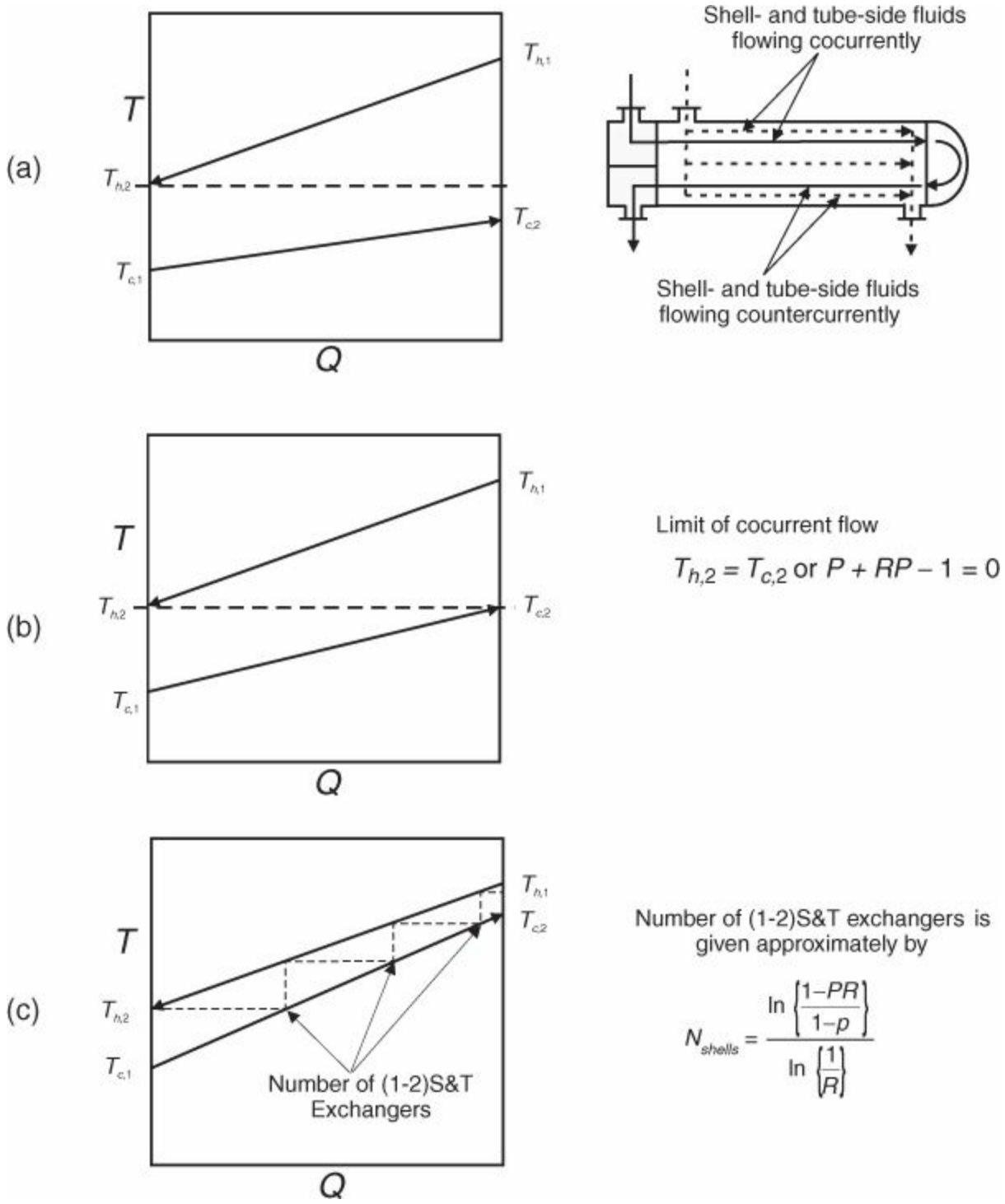


Figure 15.14. The Effect of Temperature Approach on the Number of Shells Required for a Shell-and-Tube Heat Exchanger

The line representing this equation is plotted on Figure 15.13. This line can be approximated by the condition $F = 0.8$ on the figure. If the condition of $F = 0.8$ is taken as the criterion for the limit of operation of a 1-2 S&T exchanger, then the number of shells can be calculated graphically by a McCabe-Thiele–type construction illustrated in Figure 15.14(c). The analytical expression for the number of shells using this criterion and when the specific heats of hot and cold streams are constant (this implies that the lines on the T-Q diagram are straight) is given by

$$N_{shells} = \frac{\ln\left\{\frac{1 - PR}{1 - P}\right\}}{\ln\left\{\frac{1}{R}\right\}} \quad \text{for } R \neq 1$$

or

$$N_{shells} = \frac{P}{1 - P} \quad \text{for } R = 1 \tag{15.8}$$

A more sophisticated technique, given by Smith [10] and due to Hall et al. [11], to calculate the number of shells based on using a fraction, Z, of the maximum value of P,

Equation (15.6), as the limit for using 1-2 S&T exchangers gives the following expression for the number of required shells:

$$N_{shells} = \frac{\ln \frac{1 - PR}{1 - P}}{\ln \frac{R + 1 + \sqrt{(R^2 + 1)} - 2RZP_{max}}{R + 1 + \sqrt{(R^2 + 1)} - 2ZP_{max}}} \quad \text{for } R \neq 1$$

or

$$N_{shells} = \frac{\left\{\frac{P}{1 - P}\right\}(2 + \sqrt{2} - 2ZP_{max})}{2ZP_{max}} \quad \text{for } R = 1 \tag{15.9}$$

The number of shells calculated from Equations (15.8) and (15.9) is compared in Table 15.1. The P values are chosen to coincide with the transition from one shell to two shells using Equation (15.8). According to Smith [10], a limiting value of $F = 0.75$ corresponds to $Z = 0.9$. Comparing the results in Table 15.1, it is clear that the predictions of Equation (15.8) are not drastically different from those of Equation (15.9). Unless stated otherwise, Equation (15.8) will be used to calculate the number of shells. Example 15.6 demonstrates this procedure.

Table 15.1. Predictions of the Number of Shells Required from Equations (15.8) and (15.9)

R	$P=1/(1+R)$	Eq. (15.8)	Eq. (15.9) $Z=0.8$	Eq. (15.9) $Z=0.9$	Eq. (15.9) $Z=0.95$
0.1	0.91	1	1.71	1.25	1.03
0.2	0.83	1	1.44	1.08	0.92
0.5	0.67	1	1.20	0.93	0.82
0.8	0.56	1	1.14	0.90	0.80
1.0	0.50	1	1.13	0.90	0.80
1.5	0.40	1	1.16	0.91	0.81
2.0	0.33	1	1.20	0.93	0.82
5.0	0.17	1	1.44	1.08	0.92
10.0	0.09	1	1.71	1.25	1.03

Example 15.6.

For a heat exchanger that cools a single-phase hot stream from 250°C to 60°C, using a single-phase cooling stream that is heated from 30°C to 200°C, estimate the number of 1-2 S&T heat exchangers required. Assume that the specific heats of the two streams are constant.

The *T*-*Q* diagram for this heat exchanger is given in Figure E15.6.

$R = (250 - 60)/(200 - 30) = 190/170 = 1.1176$ and $P = (200 - 30)/(250 - 30) = 170/220 = 0.7727$

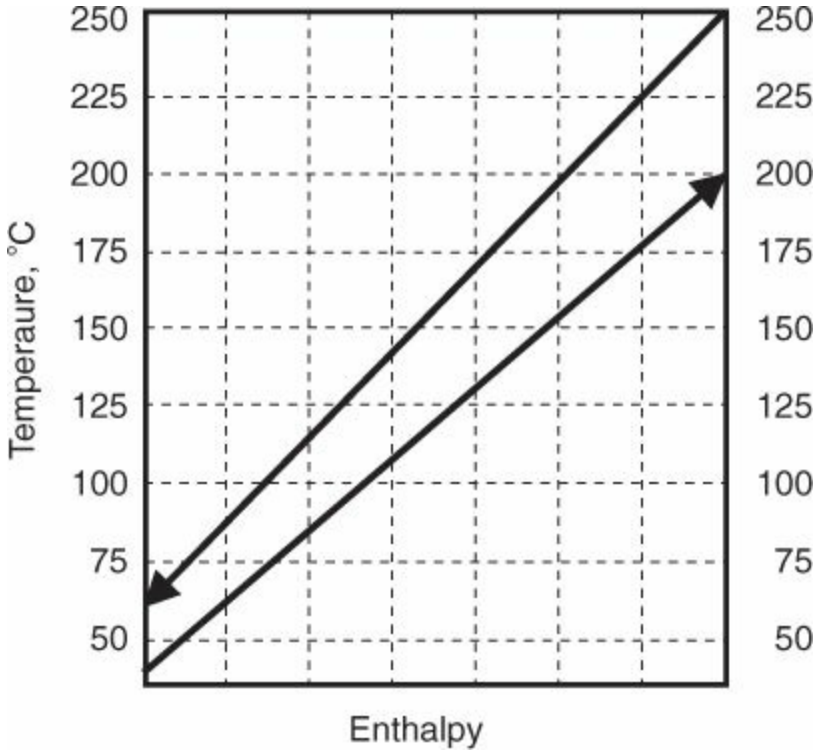


Figure E15.6. Temperature-Enthalpy Diagram for Example 15.6

From Equation (15.8),

$$N_{shells} = \frac{\ln\left\{\frac{1 - PR}{1 - P}\right\}}{\ln\left\{\frac{1}{R}\right\}} = \frac{\ln\left\{\frac{1 - (0.7727)(1.1176)}{1 - 0.7727}\right\}}{\ln\left\{\frac{1}{1.1176}\right\}} = 4.59$$

Rounding up, $N_{shells} = 5$.

From Equation (15.9),

$$N_{shells} = \frac{\ln\left[\frac{1 - PR}{1 - P}\right]}{\ln\left[\frac{R + 1 + \sqrt{(R^2 + 1)} - 2RZ}{R + 1 + \sqrt{(R^2 + 1)} - 2Z}\right]} = \frac{\ln\left[\frac{1 - (0.7727)(1.1176)}{1 - 0.7727}\right]}{\ln\left[\frac{1.1176 + 1 + \sqrt{(1.1176^2 + 1)} - 2(1.1176)(0.9)}{1.1176 + 1 + \sqrt{(1.1176^2 + 1)} - 2(0.9)}\right]}$$

Rounding up, $N_{shells} = 5$.

Both methods predict the need for an exchanger with five shell passes (and ten tube passes) requiring five 1-2 S&T exchangers stacked on top of each other. This equipment would be referred to as a 5-10 S&T exchanger.

15.7. Combining Costs to Give the Eaoc for the Network

The final step in evaluating the capital cost of the exchanger network is to estimate the number of heat-exchanger units required for the network. In Example 15.3, the individual areas of the heat exchangers were evaluated. If the number of shells required for each exchanger is calculated, the total number and areas of each 1-2 S&T exchanger required for the design can be calculated. From these data, using the cost correlations introduced in Chapter 7, the fixed capital investment for the installed network can be evaluated. It should be noted that due to the economy of scale, the cost of two 1-2 S&T exchangers placed with their shells in series to form a 2-4 S&T exchanger will be greater than the equivalent 1-2 S&T exchanger with the same total heat transfer area. The use of the correct number of shells is therefore important if an accurate estimate of the FCI of the HEN is to be obtained. This is especially true when the approach temperatures in an exchanger are small, for example, in the crude preheat train of oil refineries.

Several economic criteria introduced in Chapter 10 can be used to evaluate the profitability of a given heat-exchanger network. For this discussion, the equivalent annual operating cost (EAOC) will be used:

$$EAOC = FCI\frac{i(1+i)^n}{(1+i)^n - 1} + \Sigma(\text{utility costs}) \qquad (15.10)$$

where the fixed capital investment, *FCI*, is the total module cost of the exchanger network, the second term on the right-hand side of Equation (15.10) is the yearly cost of the hot and cold utilities, and n is the number of years over which the economic analysis is carried out. For a complete after-tax economic analysis, provision must be made for depreciating the FCI. To simplify the analysis, a before-tax hurdle rate, i, can be used to compare cases with different minimum approach temperatures.

When the composite enthalpy curves are used to estimate exchanger areas, there is no simple way of estimating the number and areas of individual exchangers. This is because no specific stream matches are made when estimating the total heat transfer area from the composite enthalpy curves. The simplest method for estimating specific heat transfer areas, which is necessary to calculate the cost of the heat-exchanger network, is to assume that all the heat exchangers have the same area. This approach tends to overestimate somewhat the cost of the network. Thus, the fixed capital investment can be estimated using $(N_{min,a}+N_{min,b})$ times the cost of a heat exchanger with an area of $A_{network}/(N_{min,a}+N_{min,b})$. The EAOC can then be estimated using Equation (15.10). Example 15.7 illustrates how the cost of the heat-exchanger network can be estimated.

Example 15.7.

Using the results from Example 15.5, estimate the EAOC for the heat-exchanger network. Assume that i (before-tax) = 10% p.a. and n = 5 years.

From Example 15.4, the total network heat transfer area (excluding utility exchangers) = 788 m^2.

The minimum number of exchangers was found to be 8.

The fixed capital investment is based on 8 exchangers each with an area of (788/8) = 98.5 m^2.

$$C_{TM,S\&T\,floating\,head\,exchanger} = \$97{,}700$$

The utility costs are estimated as follows:

Cooling water utility costs = (50×10^3)[J/s] (3600)[s/h](8000)[h/y](0.354)[$/GJ] (1×10^{-9})[GJ/J] = $510/y

HPS utility = (100×10^3)[J/s] (3600)[s/h](8000)[h/y](9.83)[$/GJ]$(1 \times 10^{-9})$[GJ/J] = $28,310/y

$$EAOC = FCI\frac{(0.1)(1+0.1)^5}{(1+0.1)^5-1} + \$28{,}310/y + \$510/y = (0.2638)(8)(97{,}000) + \$28{,}820/y = \$235{,}000/y$$

The procedure illustrated in Example 15.7 can be repeated for different minimum approach temperatures. The basic trends for utility consumption, heat transfer area, and EAOC as functions of minimum temperature approach are shown in Figure 15.15. It is clear from this figure that there will be an optimum minimum temperature approach for the heat-exchanger network. At the optimum, the increase in utility costs (usage) for an incremental change in minimum temperature approach will be just balanced by the decrease in the equivalent annual operating cost for the smaller heat-exchanger network.

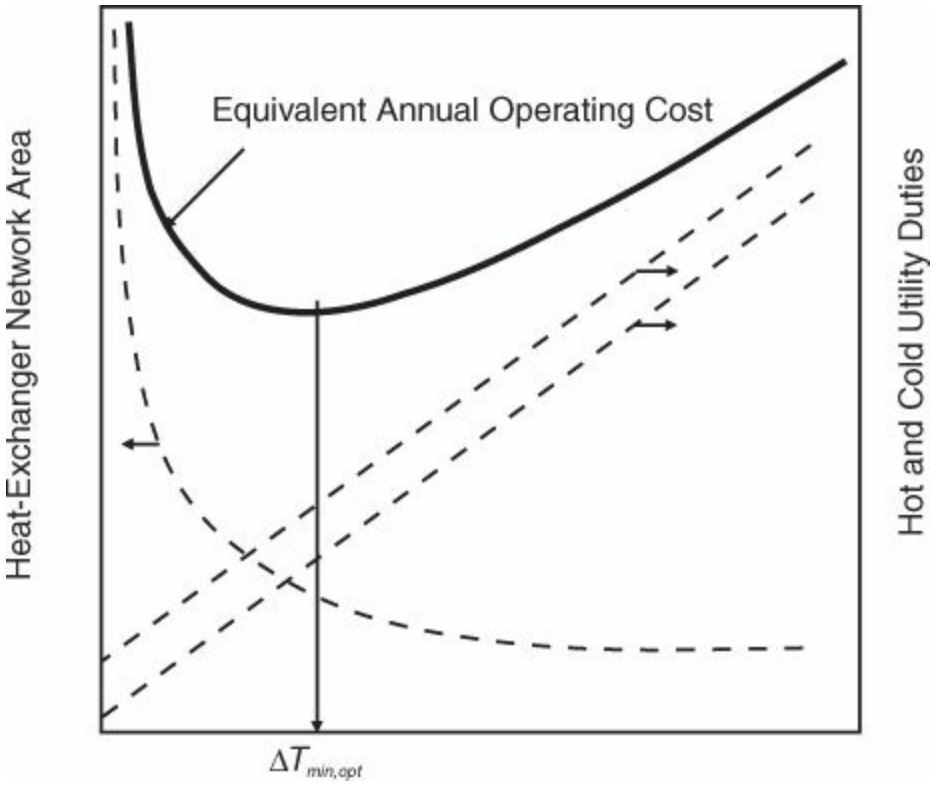


Figure 15.15. Typical Relationships for Heat Transfer Area, Utilities, and EAOC for a HEN

15.8. Other Considerations

To this point in the discussion, it has been assumed that the cost of the heat exchanger is simply a function of the heat transfer surface area. From discussions in Chapter 7, it is clear that both the materials of construction and operating pressure are important factors in estimating heat-exchanger costs. These effects must be taken into account when estimating the FCI from the composite temperature-enthalpy diagram. This problem has been addressed by Hall et al. [11] and is explained in the following section.

15.8.1. Materials of Construction and Operating Pressure Issues

Initially, it is assumed that the materials of construction and maximum operating pressures for all heat exchangers are the same. Some streams may require different materials of construction and operating

pressures, and, for these streams, the film heat transfer coefficients can be adjusted to correct for the different fixed capital cost associated with exchangers in contact with these streams. For example, assume that all but one of the streams in a HEN are at pressures less than 5 barg and require carbon steel construction. The remaining stream, however, is at a pressure of 25 barg, is corrosive, and requires all exchanger surfaces in contact with it to be made of 304 grade stainless steel. The heat exchangers that contact this fluid will be more expensive than similar sized exchangers that do not contact this fluid. Hall et al. [11] suggest using an effective film heat transfer coefficient for this stream that is lower than the true value. By doing this, the areas predicted for heat exchangers that process this stream increase, causing the costs of the exchangers also to increase. Therefore, using these effective film coefficients allows the same cost equation to be used for all exchangers in the HEN. The form of the cost equations introduced in Chapter 7 (and Appendix A) is not suitable for this analysis. Instead, the simpler form of cost relationship given in Equation (7.2) is used:

$$C_p = KA^n \tag{15.11}$$

The total module cost of the exchanger is given by combining the results of Equations (7.2), (7.15), and (A.4):

$$C_{TM} = 1.18(B_1 + B_2F_MF_P)KA^n \tag{15.12}$$

For the base conditions, operating pressure <5 barg, and carbon steel construction, F_M and F_P in Equation (15.12) are both equal to 1. Let the area of a heat exchanger operating at pressure P and using the correct materials of construction be A, and let the area of an exchanger at the base conditions that has the same total module cost as the other exchanger be A_{bc}. Using Equation (15.12) and equating total module costs gives

$$1.18(B_1 + B_2F_MF_P)KA^n = 1.18(B_1 + B_2)KA_{bc}{}^n$$

$$\frac{A_{bc}}{A} = \left[\frac{B_1 + B_2F_MF_P}{B_1 + B_2}\right]^{\frac{1}{n}} \tag{15.13}$$

From Equation (15.13), it is clear that for equal cost, the heat-exchanger area at base conditions must be greater than the true area by the factor on the right-hand side of the equation. Because the area is inversely proportional to the film heat transfer coefficient, the relationship in Equation (15.14) is obtained:

$$\frac{h}{h_{bc}} = \left[\frac{B_1 + B_2F_MF_P}{B_1 + B_2}\right]^{\frac{1}{n}} \tag{15.14}$$

By modifying heat transfer coefficients for streams requiring non-base-case operating conditions using Equation (15.14), the same cost equation can be used to calculate all exchanger costs in a given network.

The correction factors for a floating-head, shell-and-tube heat exchanger are shown in Figure 15.16. From Appendix A, the values used in Equation (15.14) are $B_1 = 1.63$, $B_2 = 1.66$, and $n = 0.573$. Examples 15.8 and 15.9 illustrate how to use this information.

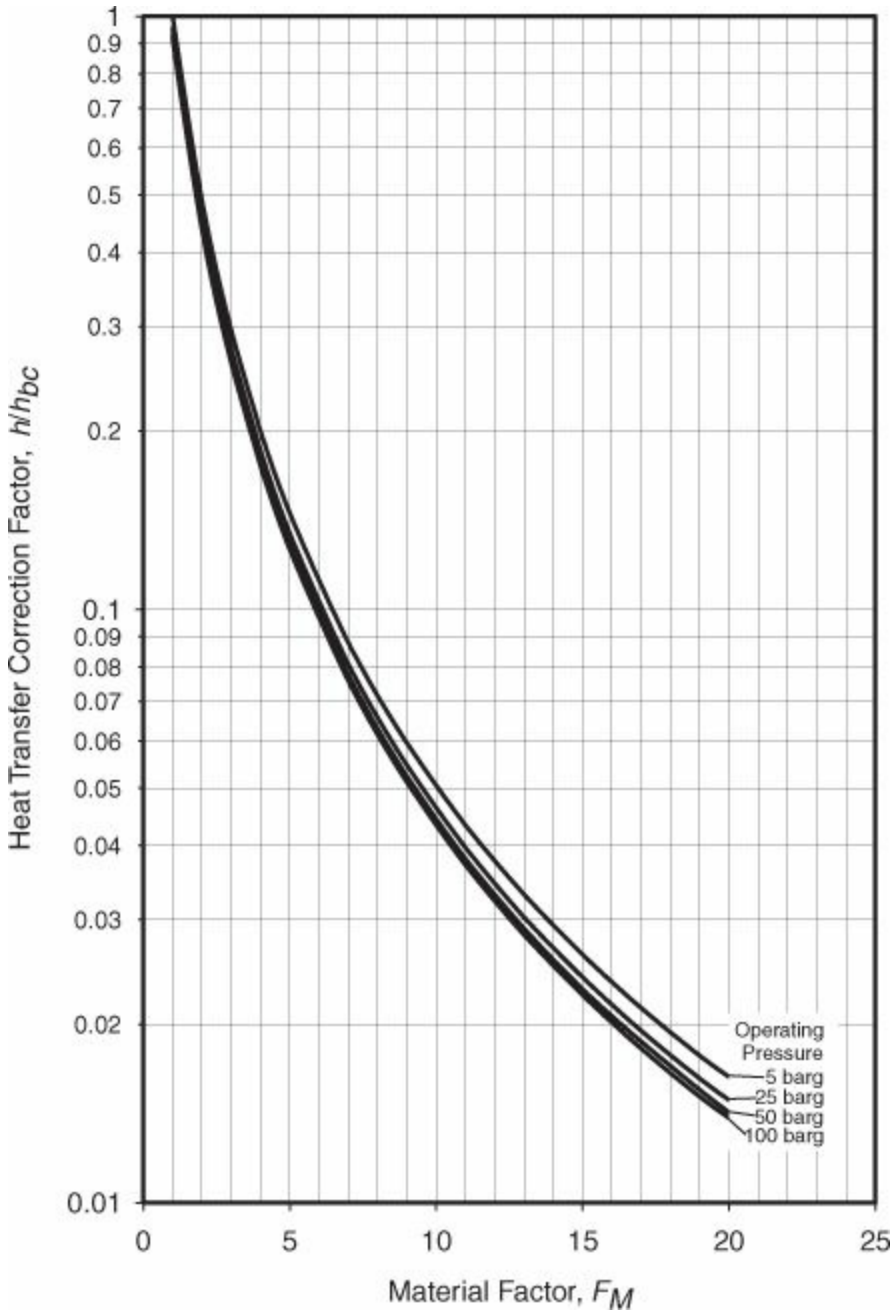


Figure 15.16. Heat Transfer Correction Factor for Shell-and-Tube, Floating-Head Heat Exchangers

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Example 15.8.

For the heat-exchanger network developed in Examples 15.2, 15.3, and 15.4, what heat transfer coefficient should be used to account for the fact that Stream 3 requires stainless steel construction and is at a pressure of 50 barg? Assume that all the streams except Stream 3 are available at pressures <5 bar and require only carbon steel construction.

In order to minimize the investment cost, Stream 3 will always be placed on the tube side of any exchanger through which it passes. From Table A.3, the material factor, F_M, for heat exchangers with carbon steel shells and stainless steel tubes is 1.81. From Figure 15.16, with an operating pressure of 50 barg and F_M of 1.81, the value of h_{bc}/h is 0.517. Therefore, a modified heat transfer coefficient of (530)(0.517) = 274 W/m^2°C should be used to estimate heat transfer areas using the cost equation for base-case conditions.

Example 15.9.

Estimate the effect of the result of Example 15.8 on the total heat transfer area and cost of the heat-exchanger network calculated in Example 15.4. The adjusted heat transfer areas for the network are shown in Table E15.9.

Table E15.9. Heat Transfer Areas for Network Adjusted for Non-Base-Case Conditions for Stream 3

Temperature Interval	$\Sigma(Q_i/h_i)$ (m^2°C)	$A_{interval}$ (m^2)
2	$\frac{80}{0.27}+\frac{120}{0.274}+\frac{200}{0.08}$ $= 3234$	$\frac{3241}{(14.43)(0.8)} = 280.1$
3	$\frac{100}{0.27}+\frac{150}{0.274}+\frac{166.7}{0.25}+\frac{83.3}{0.08}$ $= 2626$	$\frac{2626}{(21.4)(0.8)} = 153.4$
4	$\frac{400}{0.40}+\frac{150}{0.274}+\frac{366.7}{0.25}+\frac{183.3}{0.08}$ $= 5305$	$\frac{5305}{(41.2)(0.8)} = 161.0$
5	$\frac{400}{0.40}+\frac{266.7}{0.25}+\frac{133.3}{0.08}$ $= 3733.1$	$\frac{3733}{(43.3)(0.8)} = 107.8$
6	$\frac{400}{0.40}+\frac{400}{0.10}$ $= 5000$	$\frac{5000}{(43.3)(0.8)} = 144.3$
Total		847 m^2

The results in Table E15.9 show that the effect on the fixed capital investment of the HEN of using stainless steel and an operating pressure of 50 bar for Stream 3 is equivalent to increasing the HEN area from 788 to 848 m^2 using base-case costs. The fixed capital investment from Example 15.7 was (8)($97,700) = $781,600. The use of nonstandard conditions is based on 8 exchangers each of area (847/8) = 106.0 m^2, a cost of (8)(103,600) = $828,800. This is an increase of $47,200.

15.8.2. Problems with Multiple Utilities

For more complicated problems, several pinch temperatures may occur, and energy may have to be added from more than one hot utility and rejected to more than one cold utility. In general, it makes good engineering sense to add heat from the coolest "hot" utility and reject heat to the hottest "cold" utility. For example, if heat must be rejected from the process at a temperature of 190°C, it could be rejected to the cooling water utility. However, it makes more sense—that is, it is more profitable—if this excess energy can be used to make medium-pressure steam, which can be used elsewhere in the plant. Likewise, if heat needs to be added to the process at a temperature of 80°C, it makes little sense to use valuable high-pressure steam (at 250°C); rather, low-pressure steam should be used.

15.8.3. Handling Streams with Phase Changes

The area of heat integration and pinch technology, in general, is quite broad, and many topics have not been covered here. The MUMNE approach outlined above will give a reasonable first approximation to the optimum heat integration scheme for a given process and is therefore useful in the preliminary design of a process. Although not stated explicitly, the analysis for the MUMNE design assumes that the streams are single phase and that the specific heat capacities of the streams are constant over the temperature range in the process. For streams that undergo a phase change or for which the specific heat capacities are not constant, the analysis becomes more complicated. However, for such streams, dummy streams can be used that have constant heat capacities. This concept is illustrated in Figure 15.17. The left-hand diagram shows a situation where a partial phase change is occurring. In this case, the enthalpy change can be approximated by using two dummy streams with constant heat capacities as shown in the diagram. For a single component that changes phase, the *T*-*Q* diagram is a horizontal line, and for this case, an arbitrarily small ΔT of 1°C is used to get the dummy heat capacity.

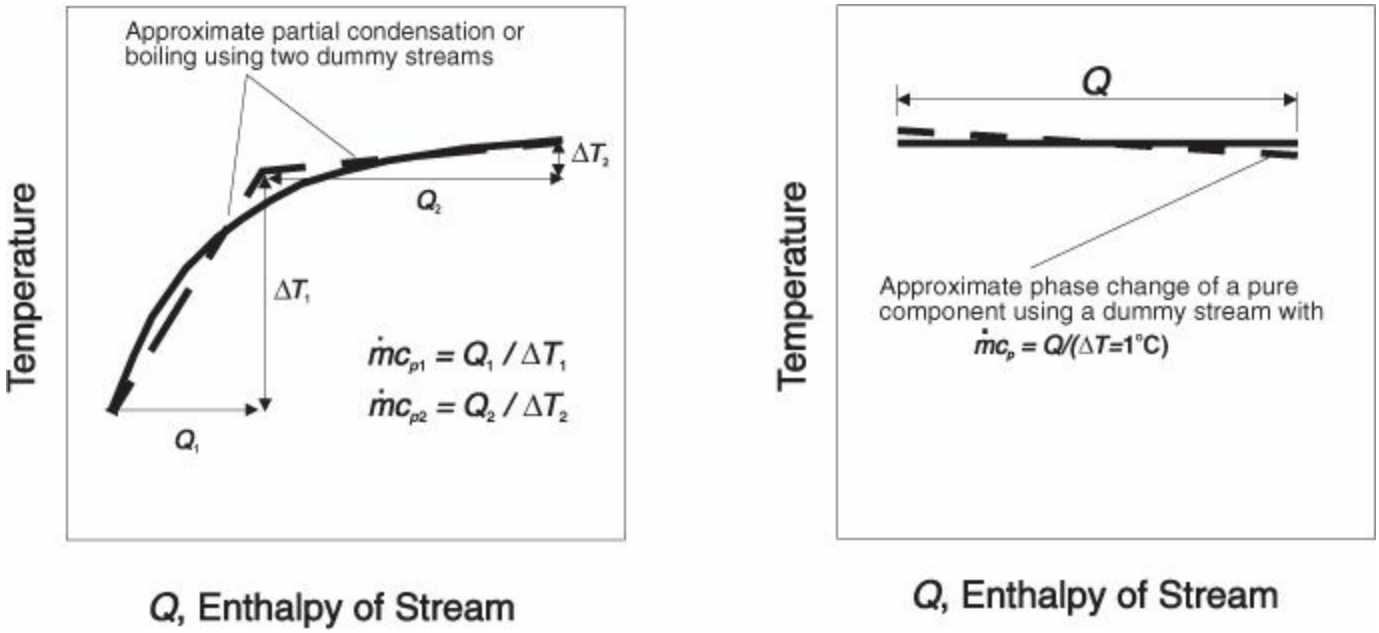


Figure 15.17. Use of Dummy Streams for Phase Changes

For large processes, the hand calculations described above become unwieldy and very time consuming. To help in these calculations, the HENSAD software has been developed and is contained on the CD accompanying the text.

15.9. Heat-Exchanger Network Synthesis Analysis and Design (HENSAD) Program

The heat-exchanger network synthesis analysis and design (HENSAD) program was developed to aid in solving the MUMNE problem previously described in this chapter. Once the feed stream information has been entered, temperature interval diagrams, cascade diagrams, and composite temperature-enthalpy plots (corresponding to Steps 1–4 introduced in Section 15.2) are calculated by the program. The design of the optimum exchanger network can also be completed using the software. However, the user must interact with the program to achieve a design that does not violate the minimum approach temperature specified for the problem. Parametric studies using the composite enthalpy diagram can also be carried out. Plots of network exchanger area, utility consumption, and EAOC as functions of minimum approach temperature can be made and printed out. The user is referred to a training video (HENSAD.AVI) that accompanies the software, which explains the

operation of the program and required user input. Although the software solves comprehensive problems, it is limited by the following assumptions:

- The specific heats of the streams are assumed to be constant.
- Problems with only one hot and one cold utility can be solved.
- For comparing the "optimal" minimum approach temperature, the before-tax EAOC is used as the objective function.
- Problems without a pinch may be analyzed, but plots of ΔT_{min} versus heat-exchanger area and EAOC are strictly correct only for situations where a pinch occurs.
- Economic analyses are valid for the range of application of the cost correlations.

In order to gain experience with the software, it is recommended that the problem studied in this chapter be entered and checked using the program after the AVI file has been viewed.

15.10. Mass-Exchange Networks

Pinch technology can be applied to the integration of mass-exchange devices in a manner analogous to how it is applied to integration of heat exchangers. A mass-exchange device is a separator. The purpose of heat integration is to use energy more efficiently. By matching hot and cold streams, the need for hot and cold utilities is minimized. This has environmental benefits in that utilities require energy, which increases pollution. Energy integration also saves the cost of these utilities, although it must be remembered that the most energy-efficient heat-exchange network is not necessarily the most economical one.

The purpose of mass-exchange networks is to use mass more efficiently. If mass is not used efficiently, the amount of waste created increases, creating more pollution. Without mass integration, raw materials also may not be used very efficiently.

As a simple example of mass integration, consider the acetone process in Appendix B, Section B.10. It is observed that process water is needed to scrub the acetone remaining in the vapor stream exiting the vessel, V-1102. It is also observed that there is a wastewater stream exiting the final distillation column, T-1103. This wastewater stream contains trace amounts of acetone and isopropyl alcohol. It should be possible to use some or all of this wastewater stream in the scrubber, T-1101, in place of process water. Because the water now contains some solute, it may be necessary to increase the size of the scrubber. In this example of mass integration, less waste is produced. Furthermore, the expenses of producing pure process water and of treating the wastewater stream are either reduced or eliminated.

The procedure for synthesis of mass-exchange networks is summarized here. Much more detailed treatments are available [12, 13], and brief discussions for pollution prevention applications are also available [14, 15]. The procedure parallels that for heat-exchange networks. There is a composition interval diagram (CID) that is analogous to the temperature interval diagram (TID). There is also a cascade diagram, a similar method for identifying the pinch and the minimum number of exchangers above and below the pinch, a composite mass-exchange diagram, and a final mass-exchange network. In the context of mass-exchange networks, a utility is the separation or addition of a solute to a sink or from a source that is not a process stream. This is similar to the hot and cold utilities in heat-exchange networks, and the analogous terms to *hot* and *cold* utilities are *rich* and *lean* utilities, respectively. Just as a hot utility adds energy to a stream, a rich utility adds mass (of a solute) to a stream. Similarly, just as a cold utility removes energy from a stream, a lean utility removes mass from a

stream (an adsorbent, for example). The term *rich* means a stream that is more concentrated in solute and hence will be losing solute to another process stream by mass transfer. The term *lean* means a stream that is less concentrated in solute and hence will be receiving solute from another process stream by mass transfer. With this analogy between hot and cold and rich and lean utilities understood, then the concept of a MUMNE (minimum utility, minimum number of exchangers) network also exists for mass-exchange networks.

However, there are several differences between heat-exchange networks and mass-exchange networks that must be understood:

1. The partition coefficient of the solute between the phases contacted in the mass-exchange devices (separators, probably absorbers, strippers, or liquid-liquid extractors) must be included. This is accomplished by plotting the mole fraction in the rich phase (denoted y) on the left side of the CID, and the mole fraction of the lean phase (denoted x) on the right side of the diagram. In a TID, the temperatures on opposite sides of the same horizontal line differ by the minimum approach temperature. In a CID, the rich- and lean-phase compositions are related by
$$y = m(x + \delta) \qquad (15.15)$$
where m is the partition coefficient and δ is the minimum approach composition based on the lean phase. The consequence of the partition coefficient is that the criterion for mass transfer from the rich phase to the lean phase is $y > mx$. If the partition coefficient, m, were unity, then this criterion would be completely analogous to that for heat transfer, where the criterion for heat transfer from hot to cold streams is $T_H > T_C$. Therefore, if $m < 1$, mass can be transferred from a rich phase with a lower mole fraction than the lean phase.
2. The rules for matching streams at the pinch are different. Above the pinch, the criterion for matching streams is
$$L \geq mR \qquad (15.16)$$
where L is the mass flowrate of the lean stream, and R is the mass flowrate of the rich stream. Below the pinch, the criterion for matching streams is
$$L \leq mR \qquad (15.17)$$
3. There is also a constraint regarding the number of streams. Above the pinch,
$$N_R \leq N_L \qquad (15.18)$$
and below the pinch,
$$N_R \geq N_L \qquad (15.19)$$
where N_L is the number of lean streams and N_R is the number of rich streams. If this criterion is not met, this means that stream splitting is required.

The procedure for synthesis of mass-exchange networks is illustrated in Examples 15.10 and 15.11. In these examples, it is assumed that there is only one solute, and it is the only component being transferred. The phases are completely immiscible; that is, no solvent is transferred between phases.

Example 15.10.

Consider the following process streams, all containing the same solute. The partition coefficient between both rich phases and the lean phase is 0.5 (i.e., $y = 0.5x$).

	kg/s	y_{in}	y_{out}
$R_1 = 1$	2	0.10	0.03
$R_2 = 2$	4	0.07	0.02
	kg/s	x_{in}	x_{out}
$L = 3$	4	0.00	0.07

Synthesize the MUMNE mass-exchange network for a minimum approach composition of $\delta = 0.01$.

The CID is shown in Figure E15.10(a). It is observed that the values on the left side represent y, the rich-stream compositions (mass fractions). The corresponding values on the right side are obtained by solving for x in Equation (15.15). The values far to the right are the total mass transferred in each interval and are obtained from the indicated equation.

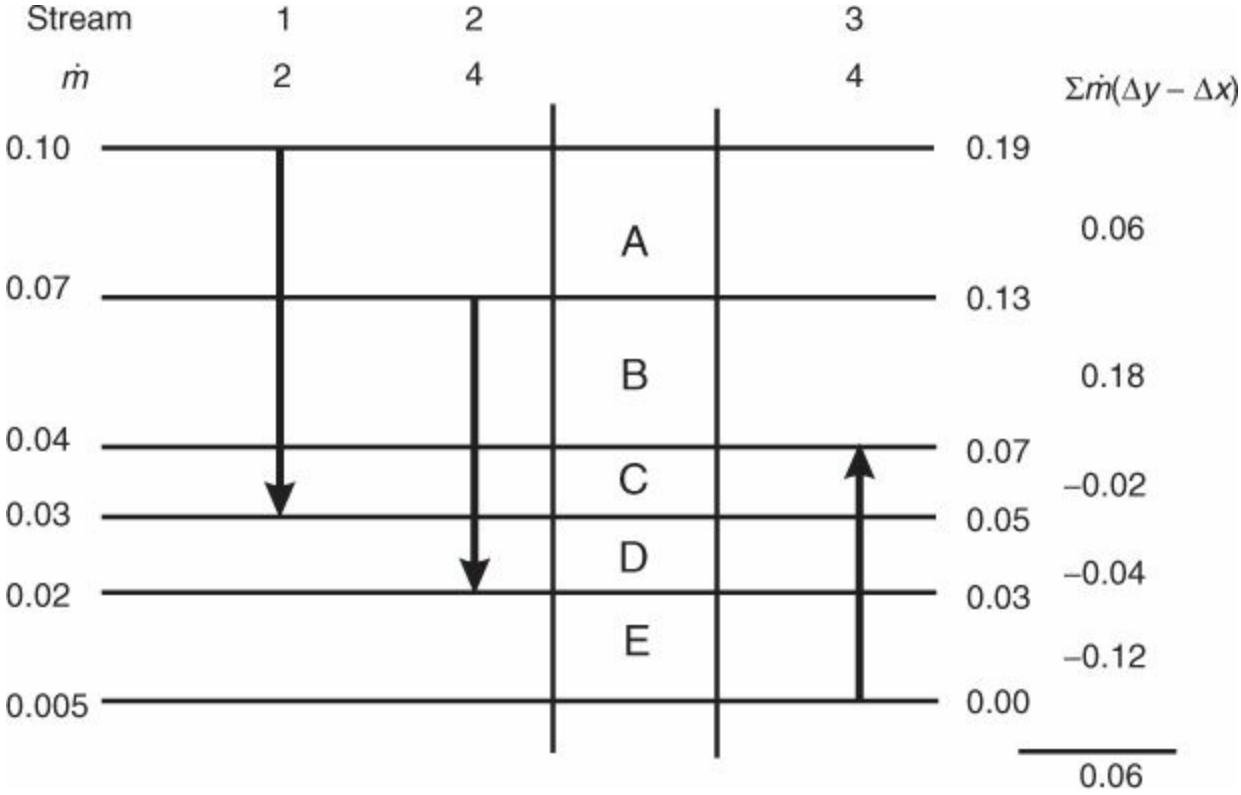


Figure E15.10(a). Composition Interval Diagram for Example 15.10

The cascade diagram is shown in Figure E15.10(b). Just as in heat-exchange networks, excess mass is cascaded through each interval. In this example, there is no pinch. At the bottom of the cascade diagram, there is excess mass requiring a lean utility (LU). An LU is a different separation unit, such as an adsorber, that removes solute.

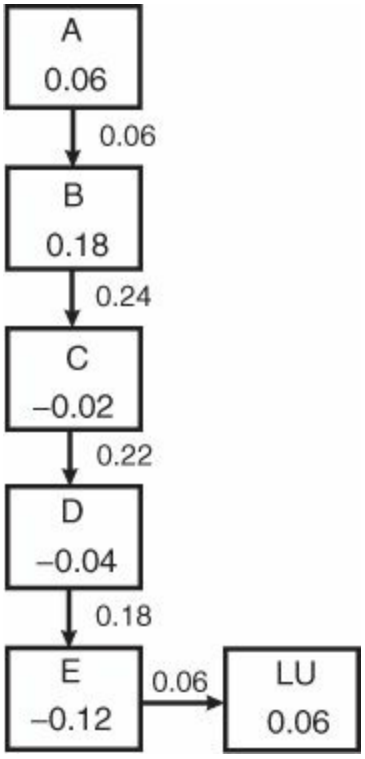


Figure E15.10(b). Cascade Diagram for Example 15.10

The minimum number of mass exchangers is shown in Figure E15.10(c). The method exactly parallels that for the minimum number of heat exchangers. In this example, three mass-exchange devices are required.

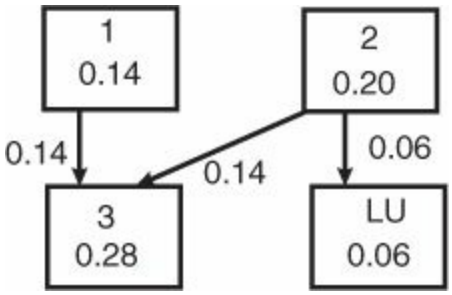


Figure E15.10(c). Minimum Number of Mass Exchangers for Example 15.10

Figure E15.10(d) shows the MUMNE network. Because there is no pinch, there are no restrictions other than mass balance and concentration gradient.

Stream	1	2	3
$\dot{m}$	2	4	4

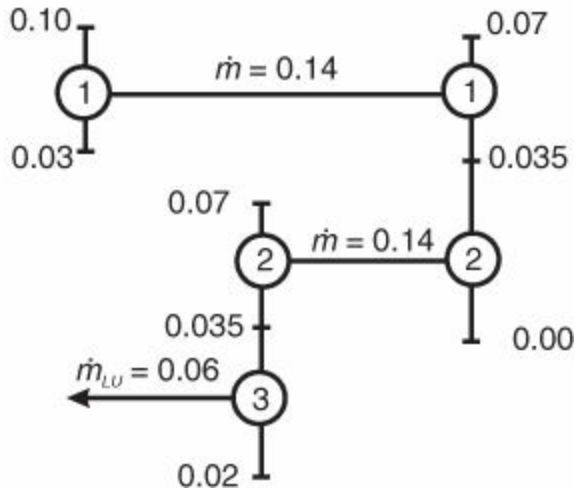


Figure E15.10(d). MUMNE Network for Example 15.10

Figure E15.10(e) shows the composite mass flow diagram. It is observed that the ordinate is the mass fraction in the lean phase. Therefore, for each rich-phase composition, Equation (15.15) is used to obtain a corresponding lean-phase value. Alternatively, the diagram could have been plotted using the mass fraction in the rich phase. There are two composite lines: one for the rich phase and one for the lean phase. The points needed to plot Figure E15.10(e) are as shown in the table on page 536.

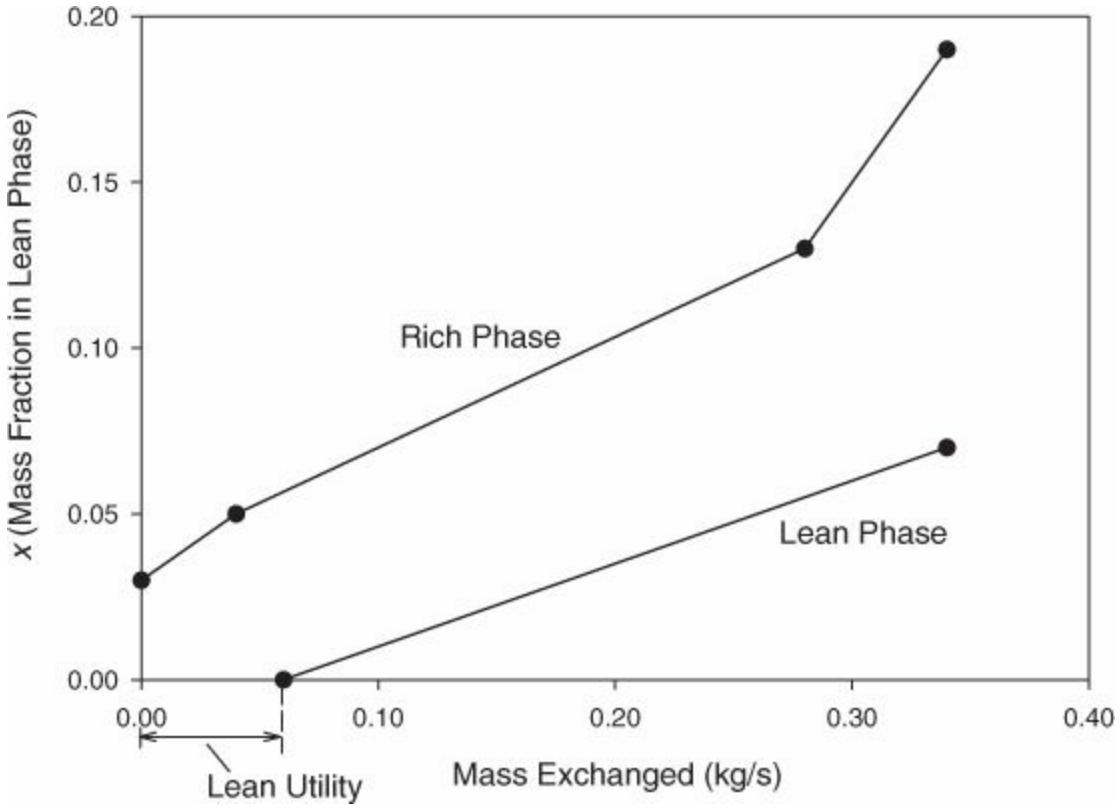


Figure E15.10(e). Composite Mass Flow Diagram for Example 15.10

Lean Streams			
Composition Interval	Mass Transferred in Interval (kg/s)	Cumulative Mass Transferred (kg/s)	Mass Fraction in Lean Phase (x)
E	0.00	0.06 (LU)	0.00
D	0.12	0.18	0.03
C	0.08	0.26	0.05
	0.08	0.34	0.07

Rich Streams			
Composition Interval	Mass Transferred in Interval (kg/s)	Cumulative Mass Transferred (kg/s)	Mass Fraction in Lean Phase (x)
E	0.00	0.00	0.03
D	0.04	0.04	0.05
C	0.02 + 0.04 = 0.06	0.10	0.07
B	0.06 + 0.12 = 0.18	0.28	0.13
A	0.06	0.34	0.19

The mass transfer in each interval is obtained by summing the mass flowrate of each stream multiplied by the composition change across the interval. It should be noted that only the points where the slope of the composite line changes are highlighted in Figure E15.10(e). The lean-stream line has been shifted to the right by the lean utility value so that the lean utility can be illustrated on Figure E15.10(e). This is so that the composite mass flow diagram is completely analogous to the composite heat flow diagram.

It is observed that there is no pinch point in Figure E15.10(e); that is, there is no point where the minimum approach composition is 0.01, as provided in the analysis. This is because there was no pinch identified in the cascade diagram (Figure E15.10[b]).

Finally, examine mass exchanger 1 on Figure E15.10(d). On the surface, it appears that this mass exchanger may not be feasible because of the mass fraction cross, which is illustrated by the lower two lines on Figure E15.10(f). However, as stated previously under the first difference between heat-exchange and mass-exchange networks, the partition coefficient must be considered when determining mass-exchanger feasibility. If the rich-stream mass fractions are divided by the partition coefficient (0.5 in this example), they are converted to the lean-stream scale. This line is so indicated on Figure E15.10(f). On the same scale, it is demonstrated that this mass exchanger is feasible; that is, there are no mass fraction crosses. An alternative, equally valid illustration of this point would have been to multiply the lean-stream mass fractions by 0.5.

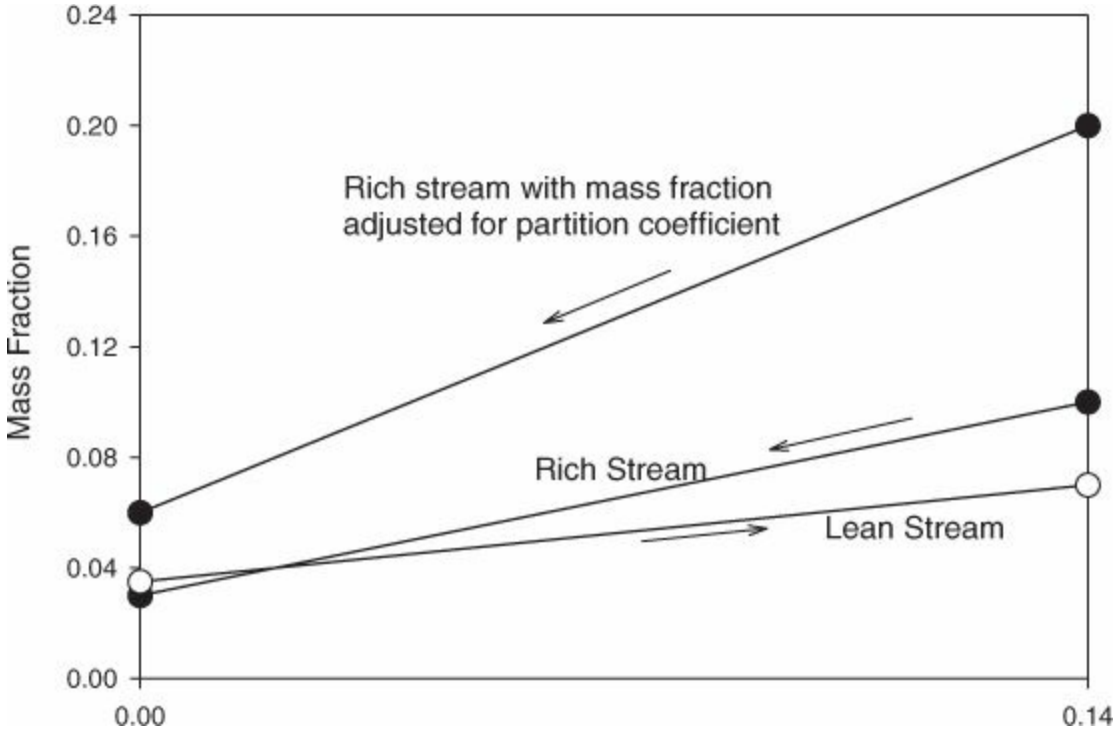


Figure E15.10(f). Illustration of Validity of Mass Exchanger 1 in Example 15.10

Example 15.11.

Consider the following process streams, all containing the same solute. The partition coefficient between both rich phases and the lean phase is 0.667 (i.e., $y = 0.667x$).

	kg/s	y_{in}	y_{out}
$R_1 = 1$	2	0.120	0.030
$R_2 = 2$	1	0.060	0.010

	kg/s	x_{in}	x_{out}
$L_1 = 3$	1	0.005	0.125
$L_2 = 4$	6	0.080	0.125

Synthesize the MUMNE mass-exchange network for a minimum approach composition of $\delta = 0.010$.

The composition interval diagram (CID) is shown in Figure E15.11(a). As in the previous example, the values on the left side represent y, the rich-stream compositions (mass fractions). The corresponding values on the right side are obtained by solving for x in Equation (15.15). The values far to the right are the total mass transferred in each interval and are obtained from the indicated equation.

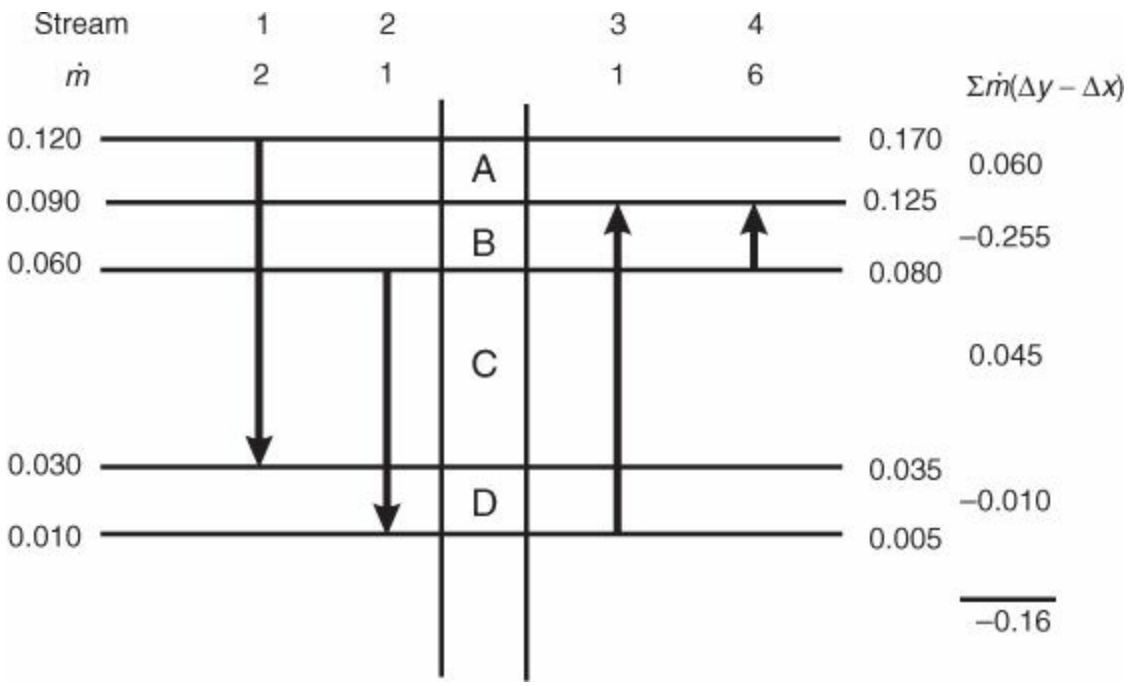


Figure E15.11(a). Composition Interval Diagram for Example 15.11

The cascade diagram is shown in Figure E15.11(b). There is a pinch in this example between intervals B and C. Therefore, the pinch compositions are 0.060 – 0.080. There is a mass deficiency above the pinch requiring a rich utility (RU). A rich utility is a separate unit in which pure solute is added to a stream. This may seem unusual. However, it must be remembered that this is not necessarily the optimum economic solution; it is the optimum solution for use of mass. There is also a mass excess below the pinch requiring a lean utility (LU). A lean utility is a separation device (such as an adsorber) that removes solute without exchanging solute with other process streams.

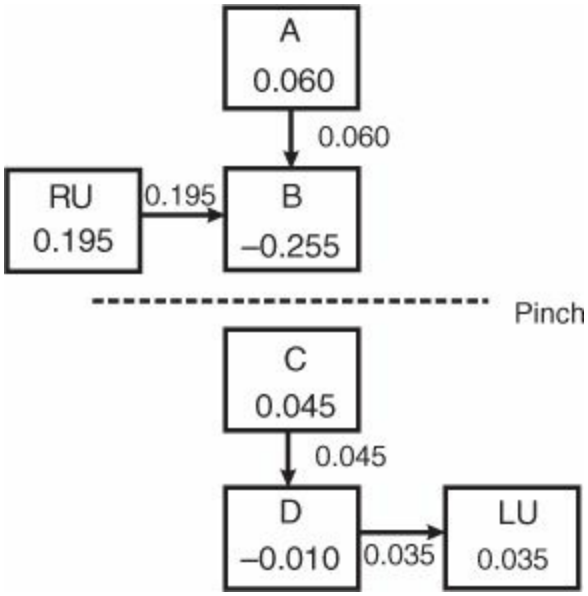


Figure E15.11(b). Cascade Diagram for Example 15.11

The minimum number of mass exchangers above and below the pinch is shown in Figure E15.11(c). In this example, three mass-exchange devices are required both above and below the pinch.

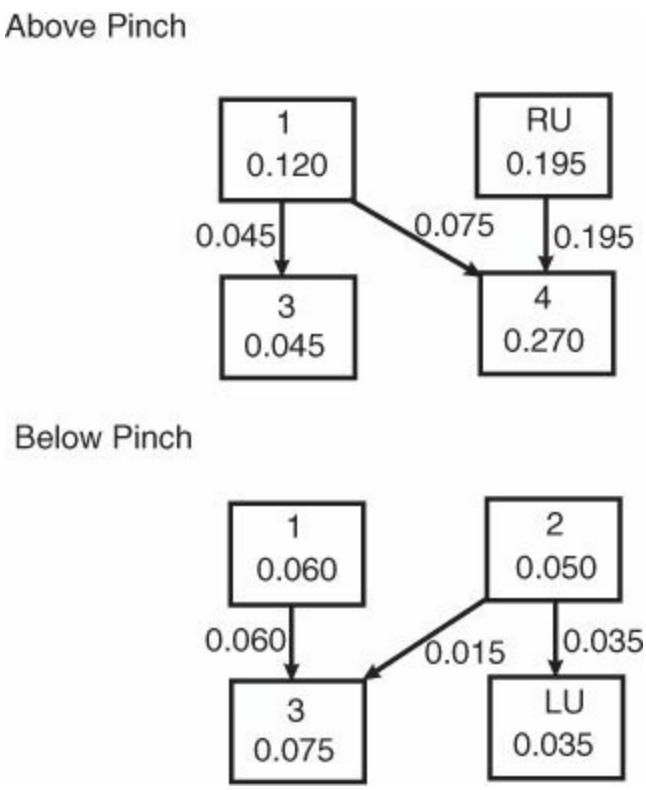


Figure E15.11(c). Minimum Number of Mass Exchangers Above and Below Pinch for Example 15.11

Figure E15.11(d) shows the MUMNE network. It is observed that the criteria in Equations (15.16) through (15.19) are obeyed.

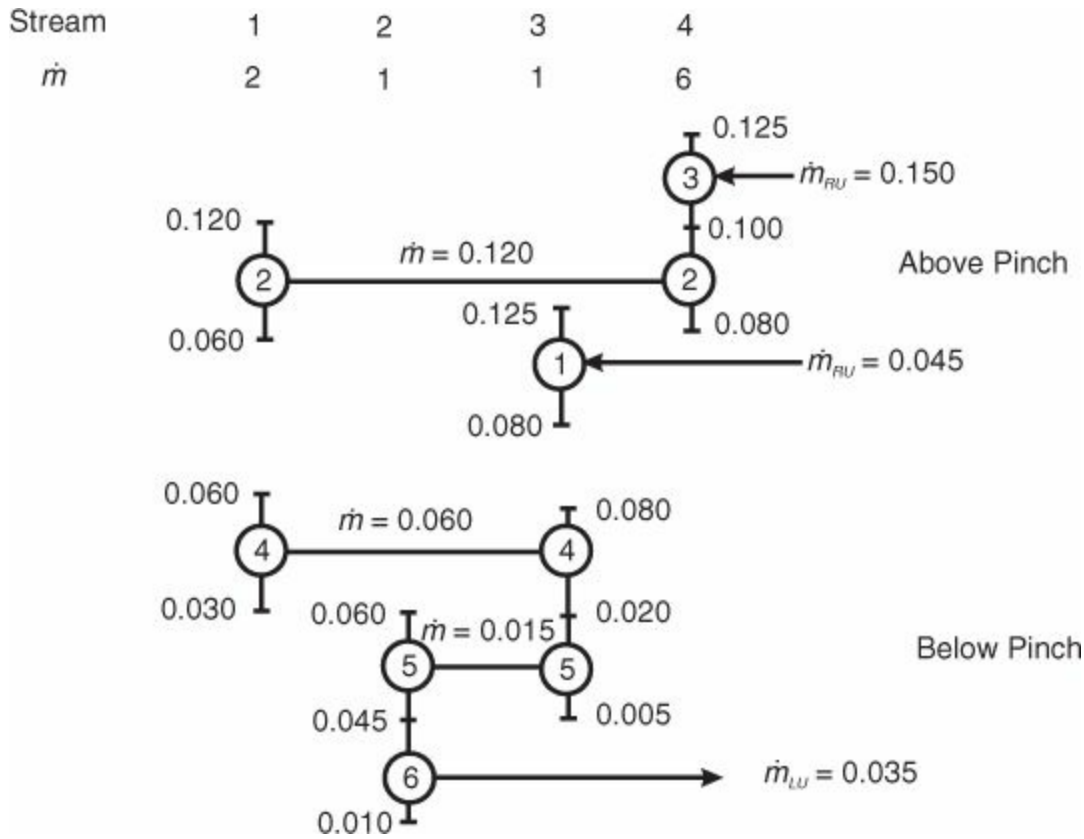


Figure E15.11(d). MUMNE Network for Example 15.11

Figure E15.11(e) shows the composite mass-exchange diagram. Once again the ordinate is the mass fraction in the lean phase. The points on Figure E15.11(e) are as shown in the table on page 541.

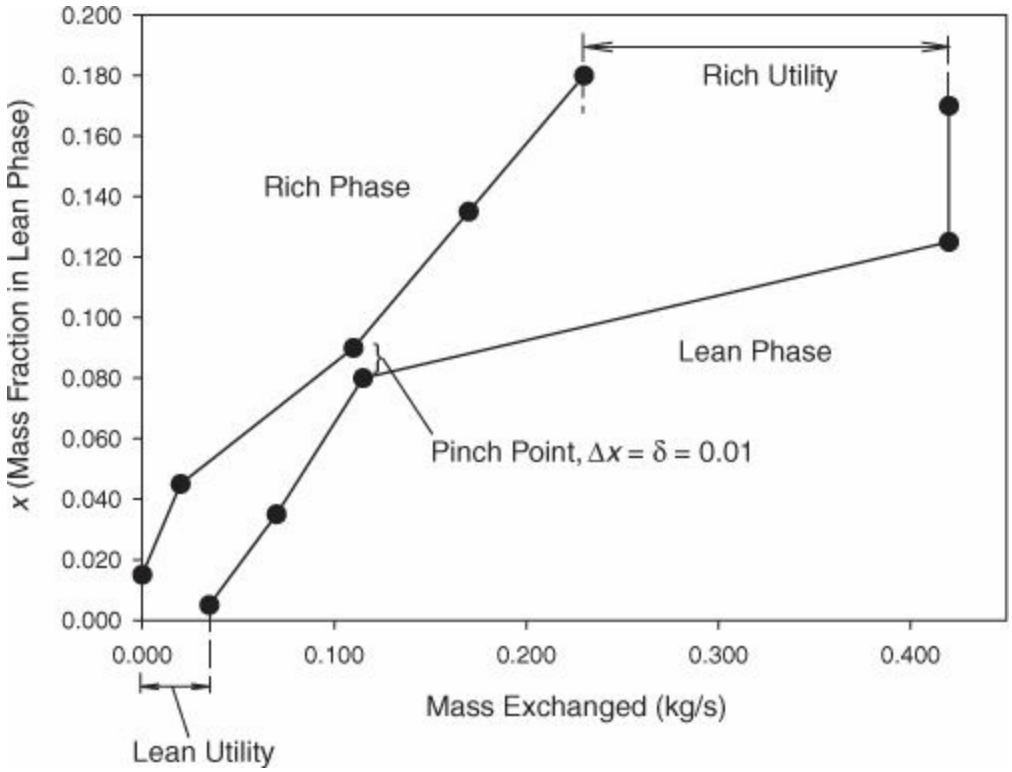


Figure E15.11(e). Composite Mass Flow Diagram for Example 15.11

Rich Streams			
Composition Interval	**Mass Transferred in Interval (kg/s)**	**Cumulative Mass Transferred (kg/s)**	**Mass Fraction in Lean Phase (*x*)**
E	0.000	0.000	0.015
D	0.020	0.020	0.045
C	0.060 + 0.060 = 0.090	0.110	0.090
B	0.060	0.170	0.135
A	0.060	0.230	0.180

Lean Streams			
Composition Interval	**Mass Transferred in Interval (kg/s)**	**Cumulative Mass Transferred (kg/s)**	**Mass Fraction in Lean Phase (*x*)**
D	0.000	0.035 (LU)	0.005
C	0.035	0.070	0.035
B	0.045	0.115	0.080
A	0.315	0.420	0.125
	0.000	0.420	0.170

The mass transfer in each interval is obtained by summing the mass flowrate of each stream multiplied by the composition change across the interval. Once again, the lean-stream curve is shifted by the lean utility value, and only the points where the slope of the composite line changes are highlighted in Figure E15.11(e).

There is a pinch point in this problem, and it is shown in Figure E15.11(e). As per the criteria, the pinch is at a composition difference of 0.010.

15.11. Summary

The applications of pinch technology to heat and mass integration were considered separately. The temperature interval diagram and cascade diagram were used to illustrate the relationship between the energy in the hot and cold streams, the relative temperatures of the streams, and the possible transfers of energy between them. The algorithm for analyzing the minimum utility, minimum number of exchangers problem (MUMNE) was outlined and was illustrated using an example. The role of the composite enthalpy diagram to determine the heat transfer area and the effect of minimum approach temperature was illustrated using several examples. The calculation of exchanger effectiveness for shell-and-tube heat exchangers was covered, and a simple expression to determine the number of shells for a given service was introduced. The effects of operating pressure and different materials of construction on the design of the heat-exchange network were illustrated with an example. Finally, the HENSAD software was introduced.

Mass-exchanger networks were discussed, and the composition interval diagram and cascade diagram for these systems were shown to parallel the development for heat-exchange networks. The role of the composite mass flow diagram was introduced, and the MUMNE design algorithm for mass-exchange networks was illustrated with two examples.

What You Should Have Learned

- The MUMNE method can be used to determine the "optimum" heat-exchange network.
- The optimum obtained from the MUMNE analysis is not necessarily the economic optimum.
- Decision variables within the MUMNE analysis can be varied to obtain an economic optimum.
- The mass integration analysis works essentially the same way as the MUMNE method.

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Short Answer Questions

1. List all the costs that are affected by changing the minimum temperature approach in a heat-exchanger network (HEN) design.
2. What are the advantages and disadvantages of decreasing the minimum approach temperature in a heat-exchange network?
3. One way to account for different materials of construction (MOCs) in heat-exchanger network design is to "adjust" the film heat transfer coefficients for streams that require MOCs other than carbon steel (CS). How would you adjust (increase or decrease) the heat transfer coefficients for streams requiring (a) MOCs cheaper than CS and (b) MOCs more expensive than CS? Briefly explain your reasoning.
4. In heat-exchanger network designs, there exists an optimum ΔT_{min} for the network. Explain carefully how capital costs and operating costs change as ΔT_{min} is increased.
5. For designing heat exchangers at the pinch, what is the criterion for matching streams above the pinch? Why is such a criterion needed?
6. Sketch a typical composite enthalpy diagram for a heat-exchanger network. On this diagram clearly label the x- and y-axes, and indicate on the diagram the values and location of the overall hot and cold utility demands and the pinch point.
7. What does the cascade diagram illustrate?
8. In general, what is the minimum number of exchangers required to design a heat-exchange network above the pinch that consists of n hot streams and m cold streams?
9. How does one deal with a stream that changes phase in a heat-exchanger network?
10. What is MUMNE? Describe it.

Problems

11. For a process, the following process streams must be cooled or heated:

Stream No.	$\dot{m}C_p$ $(10^3 BTU)/hr°F$	Temperature In °F	Temperature Out °F
1	4	600	320
2	4	470	280
3	3	340	580
4	5	300	480

Use the MUMNE algorithm for heat-exchanger networks and a minimum approach temperature of 20°F.

a. Determine the temperature interval diagram.

b. Determine the cascade diagram, the pinch temperatures, and the minimum hot and cold utilities. If there is a choice, for the sake of uniformity, choose the larger values for the pinch temperatures.

c. Determine the minimum number of heat exchangers above and below the pinch.

d. Determine the heat-exchange network above the pinch.

e. Determine the heat-exchange network below the pinch.

12. For a new process, the following process streams must be cooled or heated:

Stream No.	$\dot{m}C_p$ $(10^3 BTU)/hr°F$	Temperature In °F	Temperature Out °F
1	2	400	320
2	4	300	100
3	3	90	310
4	2	170	310

Use the MUMNE algorithm for heat-exchanger networks and a minimum approach temperature of 10°F.

a. Determine the temperature interval diagram.

b. Determine the cascade diagram, the pinch temperatures, and the minimum hot and cold utilities.

c. Determine the minimum number of heat exchangers above and below the pinch.

d. Determine the heat-exchange network above the pinch.

e. Determine the heat-exchange network below the pinch.

13. For a new process, the following process streams must be cooled or heated:

Stream No.	$\dot{m}C_p$ kW/°C	Temperature In °C	Temperature Out °C
1	3	180	100
2	5	120	80
3	3	70	140
4	2	80	160

Use the MUMNE algorithm for heat-exchanger networks and a minimum approach temperature

of 20°C.

a. Determine the temperature interval diagram.

b. Determine the cascade diagram, the pinch temperatures, and the minimum hot and cold utilities.

c. Determine the minimum number of heat exchangers above and below the pinch.

d. Determine the heat-exchange network above the pinch.

e. Determine a heat-exchange network below the pinch that has only one utility exchanger.

14. For a new process, the following process streams must be cooled or heated:

Stream No.	$\dot{m}C_p$ $(10^3 BTU)/hr°F$	Temperature In °F	Temperature Out °F
1	4	500	360
2	4	430	340
3	3	370	490
4	4	350	440

Use the MUMNE algorithm for heat-exchanger networks and a minimum approach temperature of 10°F.

a. Determine the temperature interval diagram.

b. Determine the cascade diagram, the pinch temperatures, and the minimum hot and cold utilities.

c. Determine the minimum number of heat exchangers above and below the pinch.

d. Determine the heat-exchange network above the pinch.

e. Determine a heat-exchange network below the pinch.

15. In a process design, the following process streams must be cooled or heated:

Stream No.	$\dot{m}C_p$ kW/°C	Temperature In °C	Temperature Out °C
1	3	250	200
2	5	200	40
3	4	30	200
4	3	90	200

Use the MUMNE algorithm for heat-exchanger networks and a minimum approach temperature of 10°C.

a. Determine the temperature interval diagram.

b. Determine the cascade diagram, the pinch temperatures, and the minimum hot and cold utilities.

c. Determine the minimum number of heat exchangers above and below the pinch.

d. Determine a heat-exchange network above the pinch.

e. Determine the heat-exchange network below the pinch.

16. The temperature interval diagram for a process is shown in Figure P15.16. For this process do

the following:

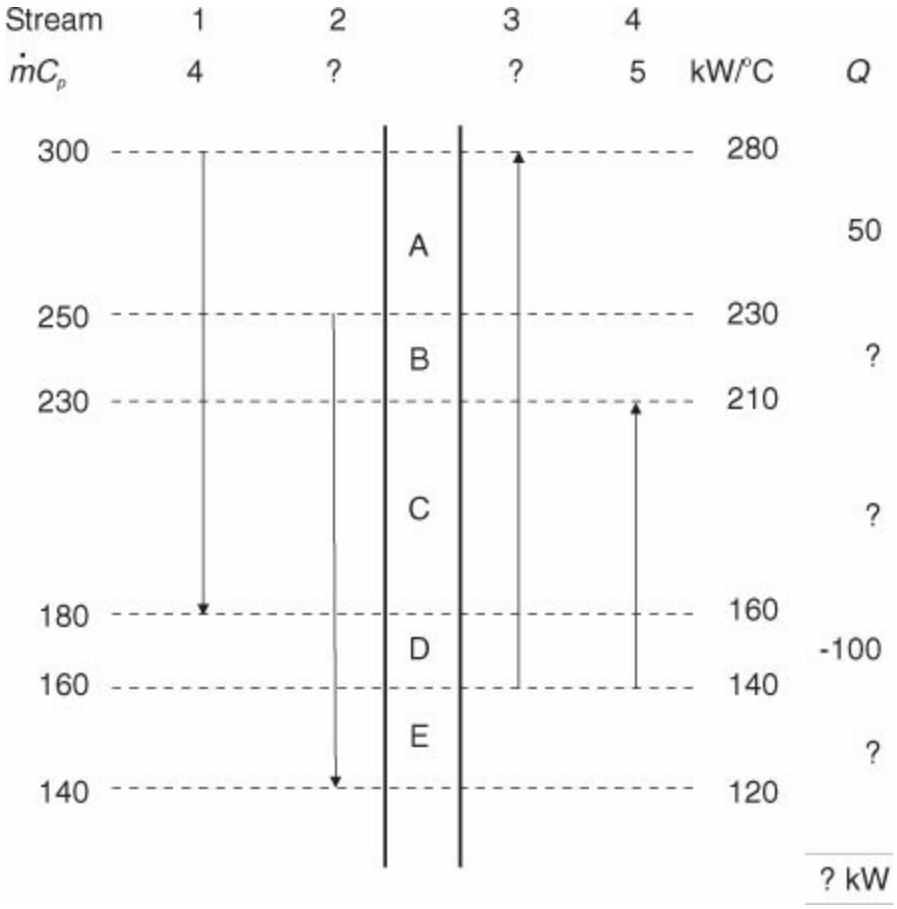


Figure P15.16. Temperature Interval Diagram for Problem 15.16

a. Compute the missing values of $\dot{m}C_p$ for Streams 2 and 3, the missing Q values for temperature intervals B, C, and E, and the total of all intervals.

b. Calculate the minimum hot and cold utility loads for this process subject to a minimum approach temperature of 20°C.

c. Calculate the pinch temperatures for this process. You may assume that there is only one hot and one cold utility available.

d. Calculate the minimum number of exchangers needed for the minimum energy case for above and below the pinch.

e. Design the MUMNE network for the process.

17. In a process design, the following process streams must be cooled or heated:

Stream No.	$\dot{m}C_p$ $(10^3$ BTU)/hr°F	Temperature In °F	Temperature Out °F
1	2	350	220
2	4	400	120
3	5	310	380
4	4	100	310

Use the MUMNE algorithm for heat-exchanger networks and a minimum approach temperature of 20°F.

a. Determine the temperature interval diagram.

b. Determine the cascade diagram, the pinch temperatures, and the minimum hot and cold utilities.

c. Determine the minimum number of heat exchangers above and below the pinch.

d. Design a heat-exchange network above the pinch.

e. Design a heat-exchange network below the pinch.

18. In a process design, the following process streams must be cooled or heated:

Stream No.	$10^{-3}\dot{m}C_p$ kW/°C	Temperature In °C	Temperature Out °C
1	4	250	180
2	5	200	160
3	4	140	230
4	3	170	210

There is an additional constraint that the only hot utility is steam at 205°C. Use the MUMNE algorithm for heat-exchanger networks and a minimum approach temperature of 20°C.

a. Determine the temperature interval diagram.

b. Determine the cascade diagram, the pinch temperatures, and the minimum hot and cold utilities.

c. Determine the minimum number of heat exchangers above and below the pinch.

d. Determine a heat-exchange network above the pinch.

e. What effect does the hot-utility constraint have on the heat-exchange network above the pinch?

f. Determine the heat-exchange network below the pinch.

19. In a process design, the following process streams must be cooled or heated:

Stream No.	$10^{-3}\dot{m}C_p$ kW/°C	Temperature In °C	Temperature Out °C
1	5	280	220
2	2	220	60
3	3	100	260
4	2	60	220

The hottest hot-utility stream is high-pressure steam at 254°C. Use the MUMNE algorithm for heat-exchanger networks and a minimum approach temperature of 20°C.

a. Determine the temperature interval diagram.

b. Determine the cascade diagram, the pinch temperatures, and the minimum hot and cold utilities.

c. Determine the minimum number of heat exchangers above and below the pinch.

d. Determine a heat-exchange network above the pinch. (Be careful!)

e. Determine the heat-exchange network below the pinch.

20. In a process design, the following process streams must be cooled or heated:

Stream No.	$10^{-3}\dot{m}C_p$ kW/°C	Temperature In °C	Temperature Out °C
1	2	250	120
2	2	260	120
3	3	110	190
4	3	150	240

Use the MUMNE algorithm for heat-exchanger networks and a minimum approach temperature of 10°C.

a. Determine the temperature interval diagram.

b. Determine the cascade diagram, the pinch temperatures, and the minimum hot and cold utilities.

c. Determine the minimum number of heat exchangers above and below the pinch.

d. Determine two alternative, correct heat-exchange networks above the pinch.

e. Determine two alternative, correct heat-exchange networks below the pinch.

21. In a process design, the following process streams must be cooled or heated:

Stream No.	$10^{-3}\dot{m}C_p$ kW/°C	Temperature In °C	Temperature Out °C
1	2	250	120
2	3	240	140
3	4	130	230
4	2	190	240

Use the MUMNE algorithm for heat-exchanger networks and a minimum approach temperature of 10°C.

a. Determine the temperature interval diagram.

b. Determine the cascade diagram, the pinch temperatures, and the minimum hot and cold utilities.

c. Determine the minimum number of heat exchangers above and below the pinch.

d. Determine a valid heat-exchange network above the pinch.

e. Determine a valid heat-exchange network below the pinch.

22. Six streams in a chemical process need to be heated or cooled. The thermal data for these streams are given in the following table:

Stream Number	$\dot{m}C_p$ (10^3BTU/hr°F)	T_{in} (°F)	T_{out} (°F)
1	1.0	620	320
2	6.0	420	120
3	3.0	420	220
4	5.0	400	600
5	2.0	200	300
6	4.0	100	400

a. Calculate the minimum hot and cold utility loads for this process subject to a minimum approach temperature of 20°F.

b. Calculate the pinch temperatures for this process. You may assume that there is only one hot and one cold utility available.

c. Calculate the minimum number of exchangers needed for the minimum energy case for above and below the pinch.

d. Design the MUMNE network for the process.

23. If the streams in Problem 15.22 have the following film heat transfer coefficients, estimate the optimum minimum approach temperature for this problem.

$h_1 = 75$ BTU/hr/ft^2°F

$h_2 = 25$ BTU/hr/ft^2°F

$h_3 = 10$ BTU/hr/ft^2°F

$h_4 = 45$ BTU/hr/ft^2°F

$h_5 = 30$ BTU/hr/ft^2°F

$h_6 = 30$ BTU/hr/ft^2°F

24. Rework Problem 15.23, for the case when the streams require special materials of construction with the following material factors:

Stream 1, $F_M = 1.0$

Stream 2, $F_M = 2.0$

Stream 3, $F_M = 3.0$

Stream 4, $F_M = 7.0$

Stream 5, $F_M = 2.5$

Stream 6, $F_M = 1.0$

25. Consider the following process streams, all containing the same solute. The partition coefficient between both rich phases and the lean phase is 0.5 (i.e., $y = 0.5x$).

	kg/s	y_{in}	y_{out}
$R_1 = 1$	2	0.10	0.03
$R_2 = 2$	4	0.07	0.02
	kg/s	x_{in}	x_{out}
$L = 3$	4	0.00	0.06

Synthesize the MUMNE mass-exchange network for a minimum approach composition of $\delta = 0.02$.

26. Ethanol can be made by fermentation of grains such as corn. It can be fermented only up to a mass fraction of about 0.15 because higher concentrations kill the yeast. A big market for ethanol made this way is as an additive to gasoline.

Suppose that you have 90 kg/h of gasoline, the lean stream, and you would like to increase its concentration of ethanol from zero mass fraction to 0.09. You have two rich ethanol-water streams from fermentation processes. One is at 60 kg/h and a mass fraction of 0.09, and the other is at 30 kg/h and a mass fraction of 0.12. It is desired to reduce the ethanol mass fraction in the rich streams to a mass fraction of 0.02. The partition coefficient between the rich and lean streams is 1.2 (i.e., $y = 1.2x$), where y is the mass fraction in the ethanol-water (rich) stream and x is the mass fraction of ethanol in the gasoline (lean) stream. Synthesize the MUMNE mass-exchange network for a minimum approach composition of $\delta = 0.01$.

27. Consider the following process streams, all containing the same solute. The partition coefficient between both rich phases and the lean phase is 0.5 (i.e., $y = 0.5x$).

	kg/s	y_{in}	y_{out}
$R_1 = 1$	4	0.10	0.06
$R_2 = 2$	6	0.07	0.05
	kg/s	x_{in}	x_{out}
$L_1 = 3$	4	0.10	0.16
$L_2 = 4$	1	0.06	0.12

Synthesize the MUMNE mass-exchange network for a minimum approach composition of $\delta = 0.02$.

28. Consider the following process streams, all containing the same solute. The partition coefficient between both rich phases and the lean phase is 0.667 (i.e., $y = 0.667x$).

	kg/s	y_{in}	y_{out}
$R_1 = 1$	4	0.100	0.060
$R_2 = 2$	6	0.070	0.050
	kg/s	x_{in}	x_{out}
$L_1 = 3$	4	0.065	0.125
$L_2 = 4$	1	0.000	0.080

Synthesize the MUMNE mass-exchange network for a minimum approach composition of $\delta = 0.010$.

29. Consider the following process streams, all containing the same solute. The partition coefficient between both rich phases and the lean phase is 0.667 (i.e., $y = 0.667x$).

	kg/s	y_{in}	y_{out}
$R_1 = 1$	1	0.100	0.060
$R_2 = 2$	6	0.070	0.020
	kg/s	x_{in}	x_{out}
$L_1 = 3$	2	0.020	0.125
$L_2 = 4$	1	0.000	0.080

Synthesize the MUMNE mass-exchange network for a minimum approach composition of $\delta = 0.010$.

Chapter 16. Advanced Topics Using Steady-State Simulators

What You Will Learn

- How user-added models can be developed to complement or enhance the capabilities of process simulators
- How and when to change the default sequence and method of solution in process simulators to aid convergence
- How to use a steady-state simulator to perform sensitivity and optimization studies
- How to use a process simulator for estimating physical property parameters

The fundamental concepts required for the basic use of steady-state process simulators were introduced in Chapter 13. These concepts should be clearly understood before proceeding with this chapter. Some of the features discussed in this chapter may not be available in a particular process simulator. Under these circumstances, there are generally three choices: to innovate an approach to mimic the desired feature or function by using the existing blocks in the process simulator of choice; to interface the simulator with other software possessing the required features, usually through a suitable interface; or to develop user models, fully or in part, with FORTRAN, C, Excel, or other proprietary programming languages and integrate them with the remaining flowsheet. Often, the choice depends upon the accuracy desired, the simulator software used, and the feature that the user wants to capture. Many of these aspects are discussed later in this chapter. The critical tasks are to find the modeling capabilities of the particular software platform for the desired fidelity of the model and to develop the model using these capabilities. This chapter discusses the various aspects of advanced modeling of which the user needs to be aware before attempting to develop such models in a simulator. In this chapter and elsewhere in the book, matrices/vectors are denoted by boldface, italicized letters, for example, $\boldsymbol{A}$ and $\boldsymbol{x}$. The entry in the i^{th} row and j^{th} column of a matrix A is denoted by A_{ij} or $A(i,j)$. The i^{th} entry of a vector x is denoted by x_i.

16.1. Why the Need for Advanced Topics in Steady-State Simulation?

With the advent of affordable, high-speed computers, computational work that was unthinkable even ten years ago can be easily performed today on a desktop computer. Future process engineers will benefit from learning these advanced topics for the following reasons:

- In a global economy, the process industries of today face steep competition from industries abroad. So, future plants should be exceptionally efficient. This type of advanced knowledge can also be used for retrofitting existing plants to improve their efficiency.
- Environmental regulations are becoming more and more stringent. The process industries are increasingly using advanced simulation techniques for modifying existing process plants and for developing advanced designs of new plants to maximize profit without violating the limits on environmental emissions. A number of examples are included in this chapter that focus on modeling acid-gas removal (AGR) plants.
- Process engineers can simulate new technologies with reasonable effort. Many of the advanced features available in the current process simulators make it possible to integrate relevant

experimental data in the process simulation. This results in a more accurate prediction over a wide range of operating conditions, something that is difficult, costly, and time consuming with an experiment-only approach.

- Large databases of thermodynamic as well as reaction data are now available. Such a database can be easily incorporated into the process model for a more accurate and more predictive model.
- There is growing interest within the process industries in understanding process systems better and benefiting from that understanding, not only by modifying the process/plant but also by monitoring the plant, predicting when problems may occur, and subsequent troubleshooting.
- Advanced modeling techniques can also help in identifying possible heat and work integration between various units of a process or between separate processes within a large chemical complex. This, in turn, helps to improve the plant profitability and operational flexibility.
- Availability of higher computational power makes it possible to simulate very complicated process plants with reasonable effort within a reasonable time. Understanding the techniques employed by the process simulators can really help in setting up large-scale simulations.
- Advanced solvers and optimization algorithms are also available in commercial process simulators that enable the optimal solution to be found quickly and efficiently.
- The implementation of advanced techniques also facilitates rapid screening between alternative and competing technologies and designs.

16.2. User-Added Models

User-added models (UAMs) can be created in a number of process simulators to overcome the following limitations:

- Even though simulators contain models of most process unit operations, the user may be interested in a higher-fidelity model, or the unit operation model is not available in the library of the process simulator.
- The required thermodynamic and/or transport models to represent a system are not available in the process simulator.
- Additional stream information is needed.
- Additional calculations are needed to complement the existing unit operation models.

In general, the UAMs need to communicate with the existing models in a flowsheet, and the simulator should be able to communicate with the UAMs. The UAMs are usually created in FORTRAN, C, Excel, VB, or some proprietary language such as Aspen Custom Modeler (ACM) in the Aspen Plus environment. Knowledge of these languages is essential, in addition to a clear understanding of the modeling requirements and the functioning of the software. Configuration of these compilers is usually simulator specific and will not be discussed here. In addition, certain rules must be followed while using a programming language in a particular simulator environment. This information is normally available in the user manual of the specific software. The software must know the location of a UAM if it is not physically connected to other blocks in the flowsheet, as is usually the case for unit operation models. Depending on the simulator environment, the user can make CAPE-OPEN-compliant UAMs, so that the process simulator can call these UAMs through suitable interfaces. The CAPE-OPEN-compliant UAMs need to follow CAPE-OPEN standards. These standards are

managed by CAPE-OPEN Laboratories Network (CO-LaN) [1] and help the computer-aided process engineering (CAPE) applications to communicate with each other.

16.2.1. Unit Operation Models

User-added unit operation models (UAUOM) can be stand-alone models, where everything needed for executing the model is part of the model itself. This includes the properties database and thermodynamic and transport models in addition to the model equations such as mass, momentum, species, energy conservation, and other constitutive relations. Then the simulator is simply used for interfacing with other models and for solving the system of relevant equations. Quite often, all or part of the properties database and thermodynamic and transport models is used. Function calls can be made to available routines in the simulator. Hence, a strategy might be to use the existing database, thermodynamic and transport models, and routines (or functions) from the simulator as much as possible and then to write equations for only those mechanisms/aspects that are not available or are unsatisfactory. The UAUOMs are often included as part of a user library, so that they can be used like other blocks available in the standard library.

For many unit operations, estimation of the phase equilibrium is one of the most important calculations. Calculation of phase equilibrium is an iterative procedure. Robust solution algorithms that can converge to a solution starting with a poor initial guess are often available in process simulators for phase-equilibrium calculations. The user can make use of these algorithms for solving user thermodynamic models. A number of options are available in the input arguments when the function call is made. If a function call is made for the phase-equilibrium calculations, it must be checked (as part of the UAUOM) to ensure that a successful solution has been reached before using the output and concluding that the simulation has been solved successfully. For calculating the phase equilibrium and mass and heat transport (momentum transport is often approximated by some constitutive law in a simulator environment), function calls can be made for calculating all or part of the thermodynamic and transport properties for the pure species and mixture by using the inbuilt models. Care must be exercised about the phase to which a model is applied and the properties that are needed for subsequent calculations. If Newton's method or a quasi-Newton method is used for solving the system of equations that requires the calculation of the partial derivatives of thermodynamic properties, the built-in routines can be used or codes can be written for calculating analytical and/or numerical Jacobians (defined in the discussion below). Note that substantial memory may be used in calculating these property derivatives, especially when a substantial number of species are present. Available options should be explored within a particular simulator for decreasing the computational cost.

For diagnostics in case of a convergence failure, special functions are available that generate some code or message from which the reason for the failure can be identified. Function calls can be made to the available mass and energy balance routines in the simulator. Again, the required inputs should be provided, and the outputs needed for the subsequent blocks should be calculated. Convergence of the unit should be checked by generating some flag/message/code.

When the user model is located in a separate Excel or FORTRAN or C file, the required inputs are passed on to that model from the simulator, the equation(s) is (are) solved in the user model, and the retrieved outputs are used for the subsequent blocks. In essence, the following steps are most often required:

Step 1: The model is developed by writing out the equations in the format required by the

simulator. If Newton's method or a quasi-Newton method is used for solving the system of equations, then a matrix is generated that contains first-order partial derivatives of the above-mentioned equations with respect to the variables. This matrix is known as the Jacobian matrix. If the vector of the system of equations is given by $\boldsymbol{f}$ and the vector of variables is given by $\boldsymbol{x}$, then the Jacobian matrix $\boldsymbol{J}$ is given by $\boldsymbol{J}_{ij} = \frac{\partial \boldsymbol{f}_i}{\partial \boldsymbol{x}_j}$.

Step 2: The built-in functions to be used must be specified. These include all thermodynamic and transport models, use of available databanks for physical properties and other parameters, and routines for mass and energy (and momentum) conservation equations and for generating diagnostic messages. The specific phase and whether pure or mixed species systems are to be used in these routines must be determined. The arguments needed must be satisfied, and it must be ensured that the correct messages are displayed when a routine or the entire system fails to solve.

Step 3: The input and output arguments in the calling sequence must be satisfied. The mapping of the input and output data must be correct. Other aspects that need attention in the calling sequence include parameter requirements, stream structure, data classification, parameter and variable data structure, types of variables and their mapping, sign conventions for heat and power, and so on.

Step 4: Any other specific requirements must be satisfied, such as specific report format and block initialization. Quite often, the variables must be scaled in magnitude for solution. The scaling and rescaling must be appropriate and correct.

Step 5: The code for the user model must satisfy the syntax requirement that is needed to compile it.

It is also important to ensure that the communication with the simulator is seamless and the calling sequence meets the requirements of the user. The robustness of the simulation should be checked by changing the input conditions. In some simulators, subroutines can be added to calculate some user-defined functions within the built-in user models, depending upon the simulator and particular unit operation model. These may include heat transfer rates, performance curves of pumps and compressors, mass and heat transfer coefficients, and tray and packing parameters in a distillation column. Example 16.1 will clarify these steps further.

16.2.2. User Thermodynamic and Transport Models

If the available thermodynamic and transport models are not satisfactory, the user can provide custom models. Properties of the pure species and species in a mixture can be calculated along with the bulk properties. For calculating the properties in a mixture, pure-component properties are usually used. Again, for pure-component properties, certain correlations may be used that depend upon other pure-component properties. For example, if the diffusivity of a species in a mixture is to be calculated using the Stefan-Maxwell or similar equations [2], then the binary diffusivities between species i and all other species j must be used. To calculate the binary diffusivities, the Chapman-Enskog formulation may be used [3], which for an ideal gas can be written as

$$D_{ij} = 0.0018583 \sqrt{T^3 \left(\frac{1}{M_i} + \frac{1}{M_j} \right)} \frac{1}{P \sigma_{ij}^2 \Omega_{ij}} \qquad (16.1)$$

where D_{ij} is the binary diffusivity (cm^2/s), T is the temperature of the system in K, M_i and M_j are the

molecular weights of species i and j respectively, P is the system pressure in atm, Ω_{ij} is the dimensionless collision integral, and σ_{ij} is the binary size parameter (Å) that appears in the Lennard-Jones potential between species i and j.

Before using this formulation, the collision integral Ω_{ij} should be known. However, this is a function of $\frac{k_B T}{\epsilon_{ij}}$. So the binary size and energy parameters σ_{ij} and ϵ_{ij} must be known.

Example 16.1 demonstrates the development of a UAM that reads the input data from a process simulator, carries out the necessary calculations, and writes the output stream data back to the process simulator for subsequent calculations.

Example 16.1.

A solvent for capturing CO_2 and H_2S is being developed in a laboratory. The K-values are known only at 20 bar and 30°C. The values are 4.68, 1.44, and 7.69×10^{-6} for CO_2, H_2S, and USR-SOL (the user solvent), respectively. Stream 1 in Figure E16.1(a) has the following properties:

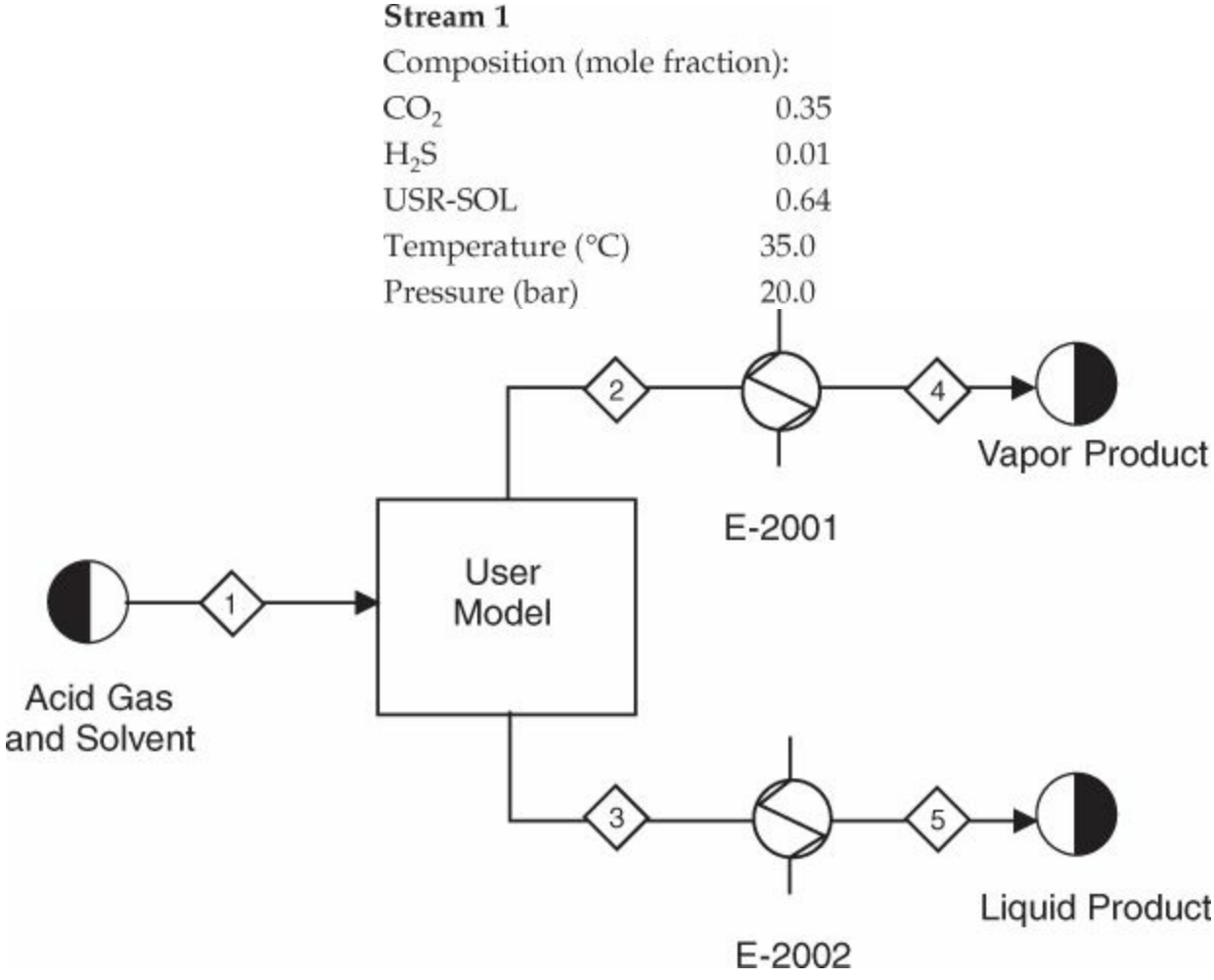


Figure E16.1(a). User Model of a Flash Vessel

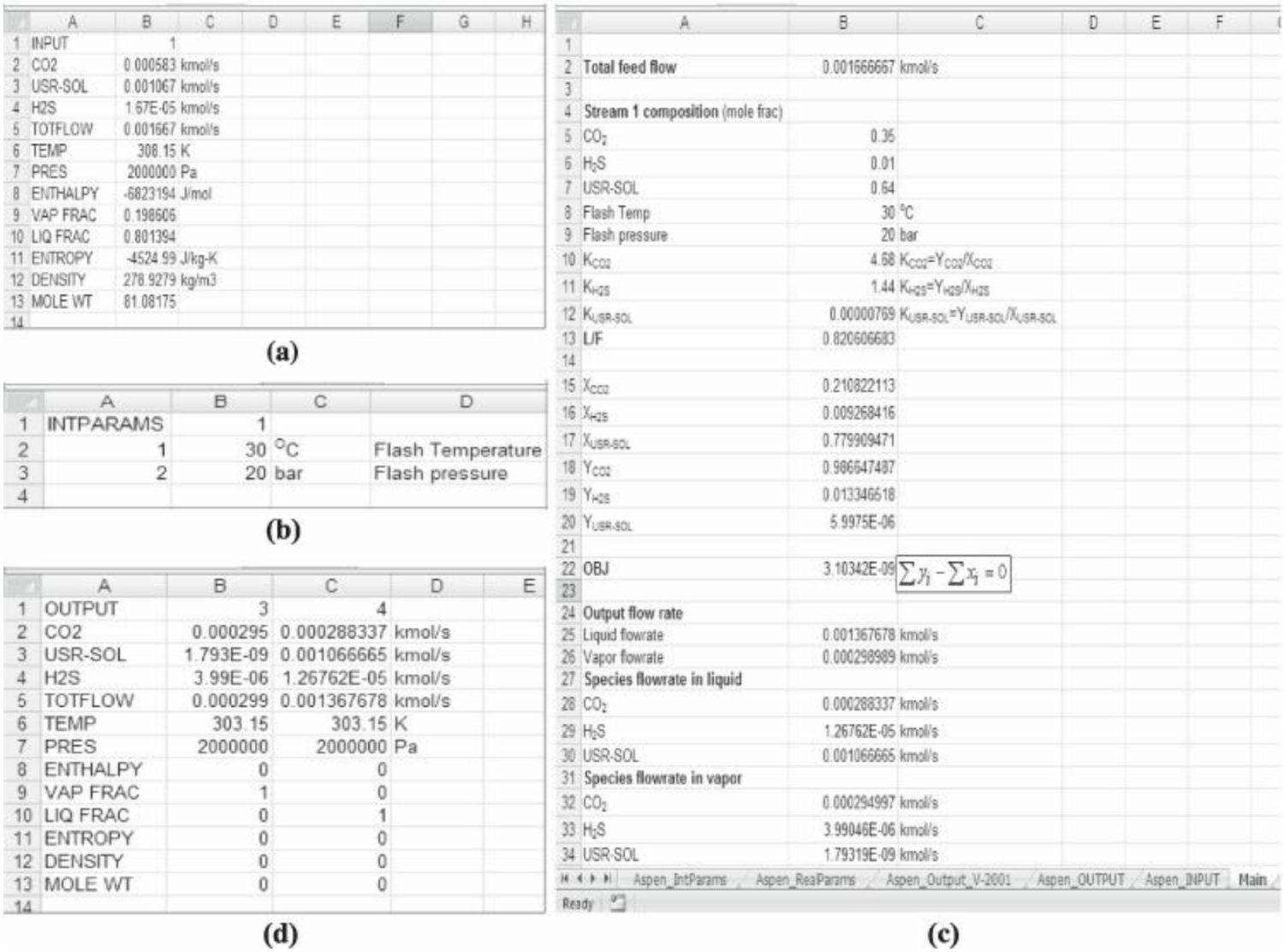
Develop a user flash model for which the temperature of the flash vessel is 30°C and the pressure is 20 bar. Write back the results of Streams 2 and 3 to the process simulator. The temperatures of Streams 4 and 5 are 50°C and 25°C, respectively. The heater blocks, E-2001 and E-2002, are included to ensure that the simulator can continue calculations with the results from the UAM.

Solution

The problem is set up in Aspen Plus V7.2, and the UAM is developed in Excel 2007. In Aspen Plus V7.2, propylene carbonate is used as the user solvent for the non-UAM Aspen Plus V7.2 blocks and for calculating other stream properties such as molecular weight, density, and enthalpy. The USER2 block in the Aspen Plus V7.2 library is used to call the UAM in Excel. A template .xls file from the Aspen Plus V7.2 USER library is used for this purpose. The template file contains a number of functions that are required for executing a UAM in Excel. In this template file, there are four sheets. The first sheet is named "Aspen_INPUT," a screen shot of which is shown in Figure E16.1(b)(a). In this sheet, Stream 1 properties such as species flowrates, total flowrate, pressure, enthalpy, vapor and liquid fraction, entropy, density, and molecular weight are passed on from Aspen Plus V7.2. In the second and third sheets, named "Aspen_Intparams" and "Aspen_Realparams," the integer and real parameters are passed on from the Aspen Plus V7.2 model of V-2001. In this example, two integer parameters, namely, the temperature (30°C) and pressure (20 bar) of V-2001, are declared under "User Arrays" in the USER2 block in Aspen Plus V7.2. Figure E16.1(b)(b) shows a screen shot of the sheet named "Aspen_Intparams." These and additional parameters can also be declared as real parameters in the sheet named "Aspen_Realparams." However, no real parameters are passed on to the user model in this example. Consequently, the sheet named "Aspen_Realparams" remains blank. Then a new sheet, called "Main," is created where the VLE calculation is carried out. A screen shot of this sheet is shown in Figure E16.1(b)(c). If F, L, V denote Stream 1, Stream 3, and Stream 2 molar flowrates, respectively, and z_i, x_i, y_i denote the respective mole fractions of the species i, then for an isothermal flash [4]

$$x_i = \frac{z_i}{K_i + \frac{L}{F}(1 - K_i)}$$

$$y_i = K_i x_i$$



	A	B	C
1	INPUT	1	
2	CO2	0.000583	kmol/s
3	USR-SOL	0.001067	kmol/s
4	H2S	1.67E-05	kmol/s
5	TOTFLOW	0.001667	kmol/s
6	TEMP	308.15	K
7	PRES	2000000	Pa
8	ENTHALPY	-6823194	J/mol
9	VAP FRAC	0.198606	
10	LIQ FRAC	0.801394	
11	ENTROPY	-4524.99	J/kg-K
12	DENSITY	278.9279	kg/m3
13	MOLE WT	81.08175	

(a)

	A	B	C	D
1	INTPARAMS	1		
2	1	30	°C	Flash Temperature
3	2	20	bar	Flash pressure
4				

(b)

	A	B	C	D	E
1	OUTPUT	3	4		
2	CO2	0.000295	0.000288337	kmol/s	
3	USR-SOL	1.793E-09	0.001066665	kmol/s	
4	H2S	3.99E-06	1.26762E-05	kmol/s	
5	TOTFLOW	0.000299	0.001367678	kmol/s	
6	TEMP	303.15	303.15	K	
7	PRES	2000000	2000000	Pa	
8	ENTHALPY	0	0		
9	VAP FRAC	1	0		
10	LIQ FRAC	0	1		
11	ENTROPY	0	0		
12	DENSITY	0	0		
13	MOLE WT	0	0		

(d)

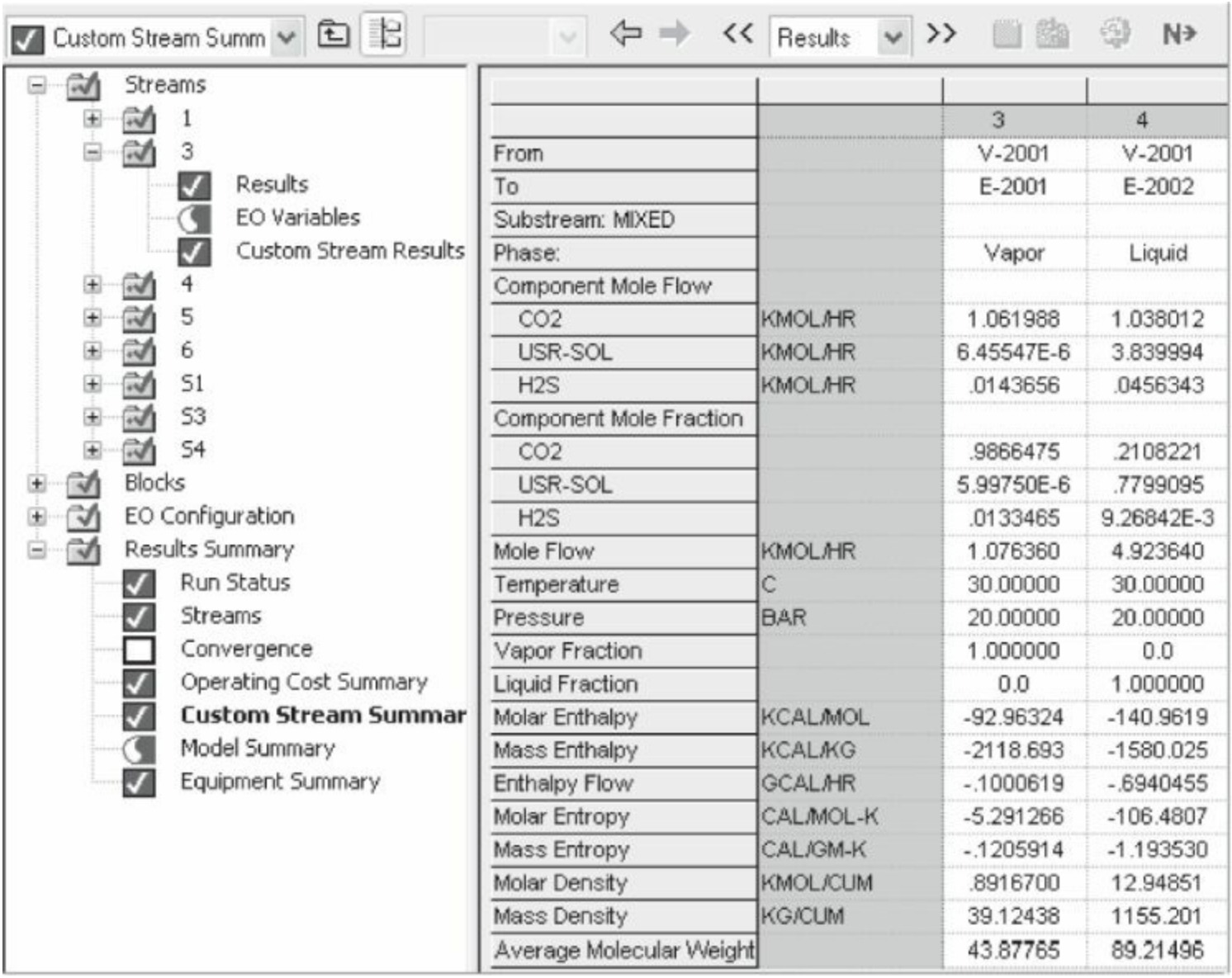
	A	B	C	D	E	F
1						
2	**Total feed flow**	0.001666667	kmol/s			
3						
4	**Stream 1 composition** (mole frac)					
5	CO_2	0.35				
6	H_2S	0.01				
7	USR-SOL	0.64				
8	Flash Temp	30	°C			
9	Flash pressure	20	bar			
10	K_{CO2}	4.68	$K_{CO2}=Y_{CO2}/X_{CO2}$			
11	K_{H2S}	1.44	$K_{H2S}=Y_{H2S}/X_{H2S}$			
12	$K_{USR-SOL}$	0.00000769	$K_{USR-SOL}=Y_{USR-SOL}/X_{USR-SOL}$			
13	L/F	0.820606683				
14						
15	X_{CO2}	0.210822113				
16	X_{H2S}	0.009268416				
17	$X_{USR-SOL}$	0.779909471				
18	Y_{CO2}	0.986647487				
19	Y_{H2S}	0.013346518				
20	$Y_{USR-SOL}$	5.9975E-06				
21						
22	OBJ	3.10342E-09	$\sum y_i - \sum x_i = 0$			
23						
24	**Output flow rate**					
25	Liquid fowrate	0.001367678	kmol/s			
26	Vapor fowrate	0.000298989	kmol/s			
27	**Species flowrate in liquid**					
28	CO_2	0.000288337	kmol/s			
29	H_2S	1.26762E-05	kmol/s			
30	USR-SOL	0.001066665	kmol/s			
31	**Species flowrate in vapor**					
32	CO_2	0.000294997	kmol/s			
33	H_2S	3.99046E-06	kmol/s			
34	USR-SOL	1.79319E-09	kmol/s			

Aspen_IntParams | Aspen_RealParams | Aspen_Output_V-2001 | Aspen_OUTPUT | Aspen_INPUT | Main

Ready

(c)

Figure E16.1(b). Screen Shots of the Excel Sheets for the VLE UAM: (a) "Aspen_Input" Sheet (b) "Aspen_Intparams" Sheet (c) "Main" Sheet Where All the Calculations Are Carried Out, and (d) "Aspen_Output" Sheet



		3	4
From		V-2001	V-2001
To		E-2001	E-2002
Substream: MIXED			
Phase:		Vapor	Liquid
Component Mole Flow			
CO2	KMOL/HR	1.061988	1.038012
USR-SOL	KMOL/HR	6.45547E-6	3.839994
H2S	KMOL/HR	.0143656	.0456343
Component Mole Fraction			
CO2		.9866475	.2108221
USR-SOL		5.99750E-6	.7799095
H2S		.0133465	9.26842E-3
Mole Flow	KMOL/HR	1.076360	4.923640
Temperature	C	30.00000	30.00000
Pressure	BAR	20.00000	20.00000
Vapor Fraction		1.000000	0.0
Liquid Fraction		0.0	1.000000
Molar Enthalpy	KCAL/MOL	-92.96324	-140.9619
Mass Enthalpy	KCAL/KG	-2118.693	-1580.025
Enthalpy Flow	GCAL/HR	-.1000619	-.6940455
Molar Entropy	CAL/MOL-K	-5.291266	-106.4807
Mass Entropy	CAL/GM-K	-.1205914	-1.193530
Molar Density	KMOL/CUM	.8916700	12.94851
Mass Density	KG/CUM	39.12438	1155.201
Average Molecular Weight		43.87765	89.21496

Figure E16.1(c). Results of Streams 3 and 4 Showing That the Missing Stream Properties from the Excel UAM Are Calculated by Aspen Plus V7.2

The VLE problem is solved when $\sum_i y_i - \sum_i x_i = 0$ by manipulating *L/F*. Cell B22 in this sheet (Figure E16.1[b][c]) shows the final value of the residual from the Excel solver. With the value of *L/F* known, the molar flowrates of the species in the liquid and vapor product can easily be obtained. All the calculations are performed in this sheet using the values in the "Aspen_INPUT" sheet. The values from the "Aspen_INPUT" sheet are called by "Aspen Helper" functions. For example, in cell B5 of this sheet, the mole fraction of CO_2 in Stream 1 is calculated by obtaining the CO_2 and total flowrates from the "Aspen_INPUT" sheet. The cell B5 entry for this calculation is

"=ahGetValue(Aspen_INPUT,"CO2",1)/ahGetValue(Aspen_INPUT,"TOTFLOW",1)"

It is observed that the values are obtained by referring to the sheet name, variable name, and stream name rather than the cell address. This is done to avoid any problem due to changes in the cell location of a variable because of the addition of more streams to the block and/or more species to the Aspen Plus V7.2 simulation. In Figure E16.1(b)(d), the Excel sheet named "Aspen_Output" shows the values of the stream variables that have been referenced to the appropriate cells in the "Main" sheet. These stream variables are the output flowrates along with the temperature and pressure. Note that in this screen shot, other stream properties such as enthalpy, entropy, molecular weight, and so forth, are

not calculated because the species flowrates along with the temperature and pressure fully define the stream, and the rest of the properties can be calculated by Aspen Plus V7.2. If the calculated values of these properties determined by Aspen Plus V7.2 are not satisfactory, then only these properties need to be calculated in the UAM. These properties are calculated in the USER2 model in Aspen Plus V7.2 by carrying out a "Stream Flash" operation. There were no issues faced in simulating E-2001 and E-2002 located downstream of the flash. The results for Streams 3 and 4 from Aspen Plus V7.2 are shown in Figure 16.1(c). It is observed that Aspen Plus V7.2 has calculated the remaining properties.

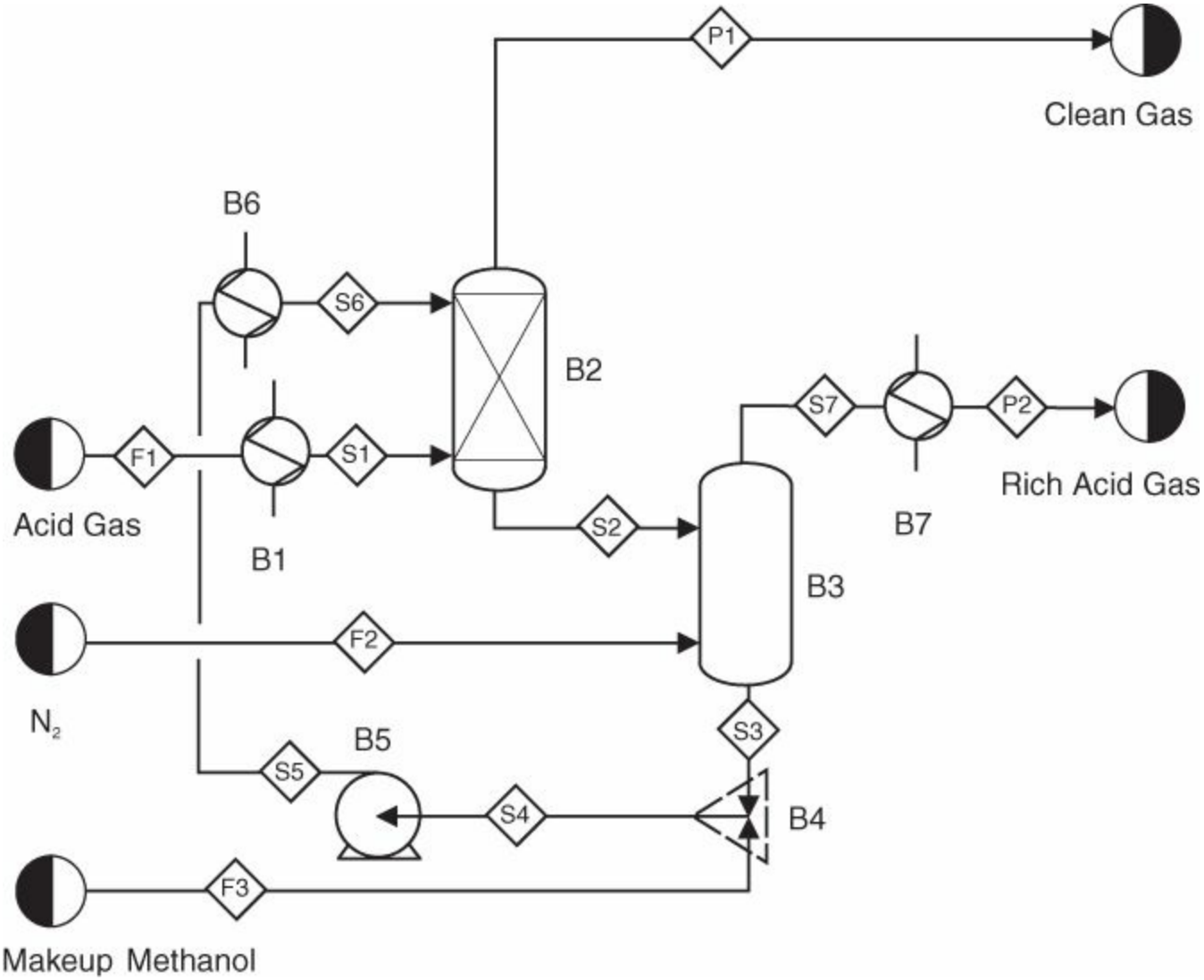


Figure 16.1. Simple Flowsheet of an Acid-Gas Removal (AGR) Process Using Chilled Methanol

16.2.3. User Kinetic Models

In process simulators, variations of power-law- and Langmuir-Hinshelwood-type expressions are available along with Arrhenius-type expressions for the pre-exponential factor. However, a specific kinetic model may be needed that is not consistent with the built-in models. While developing user kinetic models, the following items must be considered:

1. The phase(s) in which the reaction(s) takes place
2. The differences in specification between catalytic and noncatalytic reactions
3. The interpretation of signs that will depend on whether consumption or generation is considered

In addition, simulators may have some predefined units for the rate of reactions based on the phase and/or whether the reaction is catalytic or noncatalytic, and the user-added rate expressions must be consistent with these units. These requirements may vary depending on the unit operation model that calls the user-added kinetic models. For example, in a particular stage of a reactive distillation column, the temperatures used in the reaction rates are different based on the phase of the reaction, while a single temperature is used in a CSTR model. In Example 16.2, a UAM passes on specified inputs to a reactor model in a simulator, runs the model, retrieves the results, and then performs some calculations with the retrieved results.

Example 16.2.

Develop a model of a coal-fed gasifier as shown in Figure E16.2(a). The base-case properties of Streams S1 and S2 (here a different naming convention is used for reasons to be explained later) are as follows:

Properties of Stream S1	
Species Mass Flowrates (kg/s)	
H_2	0.45
O_2	0.69
N_2	0.12
S	0.25
C	6.38
H_2O	5.21
Ash	1.00
Total Flowrate (kg/s)	14.10
Temperature (°C)	100.0
Pressure (bar)	51.0
Properties of Stream S2	
Composition (mole fraction)	
O_2	0.95
N_2	0.018
Ar	0.032
Total Flowrate (kg/s)	8.28
Temperature (°C)	200.0
Pressure (bar)	51.0

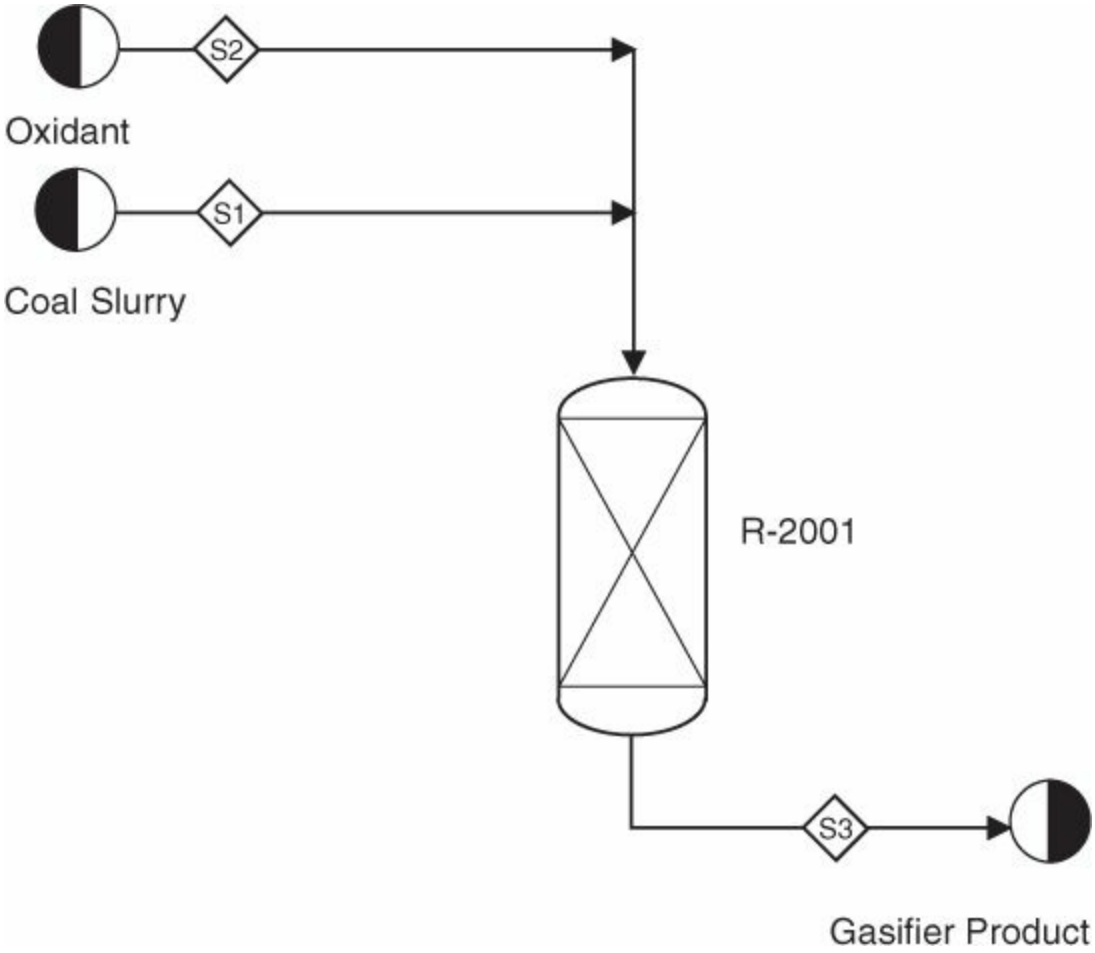


Figure E16.2(a). Flowsheet of the Gasifier

Consider ash to be pure silicon dioxide (SiO_2), and treat the ash and carbon as pure solids. Simulate the gasifier considering simultaneous physical and chemical equilibrium. The operating pressure is 50 bar and the heat duty is –4133 kW (i.e., heat loss to the surroundings). Once the base-case simulation is developed, calculate the gasifier cold gas efficiency as the water/coal and oxidant/coal ratios (both ratios are on a mass basis) are changed. The coal flowrate in these two ratios is that of the wet coal flowrate. For this study, develop a UAM in Excel or FORTRAN or C, or any other software interface from which inputs can be written to the process simulator model and outputs can be obtained. For Stream S1, 1.11 kg/s of mass flow is due to the wet coal and 4.1 kg/s is the added water for preparing the slurry. Subtracting this added water from the total flowrate of Stream S1, the wet coal flowrate in Stream S1 can be calculated to be 10 kg/s.

$$\text{Water Flowrate in Stream S1} = R_W C_W + W_C$$

$$\text{Flowrate of Stream S2} = R_{O_2} C_W$$

$$\text{Heat Duty of R–2001(kW)} = -250 - 4690 R_{O_2}$$

$$\text{Cold Gas Efficiency (\%)} = \frac{(121)F_{W,H_2} + (10.2)F_{W,CO} + (49.9)F_{W,CH_4}}{(27.151)C_W}$$

where R_W is the water/coal ratio, C_W is the wet coal flowrate (= 10 kg/s in the base case), W_C is the flowrate of water contained the wet coal (= 1.1 kg/s in the base case), and R_{O_2} is the oxidant/coal ratio. F_{W,H_2}, $F_{W,CO}$, and F_{W,CH_4} are the mass flowrates (kg/s) of H_2, CO, and CH_4 in Stream S3, respectively. For the heat-loss term, follow the convention for your simulator. The equation above is written following the convention that a negative heat duty is treated as heat loss to the environment.

The heat-loss term is not particularly accurate but is used for estimation purposes only. Calculate the gasified cold gas efficiency by varying the R_{O_2} in the range 0.678–0.928 with $R_W = 0.410$ and by varying R_W in the range 0.310–0.498 with $R_{O_2} = 0.828$.

Solution

The problem is set up in Aspen Plus V7.2 using an "RGibbs" block for simulating the gasifier. The Peng-Robinson (PR) EOS is used. The following products are considered: CO, CO_2, H_2, H_2O, O_2, C, N_2, CH_4, ash (inert), S, H_2S, NH_3, Ar (inert). Because of the presence of solids, the stream class is declared as MIXCISLD. This stream class supports conventional solids without particle size distributions along with a mixed substream to handle other liquid and gaseous species. Once the base-case model is developed and solved successfully, an Excel file is generated that can interact with the Aspen Plus V7.2 file using the COM interface. Figure E16.2(b) shows the Excel file with the calculations, the function calls, and the plot. The location of the Aspen Plus V7.2 file is shown in cell A1. For establishing a link with the Aspen Plus V7.2 file and for closing it, two buttons are created to which the macros "OpenSim" and "CloseSim" are assigned. These macros can be seen in Figure E16.2(c).

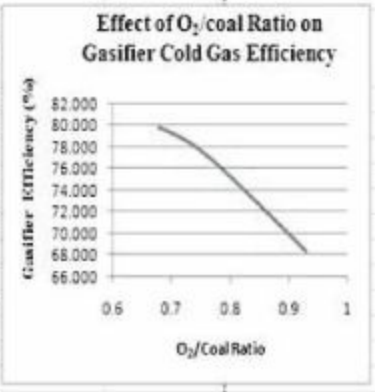
C:\Debu\IGCC\Prdriven\Book\USERMODEL\Example\Rgibbs_gasifier.bkp

Open Gasifier Simulation | Close Gasifier Simulation

coal flowrate (kg/s)	10
water in coal (kg/s)	1.11

	LHV (MJ/kg)
coal	27.151
H_2	121
CO	10.2
CH_4	49.9

Water/Coal	O_2/Coal	Oxidant (kg/s)	Water (kg/s)	Heat loss (kW)	H_2 in Stream PROD (kg/s)	CO in Stream PROD (kg/s)	CH_4 in Stream PROD (kg/s)	Gasifier cold gas efficiency (%)
0.410	0.678	6.78	5.21	-3429.82	0.661	11.602	0.369	79.837
0.410	0.703	7.03	5.21	-3547.07	0.682	11.900	0.226	79.249
0.410	0.728	7.28	5.21	-3664.32	0.691	12.138	0.115	78.503
0.410	0.753	7.53	5.21	-3781.57	0.685	12.289	0.046	77.538
0.410	0.778	7.78	5.21	-3898.82	0.666	12.356	0.016	76.373
0.410	0.803	8.03	5.21	-4016.07	0.640	12.370	0.005	75.098
0.410	0.828	8.28	5.21	-4133.32	0.613	12.355	0.002	73.779
0.410	0.853	8.53	5.21	-4250.57	0.586	12.322	0.001	72.440
0.410	0.878	8.78	5.21	-4367.82	0.560	12.275	0.000	71.091
0.410	0.903	9.03	5.21	-4485.07	0.535	12.216	0.000	69.734
0.410	0.928	9.28	5.21	-4602.32	0.510	12.146	0.000	68.370
0.310	0.828	8.28	4.21	-4133.32	0.576	12.884	0.001	74.075
0.323	0.828	8.28	4.335	-4133.32	0.580	12.819	0.001	74.039
0.335	0.828	8.28	4.46	-4133.32	0.585	12.754	0.001	74.003
0.348	0.828	8.28	4.585	-4133.32	0.590	12.688	0.001	73.966
0.360	0.828	8.28	4.71	-4133.32	0.594	12.622	0.001	73.929
0.373	0.828	8.28	4.835	-4133.32	0.599	12.556	0.001	73.892
0.385	0.828	8.28	4.96	-4133.32	0.604	12.489	0.002	73.855
0.398	0.828	8.28	5.085	-4133.32	0.608	12.422	0.002	73.817
0.410	0.828	8.28	5.21	-4133.32	0.613	12.355	0.002	73.779
0.423	0.828	8.28	5.335	-4133.32	0.618	12.286	0.002	73.740
0.435	0.828	8.28	5.46	-4133.32	0.623	12.218	0.002	73.701
0.448	0.828	8.28	5.585	-4133.32	0.628	12.149	0.003	73.662
0.460	0.828	8.28	5.71	-4133.32	0.632	12.079	0.003	73.622
0.473	0.828	8.28	5.835	-4133.32	0.637	12.009	0.004	73.582
0.485	0.828	8.28	5.96	-4133.32	0.642	11.939	0.004	73.541
0.498	0.828	8.28	6.085	-4133.32	0.647	11.868	0.005	73.499



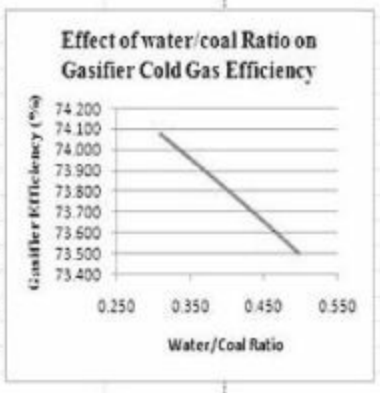


Figure E16.2(b). Excel Sheet for Writing to and Retrieving Results from a Gasifier Model Developed in Aspen Plus V7.2

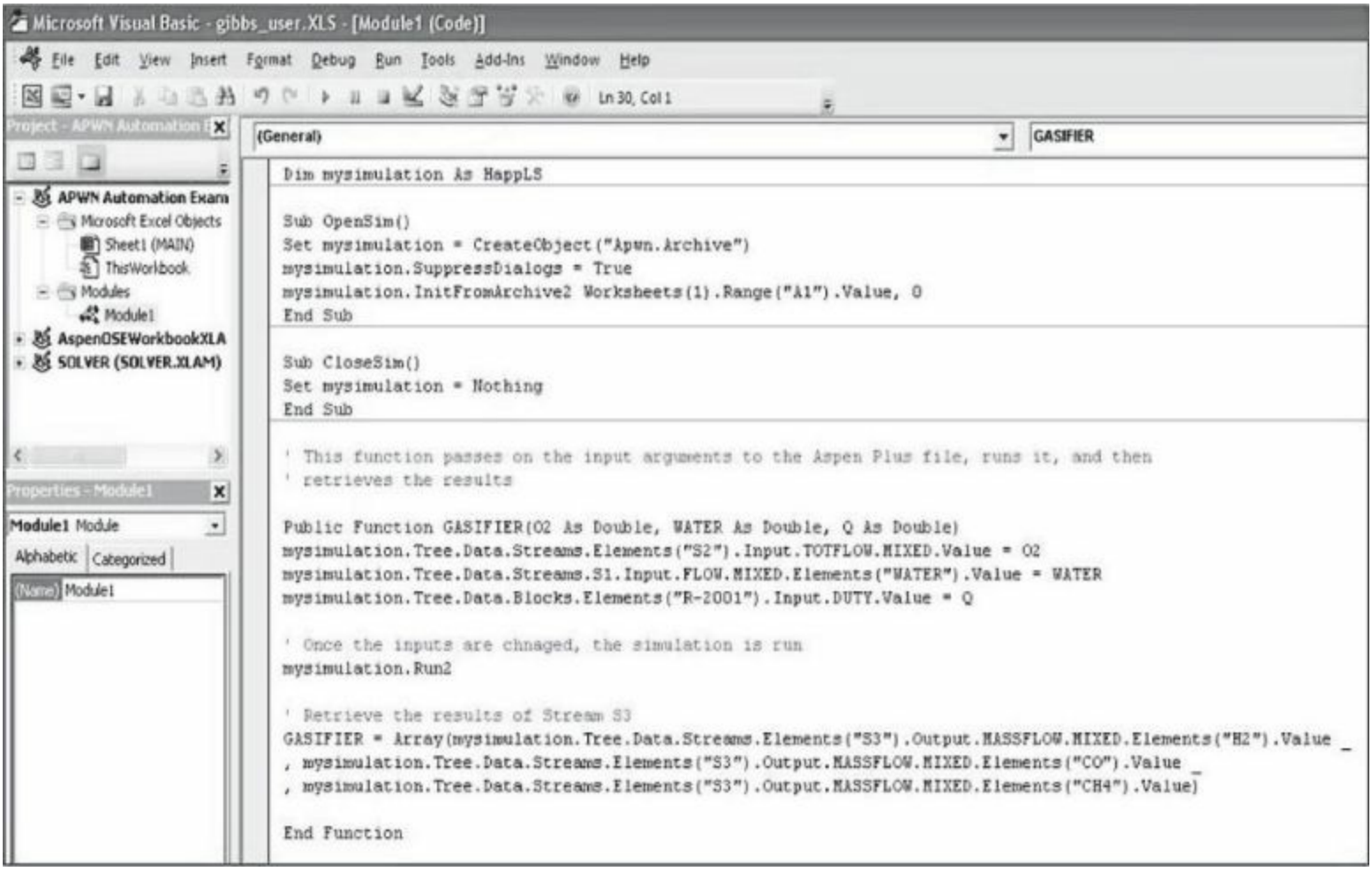


Figure E16.2(c). Screen shot of the VBA Code in Excel for Example 16.2

Along with the macros, a function named GASIFIER is created for passing on the changed oxidant flowrate (total flowrate of Stream S2), the water flowrate in Stream S1, and the heat duty to R-2001. The screen shot of the VBA code of this function is shown in Figure E16.2(c). The function runs the Aspen Plus V7.2 simulation and retrieves the flowrates of H_2, CO, and CH_4 in Stream S3. Note that the output of this function is an array of three elements. Therefore, three cells must be selected for receiving outputs from the function GASIFIER. For example, if it is desired to evaluate this function with inputs from cells C8, D8, and E8, then three cells (F8, G8, and H8 in Figure E16.2[c]) are selected, the equation "=GASIFIER(C8,D8,E8)" is inserted, and Ctrl + Shift + Enter is pressed. The gasifier cold gas efficiency is then calculated by using those results. Appropriate cells are selected for plotting the figures on the right-hand side of Figure E16.2(c).

Once the above-mentioned steps are performed, first communication with the Aspen Plus V7.2 simulation is established by pressing the "Open Gasifier Simulation" button. The values in columns A and B can be changed for calculating the gasifier cold gas efficiency and generating the plots. At the end, the "Close Gasifier Simulation" button is pressed to close the simulation. The gasifier model developed here is not very accurate. A kinetic model along with appropriate modeling of the hydrodynamics would be needed for more accurate predictions. This simple model is developed only for demonstration of the UAM.

It should be noted that in Example E16.1, the process simulator (Aspen Plus) was the master. It called the UAM and continued with other blocks after obtaining a solution from the UAM. Therefore, Aspen Plus V7.2 provided the input specification to the UAM. In Example E16.2, the Excel UAM is the master that calls the process simulator (Aspen Plus V7.2) and continues with other calculations after

obtaining a solution from the process simulator. The correct approach to use depends upon the user's interest. For complicated simulations, multiple UAMs and process simulator models can be called in a single simulation.

16.3. Solution Strategy for Steady-State Simulations

As process flowsheets become more complex, the default features of a process simulator may not be sufficient. For example, when simulating the benzene production process illustrated in Figure 1.3, which is a relatively simple process, there should be little difficulty converging on a solution. However, when simulating a far more complex process, such as the coal to higher alcohol process illustrated in Figure 1.2, the default features of the process simulator may not be sufficient to obtain a converged solution rapidly, if at all. This is because every block in Figure 1.2 is a chemical process at the level of complexity of the benzene process. There are recycle loops within each block as well as recycle loops between the blocks, so the sequence and method of solution may have to be selected.

Other than the unit operation blocks, the process simulators have two types of computational blocks that need to be solved, if implemented, along with the unit operation models. The first type satisfies the design specifications and works like a feedback controller. It satisfies a design specification by manipulating an input variable to a block or some specification of a block within some given bounds. That is why it is also called a controller in some simulators. These blocks will be called **design blocks** here. To the best of the authors' knowledge, all existing process simulators allow only one manipulated variable per design block. The second type of computational block is usually called a **calculator block**, and it calculates the value of some parameter or variable or some input condition based on user-defined calculations. These blocks can be considered to be feed-forward controllers. In addition, it may be necessary to solve an optimization problem that introduces another iterative loop, and this will be discussed in more detail later.

In Chapter 13, three types of solution methods—sequential modular, equation-oriented (simultaneous nonmodular), and simultaneous modular—were introduced along with the concept of tear streams. Under most circumstances, the sequential modular method, which is the default method in most process simulators, works very well. For large flowsheets involving multiple recycles and design and calculator blocks, other methods may be more efficient. The following discussion focuses on the advantages and disadvantages of these methods and the impacts of the various options available in the process simulator.

16.3.1. Sequential Modular (SM)

In the SM approach, the unit operation blocks, design blocks, and calculator blocks are solved sequentially. The sequence is defined by the following steps:

Step 1: The main flowsheet consisting of all the blocks is divided into independent subsystems. This is known as partitioning.

Step 2: The order in which the subsystems (partitions) will be solved sequentially is determined. This is known as precedence ordering.

Step 3: Tear streams (or tear variables for some systems) are determined for each subsystem. There can be multiple tear streams in one subsystem.

Step 4: Precedence ordering (sequencing) of the blocks in each subsystem is then determined, and the system containing one or multiple tear streams and design and calculator blocks (if any)

is solved.

These steps are discussed in more detail with examples. In this section, emphasis will be placed on solution methodologies, where the focus is on partitioning, sequencing, and tear streams. The following terminology is used for convenience of discussion: B1, B2, and so on, to denote blocks; F1, F2, and so on, to denote feed streams; P1, P2, and so on, to denote product streams; R1, R2, and so on, to denote recycle streams; and S1, S2, and so on, to denote all other streams.

Steps 1 and 2. Partitioning determines the smallest group of unit operation blocks that can be solved independently. If there are no recycles/design blocks/calculator blocks, this results in the simplest case, where each subsystem contains only one unit operation block. For partitioning and precedence ordering, the flowsheet can be represented by a directed graph (DG). Consider the flowsheet of an acid-gas removal (AGR) plant using chilled methanol, shown in Figure 16.1. The acid gas is first cooled in cooler B1 and enters the absorber, B2, where the solvent is chilled methanol. The bottom product from the column B2 goes to the stripper, B3, where nitrogen is used for stripping. A makeup stream of methanol is mixed with the bottom product from B3. It is then pumped by B5, cooled in B6, and sent back to B2. The stripper off-gas is heated in B7. Note that this is a very simple configuration of an AGR plant using chilled methanol. In reality, the plant configuration is much more complicated.

The Corresponding DG is shown in Figure 16.2.

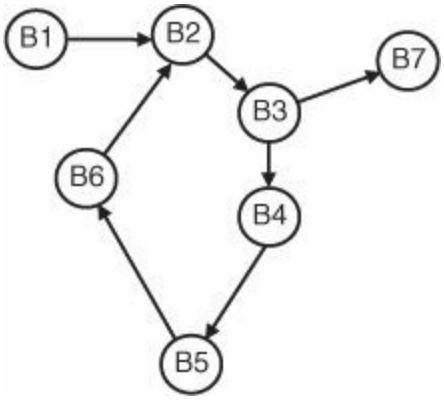


Figure 16.2. Directed Graph (DG) of the Acid-Gas Removal (AGR) Plant

In Figure 16.2, the vertices (circles) represent the units, and the edges (lines) represent connections between two units. By inspecting Figure 16.2, it can be seen that there are three strongly connected components, {B1}, {B2, B3, B4, B5, and B6}, and {B7}. So this flowsheet can be partitioned into three subsystems, and then subsystem {B1} is solved first and {B7} is solved last. Subsystem {B2, B3, B4, B5, and B6} involves a recycle loop; therefore, special techniques involving tearing and precedence ordering are applied. This will be discussed later.

For a simple system like this, the partitioning and precedence ordering can be determined manually. However, for large systems involving hundreds of unit operation blocks and numerous recycles, a graph-based approach may be difficult. Therefore, large systems are best represented by an incidence matrix. In this representation, a matrix $\boldsymbol{A}$ is formed, in which the streams are arranged in columns and the units in rows; each cell has a value of +1 for a feed, –1 for a product, and 0 otherwise. For example, since Stream S1 is connected as a feed to block B2, $\boldsymbol{A}(2, 4)$ is +1, and because S1 is connected as a product from B1, $\boldsymbol{A}(1, 4)$ is –1; otherwise $\boldsymbol{A}(3{:}\text{end}, 4) = 0$. The incidence matrix for the AGR process is

$$
A = \begin{array}{c}
\begin{array}{ccccccccccc} F1 & F2 & F3 & S1 & S2 & S3 & S4 & S5 & S6 & S7 & P1 & P2 \end{array} \\
\begin{bmatrix}
+1 & & & -1 & & & & & & & & \\
 & & & +1 & -1 & & & & +1 & & -1 & \\
 & +1 & & & +1 & -1 & & & & -1 & & \\
 & & +1 & & & +1 & -1 & & & & & \\
 & & & & & & +1 & -1 & & & & \\
 & & & & & & & +1 & -1 & & & \\
 & & & & & & & & & +1 & & -1
\end{bmatrix}
\begin{array}{c} B1 \\ B2 \\ B3 \\ B4 \\ B5 \\ B6 \\ B7 \end{array}
\end{array}
$$

where blank spaces represent 0.

In matrix A, any column with a single positive element +1 can be identified as a feed (known), any column with a single negative element –1 denotes a final product, and the block in the corresponding row must be solved to obtain its results. Many efficient algorithms are available that can consider this incidence matrix and arrange the rows to determine the partitioning and precedence ordering. Interested readers are referred to Mah [5]. One of the earliest algorithms, and a popular one, is due to Sargent and Westerberg [6]. For this example, the partitioning and precedence ordering is shown in Figure 16.3.

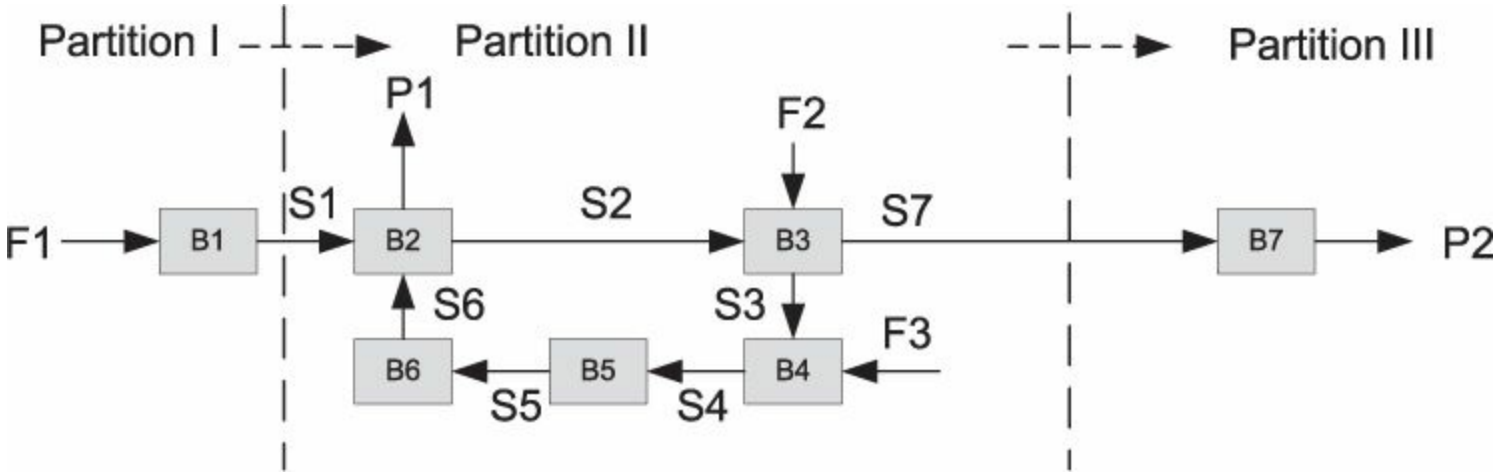


Figure 16.3. Partitioning and Precedence Ordering of the AGR Plant

Once the partitioning and precedence ordering is decided, as shown in Figure 16.3, it can be seen that the only loop that needs to be torn is in Partition II. The partitioning reduces the computation time drastically. Sometimes the number of units in a subsystem can increase (as does the computational cost) unknowingly. For example, consider implementing a calculator block to calculate the makeup solvent flowrate for the above example. The makeup flowrate can be simply calculated as

$$\text{F3 flowrate} = \frac{\text{Methanol flowrate in P1} + \text{Methanol flowrate in S7}}{\text{Methanol concentration in F3}}$$

This calculator block (C1) can be sequenced before block B4. So the sequence is (B2-B3-C1-B4-B5-B6), where the parentheses indicate that iteration will be required. It can be seen in Figure 16.4(a) that the number of partitions and the number of unit operation blocks in any partition do not change because of the calculator block. Now consider the case when "Methanol flowrate in S7" is replaced with "Methanol flowrate in P2," in the previous equation for the flowrate of F3. In principle, this should not alter the result because these flowrates are the same. While there would not be any difference in the results, the number of partitions is now two, as shown in Figure 16.4(b), block B7 being part of Partition II. The sequence is now (B2-B3-B7-C1-B4-B5-B6). Note that B7 must be

solved in each iteration, and the computational cost increases.

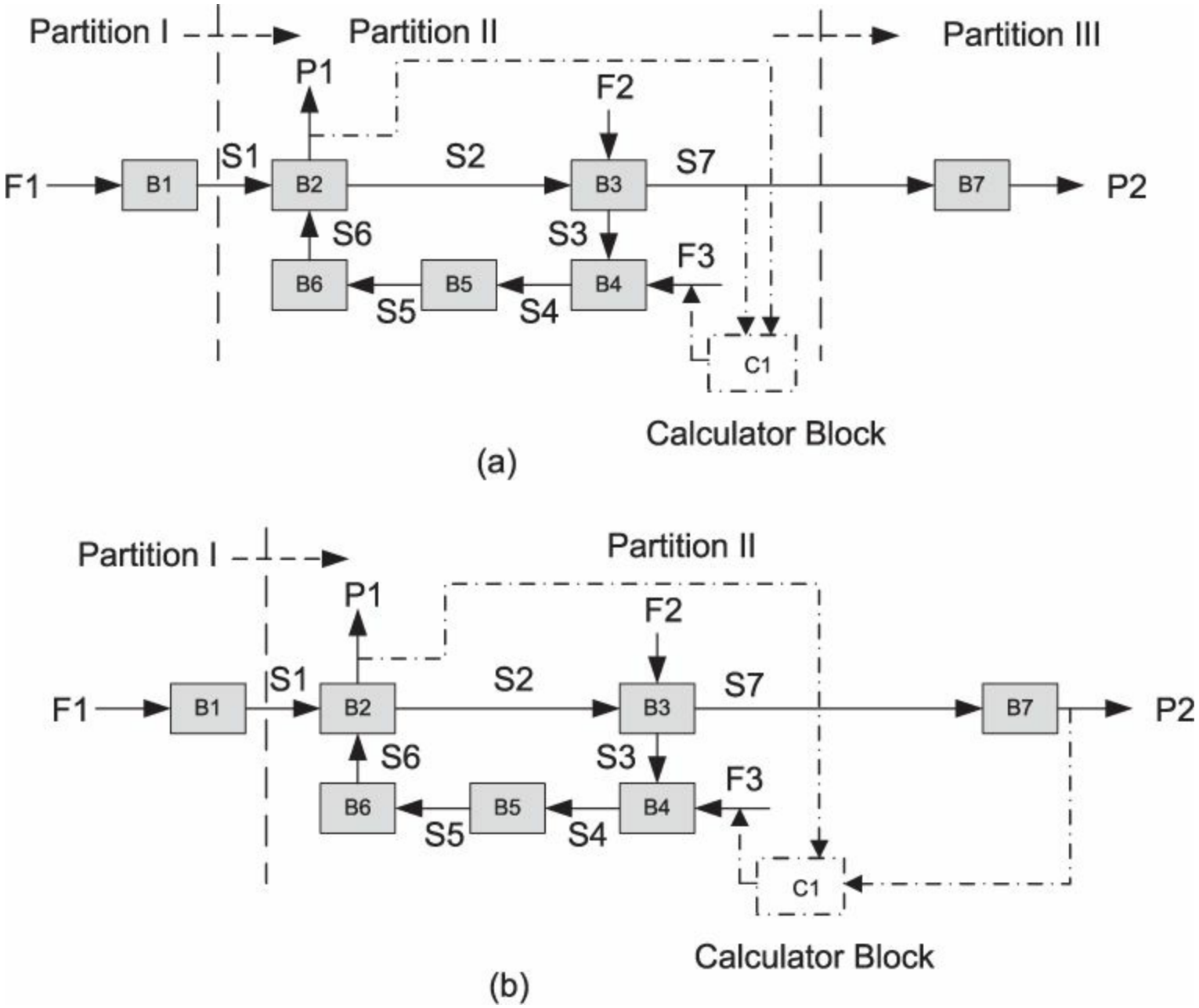


Figure 16.4. Effect of a Calculator Block on Partitioning: (a) No Change in Partition (b) Reduced Number of Partitions Increases the Computational Cost

Step 3: The partitions obtained in the previous step may contain a single unit or multiple units. When a partition contains multiple units, there exists one or multiple recycles, and the units must be solved simultaneously. However, with an SM approach, the unit operation blocks still need to be solved sequentially. So the identification and use of tear streams can facilitate this. Subsequently, an algorithm must be applied to update the stream information of the torn stream at each iteration, and then some convergence criterion is applied to ensure that the simulation has converged. Even though simulators do these tasks automatically, user intervention may be necessary to aid in the convergence, to speed up the convergence, and/or to improve the robustness for large and complicated simulations involving multiple recycles. For doing this, a clear understanding of how the required algorithms work must be obtained. The important questions to answer are: What stream(s) should be considered as tear stream(s), how is the tear stream information at each iteration to be updated, and what should be the convergence criteria?

Answering the first question can be very difficult for systems involving multiple recycle loops in a single partition. The key concept of tearing is that enough streams should be torn such that each loop is opened at least once. This is a set-covering problem that has multiple solutions. Therefore, to solve this issue, an optimization problem is formulated and solved that minimizes a criterion subject to the constraint that the solution belongs to the feasible set (one that satisfies the set-covering problem). One or more among the following four criteria should be considered:

1. The number of streams in the tear set is minimized.
2. The total number of stream variables (unknowns that are converged) is minimized.
3. Some cost function based on the difficulty in guessing the stream variables is minimized.
4. The total number of times loops are torn is minimized.

This mathematical programming problem can be written as

$$\min \sum_{i=1}^{n} w_i x_i \qquad (16.2)$$

$$\text{subject to } \sum_{i=1}^{n} C_{ji} x_i \geq 1 \ \forall j$$

where i denotes streams, j denotes cycles, w_i denotes weight of the i^{th} Stream,

$$C_{ji} = 1 \text{ if cycle } j \text{ contains } i^{th} \text{ Stream}$$
$$= 0 \text{ otherwise}$$

and

$$x_i = 1 \text{ if } i^{th} \text{ Stream is torn}$$
$$= 0 \text{ otherwise}$$

All process simulators use one or a weighted combination of some of these criteria as the objective function. Accordingly, w_i is manipulated.

Process simulators usually execute this step very efficiently. However, it may be necessary to vary the weights to aid in the convergence. Consider Figure 16.5, in which there are three recycle streams: R1, R2, and R3. At first glance, it appears that all three loops must be torn. However, if either Stream M3 or Stream M4 is torn, then the set-covering problem is solved. The question is: Which of these streams should be torn? First, it needs to be determined which stream variables are being converged. If the tear stream is a single-phase material stream, the variables are the flowrates of each of the species present in the tear stream, the pressure, and the enthalpy. Note also that if the flowrates of each species are conserved within reasonable accuracy, the total mass balance will be automatically satisfied. If the tear stream is an energy or work stream, then the only variable that needs to be considered is enthalpy/work. If Streams M3 and M4 are material streams, is it easier to provide a better initial guess for one than for the other? As an example, assume that block U4 is a heat exchanger for which the temperature has been specified. Therefore, an exact initial guess for temperature of M4 can be provided. Further, assume that the block U3 is a mixer block. This means that a good initial guess for Stream M3 is probably not available. Per Criterion (3), M4 should be selected as the tear stream. When this system is simulated in Aspen Plus V7.2, it identifies M3 as the tear stream. This is because Criteria (2) and (3) are used by default in Aspen Plus for identifying the tear stream(s).

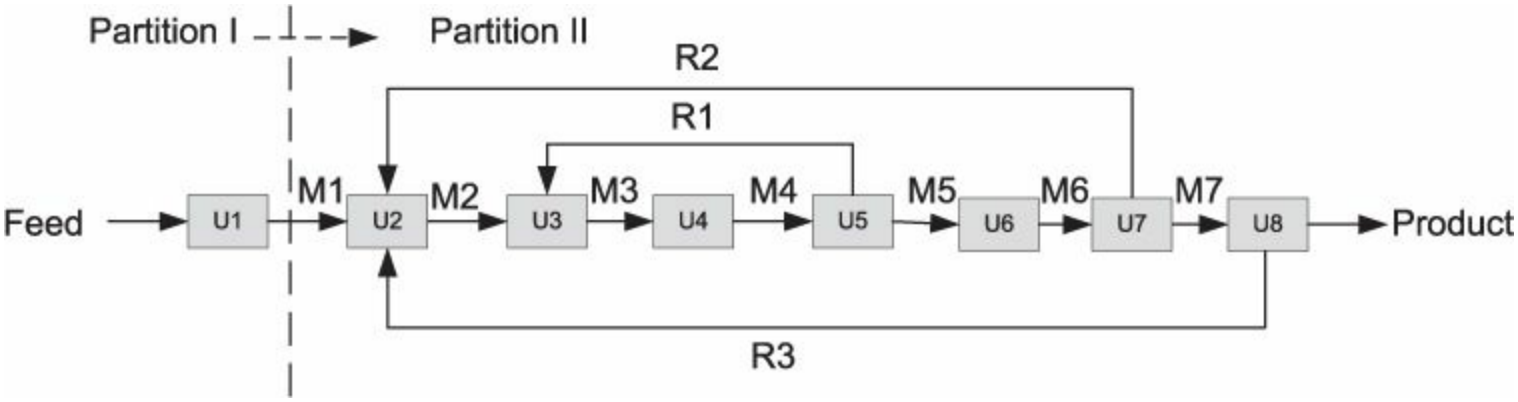


Figure 16.5. Flowsheet of a Process Containing Multiple Recycle Streams in a Given Partition

For complicated flowsheets, where the value of the initial guess of the tear stream is very important for convergence, which is basically Criterion (3), user intervention may be necessary. As another example, consider an electrolyte system as discussed in Section 13.6. If the option is to tear either a liquid or a vapor stream, then tearing a vapor stream will reduce the number of variables needed to converge, since the vapor stream does not contain any ions. Another issue, which is often neglected in steady-state simulation, is pressure drop. Consider the flowsheet in Figure 16.5. Assume that the pressure drop in each of the blocks is 0.1 bar. This yields a total pressure drop of 0.7 bar in the first iteration. If there are multiple inlet streams connected to the inlet of a unit operation, most simulators will consider the inlet pressure to be equal to the pressure of the lowest pressure stream. If that is the case, then for each iteration, the net system pressure will keep decreasing until it reaches a value of zero. At this point, the simulator will declare convergence failure for the simulation. To solve this problem, a pressure-changing device such as pump, compressor, or valve should be used, to keep the problem well posed by resetting the pressure at every iteration.

In many circumstances, multiple tear streams are unavoidable. In addition, design specifications (which can be thought of as feedback control loops) introduce additional loops. Some calculator blocks may also introduce additional loops. For example, consider the flowsheet in Figure 16.1. The makeup can be added to block B3 instead of B4. However, this creates another loop for the calculator block, since one of the variables (the methanol flowrate in S7) is downstream of where the makeup is being added. Whenever possible, such loops should be avoided. The design blocks and the calculator blocks along with the tear variable(s) can be solved by setting up a nested iteration or by solving the tear stream(s), design specifications, and calculator blocks simultaneously. Combinations of nesting and simultaneous approach are, of course, possible and are available in many simulators. However, nested iterations are usually more computationally expensive. In addition, the default nesting that specifies whether the tear streams (or design blocks/calculator blocks) will be nested inside or outside of a convergence loop may not be appropriate. One suggestion, when considering nested loops, is to tighten the tolerances for convergences of the inner nested loops, so that the cumulative errors do not result in failure of convergence of the outer nested loops. In a simultaneous solution approach, all the variables (tear stream variables, the manipulated variables of the design specs, and the output variables of the calculator blocks) are updated simultaneously. A simultaneous solution approach is usually very effective in the case of a large number of recycle streams, design blocks, and/or calculator blocks (the ones that create loops). This approach is also effective when good initial guesses for the tear streams, the manipulated variables of the design specs, and the output variables of the calculator blocks are available. In addition, a simultaneous approach is also preferred when there is strong interaction between the tear streams, design blocks, and/or calculator blocks in a partition. Examples 16.3 and 16.4 demonstrate these points.

Step 4: Once the flowsheet is made acyclic (without recycles) in Step 3, the precedence ordering of the acyclic system can be implemented in a similar way to Step 2. The solution of this acyclic system along with the design and calculator blocks, if any, is then achieved. The key question for this step is how to update the initial guess at each iteration. Consider Figure 16.6, which shows the previous flowsheet after Stream M4 has been torn. Once the tearing and precedence ordering have been implemented, the simulator can solve for M4 given an initial guess for M4' following the sequence U5-U6-U7-U8-U2-U3-U4. Assuming that M4 and M4' are material streams, and if the stream variables (usually flowrates of each of the species present in the tear stream, the pressure, and the enthalpy) of M4 and M4' are denoted by vectors $\boldsymbol{y}$ and $\boldsymbol{x}$, respectively, then the problem is to find a solution of the equation

$$\boldsymbol{x} - \boldsymbol{y} = 0 \qquad (16.3)$$

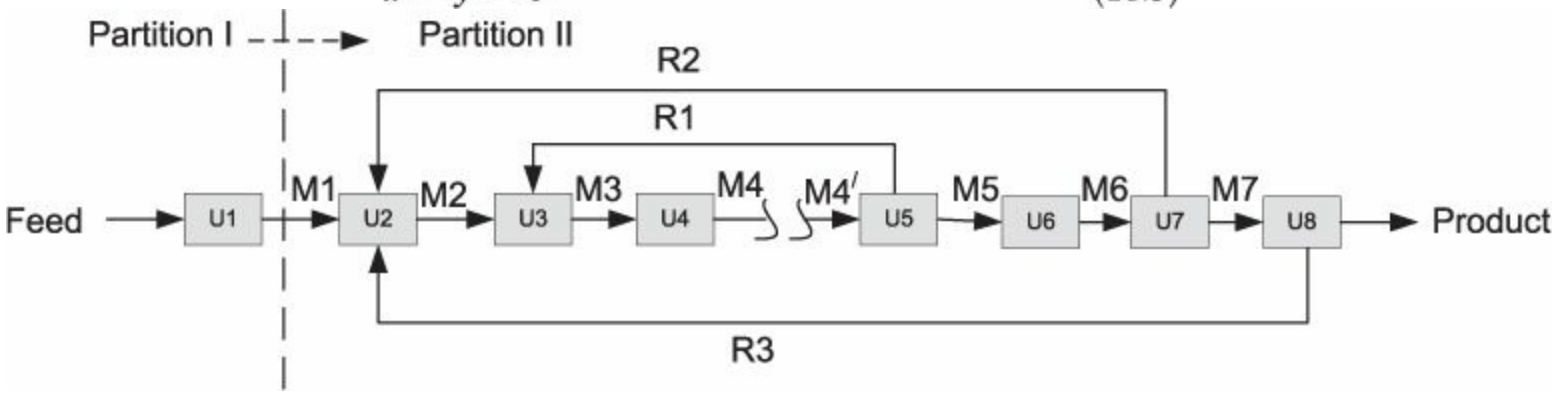


Figure 16.6. Flowsheet in Figure 16.5 after Being Torn

During a given iteration, denoted by k, values of $\boldsymbol{x}^k$ are guesses, and the corresponding value of $\boldsymbol{y}^k$ is obtained by solving all the blocks in the sequence. This information (i.e., $\boldsymbol{y}^k$) is used in calculating the next initial guess for x, that is, $\boldsymbol{x}^{k+1}$. The solution algorithms will vary depending on how $\boldsymbol{x}^{k+1}$ is calculated given $\boldsymbol{y}^k$.

A number of algorithms are usually available in the simulators, and choosing an appropriate algorithm may become critical for convergence under certain circumstances. Making the best choice requires an understanding of these algorithms. A quick review of the common algorithms will make clear their limitations and their applicability under most circumstances.

Direct Substitution: This is the simplest algorithm in which $\boldsymbol{y}^k$ is directly used to update $\boldsymbol{x}^{k+1}$:

$$\boldsymbol{x}^{k+1} = \boldsymbol{y}^k \qquad (16.4)$$

It is clear that this approach does not take care of any interaction between different variables and different tear streams and, therefore, is usually not a good candidate for processes containing multiple tear streams (possibly with design and/or calculator blocks) with a number of variables to converge. The convergence is linear and is therefore slow. In addition, it can be shown that for this algorithm to converge, $|\lambda|^{max}$ (the absolute value of the maximum eigenvalue) of the Jacobian matrix $\frac{\partial y}{\partial x}$ evaluated at the solution should be less than 1 and the initial guess should be close to the solution. The speed of convergence depends upon how close $|\lambda|^{max}$ is to 0. The number of iterations (n) needed to reach a given tolerance of ϵ is

$$n \geq \frac{\ln[\epsilon/\|\Delta \boldsymbol{x}^0\|]}{\ln|\lambda|^{max}} \qquad (16.5)$$

where $\|\Delta \boldsymbol{x}^k\|$ is some norm of $\Delta \boldsymbol{x}^k$ with $\Delta \boldsymbol{x}^k = \boldsymbol{x}^k - \boldsymbol{x}^{k-1}$. Consider a system where $|\lambda|^{max}$ is 0.996. In comparison to a system where $|\lambda|^{max} = 0.02$, there will be at least In(0.02)/In(0.996) ≈ 976 times more iterations needed (assuming ϵ and $\|\Delta \boldsymbol{x}^0\|$ remain the same).

Accelerated Successive Substitution (or Relaxation) Methods: It was shown before that as $|\lambda|^{max}$ moves closer to unity, the direct substitution method converges very slowly. Accelerated successive substitution methods seek to accelerate the convergence by using a relaxation parameter q. The new estimate is calculated by the equation

$$\boldsymbol{x}^{k+1} = q\boldsymbol{x}^k + (1 - q)\boldsymbol{y}^k \tag{16.6}$$

Note that when $q = 0$, the method collapses to the direct substitution algorithm. If $q < 0$, the method helps to accelerate the convergence. If $0 < q < 1$, the method helps convergence stabilization by damping. The common methods to choose q are the dominant eigenvalue method and Wegstein's method.

Dominant Eigenvalue Method (DEM): In this approach, $|\lambda|^{max}$ is estimated as

$$|\lambda|^{max} \approx \frac{\|\Delta \boldsymbol{x}^k\|}{\|\Delta \boldsymbol{x}^{k-1}\|} \tag{16.7}$$

The optimal value of q is then found by assuming that $\lambda^{min} \approx \lambda^{max}$ and $\lambda^{min} > 0$:

$$q = \frac{|\lambda|^{max}}{|\lambda|^{max} - 1} \tag{16.8}$$

The problem with this approach is that if the minimum and maximum eigenvalues are wide apart or one of the eigenvalues is negative, the approach may fail to converge.

Wegstein's Method: The DEM uses a single acceleration parameter for all the variables. However, for some systems, separate acceleration parameters for each variable are desired to speed up the convergence. This method applies a secant method to each tear variable. The acceleration parameter is given by

$$q_i = \frac{s_i}{s_i - 1} \tag{16.9}$$

where

$$s_i = \frac{y_i^k - y_i^{k-1}}{x_i^k - x_i^{k-1}} \tag{16.10}$$

As before, x_i and y_i are the elements of $\boldsymbol{x}$ and $\boldsymbol{y}$, respectively. This method works well for subsystems with low interactions.

These relaxation methods may lead to instability if q_i is unbounded. Usually, $q^{min} \le q_i \le 0$ and the usual value of q^{min} is about –5. However, this value can be further relaxed to accelerate convergence on a case-by-case basis, as will be shown later. Another option is to apply the acceleration after every few direct substitution steps.

Newton's Method: In this approach, the following set of equation(s) is solved:

$$f(\boldsymbol{x}) = \boldsymbol{x} - \boldsymbol{y} = 0 \tag{16.11}$$

Iterations using Newton's method yield a step algorithm given by

$$\boldsymbol{x}^{k+1} = \boldsymbol{x}^k - (\boldsymbol{J}^k)^{-1} f(\boldsymbol{x}^k) \tag{16.12}$$

where the Jacobian matrix $J_{ij} = \frac{\partial f_i}{\partial x_j}$.

The advantage of this method is the quadratic convergence rate obtained in the vicinity of the solution, and this approach is very useful for highly interacting systems. However, a good initial guess is required. This approach is computationally expensive because of the calculation of the Jacobian. In general, as there is no explicit functional form for $\boldsymbol{y}$, a numerical Jacobian is calculated by perturbing the system

$$\boldsymbol{J}_{ij} = \frac{\partial \boldsymbol{f}_i}{\partial \boldsymbol{x}_j} = \frac{\boldsymbol{f}_i(\boldsymbol{x}^k + \Delta \boldsymbol{x}_j) - \boldsymbol{f}_i(\boldsymbol{x}^k)}{\Delta \boldsymbol{x}_j} \qquad (16.13)$$

where $\Delta \boldsymbol{x}_j$ is a small scalar by which $\boldsymbol{x}_j$ is perturbed. For N variables, this requires N flowsheet passes (plus one for calculating $\boldsymbol{f}(\boldsymbol{x}^k)$), which increases the computational cost.

Broyden's Method: In Broyden's method, which is a quasi-Newton method, evaluation of the Jacobian is avoided by approximating it based on differences in $\boldsymbol{x}$ and $\boldsymbol{f}(\boldsymbol{x})$:

$$(\boldsymbol{J}^k)^{-1} = (\boldsymbol{J}^{k-1})^{-1} + \frac{(\boldsymbol{s}^k - (\boldsymbol{J}^{k-1})^{-1}\boldsymbol{r}^k)(\boldsymbol{s}^k)^T(\boldsymbol{J}^{k-1})^{-1}}{(\boldsymbol{s}^k)^T(\boldsymbol{J}^{k-1})^{-1}\boldsymbol{r}^k} \qquad (16.14)$$

where $\boldsymbol{s}^k = \boldsymbol{x}^k - \boldsymbol{x}^{k-1}$ and $\boldsymbol{r}^k = \boldsymbol{f}(\boldsymbol{x}^k) - \boldsymbol{f}(\boldsymbol{x}^{k-1})$.

Equation 16.14 can be evaluated in a single pass since it depends upon $\boldsymbol{x}^k$, $\boldsymbol{x}^{k-1}$, $\boldsymbol{f}(\boldsymbol{x}^k)$, and $\boldsymbol{f}(\boldsymbol{x}^{k-1})$, and all of these values are available from previous iterations. This approach also avoids inverting the Jacobian. Therefore, it is less computationally expensive than Newton's method, especially for systems with dense matrices and containing large numbers of tear variables. However, the rate of convergence is slower than the quadratic rate achieved using Newton's method. It should also be noted that this method can fail to converge with a poor initial guess for $\boldsymbol{x}^0$ and $(\boldsymbol{J}^0)^{-1}$. $(\boldsymbol{J}^0)^{-1}$ is often approximated as $(\boldsymbol{J}^0)^{-1} = \boldsymbol{I}$ or calculated in the same manner as Newton's method, which again increases the computational cost.

The previous discussion shows that for noninteracting systems, Wegstein's method with properly chosen acceleration parameters can be a very good choice. For highly interacting systems, Broyden's method is a very good compromise between speed of convergence and computational cost. If this approach fails, Newton's method can be tried. However, all of these methods may fail to converge if a poor initial guess is provided. The use of these methods is examined in Example 16.3.

Example 16.3.

Consider the flowsheet in Figure 16.5. Simulate the blocks U1, U4, and U6 as heat exchangers with outlet temperatures of 200°C, 300°C, and 400°C, respectively. Simulate all other blocks as mixers/splitters as appropriate. Pure H_2 enters the system at 30°C temperature at a flowrate of 100 kmol/h and a pressure of 12 bar. Assume that the pressure drop is zero in all the blocks. Compare the performance of the following tear stream convergence methods: direct substitution, Wegstein's method (with various values for q^{min}), Broyden's method, and Newton's method.

Solution

This flowsheet is simulated in Aspen Plus V7.2. The performance comparison is shown in Table

E16.3.

Table E16.3. Impact of Initial Guess on Tear Stream Convergence

Method	No Initial Guess for the Tear Stream		Good Initial Guess for the Tear Stream	
	No. of Iterations	No. of Flowsheet Passes	No. of Iterations	No. of Flowsheet Passes
Direct Substitution	2645	2645	5	5
Wegstein's Method ($q^{min} = -5$)	394	394	4	4
Wegstein's Method ($q^{min} = -40$)	62	62	3	3
Wegstein's Method ($q^{min} = -175$)*	12	12	2	2
Broyden's Method	14	14	2	2
Newton's Method	6	36	1	3

* Such a low value is not usually advisable because of instability.

For this flowsheet, there are only three tear variables, namely, the flowrate of the single species, the pressure, and the enthalpy. As mentioned before, the required number of flowsheet passes for calculating the Jacobian for Newton's method will keep increasing as the number of tear variables increases. This example demonstrates the importance of providing a good initial guess. Unfortunately, there is no "perfect" approach for generating the initial guesses. Once again, all options for tear streams must be considered to see if there is a preferred way to generate "good" initial guesses using process considerations.

It has been mentioned before that a single simulation can have one or more design and calculator blocks along with one or more tear variable(s). In such cases, the nesting option can play a crucial role, along with the solver algorithms, in obtaining a converged solution. Example 16.4 will illustrate these points.

Example 16.4.

Consider the flowsheet in Figure E16.4(a).

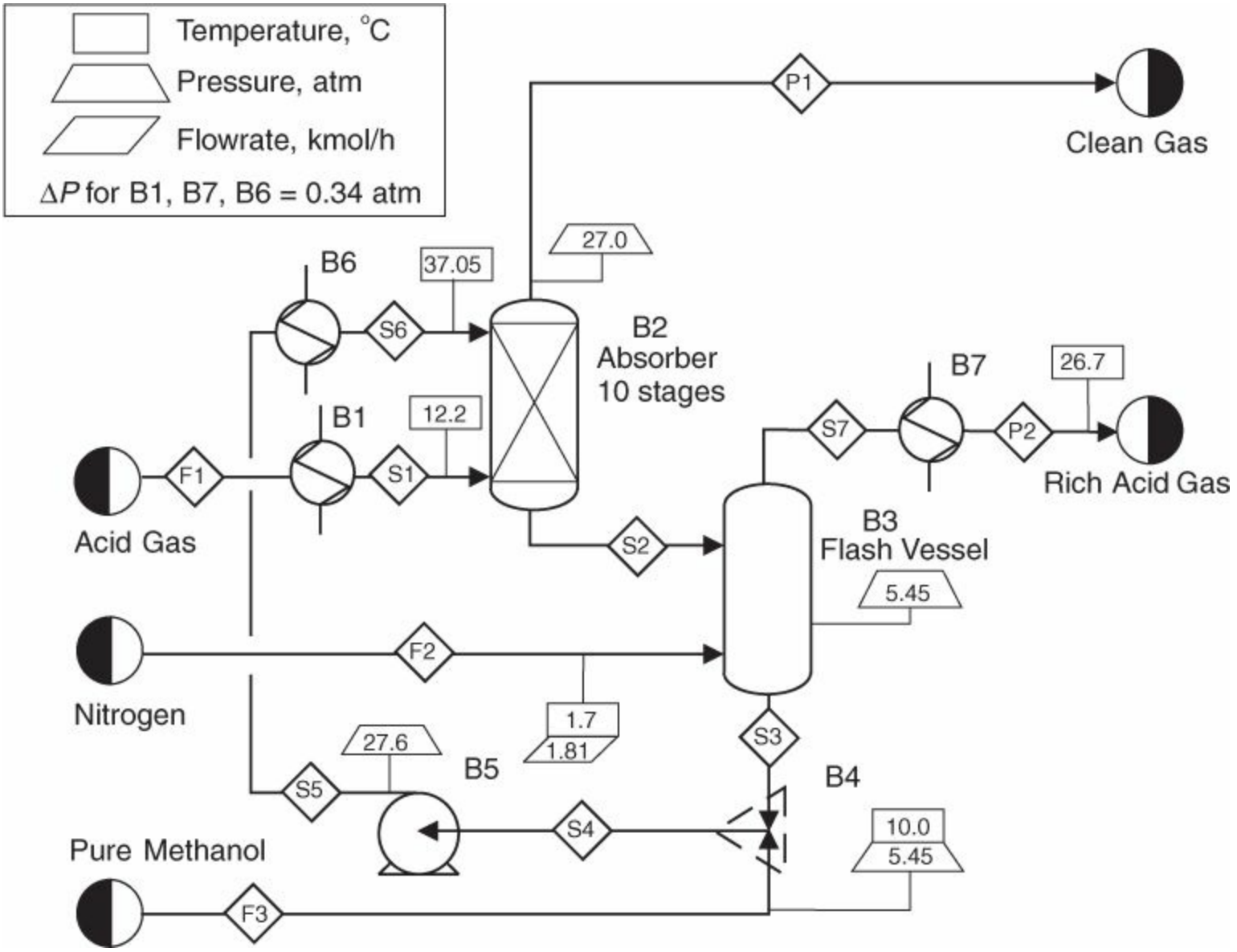


Figure E16.4(a). Flowsheet of an AGR Plant Using Chilled Methanol

Stream F1 has the following properties:

Composition (mol%):	
CO_2	28.02
H_2S	0.807
CO	20.2
N_2	15.7
COS	0.045
H_2	33.19
CH_4	2.0
Temperature (°C)	37.8
Pressure (atma)	27.56
Total Flow (kmol/h)	0.984

Set up the absorber as an equilibrium-stage column containing ten theoretical stages with the solvent being fed to the top stage and the acid gas below the bottom stage. Note that any of S4, S5, S6 . . . can be chosen as a tear stream or may be identified by the simulator as a tear stream. However, in this problem, use S6 as the tear stream, since its temperature and pressure are known to be exactly –37.05°C and 27.26 atm, respectively. As mentioned before, this system will have an infinite number of solutions based on the initial guess provided for the tear stream (S6 here) because the system is

underspecified. To converge to a unique solution, a design block must be implemented that manipulates the circulation rate to satisfy some desired specification for the clean syngas. Some changes in the plant configuration are also needed. That particular problem is solved later in Example 16.6. For the current example, an initial guess for S6 = 13.74 kmol/h is provided, and it is assumed to be pure methanol.

For this system, do the following:

a. First, implement a calculator block that will calculate the makeup solvent flowrate based on the methanol loss in Streams P1 and S7. Where in the sequence should the calculator block be executed? What are the compositions of P1 and S7? What happens if the calculator block is deleted? Why?

b. Second, implement a design specification that manipulates the flowrate of F2 (N_2 stream) to block B3 to ensure that the methanol purity in the bottom product of block B3 is 98%. What is the convergence sequence? Change the nesting option and check whether the simulation converges.

c. Finally, connect F3 (makeup stream) to block B3. Does the simulation converge as the nesting options are changed? Why or why not?

Solution

The simulation is developed in Aspen Plus V7.2 by modifying one of the example methanol absorbers available in its example flowsheet. This is available in Program Files\AspenTech\Aspen Plus V7.2\GUI\App\Physical solvents. When simulating using other platforms, note that the perturbed-chain statistical associating fluid theory (PC-SAFT) property method is used. In this model, the thermophysical property models have been validated against DIPPR correlations for species vapor pressure and liquid density and literature data for liquid heat capacity, heat of vaporization, and VLE. Because equilibrium-tray calculations are used in this simulation, any differences in transport parameters will not make a significant difference to the solution.

a. The calculator block is implemented by calculating the makeup flowrate = methanol flowrate in P1 + methanol flowrate in S7. In the automatically generated convergence sequence, as expected, the calculator block is executed just before block B4. So the sequence is B1-(B2-B3-C1-B4-B5-B6)-B7. As the value of the variables in the right-hand side of the previous equation is known before executing block B4, no additional loop is created by the calculator block. The initial value for the makeup flowrate is 1.36 kmol/h. Note that the initial value is not important for this case as the calculator block is not solved iteratively. Table E16.4(a) shows the performance results for each of the methods.

Table E16.4(a). Performance of Various Methods for Tear Stream Convergence

Method	No. of Iterations	No. of Flowsheet Passes	Time Taken (s)
Direct Substitution	35	35	2.8
Wegstein's Method	35	35	2.81
Broyden's Method	13	13	1.2
Newton's Method	8	107	10.77

Based on the number of iterations and solution time, Broyden's method is found to be the

most economical. Newton's method is the most expensive because of the much higher number of flowsheet passes (iterations). Note that there are ten tear variables here (eight species flowrates, one pressure, and one enthalpy), and they are perturbed individually (generating one flowsheet pass for each perturbation) to generate the Jacobian matrix. To generate the results shown in Table E16.4(a), the results from one method must be purged prior to resimulating using another convergence method. Otherwise, by default, the solver will start with the results from the previously converged solution and converge without any further iteration. Table E16.4(b) shows the compositions of Products 1 and 2.

Table E16.4(b). Composition of Streams P1 and S7

Species	P1 (mole fraction)	S7 (mole fraction)
Methanol	1.04×10^{-4}	6.58×10^{-4}
CO_2	0.024	0.121
H_2S	6.8×10^{-4}	3.47×10^{-4}
CO	0.245	0.020
N_2	0.236	0.841
COS	3.79×10^{-5}	1.94×10^{-4}
H_2	0.485	8.34×10^{-3}
CH_4	9.62×10^{-3}	6.27×10^{-3}

When the calculator block is removed, the simulation fails to converge no matter what method is used. The actual flowrate of F3 (makeup) is about 0.0015 kmol/h, whereas the initial value (guess) for F3 is 1.36 kmol/h. When the calculator block is included, it manipulates the flowrate of F3 based on the losses from the system. In the absence of the calculator, there can be mass buildup or loss in the system based on the flowrate of F3. To satisfy the mass balance, losses of methanol in P1 and S7 have to be balanced by the methanol added through the makeup stream. By tracking the progress of the solver at each iteration, it is seen that the flowrate of the tear stream (S6) keeps increasing when the calculator block is not present. Finally, the column fails to converge because of a very high solvent/gas ratio. The mass imbalance problem is a key issue. Each species that comes into the system must have a way to leave. Any mass accumulation or depletion will eventually lead to failure in convergence, and the reason for the convergence failure will generally not be identified by the solver. For a large flowsheet, such an ill-posed problem can be extremely difficult to identify. The solution of the calculator block from previous simulation is now considered. By using this flowrate in the input specification for the makeup flowrate, the simulation will now converge even in the absence of the calculator block because of the exact initial guess corresponding to the circulating flowrate.

b. A design block, named DS1, is implemented in Aspen Plus V7.2 by creating a design specification under the Data|Flowsheeting Options|Design Spec. The bounds for the manipulated variable (flowrate of F2) are 0.45–4.5 kmol/h. This design block creates another loop. First, the design specification is solved by nesting it inside the tear stream. The following sequence is automatically generated by Aspen Plus V7.2: B1-(B2-{B3}-C1-B4-B5-B6)-B7. The parentheses and the curly brackets denote the outer and inner convergence loops, respectively. Both the loops are solved using Broyden's method. The converged flowrate of N_2

is 1.93 kmol/h, and this approach takes 1.63 s to solve. Next, the design specification is nested outside the tear loop, again using Broyden's method. The convergence sequence is B1-({B2-B3-C1-B4-B5-B6})-B7. Notice that the innermost convergence loop now has six blocks instead of the one it had previously. It takes 5.53 s to solve this problem. Finally, the design specification and tear streams are converged simultaneously. The sequence is B1-(B2-B3-C1-B4-B5-B6)-B7, and this approach takes about 2.42 s to solve. For this particular simulation, solving the tear streams and design specifications simultaneously is not advantageous as the interaction is not very strong. Even though all the approaches converge, the times taken are very different. This may not matter for such a small simulation, but for large simulations, this can make a substantial difference.

c. The changed configuration made by connecting the makeup to block B3 is shown in Figure E16.4(b). In this case, the calculator block creates a loop as the value of methanol flowrate in S7 can be obtained after solving B3. Because of this, the calculator export variable (flowrate of Stream F3) should be torn in Aspen Plus V7.2 by clicking the appropriate check box under Data|Convergence|Conv Options|Sequencing. For this approach, it is assumed that the initial value is kept the same as the old initial value, that is, 1.36 kmol/h. When the design specification is nested inside the convergence block that solves the tear stream and the calculator block, the sequence is B1-(B2-{B3}-B4-B5-B6-C1)-B7. Here, as before, the convergence block that solves the design specification has only B3 in it. Notice that the sequence in which the calculator block C1 is considered is automatically generated by Aspen Plus V7.2, since the calculator tear is being converged simultaneously with the tear stream and the tear stream is updated at the end of the sequence. This approach fails to solve when Broyden's method is used for both convergence blocks. Since both F2 (manipulated by the design spec) and F3 (manipulated by the calculator block) go to the same block, and both affect the purity of the solvent, the system becomes strongly interacting. When the design specification is solved by Newton's method, with Broyden's method for the other convergence block, it solves in 1.61 s. When the design specification is nested outside the convergence block that solves the tear stream and the calculator tear, the sequence is B1-({B2-B3-B4-B5-B6-C1})-B7. This approach takes 5.19 s to converge when Broyden's method is used for both convergence loops and 4.85 s when the design convergence loop is converged by Newton's method. When the design specification, tear variable, and calculator blocks are all simultaneously converged, it takes Broyden's method 2.48 s to converge, while Newton's method takes 18.37 s to converge.

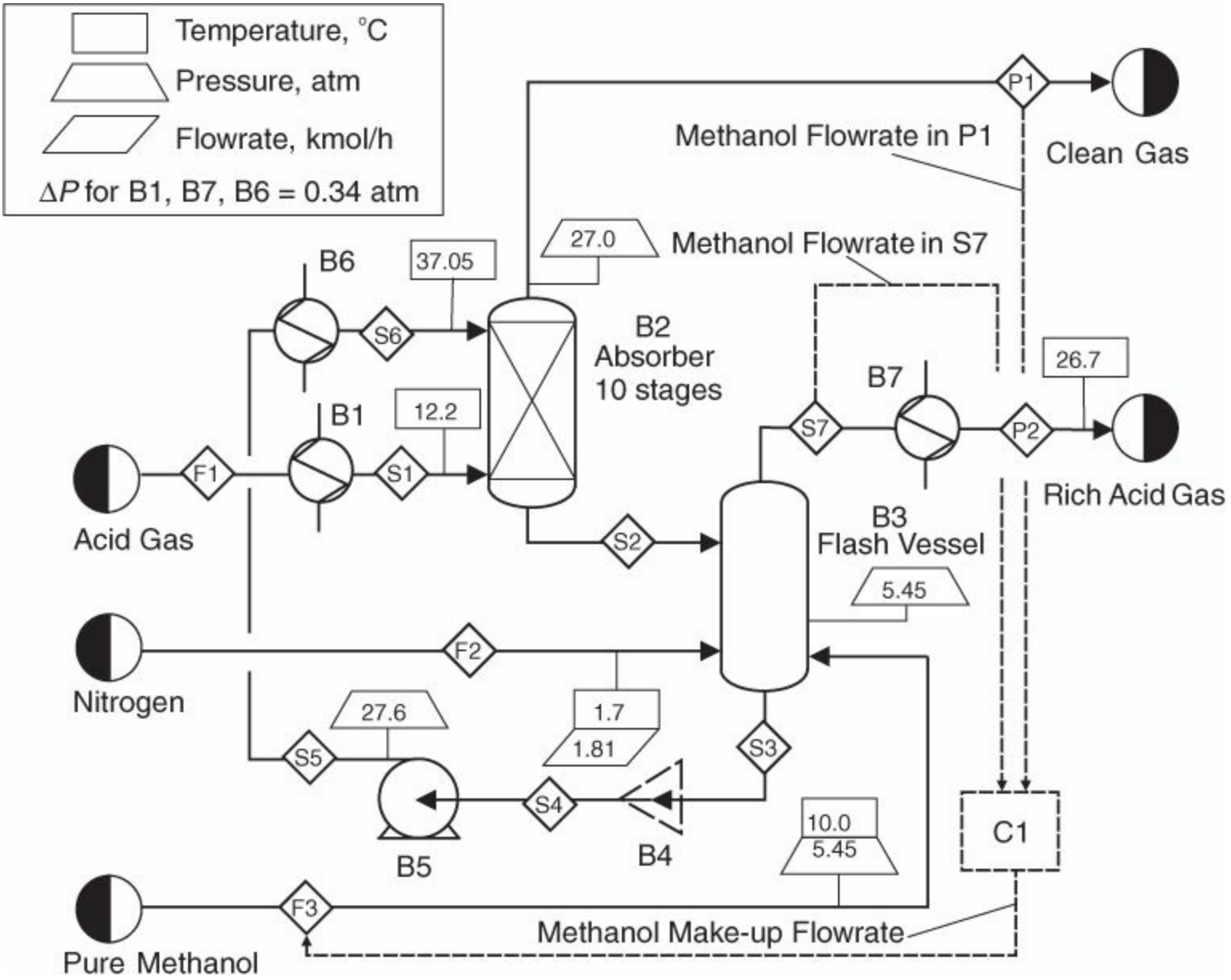


Figure E16.4(b). Modified Flowsheet of the AGR Plant When F3 (the Makeup Stream) Is Connected to B3

Example 16.4 demonstrates that when multiple tear streams, design blocks, and calculator blocks are present, an appropriate nesting along with an appropriate solution method is very important and can significantly affect the time to obtain a solution and the ability to get a solution.

16.3.2. Equation-Oriented (EO)

In the EO approach, all the equations are collected together and solved simultaneously. This approach is preferable to the SM strategy for highly heat- and/or mass- and/or work-integrated systems. This approach is also advantageous in the presence of highly interacting, multiple-design specifications and calculator blocks (that create additional loops). As the number of flowsheet passes keeps increasing, the SM approach becomes computationally very expensive. In the case of process optimization, when the flowsheet is solved many times, the EO approach is clearly beneficial for complicated flowsheets. In addition, the first- and second-order derivatives are usually needed for optimization. Because of the limitations in the approach, these derivatives are calculated numerically. However, because in an EO approach all the model equations are available, an analytical first and second derivative can be calculated, which improves the accuracy. There are exceptions to this for

models whose equations are not supported by EO solvers or for certain user models or for units handling solids. The downside of the EO strategy is that the initial guesses are usually generated by solving an SM problem or iterating the SM problem at least once. If this initial guess is "bad," then the EO approach may fail to converge. Generation of a "good" initial guess is the most critical deciding factor for the success of the EO approach. If an EO approach fails to converge, the failure can be very difficult to troubleshoot. In the case of an SM strategy, the convergence failure usually can be easily identified, since the particular unit operation block, tear stream, design block, or calculator block that fails will be identified. This facilitates troubleshooting the problem by focusing on that block or on its inputs by tracking the progress of the solver from iteration to iteration.

The workhorse of the solvers used in the EO approach is still Newton's method or a quasi-Newton method. Newton's step has been mentioned before. In practice, instead of inverting the Jacobian, the following equations are solved:

$$x^{k+1} = x^k + \alpha^k d^k$$
$$J^k d^k = f(x^k) \qquad (16.15)$$

These equations are solved by exploiting the sparsity of the Jacobian matrix, typical of large process simulations. A block-decomposition algorithm is applied to the incidence matrix that permutes the rows (equations) and columns (variables) to generate a block lower-triangular structure with minimal blocks, as shown in Figure 16.7. This approach decomposes the system into a series of subproblems that can be solved faster than the original problem. In addition, derivative calculation for the off-diagonal blocks is never needed, which again increases the speed.

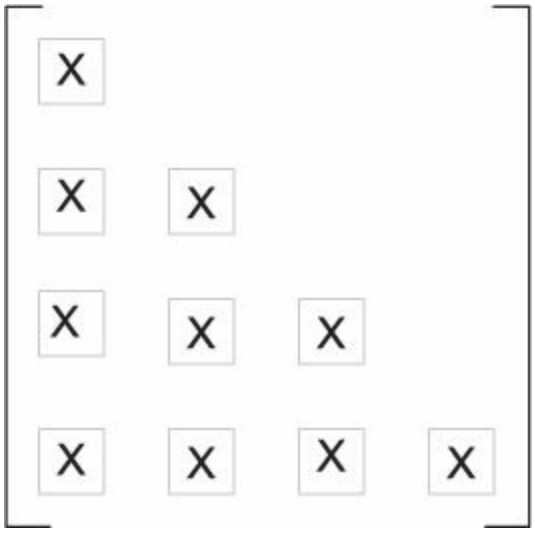


Figure 16.7. Structure of the Block Lower-Triangular Matrix

Other than the equations declared explicitly in the simulation, the EO solver usually has to solve equations where a function call is made to a subroutine written in C, FORTRAN, or another language. It is possible that the subroutine itself needs an iterative solution to converge. For example, consider a subroutine for an isothermal flash calculation where the current pressure, temperature, and feed composition are passed to the subroutine, which then iteratively solves and returns the values for liquid and vapor compositions and the liquid/feed ratio. In such a case, this creates an inner loop that must be solved in each iteration. Examples of such function calls are those made to physical property subroutines.

Rather than using Newton's method or the quasi-Newton methods discussed before, the system of nonlinear algebraic equations can be solved using an optimization approach. In an optimization

problem, in general, the minimum (or maximum) of an objective function is calculated:

$$\min_{x \in R^n} g(x) \qquad (16.16)$$

For finding the minima, the problem that is solved is $g'(x) = 0$. Note again that this is similar to a root-finding problem for a system of nonlinear algebraic equations, $f(x) = 0$. Therefore, there are a number of optimization algorithms that can be used to solve these nonlinear equations. A detailed discussion about all the methods available to solve these problems is beyond the scope of this text. Instead the interested reader is referred to comprehensive publications in this area [7, 8]. However, it should be noted that the real advantage of using an optimization problem lies in the possibility of evaluating the objective function and forcing it to decrease as the iteration continues along with the availability of powerful and efficient algorithms to achieve this aim.

In summary, it is noted that a solution is not guaranteed for any arbitrary system, no matter what approach is taken. In addition, it is essential to reiterate the importance of a good initial guess, especially when using an EO approach. The main advantages of the SM approach are easier initialization and reduced effort in problem formulation. However, for complicated problems with a large number of tear streams, design blocks, and calculator blocks, and for optimization problems, the SM approach not only becomes computationally expensive but may also fail. For such systems, the EO approach becomes a real advantage, provided that some reasonable initial guess can be provided.

16.3.3. Simultaneous Modular (SMod)

This is basically a hybrid between the SM and EO approaches, exploiting their strengths in respective areas. In the SMod approach, SM is used for subsystems with low to medium levels of interaction, while the EO approach is used for highly interactive subsystems. To illustrate the effect of the various sequences, algorithms, and approaches on the convergence of a simulation, Example 16.5 is provided.

Example 16.5.

Consider the flowsheet in Figure E16.5. This is modified Example 16.4(b). At the end of Example 16.4(b), the flowsheet has a design block, DS1, that manipulates the F2 flowrate to block B3 and a calculator block, C1, that calculates the F3 flowrate. For this new system, do the following:

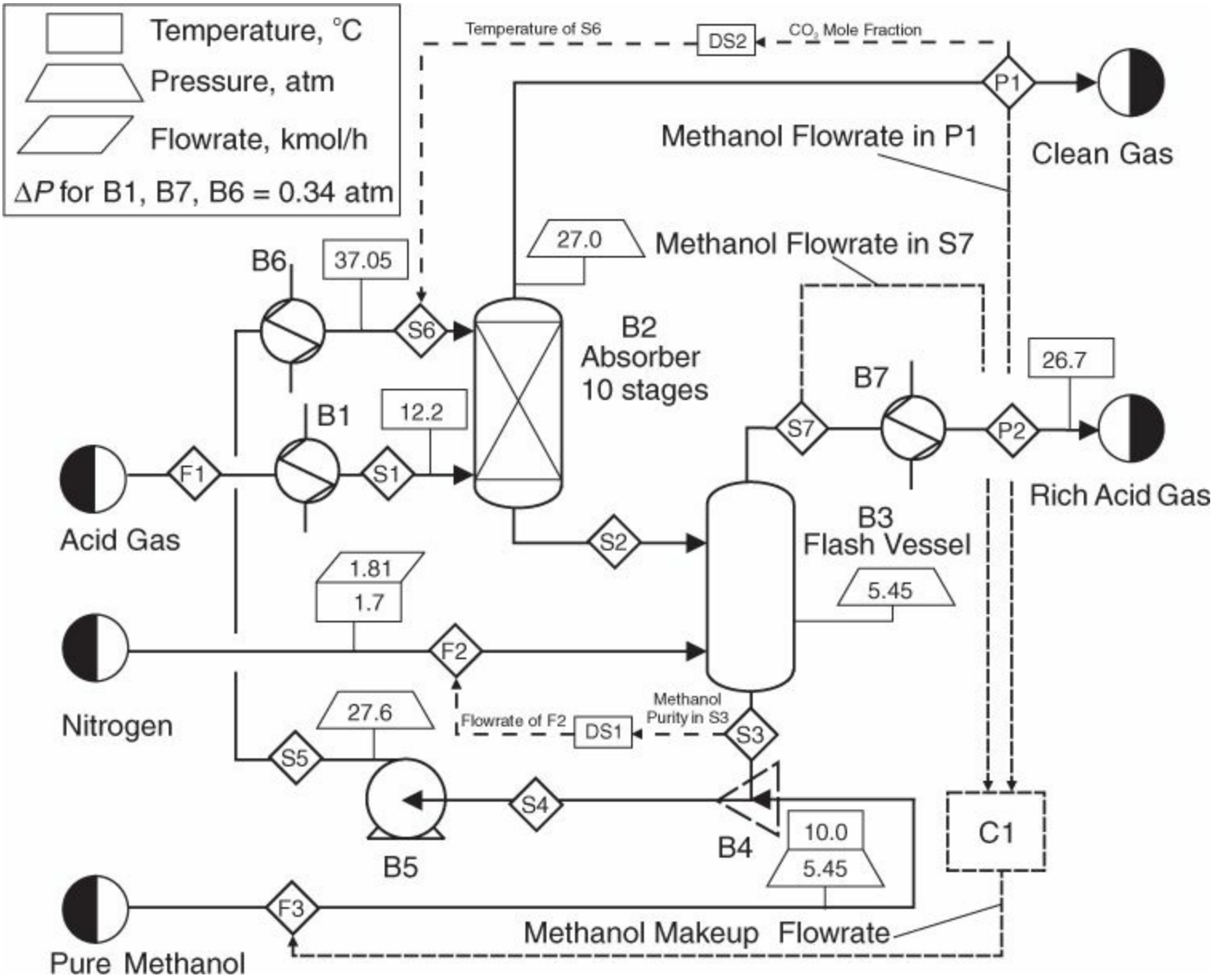


Figure E16.5. Modified Flowsheet of an AGR Plant Using Chilled Methanol

a. As shown in Figure E16.5, implement another design specification, DS2, that manipulates the temperature at the outlet of the cooler, B6, to satisfy a CO_2 mole fraction of 0.02 in P1 from the absorber, B2. Obtain a converged solution for this simulation using various algorithms with an SM approach. In addition, converge this problem using an EO approach and compare the convergence results with those from the SM approach.

b. Connect Stream F3 to block B3. Determine if the simulations converge in all the SM and EO approaches. Try various nesting options and algorithms.

Solution

a. This problem is simulated in Aspen Plus V7.2. Table E16.5(a) shows the results for three SM approaches and one EO approach. When the design specifications are nested inside and all the design specifications are solved simultaneously, all the available algorithms fail. Table E16.5(a) shows the best times achieved using any combination of the available algorithms for the solution approach. Note that the EO approach takes about 0.18 s compared to 2.61 s for the best SM approach achieved by converging the tear streams and design specifications (Case 3), simultaneously.

Table E16.5(a). Effect of Various Solution Approaches, Sequence, and Algorithms on the Convergence

Case	Solution Approach	Sequence	Algorithm	Time Taken
1	SM	Design blocks nested inside, all design blocks solved simultaneously	All algorithms available	Failed
2	SM	Design blocks nested outside, all design blocks solved simultaneously	Design block—Wegstein's method; tear stream—Broyden's method	7.31 s
3	SM	Design blocks and tear streams solved simultaneously	Broyden's method	2.61 s
4	EO		LSSQP	0.18 s (+0.39 s for one pass of the SM)

b. The results after Stream F3 is connected to block B3 are shown in Table E16.5(b).

Table E16.5(b). Performance of Various Solution Approaches, Sequence, and Algorithms after Stream F3 Is Connected to Block B3

Case	Solution Approach	Sequence	Algorithm	Time Taken
1	SM	Design blocks nested inside, all design blocks solved simultaneously	All algorithms available	Failed
2	SM	Design blocks nested outside, all design blocks solved simultaneously	Design block—Wegstein's method; tear stream—Broyden's method	Failed
3	SM	Design blocks and tear streams solved simultaneously	Broyden's method	7.7 s
4	EO		All algorithms available	Failed

Even though convergence is achieved in Case 3, the solvent circulation flowrate (flowrate of S6) is 1.87 kmol/h compared to 14 kmol/h obtained in Part (a) of this problem. On further investigation of the reason for the failure of most of the approaches for Part (b) and the convergence to a different solution, it is observed that Aspen Plus has now automatically selected S2 as the tear stream instead of S6 for which an initial guess was provided. Since there is no initial guess for S2, Aspen Plus V7.2 will start with a flow of zero. In the next iteration, the initial value of the makeup flow is added to it, and the flow will be positive, but small, and far away from the desired solution. This flow does not increase much, since the makeup flow is reduced at the next iteration based on the losses. In the case of the SM solution with simultaneous convergence of the design specifications and tear streams, this converges to

a solution nearest to the initial guess of the makeup stream. The absorber column, B2, fails to solve with all other approaches. This problem can be solved by taking any of the following three approaches:

1. Stream S6 is declared as the tear stream.
2. An initial guess is provided for Stream S2 (similar to S6).
3. A higher initial guess is provided for the makeup stream (similar to the flow of Stream S6).

With any of these approaches, the EO solver (solver LSSQP was used) now converges in 0.2 s after an initial pass through the SM approach. These results compare very favorably to the best of 3.49 s achieved with the SM approach when the design blocks and the tear streams are converged simultaneously.

Note on the solution to Example 16.5: Actually, this problem is structurally singular and has multiple solutions, since the recycle flow can have any arbitrary value, and a converged solution can be obtained with that arbitrary value as long as the most critical equipment, B2 (the absorber), can be converged. In other words, as long as a bound for the solvent-to-gas ratio is satisfied, a converged solution can be obtained. To avoid converging to an arbitrary solution (making the problem nonsingular), various approaches can be used. A design block can be implemented to manipulate the circulation flowrate (instead of the temperature of the solvent from block B6) to satisfy a desired CO_2 concentration in P1. A splitter block can be considered in the path of the solvent (preferably at the bottom of block B3) that has a specification for fixed solvent flow. This fixed flow can be used as a manipulated variable in the design block for satisfying the CO_2 specification. The other stream from the splitter block is a purge stream. This provides another degree of freedom. See Figure E16.6 and Example 16.6 for this configuration.

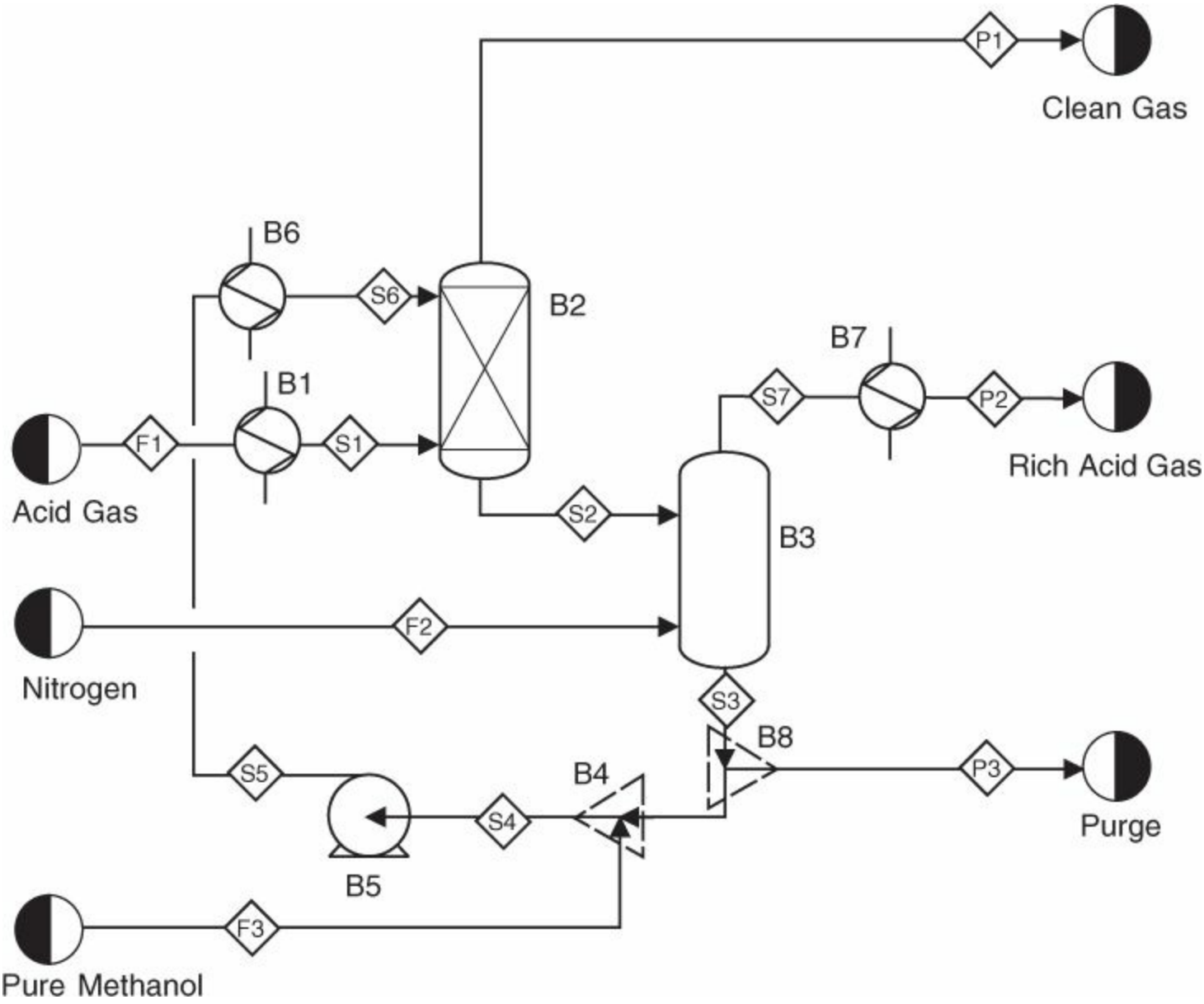


Figure E16.6. Modified Flowsheet of the AGR Unit with a Purge Stream and a Splitter Block

16.4. Studies with the Steady-State Simulation

Once a steady-state model has been developed, it can be used for a number of studies. One of the most useful of these is a sensitivity study, which gives the user insight into the process. The other common type of study is optimization.

16.4.1. Sensitivity Studies

In a sensitivity study, the key input variables and process specifications are varied to generate results for the key outputs. These studies were traditionally done manually. However, in current process simulators, a sensitivity study can be done automatically and involves identifying multiple input specifications that can be changed simultaneously. Subsequently, a loop is generated automatically that spans all the input variables of interest. Sensitivity analysis is very useful for process operability studies and simple process optimization, which can provide a bound for the decision variables or give insight into the possible existence of an optimum. As the process flowsheet must be converged for each combination of the manipulated inputs, it can be computationally expensive to evaluate many such combinations for processes with multiple recycles and/or design blocks and/or loop-creating calculator blocks. The EO approach is often a very good solution methodology for such problems.

16.4.2. Optimization Studies

A detailed discussion of various uses of optimization studies has been provided in Chapter 14. The reader should be comfortable with the material in that chapter before proceeding with the material presented here.

Optimization studies done for a complete process flowsheet are almost always nonlinear, constrained optimization problems. The constraints naturally arise as the unit operations must be converged (i.e., process model equations become equality constraints), and the bounds for the process variables must be satisfied (i.e., inequality constraints). Moreover, the process model equations are often nonlinear. In addition, the objective function can also be nonlinear. Finally, there can be additional constraints to ensure that the physics of the process system is not violated.

In process simulators, usually a single-objective, nonlinear-programming (NLP) problem is solved. A general formulation of this problem is

$$\begin{aligned} &\min_{x \in R^n} \gamma(x) \\ &\text{subject to } \boldsymbol{h}(\boldsymbol{x}) = 0 \\ &\boldsymbol{v}(\boldsymbol{x}) \geq 0 \\ &\boldsymbol{x}^L \leq \boldsymbol{x} \leq \boldsymbol{x}^U \end{aligned} \tag{16.17}$$

Here, the equality constraints are imposed by the process-model equations, design blocks, and calculator blocks. For an SM approach, this also includes the tear streams. The inequality constraints are imposed by the bounds on the variables and additional bounds on the manipulated variables of the design blocks. In the following discussions, the term *feasible point* is used to describe a point that satisfies all the constraints of the NLP problem. The solution of the optimization problem in a process flowsheet environment can be obtained using one of two methods. In the first method, called the feasible-path method, all the tear streams and the constraints are converged at each iteration. This is a major disadvantage of this approach because finding a feasible point at each iteration in the presence of nonlinear constraints is computationally expensive. In addition, for cases with multiple recycles, design specifications, and loop-creating calculator blocks, the computational expense further increases as they are usually converged in a separate, inner loop. Various algorithms such as the COMPLEX algorithm [9] exist for the feasible-path approach. The advantage is that these methods, in general, do not require derivative calculations. In the infeasible-path method, all the equality and inequality constraints, including the tear streams in the case of an SM problem, are converged simultaneously with the optimization problem. The most widely used method in this category is the sequential quadratic programming (SQP) method. In this iterative method, the NLP problem in Equation (16.17) is modeled as a quadratic programming (QP) sub-problem, and then the solution to that subproblem is used to obtain a better estimate of the variables. The quadratic subproblem is constructed such that it reflects the nonlinearities of the original problem.

$$\begin{aligned} &\min_{\boldsymbol{d}} \nabla\gamma(\boldsymbol{x}^k)^T\boldsymbol{d} + \frac{1}{2}\boldsymbol{d}^T\nabla^2 L(\boldsymbol{x}^k, \boldsymbol{\lambda}^k)\boldsymbol{d} \\ &\text{subject to} \quad \nabla\boldsymbol{h}(\boldsymbol{x}^k)^T\boldsymbol{d} + \boldsymbol{h}(\boldsymbol{x}^k) = 0 \\ &\nabla\,\boldsymbol{v}(\boldsymbol{x}^k)^T\boldsymbol{d} + \nabla\,\boldsymbol{v}(\boldsymbol{x}^k) \leq 0 \end{aligned} \tag{16.18}$$

where $L(\mathbf{x}^k, \lambda^k)$ is the Lagrangian function and λ is the Lagrangian multiplier vector. The main advantage of this approach is that the quadratic subproblem is easier to solve, and very efficient

algorithms exist for solving such problems, including Newton's and the quasi-Newton algorithms that were discussed previously. The SQP algorithms vary in their approach to handling bounds and inequality constraints, Hessian approximation, various merit functions, global convergence, and so on. The nuances of these approaches and algorithms will not be discussed here, but some salient points that may be useful for troubleshooting issues relating to convergence failures will be discussed.

1. For the SQP method to be successful, it is necessary that the resulting QP subproblem have a solution. Starting from an arbitrary initial guess, the iterative process finds a search direction and a step length with the hope that it will eventually converge to a solution. The step length is chosen such that sufficient progress is made in a merit function. A line search or a trust region algorithm is used for this criterion. In a line search method, the next iteration is calculated as

$$x^{k+1} = x^k + \alpha^k d^k \qquad (16.19)$$

   where $\alpha \in [0, 1]$ is the step size. This approach is usually efficient when the QP subproblem is well conditioned and the initial guess is good. Conversely, the trust region algorithms are very efficient for ill-conditioned problems and when the initial guess is poor. In this approach, an additional constraint is imposed. As this constraint results in a bounded feasible region, the QP subproblem is guaranteed to have a solution (for this the feasible reason must be nonempty). So, if the optimizer reports that the quadratic subproblem is infeasible, different initial guesses should be tried, and switching to the trust-region-based method along with the relevant approaches listed below is recommended.
2. It must be ensured that an optimum exists in the feasible region. This is possibly the most frequent reason for failure of an optimization problem. For simple problems, a good idea can be obtained by sensitivity studies as mentioned before.
3. It needs to be ensured that the process flowsheet is being converged to the desired tolerances. High errors in the underlying flowsheet can lead to convergence failure.
4. If a higher or lower bound is being hit by some decision variables, it needs to be determined whether the bounds can be relaxed.
5. It must be determined that the underlying process flowsheet can be solved in the extreme values of the decision variables and some arbitrary combinations. Again, sensitivity studies can be helpful.
6. It must be determined whether additional constraints are needed or whether the constraints can be relaxed or tightly bound based on a particular case. This again modifies the feasible region and can help in solution.
7. The constraints must be consistent.

For more details, interested readers are referred to an excellent review of the optimization methods and associated references in Biegler et al. [10].

In flowsheet optimization, the degrees of freedom are exploited to find the optima of some objective or cost function. As an example, the objective function can be the minimization of auxiliary power consumption, minimization of operating cost, maximization of power production, maximization of product yield, minimization of chemical consumption, maximization of profit, and so on. These objective functions can include some or all of the design specifications being considered earlier. There can be additional design specification and calculator blocks that satisfy other criteria.

In the SM approach for optimization, the tear streams can be converged in an inner loop. This results in a sequential approach where, given the values of the decision variables, the tear streams along with the design specification and calculator blocks, if any, are converged separately in an inner loop. After the solution of this loop is achieved, the objective function is recalculated with the current values of the variables. This process continues until the optimum is reached. If the tear stream is converged simultaneously, this is usually treated as an additional constraint. Traditional SQP algorithms (which are usually available in the process simulators) require calculation of first- and second-order derivatives with respect to all decision variables (and tear variables, if present, and being simultaneously converged with the optimization problem), along with other derivatives calculated for solving the process flowsheet, as discussed before. This adds to the computational cost. Note that with an infeasible-path approach, the tear streams and other equality and inequality constraints do not have to be converged at each iteration.

An EO approach can be really helpful for optimization in large flowsheets containing multiple tear streams and design and loop-creating calculator blocks. Similar to the flowsheet convergence with the EO approach, the sparse structure of the underlying problem should be exploited for efficient computation. The usual drawbacks of an EO approach such as initialization, problem formulation, troubleshooting, and so on, remain for the optimization problems as well.

Example 16.6 demonstrates the use of the SM and EO approaches for optimization of a cost function in a process flowsheet.

Example 16.6.

Consider the modified flowsheet in Figure E16.6 as suggested in the last paragraph of Example 16.5. In this problem, both the circulation rate (flowrate of S3) and the temperature at the exit of the cooler, B6, can be manipulated to satisfy a desired CO_2 specification in P1. A decrease in the solvent temperature results in a reduced circulation rate and lower solvent loss. This increases the refrigeration cost at the cooler, B6, decreases the pumping cost in the pump, B5, and decreases the cost of the makeup solvent. Therefore, there is a trade-off between these factors. Now consider the formulation of the constraints. The solvent/gas ratio to the absorber should be maintained within a bound to avoid drying or flooding that would eventually lead to convergence failure of the absorber block. The solvent purity at the exit of the flash block, B3, should be maintained to ensure that it is feasible to maintain the specification of P1. In addition, there will be a constraint for the temperature at the exit of the cooler, B6, based on the refrigerant used. The other design block manipulates the F2 flowrate for a desired solvent purity. An optimization problem can be formulated where the objective is to minimize the operating cost by considering the pumping cost, the cost of refrigeration, and the cost of makeup solvent. The decision variables are the solvent circulation rate, the temperature at the exit of B6, and the makeup solvent. As there is a desired specification for P1, an equality constraint should also be imposed. Note that algorithmically, this can be declared as an inequality constraint since a higher purity will result in a higher operating cost. So at the optimum, this inequality constraint will be active. But this can make the solution of the problem easier for intermediate steps where this is inactive. In this formulation, the design specification for maintaining the solvent purity, by manipulating the flowrate of N_2 used for stripping, is left at the flowsheet level. The cost of N_2 can be included in the cost function, and then the N_2 flowrate can be considered as a decision variable. In this case, a bound in the solvent purity must be considered to avoid infeasibility in the problem specification, as mentioned previously. There are additional implications for the hardware cost, since

the solvent flow and temperature change. For simplicity, only the operating cost will be considered here. Based on the above discussion, formulate an optimization problem. The operating cost, C_{op}, should be minimized, where

C_{op} ($/y) = Cost for electric power in pump B5 + Refrigeration cost in cooler B6 + Cost of makeup solvent

Assume that the cost of electricity is $0.20/kWh (consistent with the AGR plant being located in the northeastern United States), the refrigeration cost is $0.224/kWh, and the solvent cost is $0.75/kg. The decision variables are the solvent circulation rate (flowrate of S3; note that this additional DOF is provided by introducing block B8), the temperature at the exit of cooler B6 (temperature of S6), and the F3 (makeup) flowrate. Consider the following inequality constraints and bounds on variables: mole fraction of CO_2 in P1 < 0.02, –54°C < solvent temperature < 0°C, 4.5 kmol/h < S3 flowrate < 23 kmol/h, 0.045 kmol/h < F3 flowrate < 13.6 kmol/h. The bounds on the S3 flowrate ensure that the solvent/gas ratio is within the feasible operating region of the absorber. The lower bound in the F3 flowrate ensures that there is some minimum purge from the system that is needed to avoid buildup degradation and undesired species in the system. A design block should be implemented that maintains the methanol mole fraction in Stream S3 at 0.98 by manipulating the flowrate of N_2.

a. Solve this optimization problem using the SM approach.

b. Converge this problem using the EO approach.

Solution

a. This problem is simulated in Aspen Plus V7.2. The SM problem failed to converge after more than 3 hours when all three decision variables were considered. For ease of convergence, the F3 flowrate was removed from the list of decision variables. The calculator block that was being used previously for calculating the F3 flowrate based on the solvent loss was again implemented here. With these changes, the simulation then converged using the SQP algorithm in about 25 minutes. Because of repeated failure, the maximum number of iterations for converging the tear stream was increased from the default value of 3 to 15. Note that the large computational effort needed to converge the tear stream at each iteration increased the computational cost and converted this method from an infeasible-path approach to a feasible-path approach. The results are shown in Table E16.6.

Table E16.6. Optimal Values of the Decision Variables from the SM and EO Methods

Optimal Values of the Decision Variables	Optimization by SM Method	Optimization by EO Method
Flowrate of S3 (kmol/h)	0.045	0.045
Flowrate of F3 (kmol/h)	6.02	6.183
Temperature of S6 (°C)	–47.23	–44.81

b. In the EO approach, the optimization took 10.8 s using the DMO solver in Aspen Plus V7.2. This solver is a variant of the SQP algorithm. For the EO approach, all the decision variables are considered. The results are shown in Table E16.6. Some minor differences can be observed in the results for the EO approach compared to the SM approach. The results in the SM and EO approaches can be made similar by tightening the tear stream tolerances and

tolerances of individual blocks. But this is computationally expensive. The optimal temperature at the outlet of B6 is –44.8°C compared to the base-case value of –37.05°C. The optimal solvent flowrate is 6.2 kmol/h. Because of the comparably high cost of the makeup solvent, it always hits the lower limit. In practice, the solvent is refrigerated to reduce the solvent loss. Therefore, the results are intuitive. If the cost of refrigeration is increased, then the optimizer will increase the solvent temperature and the recycle flowrate. This problem demonstrates that the EO approach can really save time for large and complicated simulations. However, they are difficult to formulate and troubleshoot, as mentioned before.

16.5. Estimation of Physical Property Parameters

A detailed discussion of choosing thermodynamic models was provided in Chapter 13. If the required parameters of the chosen thermodynamic and/or transport property models are not available in the simulator databank or if the user is not satisfied with the performance of the available parameters, they need to be estimated.

While estimating the physical property parameters, the variables are divided into two categories, dependent and independent variables. It is usually assumed that the values of the independent variables are true values. For example, the model of the specific heat of a pure species can be written as

$$C_p = a + bT + cT^2 + dT^3 \tag{16.20}$$

T is considered to be the independent variable and C_p is the dependent variable. The estimation method depends upon the desired statistical accuracy of the fit, experimental information, the particular model, and any constraints that need to be considered. If a dependent variable can be explicitly expressed in terms of the independent variables for a linear-in-parameter (LIP) model and no constraints need to be considered, the least-squares estimate of the parameter vector (θ) can be obtained as

$$\hat{\boldsymbol{\theta}} = (\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{y} \tag{16.21}$$

where $\boldsymbol{y}$ is the vector of the experimental data of the dependent variable and $\boldsymbol{X}$ is the matrix of the independent variables. In many parameter estimation problems, the dependent variables cannot be explicitly expressed in terms of the independent variables. Besides, there may be additional constraints that must be satisfied. In these cases, an optimization problem is solved. For brevity, the estimation of binary interaction parameters of a thermodynamic model for VLE calculation will be considered here. This is one of the important and complex problems in parameter estimation.

The first question to be addressed is what should be the objective function that must be minimized (or maximized) to find the optimal values of the parameters. Usually, two criteria are used. In the least-squares criterion, a quadratic error between the experimental data and the model results is minimized over the entire experimental data range, where the decision variables are the binary interaction parameters. Some typical objective functions are

$$\min \sum_{i=1}^{N}\sum_{j=1}^{C}(K_{i,j}^{est}x_{i,j}^{exp} - y_{i,j}^{exp})^2 \tag{16.22}$$

$$\min \sum_{i=1}^{N}\sum_{j=1}^{C}\left(\frac{y_{i,j}^{est} - y_{i,j}^{exp}}{y_{i,j}^{exp}}\right)^2 \tag{16.23}$$

$$\min \sum_{i=1}^{N} \left(\frac{P_i^{est} - P_i^{exp}}{P_i^{exp}} \right)^2 \tag{16.24}$$

Various combinations of these objective functions are also considered. Here N is the number of data points, C represents the number of species, and P is the bubble point pressure. Other nomenclatures have their usual meaning.

In the second criterion, known as the maximum likelihood criterion, all the experimental data (both dependent and independent variables) and their statistical variances are considered. The objective function is

$$\min \sum_{i=1}^{N} \left[\left(\frac{P_i^{est} - P_i^{exp}}{\sigma_{P,i}} \right)^2 + \left(\frac{T_i^{est} - T_i^{exp}}{\sigma_{T,i}} \right)^2 + \sum_{j=1}^{C-1} \left(\frac{x_{i,j}^{est} - x_{i,j}^{exp}}{\sigma_{x,i,j}} \right)^2 + \sum_{j=1}^{C-1} \left(\frac{y_{i,j}^{est} - y_{i,j}^{exp}}{\sigma_{y,i,j}} \right)^2 \right] \tag{16.25}$$

Using this criterion requires the statistical variances, σ, to be known. In addition, the measurements should be subject only to random errors, and the model should be able to represent the measurements within an order of magnitude (approximately) less than the order of the experimental uncertainties.

The constraints depend upon the thermodynamic model used for the VLE calculations. If an EOS is used for both phases, then the constraint for the VLE is

$$y_i \hat{\phi}_i^{v} P - x_i \hat{\phi}_i^{l} P = 0 \tag{16.26}$$

where $\hat{\phi}_i^{v}$, and $\hat{\phi}_i^{l}$ are the fugacity coefficient of species i in the vapor and liquid phases, respectively. The fugacity coefficients are calculated from the chosen EOS:

$$\hat{\phi}_i^{v} = \phi^{v}(T, P, y) \tag{16.27}$$

$$\hat{\phi}_i^{l} = \phi^{l}(T, P, x) \tag{16.28}$$

Note that these constraints are considered for each C -1 species for all N data points.

In addition, the summation equations are treated as constraints for all N data points:

$$\sum x_i = 1 \tag{16.29}$$

$$\sum y_i = 1 \tag{16.30}$$

If an activity coefficient model is used for the liquid phase, the constraints are

$$y_i \phi_i P = x_i \gamma_i P_i^{*} \tag{16.31}$$

where $\phi_i = \frac{\hat{\phi}_i^{v}}{\phi_i^{*}} \exp\left[\frac{v_i^{l}(P_i^{*} - P)}{RT} \right]$. Here $\hat{\phi}_i^{v}$, γ_i, ϕ_i^{*}, P_i^{*}, and v_i^{l} are the fugacity coefficient of species i in the vapor phase, the activity coefficient of species i in the liquid phase, the fugacity coefficient of saturated vapor, the saturation pressure, and the molar volume of the saturated liquid for the pure species i, respectively. The ratio of the fugacity coefficients, $\frac{\hat{\phi}_i^{v}}{\phi_i^{*}}$, is calculated from the chosen EOS, γ_i is calculated from the activity coefficient model, and P_i^{*} is calculated using some appropriate equation such as the Antoine equation as shown in Equations (16.32) through (16.34), respectively:

$$\frac{\hat{\phi}_i^{v}}{\phi_i^{*}} = \phi^{v}(T, P, P_i^{*}, y) \tag{16.32}$$

$$\gamma_i = \gamma(T, x) \tag{16.33}$$

$$P_i^{*} = P^{*}(T) \tag{16.34}$$

In addition, the summation equations are also considered. Additional equations can be considered as part of this optimization problem. For example, the molar volume v_i^l can be treated as a constant for a species *i*. If it is calculated from some model, for example, the Rackett [11] equation, then additional parameters such as critical volume and critical compressibility factor are needed. Now, the critical compressibility factor can be a constant or an acentric factor. These additional calculations are automatically done by the simulator. So it must be remembered that the accuracy of a VLE model is also a strong function of the additional parameters. These additional parameters may need to be regressed/calculated/estimated first, especially when these parameters are missing in a process simulator.

Similar approaches can be used for estimating other parameters in the thermodynamic and transport models. One point of caution is that the experimental data used for such purposes must represent the operating region of interest and should be taken from a number of data sources, if possible, so that extrapolation outside of the known experimental regions is not required and so that experimental errors are averaged over multiple data sets.

Example 16.7 demonstrates the use of data regression systems in a process simulator for estimating the binary interaction parameters of a thermodynamic model for a VLE calculation.

Example 16.7.

Using VLE data for a methanol-CO_2 system from the existing literature, estimate the binary interaction parameters considering an EOS model and an activity-coefficient model. Compare their performances.

Solution

The VLE data are obtained from Weber et al. [12]. This paper reports the *T*-*P*-*x* VLE data for the system at various temperatures. In this example, data are considered at four temperatures, –40°C, –20°C, 0°C, and 25°C. The estimation is carried out in Aspen Plus V7.2 using its data regression system. A minimum-likelihood objective function is considered with all the default settings. The standard deviations in the pressure and mole fraction data are considered to be 0.1%. For the example of an EOS model, the Peng-Robinson (PR) model (PENG-ROB in Aspen Plus V7.2) is used. The binary parameters k_{ij} (PRKBV in Aspen Plus V7.2) are estimated. For the example of an activity-coefficient-based model, the nonrandom two-liquid (NRTL) model with Redlich-Kwong EOS (NRTL-RK in Aspen Plus V7.2) is used. It can be seen in Figures E16.7(a) and E16.7(b) that both models represent the data reasonably well over the entire data range, although the prediction of the NRTL model is a little better than that of the PR model. The root-mean-square errors of the residuals of the PR and NRTL models are 135.26 and 122.82, respectively. In this example, the results from the EOS model and the activity-coefficient model are similar, but the performance of the EOS model is expected to be inferior as the solution deviates further from ideality.

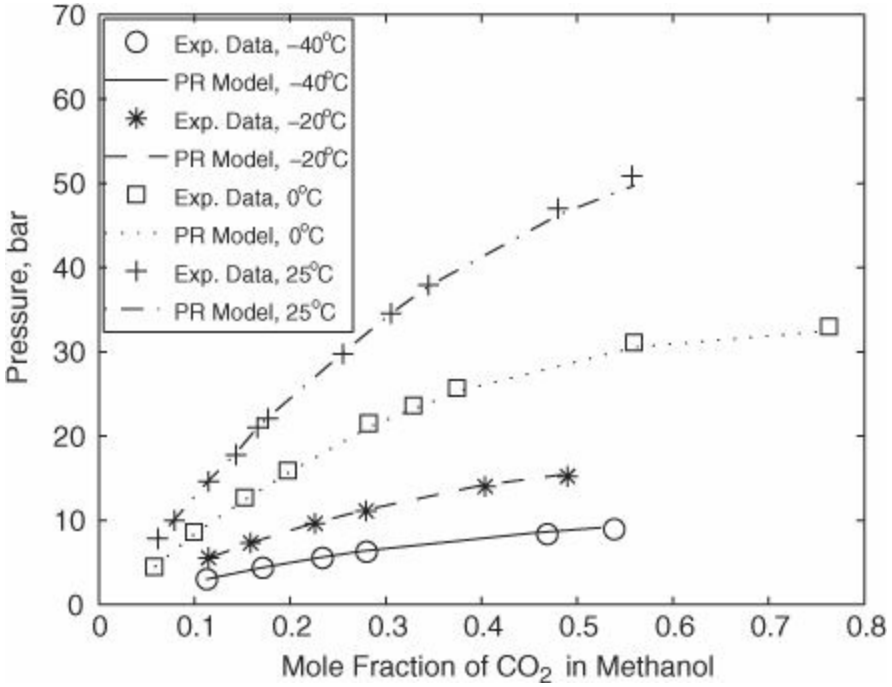


Figure E16.7(a). VLE Comparison between the Experimental Data [12] and the PR Model Using Estimated Binary Parameters for a CO_2-Methanol System

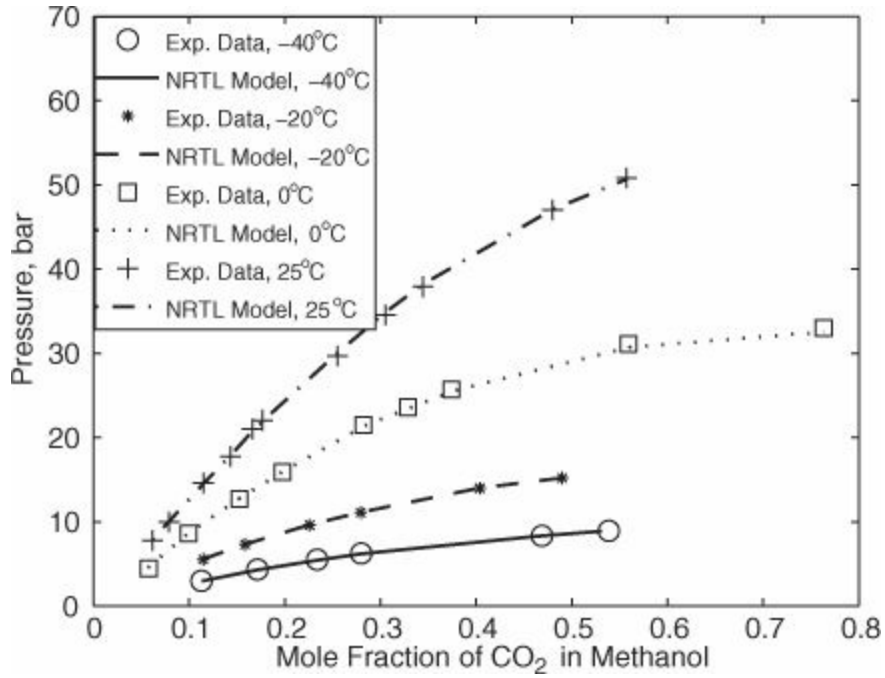


Figure E16.7(b). VLE Comparison between the Experimental Data [12] and the NRTL Model Using Estimated Binary Parameters for a CO_2-Methanol System

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16.6. Summary

With the increase of computational power and availability of advanced features in the current simulators, the power of steady-state simulators can be leveraged further. With this motivation, this chapter has focused on four advanced topics: user-added models (UAM); a solution strategy for steady-state simulation using the SM, EO, and SMod approaches; studies with steady-state simulation; and estimation of physical property parameters. A detailed discussion of the various solution strategies was provided as a theoretical background for troubleshooting convergence failure of large, complex simulations. Even though the steady-state simulation can be used for a number of studies, the focus was on optimization studies. The advantage of EO methods for optimization of

complex and highly interacting process systems was demonstrated through an example. In this chapter, discussions of the theoretical background of some of the topics, even though not exhaustive, were provided to enhance the reader's understanding of what happens in the background when using a process simulator. This understanding can help in better utilization and efficient troubleshooting of steady-state process simulations.

What You Should Have Learned

- User-added models should follow simulator guidelines so that they can be integrated with other unit operation models.
- Proper selection of a solution method among sequential modular (SM), equation-oriented (EO), and simultaneous modular (SMod) coupled with the appropriate algorithm(s) may be required to solve large, complicated, and highly integrated process simulations.
- For troubleshooting convergence failure of optimization problems, it is necessary to ensure that an optimum exists in the feasible region.
- To ensure the highest accuracy of simulation results, thermodynamic models should be compared to actual data and, if necessary, parameters should be estimated by using the data regression tool available in a process simulator.

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Short Answer Questions

1. How are partitioning and precedence ordering carried out by a process simulator?
2. Consider a flowsheet containing a number of process loops for which a single tear stream is sufficient to ensure that each loop is opened at least once. Assume that you have a choice of two tear streams. One stream has ten nonzero species, but a precise guess of its temperature, pressure, and flowrates of two of the species is available. The other stream has five nonzero species, but it is difficult to provide a good initial guess for this stream. Which stream will you choose as the tear stream? Why?
3. In a flowsheet, a material stream consisting of six species is used as the tear stream. If Newton's method is used for converging this stream, how many more flowsheet passes are required at each iteration in comparison to Broyden's method?
4. A process flowsheet contains some sections that have a number of recycle streams with strong interactions while the other sections have very few recycle streams. What is the appropriate solution method for this system?
5. In an optimization study with a flowsheet, how is the feasible region defined? Why is it important?

6. If you are estimating the binary interaction parameters of an SVE problem, what constraints are considered?

Problems

7. The stripper off-gas in Problem 13.29 is typically sent to a Claus unit for sulfur recovery. For maintaining the minimum flame temperature in the Claus furnace, it is necessary to maintain the H_2S concentration in excess of about 25 mol%. Implement a design block that manipulates the bottoms/feed ratio in T-2002 to maintain the H_2S concentration in the stripper off-gas at 40 mol%. Did you face any convergence problems? How did you solve them? (*Hint*: Make a considerable change in the bottoms/feed ratio in the absence of the design block. Did it converge? What should you have done to aid in the convergence for a large change in any of the operating variables?)
8. Modify the preceding problem to develop a flowsheet as shown in Figure P16.8. Replace the heat exchanger, E-2001, with a countercurrent heat exchanger between the feed to and product from the stripper. Assume that about 0.5% of the solvent circulation rate is purged from SP-2001. The purging (and other methods such as thermal reclaiming, mechanical filtration, washing of the solvent, etc.) helps to reduce the buildup of undesired contaminants in the system. Stream 11, makeup MDEA, and Stream 12, makeup water, are pure. The discharge pressure of P-2001 is 2.6 atm. The solvent is cooled to 38°C in E-2002 and sent to T-2001. You can manipulate the temperature specifications in E-2001, satisfying a minimum temperature approach of about 10°C. Implement two calculator blocks. One calculator block calculates the flowrate of Stream 11 based on the solvent loss. Another calculator block calculates the water makeup to maintain the water concentration in Stream 13 at 66.6 mol%. Note that this water concentration is much different compared to what was considered in Problem 13.29. Finally, this system will have one design block, two calculator blocks, and a recycle stream.

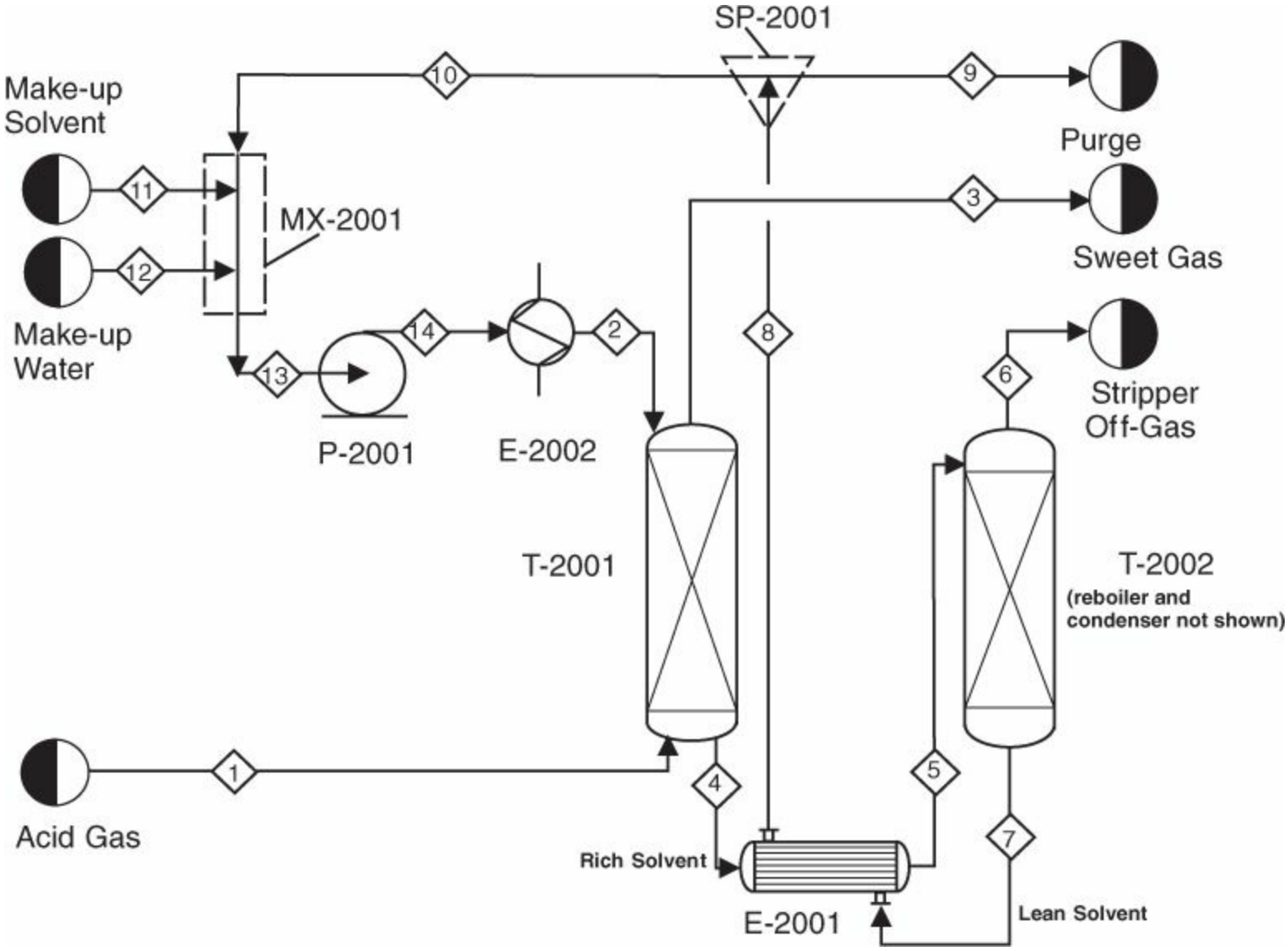


Figure P16.8. Schematic of the AGR Plant Using MDEA as the Solvent

a. Did you face any convergence problem? (*Hint*: In Example 16.5, a similar problem has been solved, but here it is an electrolyte system, which is harder to solve. What are different techniques for solving convergence issues of electrolyte systems with recycle streams?)

b. What are the compositions of Streams 3 and 6? What is the reboiler and condenser duty of T-2002? What is the flowrate of Stream 11?

9. Consider the process described in Problem 16.8.

a. Considering the various criteria discussed in the text for tear stream selection, which stream would you like to consider as tear stream?

b. What is the tear stream selected by the simulator that you used?

c. Now simulate the system with the tear stream you selected and note the differences in computational expense (time to reach the solution). If your selection matches that of the process simulator, consider another feasible tear stream and carry out this analysis.

10. Consider the process described in Problem 16.8. Implement a design block that manipulates the solvent circulation rate to achieve an H_2S concentration of 5 ppmv in Stream 3. So now there are two design blocks, two calculator blocks, and one recycle stream. Solve this problem with various combinations of solution approaches (SM and EO), sequences (design blocks nested inside/outside of the convergence block that solve the tear streams and design blocks and tear

streams solved simultaneously), and various algorithms. Compare the performance of all the combinations.

11. Formulate an optimization problem considering the flowsheet in Problem 16.8. One design block and two calculator blocks are active. Minimize the operating cost of this AGR unit:

    Operating Cost ($) = Heating cost in the reboiler of T-2002
    + Cooling cost in the condenser of T-2002
    + Pumping cost in pump P-2001
    + Cooling cost in E-2002 + Cost of makeup MDEA

    Assume the cost of electricity is $0.10/kWh, the cooling cost is $0.02/kWh, the heating cost is $0.05/kWh, and the solvent cost is $1.0/kg. The decision variables are the solvent circulation rate, reflux ratio (RR) in T-2002, and the temperature at the exit of E-2002. Consider the following constraints and bounds on variables:

    • Mole fraction of H_2S in Stream 3 < 5 ppmv

    • 30°C < Stream 2 temperature < 70°C

    In addition, consider bounds in the circulation flowrate to ensure that the solvent/gas ratio is within the feasible operating region of T-2001 and T-2002. Also, ensure that the purge from the system is 0.1%–3% of the solvent circulation rate. The minimum purge is to avoid buildup of the undesired species in the system. The high limit on the purge is imposed to avoid disposal costs that are not accounted for in the objective function.

    Solve this optimization problem with both the SM and EO approaches, and note the differences in the results, if any, and the computational expense. While using the EO approach, ensure that the design block and the calculator blocks are also considered as constraints. (*Hint*: You may find it useful to consider an additional constraint: mole fraction of H_2S in Stream 7 < 1 ppmv. This constraint, especially in the SM approach, will help to eliminate many infeasible combinations due to a lower RR, in which the required specification of Stream 3 cannot be achieved. This constraint can be relaxed after achieving initial solution.)

12. Ethylene and air react in a vapor-phase catalytic reaction to form ethylene oxide.

$$C_2H_4 + 0.5O_2 \rightarrow C_2H_4O$$

    The system can be modeled by the PR EOS. The rate law is given by Wan [13]:

$$-r_{C_2H_4} = k p_{C_2H_4}^{1/3} p_{O_2}^{2/3} \frac{\text{kmol}}{\text{kg cat s}}$$

$$k = 324 \exp\left(\frac{-19{,}300\left[\frac{\text{cal}}{\text{mol}}\right]}{RT\,[K]}\right)\left[\frac{\text{kmol}}{\text{atm kg cat s}}\right]$$

$$E = 19{,}300\,\frac{\text{cal}}{\text{mol}}$$

    a. Develop a base-case simulation considering a feed stream with ethylene and O_2 flowrates of 4 kmol/s and 2 kmol/s, respectively. The streams are available at 25 bar and 230°C. Simulate the reactor as a PFR with a constant temperature of 260°C. Consider using a total of 7500 carbon steel, catalyst-filled tubes, each with an inside diameter of 0.0254 m. Consider the bed voidage to be 0.45 and the density of the catalyst particles to be 1922 kg/m^3. Consider an

appropriate correlation for calculating the pressure drop through the reactor. What is the length of individual tubes for achieving 40% conversion of ethylene?

b. Now consider that the heat of reaction is being used for generating steam at a constant temperature of 230°C. Modify the previous reactor model to a nonisothermal reactor, calculating the heat transfer coefficient in a UAM. The UAM can be developed in FORTRAN, C, or Excel or by using any other suitable interface supported by your simulator. The UAM will retrieve the stream conditions (such as flowrates of the reactants) and physical properties (such as viscosity, density, specific heat, thermal conductivity) of the feed calculated by the process simulator. Use the inlet condition data for calculating the heat transfer coefficient with the Gnielinski [14] correlation:

$$Nu = \frac{(\mathrm{Re} - 1000)\,\mathrm{Pr}(\phi/8)}{1 + 12.7\sqrt{\phi/8}\,(\mathrm{Pr}^{2/3} - 1)}$$

$$\phi = [0.79\ \mathrm{In}(\mathrm{Re}) - 1.64]^{-2}$$

Automatically insert the calculated heat transfer coefficient in the specification of the reactor. The reactor temperature must be maintained below 270°C to avoid explosion [13]. Retrieve the maximum temperature of the reactor to the UAM and the amount of unreacted ethylene in the outlet stream. What is the maximum temperature?

c. Now modify the reactor design (number of tubes, tube diameter, and length) so that you can achieve 40% conversion of ethylene without the maximum temperature exceeding 270°C. The maximum temperature is expected to occur somewhere along the length of the reactor, not necessarily at the outlet. The reactor design parameters should be automatically inserted by the UAM into the process simulator along with the recalculated heat transfer coefficient. What are the final values of your design parameters?

d. Consider the previous UAM. Keep the reactor design parameters constant. From the UAM, vary the ethylene flowrate by +/–30%, keeping the stoichiometric ratio of O_2 constant. How much conversion of ethylene did you achieve in the extreme conditions? Could you satisfy the temperature limit? If not, modify the reactor design so that you can satisfy the temperature limit in this operating range. Note that you will still need to ensure that 40% conversion of ethylene is achieved when the flowrates are at their base-case values.

13. In a process for producing methanol, synthesis gas composed of CO, CO_2, H_2, and H_2O is sent through a heat exchanger, E-2001, to a plug-flow reactor, R-2001, as shown in Figure P16.13. In addition to the desired methanol synthesis, some undesired reactions also take place [15, 16]:

$$CO + 2H_2 \rightleftharpoons CH_3OH \qquad \text{(P16.7a)}$$
$$CO + H_2O \rightleftharpoons CO_2 + H_2 \qquad \text{(P16.7b)}$$
$$CH_3OH \rightarrow CH_2O + H_2 \qquad \text{(P16.7c)}$$

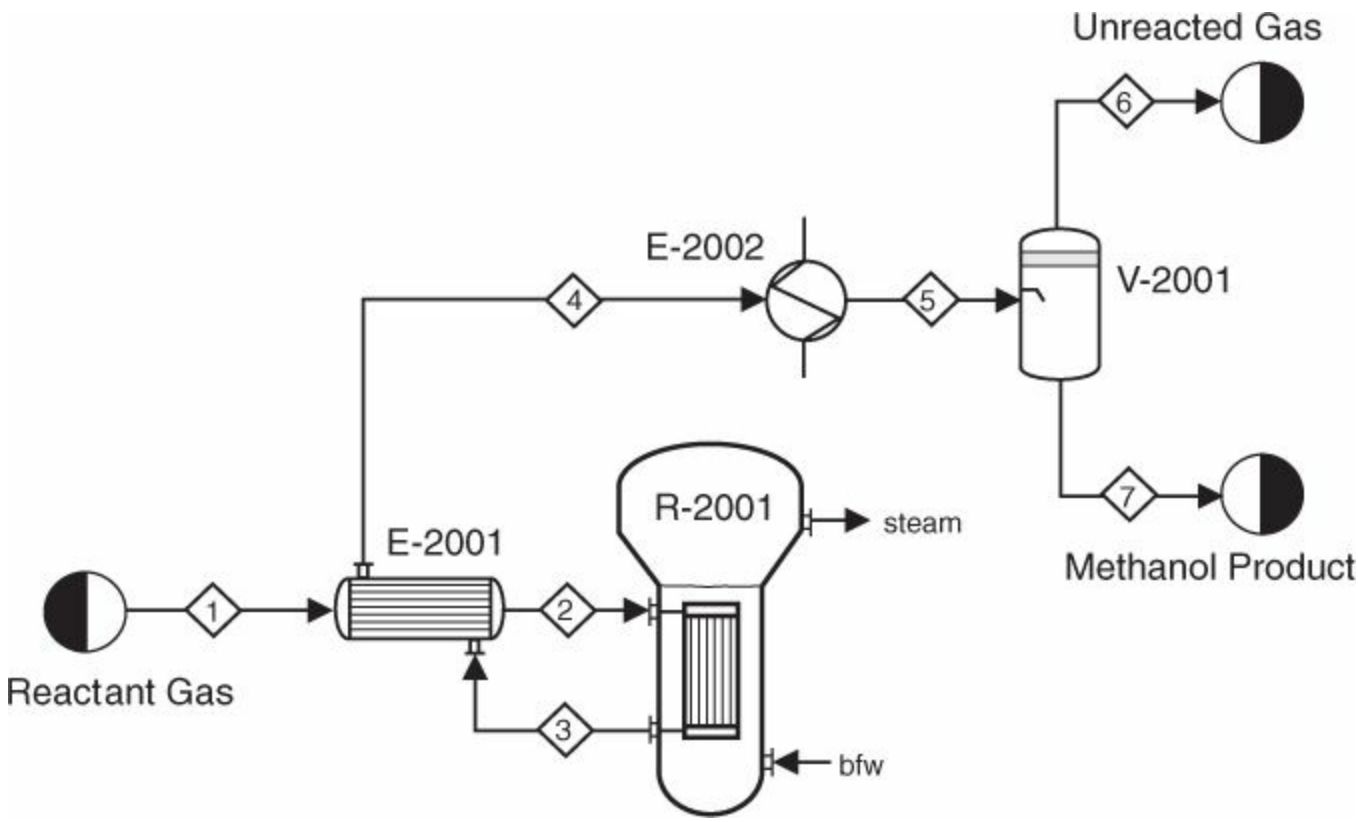


Figure P16.13. Flowsheet of a Methanol Production Unit

The corresponding rate laws for these reactions are [15, 16]

$$r_{CH_3OH} = 6.4278 \times 10^{8}\left[\frac{\text{kmol}}{\text{kg cat s}}\right]\exp\left(\frac{-105.5\left[\frac{\text{kJ}}{\text{mol}}\right]}{RT\,[K]}\right)\left(C_{CO}C_{H_2}^{2} - \frac{C_{CH_3OH}}{K_{eq,CH_3OH}}\right)$$

$$-r_{CO} = 4.189 \times 10^{-8}\left[\frac{\text{kmol}}{\text{kg cat s}}\right]\exp\left(\frac{-40\left[\frac{\text{kJ}}{\text{mol}}\right]}{RT\,[K]}\right)\left(y_{CO}y_{H_2O} - \frac{y_{CO_2}y_{H_2}}{K_{eq,WGS}}\right)$$

$$-r_{CH_3OH} = 6.314 \times 10^{-7}\left[\frac{\text{kmol}}{\text{kg cat s}}\right]\exp\left(\frac{-58.65\left[\frac{\text{kJ}}{\text{mol}}\right]}{RT\,[K]}\right)C_{CH_3OH}$$

where C_i is the concentration of the species i in kmol/m^3.

In R-2001, steam is being generated at a temperature of 350°C. Consider an overall heat transfer coefficient of 80 W/m^2°C between the process stream and the boiling water. The reactor effluent is sent to E-2001 and then further cooled in E-2002 to 40°C before being sent to the flash separator, V-2001. Unconverted reactants are recovered from the top of V-2001. Assume that the feed composition (mole fraction) and rate are

H_2	0.42
H_2O	0.16
CO	0.2
CO_2	0.22

Flowrate = 1 kmol/h

The minimum temperature approach in E-2001 is 15°C. Further assume that the pressure drops in both the shell and tube sides of E-2001 are 0.1 bar. The catalyst particle density is 1800

kg/m^3 and the bed voidage is 0.45. Assume the pressure drop in R-2001 is 0.2 bar. Maximize the yield of methanol in this process, where the decision variables are the inlet temperature, the pressure of Stream 1, and the dimensions of R-2001 (length and diameter). What bounds on the decision variables did you consider? Why? You can solve this problem with either the SM or EO approach.

14. In the preceding problem, the composition of the feed was assumed to be constant. However, the CO/H_2 ratio in the feed can be manipulated as these streams are usually supplied from different sources. Solve the preceding optimization problem by considering the CO/H_2 ratio as another decision variable. Did you have to consider any additional constraints? Why? Compare the results with the results that you obtained in Problem 16.13.

15. Consider Problem 16.14, but for the case when the unconverted reactants are recycled to the reactor, as shown in Figure P16.15. Consider the purge-stream flow to be 2% of the total flow of Stream 6, and assume that compressor C-1001 has an isentropic efficiency of 80%. Maximize the following objective function:

$$Max\ C_{CH_3OH}F_{CH_3OH} - C_{UC}P_{UC}$$

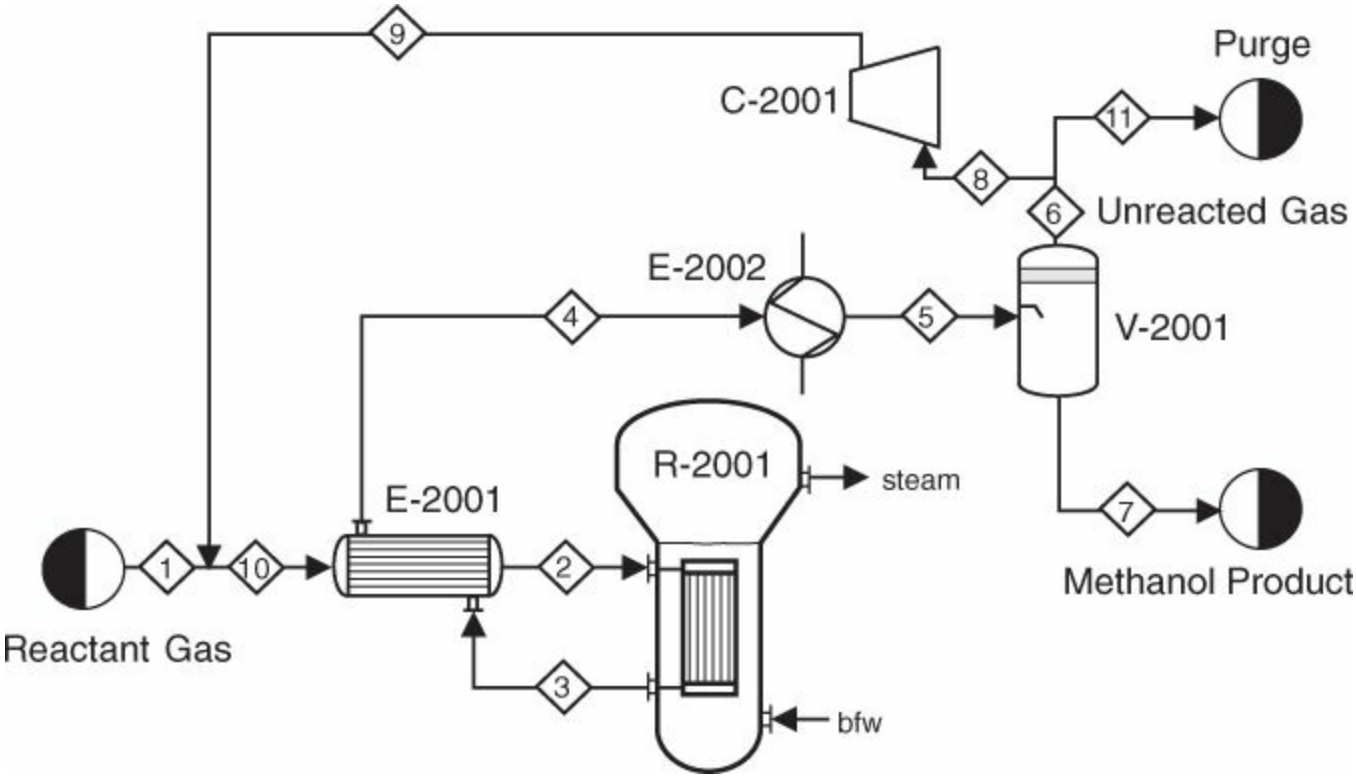


Figure p16.15. Flowsheet of the Methanol Production Unit by Considering the Recycle of the Unreacted Reactants

where C_{CH_3OH} = \$0.42/kg methanol and F_{CH_3OH} is the hourly flowrate of methanol in Stream 7. C_{UC} = \$0.15/kWh is the cost of electricity, and P_{UC} is the hourly power consumption in C-2001. The decision variables are inlet temperature and pressure of Stream 1, dimensions of R-2001, and CO/H_2 ratio in Stream 1. Solve this optimization problem with the SM and EO approaches and compare the optimal values of the decision variables with the values that you obtained in Problems 16.13 and 16.14. Did you have to consider any additional constraints for this optimization problem? Why?

16. Experimental solubility data of H_2S in diglycolamine (DGA) have been provided by Martin et

al. [17]. The DGA solution used in their experiment had 60 wt% DGA, and the remainder was water. Equilibrium data, reported at two temperatures, 50°C and 100°C, are shown in Table P16.16.

Table 16.16. Equilibrium Data for Problem 16.16

$T = 50°C$		$T = 100°C$	
p_{H_2S} (kPa)	Moles H_2S / Moles DGA	p_{H_2S} (kPa)	Moles H_2S / Moles DGA
2.5	0.221	4.9	0.057
3.9	0.262	9.3	0.071
5.4	0.291	13.4	0.095
8.9	0.344	16.5	0.100
11.5	0.381	17.5	0.116
18.9	0.452	48.2	0.182
28.3	0.508	55.1	0.210
53.1	0.543	65.3	0.217
46.2	0.577	126.0	0.316
63.1	0.608	273.0	0.456
72.9	0.654	396.0	0.522
86.1	0.657	509.0	0.571
121.0	0.699	620.0	0.639
121.0	0.711	662.0	0.640
217.0	0.778	987.0	0.712
414.0	0.877	1460.0	0.806
679.0	0.929	1660.0	0.849
1140.0	1.001	1890.0	0.909
1480.0	1.043		
1730.0	1.052		
1490.0	1.068		
1730.0	1.091		

Estimate the binary interaction parameters, considering an EOS model, a nonelectrolyte activity-coefficient model, and an electrolyte activity-coefficient model. Compare their performances.

17. n-Methyl-2-pyrrolidone (NMP) is a physical solvent that is widely used for acid-gas removal. For improving the accuracy of the VLE calculation using an activity-coefficient model, it is desired that the parameters of the vapor-pressure model be estimated first.

    a. Assume that the Antoine equation will be used for calculating the vapor pressure. Using the vapor-pressure data [18, 19, 20] in Table P16.17(a), estimate the parameters of the Antoine equation.

Table P16.17(a). Vapor-Pressure Data for Problem 16.17(a)

T(°C)	P^*(kPa)	T(°C)	P^*(kPa)
25.00	0.046	170.05	41.475
40.00	0.133	177.77	51.630
63.73	0.517	184.54	62.166
75.59	1.024	190.34	72.425
94.03	2.595	195.60	82.826
109.80	5.160	200.26	93.043
127.59	10.329	202.09	97.304
147.56	20.701	204.21	102.432
160.31	31.022		

b. Solubility data of CO_2 in NMP at 25°C, 50°C, and 100°C [21] are shown in Table P16.17(b). Estimate the binary interaction parameters, considering an EOS model and an activity-coefficient model using the Antoine parameters estimated before. Compare the results from these models with the results from the corresponding EOS and activity-coefficient models with default parameters from the simulator databank, if these parameters are available in the simulator you are using.

Table P16.17(b). Vapor-Pressure Data for Problem 16.17(b)

T = 25°C		T = 50°C		T = 100°C	
p_{CO_2}(kPa)	x_{CO_2}	p_{CO_2}(kPa)	x_{CO_2}	p_{CO_2}(kPa)	x_{CO_2}
184.8	0.0289	204.1	0.0206	251.3	0.0105
395.7	0.0611	419.0	0.0412	522.8	0.0240
641.5	0.0948	639.3	0.0615	883.0	0.0410
859.5	0.1272	862.4	0.0841	1183.3	0.0562
1145.4	0.1675	1084.1	0.1071	1438.5	0.0700
1407.8	0.2048	1421.0	0.1439		

Chapter 17. Using Dynamic Simulators in Process Design

What You Will Learn

- Dynamic simulation has a number of uses and is an important tool for both design and simulation purposes.
- Setting up a dynamic simulation may require significant changes to a steady-state simulation.
- Solver algorithms should be carefully chosen.
- Control system design plays a key role in obtaining a stable dynamic simulation.

In Chapters 13 and 16, various aspects of steady-state simulation were discussed. In this chapter, various aspects of dynamic simulation, ranging from its development to its utility in process design, will be discussed. As the steady-state design of a process forms the basis for its dynamic simulation, it is desired that the reader be conversant with Chapters 13 and 16 before proceeding with this chapter. In this chapter and elsewhere in the book, matrices/vectors are denoted by boldface, italicized letters, for example, $\boldsymbol{A}$ and $\boldsymbol{x}$. To aid the discussion presented in this chapter, some terms need to be defined:

Input variables or simply **inputs:** These are the variables that can affect the process independently. These variables can change externally (to the process) and, as a result, affect the process. It should be noted that input variables are not necessarily related to the inlet streams. Input variables that can be manipulated are called manipulated variables (MVs). Input variables that cannot be manipulated are called disturbance variables (DVs).

State variables: These are the minimum set of variables that can completely describe the internal condition of a system.

Output variables or simply **outputs:** These are the variables that depend upon the internal condition of a process. The output variables are the process response to the input variables. The latter can be considered as the cause for the changes in the process.

A steady-state simulation reveals important information about the steady-state operating conditions of a process, but it does not provide any information about the trajectory that the process takes in moving from one steady state to another one. Consider, for example, that an exothermic reaction is taking place in a catalytic reactor. At steady state, the reactor outlet temperature is at T_0 as shown in Figure 17.1. At time t_1, the feed concentration is changed such that the reactor outlet temperature reaches its new steady state T_F after some time. Note that there are an infinite number of trajectories that the temperature can take to reach its steady state. In Figure 17.1, a few trajectories are shown. In trajectory TR1, the temperature gradually reaches its new steady state. But in trajectory TR2, not only is the response oscillatory, but the overshoot in temperature may be unacceptable. It is possible that the overshoot temperature is beyond the softening temperature of the materials of construction of the reactor or above the sintering temperature of the catalyst. In trajectory TR3, there is a time delay that may be unwanted. In trajectory TR4, the temperature first goes in the reverse direction, changes direction, and then goes to the steady state. This is known as an inverse response. A single (or multiple) steady-state simulation(s) of this reactor gives no information about which trajectory the

process will take to reach T_F, if it reaches there at all. Traditionally, this information about the trajectory of a process is used for studying the transient response of a process in response to various DVs and MVs and for designing an efficient control system. However, dynamic simulations can be more effectively used by integrating them into the design phase itself to satisfy an optimal process operation in the face of disturbances, which are typical but unavoidable for any process system.

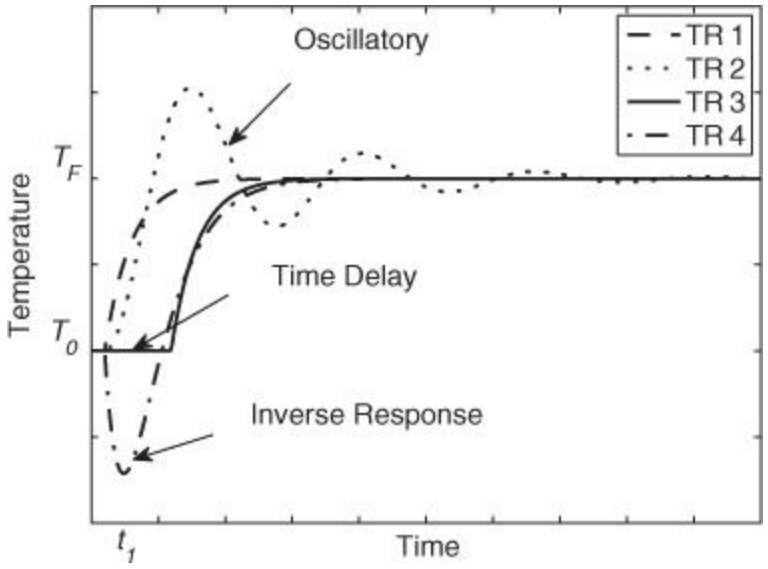


Figure 17.1. Example of Various Trajectories from T_0 to T_F

17.1. Why is there a Need for Dynamic Simulation?

Dynamic simulations can be used to accomplish one or more of the following:

- Dynamic simulations can be used to study the transient response of a process. The transient response can change due to different inputs to the system, both MVs and DVs, and uncertain and time-varying parameters. Dynamic simulations also provide information on system characteristics, such as time delay, inverse response, and oscillatory response, that not only are undesired but also pose significant operational challenges.
- One of the very important applications of a dynamic simulation is in control system design. Two types of control problems are encountered: servo control and regulatory control. In servo control, the control objective is that the output(s) should follow a desired trajectory. In the regulatory control problem, the objective is to maintain the output(s) at a desired set point by rejecting the effect of the disturbances. In both cases, the MVs are the degrees of freedom of a process that are manipulated to satisfy the desired control objective. The control system design must ensure that the constraints on state, manipulated, and output variables are not violated. An efficient control system design ensures that the plant operation is efficient, safe, satisfies environmental regulations, and results in extended equipment life and improved plant availability.
- Not all the state variables and DVs can be measured or can be measured within desired accuracy. The dynamic simulation can be used for estimating these variables. This helps in improving process monitoring and improving the performance of the control system.
- Dynamic simulation is also very useful in process performance monitoring and fault diagnosis and identification (FDI). Not only does the transient response provide valuable information that can be used in FDI algorithms, but so does the temporal evolution of the process variables.
- Dynamic modeling can be used to identify complex, multivariable interactions of dynamic

systems. This information is useful for control system design and FDI.

- Dynamic modeling also helps to identify and to show where to take appropriate action for unstable systems. These systems grow without bounds when an input variable is perturbed.
- Dynamic modeling can be used for plant start-up and shutdown simulations and can be used to develop faster start-up/shutdown procedures without damaging the plant equipment.

17.2. Setting Up a Dynamic Simulation

For a dynamic simulation, it is necessary to know the initial values of the state and input variables. One common approach to do this in the process simulator environment is to start with the steady-state simulation and use the steady-state solution as the initial condition of the dynamic simulation. However, a dynamic simulation intended for studying start-up of a plant must have the appropriate initial conditions. In the following discussion, it is assumed that an existing steady-state simulation will be modified to generate a dynamic simulation. The necessary steps will be outlined and an example given to illustrate the procedure.

17.2.1. Step 1: Topological Change in the Steady-State Simulation

Topological changes from the steady-state simulation become necessary for the following reasons:

Valid Pressure-Flow Network. The pressure drop in a unit operation with holdup, called pressure nodes, depends upon the flow into and out of the unit. In a steady-state simulator, the flow into a unit operation model is based on user input or depends upon the upstream unit, but not on the operating pressure of the unit operation block. The flow out of a unit does not depend upon the pressure of the downstream equipment. However, in the real world, the flow between units is governed by the pressure difference between them. This is an important feature of a dynamic simulation; namely, the flow into and out of the pressure nodes depends upon upstream and downstream pressures. This requires the solution of coupled, pressure-flow equations. To make the system of equations well defined, the pressure nodes are connected through flow devices (devices that possess frictional resistance). These flow devices are described by equations that relate the flow through the device to the pressure drop across it, such as

$$\dot{v} = C_o\sqrt{\frac{\Delta P}{\rho}} \qquad (17.1)$$

where C_O is the conductance, ρ is the stream bulk density, $\dot{v}$ is the volumetric flowrate, and ΔP is the pressure drop through the flow device. As an example, consider the case of turbulent flow through a pipe. Equation (20.11) can be written

$$\Delta P = -\frac{2\rho f L_{eq} u^2}{D} \Rightarrow \Delta P = -\frac{2\rho f L_{eq}\left(\frac{\pi}{4}D^2\right)^2 u^2}{\left(\frac{\pi}{4}D^2\right)^2 D} = \frac{2\rho f L_{eq}\dot{v}^2}{\frac{\pi^2}{16}D^5} \Rightarrow \dot{v} = C_o\sqrt{\frac{\Delta P}{\rho}} \qquad (17.2)$$

Therefore, for turbulent flow in a pipe, the conductance is given by

$$C_o = \frac{\pi^2 D^5}{32 f L_{eq}} \qquad (17.3)$$

For a dynamic simulation to model the pressure-flow relationship for all equipment properly, it requires two pressure nodes to be always connected through a flow device for developing a valid

pressure-flow network. Therefore, a direct connection between two pressure nodes without a connecting flow device is not allowed. This will be explained through an example.

Figure 17.2 shows a flash vessel. For simplicity, the system is considered to be isothermal. The species conservation equation can be written as

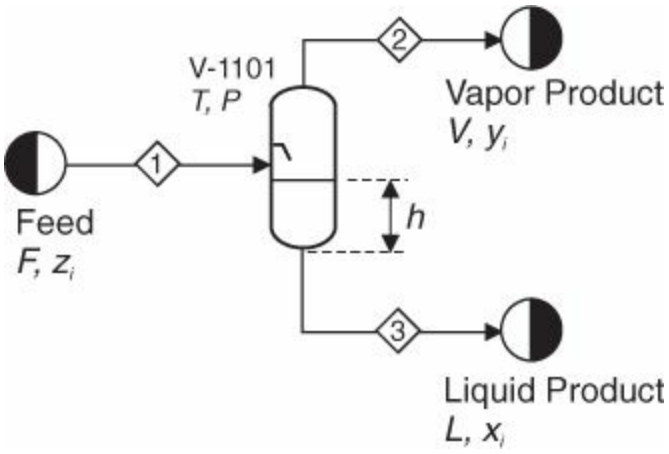


Figure 17.2. Schematic of a Flash Vessel

$$\frac{dN_i}{dt} = Fz_i - Vy_i - Lx_i \qquad (17.4)$$

where N_i is the molar holdup of species i; F, V, and L are the flowrates of the feed, vapor product, and liquid product, respectively; and z_i, y_i, and x_i are the mole fractions of species i in the feed, vapor product, and liquid product, respectively. Noting that holdup of the species occurs in both liquid and vapor phases, an expression for N_i can be developed:

$$N_i = N^v y_i + N^l x_i = V^v C^v y_i + V^l C^l x_i = A(H - h)C^v y_i + AhC^l x_i \qquad (17.5)$$

where N^v and N^l are the total molar holdups in the vapor and liquid phases, respectively; V^v and V^l are the volume of the vapor and liquid phases, respectively; C^v and C^l are the molar density of the vapor and liquid phases, respectively; A and H are the cross-sectional area and height of the vessel, V-2001, respectively; and h is the height of the liquid at time t inside the vessel. Substituting Equation (17.5) in Equation (17.4) gives

$$A\frac{d[(H - h)C^v y_i + hC^l x_i]}{dt} = Fz_i - Vy_i - Lx_i \quad i = 1 \ldots n \qquad (17.6)$$

The phase-equilibrium equations are written as

$$y_i = K_i x_i \quad i = 1 \ldots n \qquad (17.7)$$

The summation equations can be written as

$$\sum_{i=1}^{n} y_i - 1 = 0 \qquad (17.8)$$

$$\sum_{i=1}^{n} x_i - 1 = 0 \qquad (17.9)$$

Additional equations are required for calculating physical properties such as C^v, C^l, and K.

Summing up the total number of equations listed in Equations (17.6) through (17.9) for n species gives a total of $2n + 2$ equations. However, the unknown variables are n vapor mole fractions, y_i, n liquid mole fractions, x_i, molar flowrates F, V, and L, vessel pressure P, and the height of the liquid

in the vessel, h. Therefore, the total number of unknown variables is $2n + 5$. It should be noted that the variables F and h are not calculated in the steady-state simulation of the flash block because F is known, either specified by the user or obtained from the upstream block, and h is not required in the steady-state solution. Therefore, P can be calculated in a steady-state simulation by a user-specified correlation or other detailed momentum balance equation, or it can simply be a constant specified by the user. The dynamic description given previously is underdefined. To make this system square (i.e., the number of equations is equal to the number of unknowns), the flash block, which is a pressure node, must be connected via flow devices as shown in Figure 17.3.

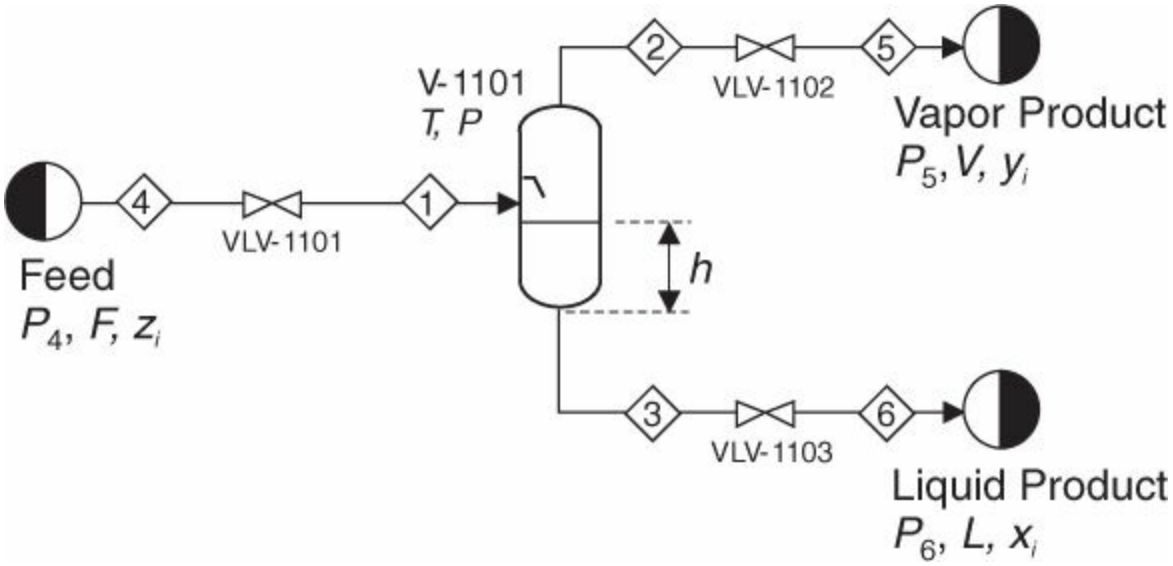


Figure 17.3. The Modified Schematic of the Flash Vessel Connected with the Flow Devices

In Figure 17.3, the flow devices are the valves, VLV-1101, VLV-1102, and VLV-1103. Assuming linear characteristics for the valves, the corresponding flow/pressure equations are

$$F = C_{o,1} VS_1 \sqrt{\frac{P_4 - P}{\rho_F}} \tag{17.10}$$

$$V = C_{o,2} VS_2 \sqrt{\frac{P - P_5}{\rho_V}} \tag{17.11}$$

$$L = C_{o,3} VS_3 \sqrt{\frac{P + \rho_L g h - P_6}{\rho_L}} \tag{17.12}$$

where F, V, and L are the feed, vapor, and liquid volumetric flowrates entering/leaving V-1101; and $C_{O,1}$, $C_{O,2}$, and $C_{O,3}$ are control-valve sizing coefficients for VLV-1101, VLV-1102, and VLV-1103, respectively. It should be noted that in the above formulation there is no pressure drop assumed across V-1101; therefore, the pressures of Streams 1, 2, and 3 (P_1, P_2, and P_3) are related by $P = P_1 = P_2$ and $P_3 = P + \rho_L g h$. The mass density of Streams 1, 2, and 3 is given by ρ_F, ρ_L, and ρ_V, respectively, and VS_1, VS_2, and VS_3 are the valve-stem positions (expressed as a fraction) of VLV-1101, VLV-1102, and VLV-1103, respectively. To make the system of equations consistent, the pressures at the system boundaries, P_4, P_5, and P_6, are considered constant. The system of equations now becomes well defined. This example shows why the pressure nodes are to be connected to the flow devices to make the system well defined. If a pressure drop in the vessel is considered, then the pressure of Stream 1 is no longer equal to P, the vessel pressure. The previous equations must be modified accordingly. An additional equation is now required to calculate the pressure drop to make the system well defined. For a nonisothermal, flash block model, the temperatures of the streams

entering and leaving the flash are additional variables, and the additional equation is the energy conservation equation.

Unsupported Blocks. Certain types of blocks can be supported in a steady-state simulation, but these blocks may not be supported in a dynamic simulation. Such blocks do not usually represent any real unit operation or may be unsupported blocks for which the dynamic model is not available. For example, a "component separator" block is supported in Aspen Plus, but not in Aspen Plus Dynamics. In a steady-state model, this block can be used to split a feed into two or more products based on user-specified composition(s). While such a composition can be obtained from the experimental or literature data at a given operating condition, it is expected to vary during the transients, and, therefore, such blocks cannot be appropriately represented in a dynamic model. In addition, there may be unsupported blocks, such as the blocks handling solids, for which the dynamic model is not yet available. The simulator manual should be consulted for this information. All unsupported blocks must be replaced by appropriate supported blocks.

17.2.2. Step 2: Equipment Geometry and Size

First-principles models are based on conservation equations. The conservation equations for a dynamic model are written as

$$\begin{aligned}\text{Rate of accumulation} = {} & \text{Rate of inputs} + \text{Rate of addition/generation} \\ & - \text{Rate of outputs} - \text{Rate of consumption}\end{aligned} \tag{17.13}$$

Note that the term on the left-hand side of Equation (17.13) does not appear in a steady-state model. This term is expressed as

$$\text{Rate of accumulation} = \frac{d[(\text{holdup volume})\ (\text{appropriate terms})]}{dt} \tag{17.14}$$

The "appropriate terms" in Equation (17.14) depend upon the conserved variable. Equation (17.14) shows that the volume information plays a key role in calculating the rate of accumulation or mass or momentum or energy. The equipment should be sized appropriately, mainly based on the steady-state results. Most steady-state process simulators provide sizing routines for the trays and packings in distillation columns. Other equipment can be sized using appropriate software, heuristics, or following this and other books in this area [1–3]. Some useful information about equipment sizing from the perspective of dynamic simulation can be found elsewhere [4].

The vessel size, the equipment geometry, and the equipment orientation can have a significant impact on the transient response of certain types of equipment. For example, the orientation of a flash vessel can be horizontal or vertical, as shown in Figures 17.4(a) and 17.4(b). For a given length L, radius r, and height of liquid h, the holdup volume of the vertical and horizontal vessels is given by (neglecting the volume of the heads)

$$V_{vertical} = \pi r^2 h \tag{17.15}$$

$$V_{horizontal} = L\left[r^2 \cos^{-1}\left(\frac{r-h}{r}\right) - (r-h)\sqrt{2rh - h^2}\right] \tag{17.16}$$

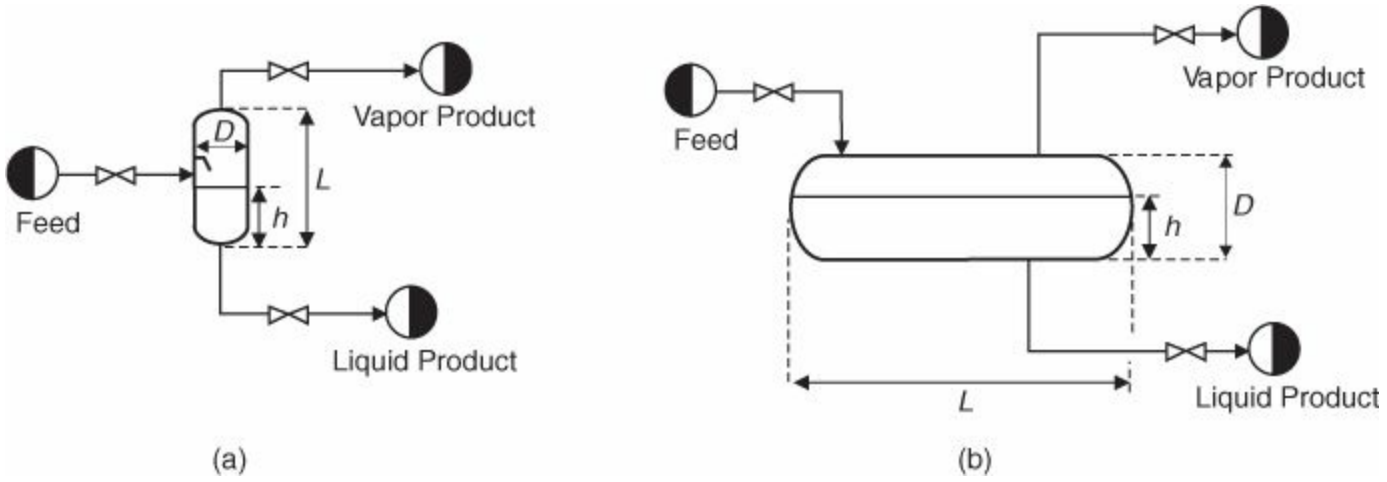


Figure 17.4. Vessels with Different Orientations: (a) Vertical Orientation (b) Horizontal Orientation

As shown by Equations (17.15) and (17.16), the holdup volumes, and therefore the transient response, can be significantly different when the liquid level heights are the same in both types of vessel. If the holdup volumes are the same in two such vessels, the height can be significantly different, which affects the pressure at the upstream of the discharge liquid control valve at a given vessel pressure.

In addition, the equipment geometry can have an effect on the transient response. For example, if the flash vessel is vertical, as in Figure 17.4(a), and the liquid level at any time is above the vessel tangent line (the hypothetical line that passes through the points of contact between the cylinder and the knuckle portion of the vessel head), the geometry of the vessel head has no effect on the rate of accumulation. However, for a horizontal vessel, the head geometry has an effect (albeit small in most cases) on the transient no matter where the level is being maintained. The geometry can have an effect on the heat loss from a vessel to the environment or on the heat transfer to or from a vessel if a heating/cooling jacket is considered. Two vessels having the same volume and the same wall thickness but different L/D ratios will have different surface areas, which affects their temperature transients. For tray distillation columns, the tray geometry, such as the diameter, spacing, weir height, downcomer dimension, and type of tray, can have a significant effect on the dynamics of holdup, and residence time, for both equilibrium- and nonequilibrium-stage models and on the overall dynamics of mass transfer for cases using nonequilibrium-stage models.

17.2.3. Step 3: Additional Dynamic Data/Dynamic Specification

The additional data/dynamic specifications required for transient simulation are equipment specific. In the following discussion, the key dynamic information for commonly occurring equipment will be presented. Before the discussion of equipment-specific dynamic data, a discussion that is applicable to most equipment is presented.

The effect of the ambient conditions, such as the temperature, pressure, and humidity, on the dynamic model depends on the type of equipment used and its fidelity. For example, the heat loss to the environment depends upon the ambient temperature. The operation of an air compressor that uses atmospheric air is highly affected by the ambient pressure, temperature, and humidity. In addition, the metal mass of a piece of equipment plays a key role in its temperature transients. The metal mass includes the mass of the entire equipment including the internals, if any. To clarify further, it can be noted that the accumulation term in the energy conservation equation is written as

$$\text{Rate of accumulation of energy} = \frac{dU}{dt} \qquad (17.17)$$

where U is the internal energy of the system. Equation (17.17) has been written neglecting the change in kinetic and potential energy. Since

$$H = U + PV \tag{17.18}$$

where H is the enthalpy, Equation (17.17) can be written as

$$\frac{dU}{dt} = \frac{dH}{dt} - P\frac{dV}{dt} - V\frac{dP}{dt} \tag{17.19}$$

The expression for H depends upon the equipment type, the number of phases within the equipment, whether their temperatures are considered to be equal, and other assumptions. Considering the example of the flash block shown in Figure 17.2, H can be calculated by

$$H = N^v M^v h^v + N^l M^l h^l + M_{eq} h_{eq} \tag{17.20}$$

In Equation (17.20), M^v and M^l are the average molecular weights of the vapor and liquid phases, respectively, and h^v and h^l are the specific enthalpy of the vapor and liquid phases, respectively. Calculation of h^v and h^l depends on the properties package used in the process simulator. M_{eq} and h_{eq} are the metal mass and the specific enthalpy of the metal, respectively. With further simplification, it can be seen that

$$\frac{dH}{dt} = \frac{d(N^v M^v h^v)}{dt} + \frac{d(N^l M^l h^l)}{dt} + M_{eq}\frac{d(C_{p,eq}T)}{dt} \tag{17.21}$$

where $C_{p,eq}$ is the equivalent heat capacity of the metal in the vessel.

Equation (17.21) shows why the metal mass plays a key role in the temperature transient. This term is usually the dominant term during start-up and shutdown of a plant and, therefore, should be considered in the models intended for simulating plant start-up and shutdown.

A representative design of the equipment and the materials of construction is needed to calculate the metal mass. This is usually done in Step 2 as part of the equipment design.

Heat Exchangers. The dynamic models for heat exchangers in process simulators are usually lumped-parameter models. In a lumped-parameter model, the process variables are assumed to vary only with time; therefore, their spatial variation is neglected. However, in a heat exchanger, the temperature of the fluids, and, therefore, the thermodynamic and transport properties, vary with position. Therefore, a rigorous heat-exchanger model should be a distributed-parameter model, where the process variables are considered to vary with space and time. Such models quickly become intractable in dynamic simulations of large process systems and are rarely used. Various simplifications are also made in the lumped-parameter models for easier solution of the equations. These points will be discussed below. In the following discussion, whenever rigorous models are mentioned, it is assumed that these refer to rigorous, lumped-parameter models and not to distributed-parameter models. In process flowsheets, both utility heaters/coolers and process heat exchangers are used.

Utility Heaters/Coolers. For heaters/coolers, where a utility is used for heating/cooling a process stream, a temperature or heat duty is provided in the steady-state model. A simple lumped-parameter, dynamic model of a utility heater/cooler can be written as

$$\frac{d(\rho C_p V T_{out})}{dt} = \dot{m} C_p (T_{in} - T_{out}) + \dot{Q} \qquad (17.22)$$

Where ρ, V, T_{in}, T_{out}, and $\dot{m}$ represent density, volume, inlet temperature, outlet temperature, and mass flowrate of the process fluid, respectively. $\dot{Q}$ is the heat transfer rate. The dynamic heater/cooler models vary depending on how $\dot{Q}$ is calculated. The appropriate option for calculating $\dot{Q}$ should depend upon the actual process configuration. Even though the number of possible options varies with the process simulator of choice, four common options will be discussed here. The first option, called the "constant duty" option here, is the simplest case, where the heat duty can be an input variable that can be used as an MV in the dynamic simulation for maintaining the temperature. This option is suitable for processes where a heating fluid (such as steam) or a cooling fluid (refrigerant) is being used such that the process temperature is far from the heating/cooling-medium temperature, and it is not expected that the system will ever reach the minimum temperature approach. The underlying assumption of this option is that the dynamics in the heating/cooling medium are very fast and, therefore, can be neglected. With this option, if a temperature controller is not considered and the process-stream flowrate, specific heat, or inlet temperature drastically changes in comparison to its steady-state design conditions, the outlet temperature can be unrealistic and the simulation may fail to converge. In the second option, called the "constant medium temperature" option here, the heat transfer is calculated based on the difference in the temperature of the process stream and the heating/cooling medium. Simply put,

$$\dot{Q} = U_h A (T_{out} - T_m) \qquad (17.23)$$

where T_m is the temperature of the heating/cooling medium. This option is appropriate when the change in the heating/cooling-medium temperature along the length of the separator/vessel is negligible, and its flowrate is kept constant in the dynamic simulation. The first two options do not take into account the cooling/heating-medium flowrate and the change in the utility temperature due to heat exchange. Therefore, they cannot be used in dynamic simulations where the flowrate of the medium varies (i.e., it is a DV or an MV) and/or the utility flow must be accounted for. Therefore, in the third option, called the "LMTD" option here, the effect of the flowrate of the medium and its temperature change due to heat exchange are considered. The equation for $\dot{Q}$ is

$$\dot{Q} = U_h A \Delta T_{lm} \qquad (17.24)$$

Neglecting the temperature dynamics of the medium,

$$\dot{Q} = \dot{m}_m C_{p,m} (T_{m,out} - T_{m,in}) \qquad (17.25)$$

Where $\dot{m}_m$, $C_{p,m}$, $T_{m,out}$, and $T_{m,in}$ are the flowrate, specific heat, and inlet and outlet temperatures of the medium, respectively. In this option, the holdup of the medium is not considered.

If the heat duty is provided by evaporating/condensing a medium, then the option (fourth option) is to model the heat duty by

$$\dot{Q} = \dot{m}_m \lambda \qquad (17.26)$$

where λ is the specific latent heat of the evaporating/condensing medium.

Example 17.1 demonstrates how the option chosen for a cooler affects its transient response and the final steady-state temperature.

Example 17.1.

Steam is being condensed in a surface condenser of a steam turbine under vacuum using cooling water. The flowrate of the steam to the condenser is 50 kmol/h at a temperature and pressure of 55°C and 0.12 bar, respectively. The pressure drop in the condenser is 0.02 bar. At the outlet of the condenser, the steam is completely condensed without any subcooling. Cooling water is available at a temperature and pressure of 25°C and 5 bar, respectively. Design the cooler such that the cooling water temperature at the condenser outlet is 35°C. The maximum allowable pressure drop of the cooling water is 0.5 bar. Develop three dynamic models of this condenser using the "constant duty" option, the "constant medium temperature" option, and the "LMTD" option. Compare the transient response of the process outlet temperature for each of the options when the flowrate of the steam is step decreased to 45.5 kmol/h.

Solution

The problem is set up in Aspen Engineering Suite (AES) using Aspen Plus V7.2, Aspen Plus Dynamics V7.2, and Exchanger Design and Rating (EDR) V7.2. In Aspen Plus, the heater/cooler volume can be provided under "dynamic options." The volume can be distributed between inlet and outlet volumes. In addition, the quantity of the metal mass can be provided. Considering that the steam is in the shell side, the shell volume and the shell mass are calculated using Aspen EDR. In Aspen EDR, the design objective for optimization is considered to be minimization of cost. The default design options for shell-and-tube heat exchangers in EDR are used. The designed heat exchanger has one shell of diameter 0.337 m, tube OD of 0.019 m, tube ID of 0.015 m, tube length of 2.44 m, 117 tubes, and a shell weight (including the heads) of 392 kg. The material of construction is carbon steel. As mentioned before, the shell- and tube-side volumes can be provided under "dynamic options" in Aspen Plus, with options for providing separate inlet and outlet volumes. In this simulation, the shell-side and tube-side volumes are calculated from the heat-exchanger design mentioned above and then divided into two equal volumes for the inlet and outlet volumes. A similar approach is taken for the metal mass. Three condenser models are considered in Aspen Plus, all with the same steady-state specifications, but the dynamic specifications are as per the problem statement. The converged Aspen Plus simulation is exported to Aspen Plus Dynamics, and after running the dynamic simulation for about 0.08 h, the flowrate of steam is decreased from 50 kmol/h to 45.5 kmol/h. No controller is implemented; that is, neither the heat duty, the medium temperature, nor the medium flowrate is changed. The transient response of the process stream at the outlet of the condensers is shown in Figure E17.1. The temperature at the outlet of the condenser with the "constant duty" option reaches a negative value. Even with this severe temperature cross, the simulation continues without any warning. When the steam flowrate is decreased, it would be expected that the cooling water outlet temperature would decrease. Thus, the condenser with the "LMTD" option shows a lower condenser outlet temperature than the condenser with "constant medium temperature" option, that is, a few degrees of subcooling. The temperature response of the exchanger with the "LMTD" option is as expected. This example demonstrates that the user needs to be careful about the choice of the heat-exchanger blocks to avoid unrealistic results from a dynamic simulation.

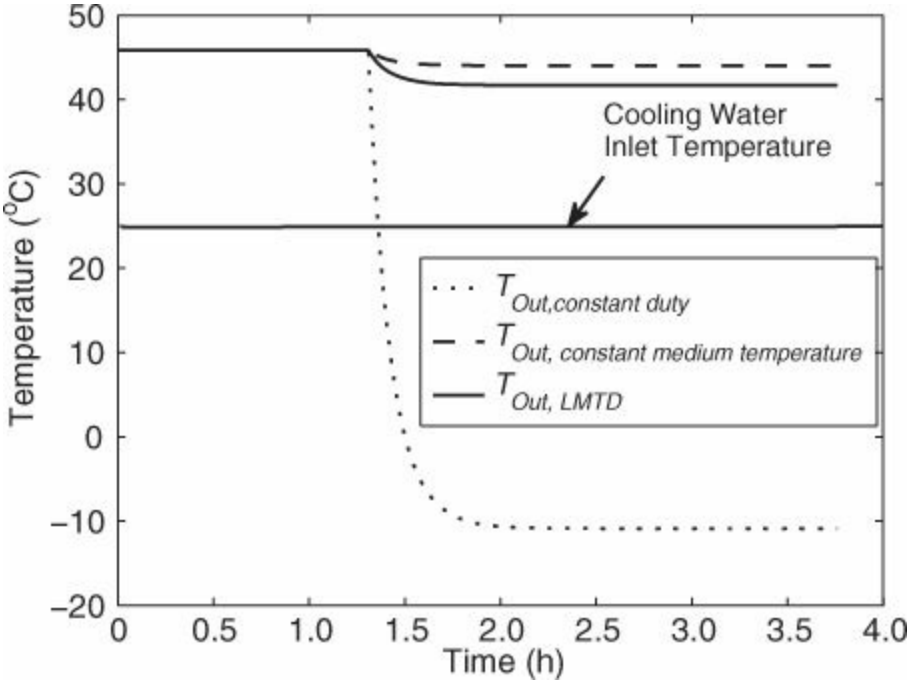


Figure E17.1. Transient Response of the Condenser Outlet Temperature with "Constant Duty" Option, "Constant Medium Temperature" Option, and "LMTD" Option

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Process Heat Exchanger. For simulating process heat exchangers, two options will be considered. In the first, which will be called the "simple" option, the process heat exchangers will be simulated simply by combining a heater with a cooler and equating their heat duties, as shown in Figure 17.5(a). This option is widely used in steady-state simulation. In a steady-state simulation, the outlet temperature of E-1101A/E-1101B or its heat duty can be specified, ensuring that the minimum temperature approach is not violated. However, if the flowrates and/or the temperatures of the hot and cold streams vary in the dynamic simulation, there can be a temperature cross. Even though this is physically impossible, the simulation may not report this error and continue. This can result in completely unrealistic transient response and steady-state results as seen in Example E17.2. The second option is to consider a heat exchanger as shown in Figure 17.5(b). This will be called a "rigorous exchanger," in the sense that this option is a rigorous lumped-heat-exchanger model with appropriate methods for calculating heat transfer coefficients.

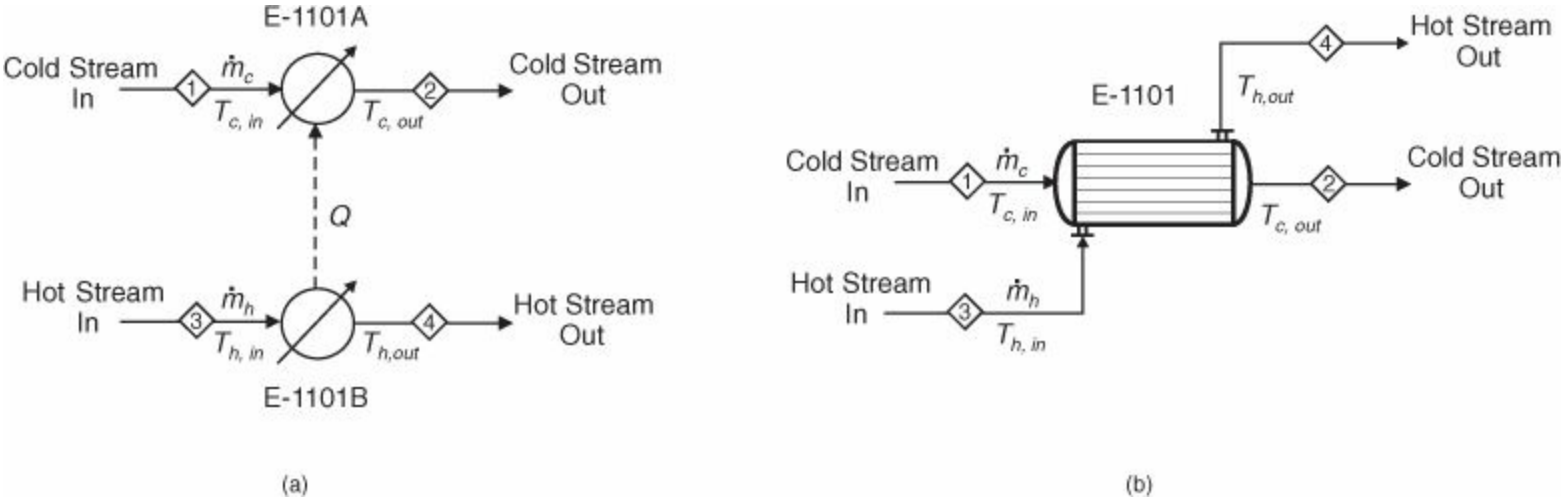


Figure 17.5. Configurations of Process Heat Exchangers: (a) Simple Configuration; (b) Rigorous Configuration

A simple model of a rigorous heat exchanger can be written as

$$\frac{d(\rho_c C_{p,c} V_c T_{c,out})}{dt} = \dot{m}_c C_{p,c}(T_{c,in} - T_{c,out}) + \dot{Q} \quad (17.27)$$

$$\frac{d(\rho_h C_{p,h} V_h T_{h,out})}{dt} = \dot{m}_h C_{p,h}(T_{h,in} - T_{h,out}) - \dot{Q} \quad (17.28)$$

$$\dot{Q} = UA\Delta T_{lm} \quad (17.29)$$

In the process-heat-exchanger and utility heater/cooler models, the effect of the metal mass can also be considered. As mentioned before, such considerations play a key role in the transient response of the models intended for simulating plant start-up/shutdown. Based on the expected skin temperature of a heat exchanger, it may be important to consider the heat loss to the environment.

Example 17.2 shows that a simple process heat exchanger can give unrealistic results under certain process conditions. In this and other examples in this chapter, the specifications shown in the flowsheet are the steady-state values.

Example 17.2.

Develop two dynamic models of the process heat exchanger shown in Figures E17.2(a)(a) and E17.2(a)(b), one with the simple option and another with the rigorous option. In this process heat exchanger, at the design condition, Stream 1, a mixture of methane and ethane, is to be heated to 200°C by a hot stream of ethane. Initially the process is at steady state. Then the flowrate of Stream 1 is decreased by a step change to 45 kmol/h. Show the transient response of the outlet temperatures of the hot and cold streams from both the heat-exchanger models. Assume heat loss to the environment to be negligible.

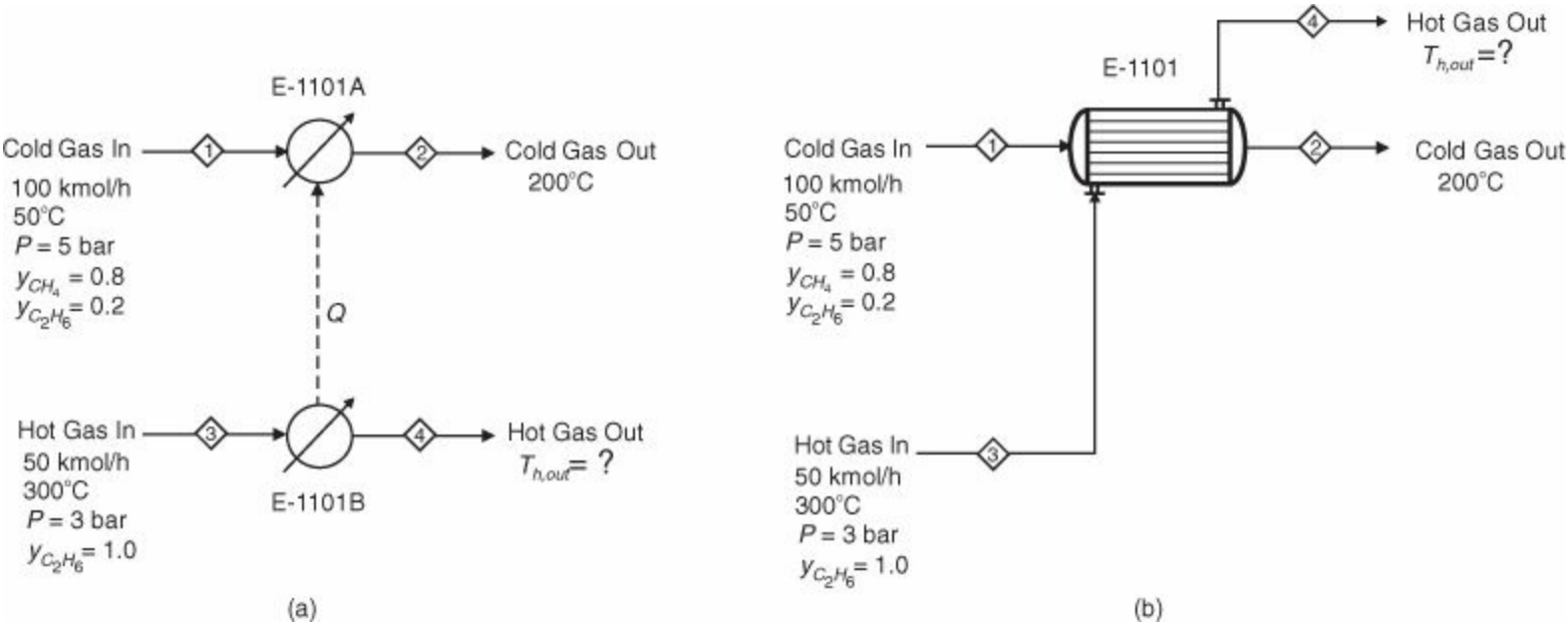


Figure E17.2(a). (a) Simple Configuration of a Heat Exchanger; (b) Rigorous Configuration of a Heat Exchanger

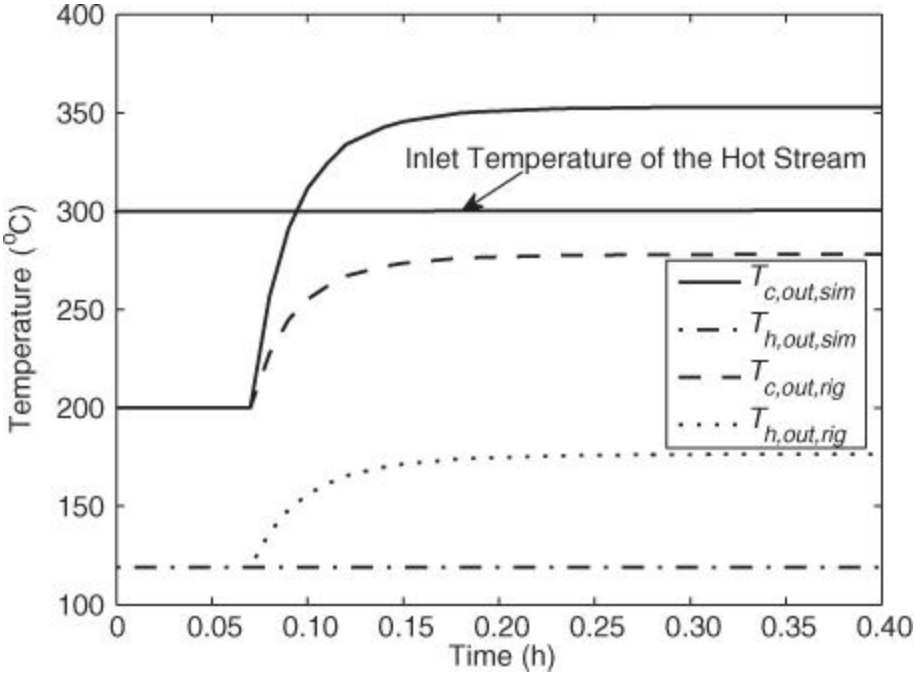


Figure E17.2(b). Transient Response of the Hot and Cold Stream Temperatures for the Simple Heat-Exchanger Configuration and the Rigorous Heat-Exchanger Configuration

Solution

The problem is set up in Aspen Engineering Suite (AES) using Aspen Plus V7.2, Aspen Plus Dynamics V7.2, and Exchanger Design and Rating (EDR) V7.2. In Aspen Plus, the shell- and tube-side volumes of both heat-exchanger models are provided. The volumes are equally distributed between the inlet and outlet volumes. In addition, the quantity of metal mass is provided. For calculating the shell-side and tube-side volumes and the metal mass, Aspen Exchanger Design and Rating V7.2 is used. In this design of a floating-head, shell-and-tube heat exchanger, the hot fluid is located on the shell side. Predictive SRK (PSRK in Aspen Properties) EOS is used for designing the exchanger in EDR and for simulating it in Aspen Plus and Aspen Plus Dynamics. The design objective for the heat-exchanger design is to minimize the cost. The default design options for shell-and-tube heat exchangers in EDR are used. The designed heat exchanger has one shell of diameter 0.205 m, a tube OD of 0.019 m, a tube ID of 0.015 m, a tube length of 4.877 m, 40 tubes, a shell weight (including the heads) of 356 kg, and a tube-bundle weight of 205 kg. The material of construction for both the shell and tubes is carbon steel. For the simple heat exchanger, the pressure drops on both the shell and tube sides are assumed to be 0.1 psi. For the rigorous heat exchanger, the EDR file is inserted in the heat-exchanger specification sheet. The converged Aspen Plus simulation is then exported to Aspen Plus Dynamics, and after running the dynamic simulation for about 0.08 h, the flowrate of Stream 1 is decreased from 100 kmol/h to 45 kmol/h. The transient response of the hot and cold streams at the outlet of the heat exchangers is shown in Figure E17.2(b). The hot stream temperature in the simple configuration does not change at all, since the heat-exchanger duty remains the same and the inlet condition of the hot stream does not change. There is a temperature cross in the cold stream outlet temperature, because it exceeds 300°C, the inlet temperature of the hot stream. However, the simulation continues without any warning. The temperature response of the rigorous exchanger is as expected. It should be noted that in Aspen Plus Dynamics, the response of the simple exchanger can be made similar to that of the rigorous exchanger by writing "scripts."

Flash Separators and Storage Vessels. Equations (17.6) through (17.9) describe the dynamic model

of a flash vessel. For a storage vessel, a single phase is considered; thus, Equations (17.6) through (17.9) can be modified accordingly. As mentioned previously, the geometry/size information should be provided for the flash separators and storage vessel. In the case of a nonisothermal model, an energy balance equation is also needed. The energy balance equation is written as

$$\frac{dU}{dt} = Fh_{in} - Vh^{v} - Lh^{l} + \dot{Q}_{in} - \dot{Q}_{loss} \qquad (17.30)$$

where h_{in}, h^{v}, and h^{l} are the molar enthalpies of the feed stream, vapor outlet, and liquid outlet, respectively. $\dot{Q}_{in}$ is the rate of heat transfer to the vessel and is considered to be nonzero for a vessel with a heating or cooling jacket. $\dot{Q}_{loss}$ is the rate of heat loss to the environment and can be considered to be zero for a well-insulated vessel and/or when the vessel temperature is close to the temperature of the environment. For the left-hand term of Equation (17.30), appropriate forms of Equations (17.19) and (17.21) are used. For calculating $\dot{Q}_{in}$ in the dynamic simulation, the options are similar to what has been discussed in the section on utility heaters/coolers. Any of the four options discussed there can be used with the most appropriate option chosen for the situation under consideration. The heat transfer option, whenever applicable, plays a key role in the transient response of the temperature. Example 17.3 shows how the heat transfer option affects not only the temperature of the system but also other state variables.

Example 17.3.

Figure E17.3(a) shows the schematic of a jacketed flash vessel in which a mixture of CO_2 and methanol is being separated. The inlet temperature of the heating medium stream is 90°C and its specific heat is similar to that of water. There is no phase change of the heating medium in the jacket. Compare the transient response of the flash vessel outlet temperature and its level for the "constant duty" and "LMTD" options when the inlet feed flowrate is reduced to 10 kmol/h. Assume no change in the inlet temperature and flowrate of the heating medium. The vessel is well insulated; that is, heat loss to the environment may be assumed to be negligible.

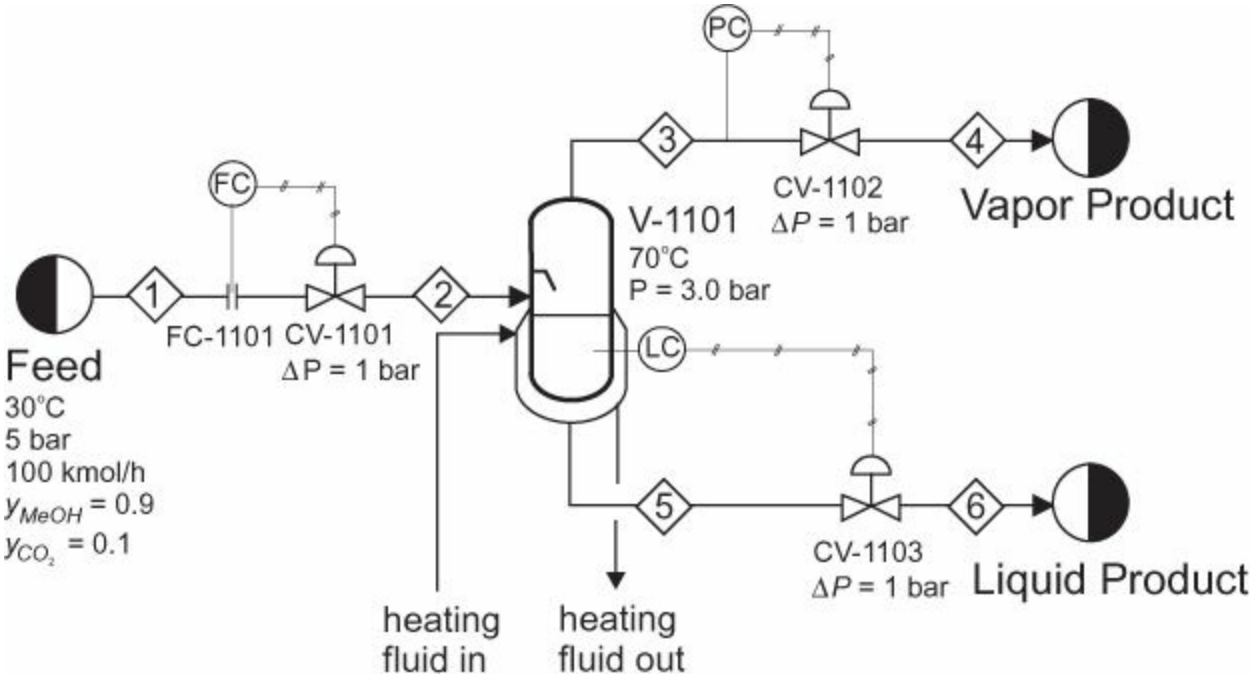


Figure E17.3(a). Configuration of the Jacketed Flash Vessel for Separating CO_2 and Methanol

Solution

The problem is set up in Aspen Engineering Suite (AES) using Aspen Plus V7.2 and Aspen Plus Dynamics V7.2. The Aspen Plus V7.2 simulation is developed by modifying one of the examples for methanol absorbers available in the example flowsheet under Program Files\AspenTech\Aspen Plus V7.2\GUI\App\Physical solvents. For users simulating it in other platforms, it should be noted that the perturbed-chain statistical associating fluid theory (PC-SAFT) EOS is used. In this model, the thermophysical property models have been validated against DIPPR correlations for species vapor pressure and liquid density and against literature data for liquid heat capacity, heat of vaporization, and VLE. The vessel size is calculated considering both liquid holdup and vapor velocity following the heuristics laid out in Table 11.6. Holdup time is considered to be 5 min for the half-full flash vessel. For calculating the gas velocity, the flash vessel is considered to have a mesh demister. It is assumed that $L/D = 3$. The values of length and diameter are found to be $L = 1.92$ m and $D = 0.64$ m. The thickness of the wall is found using carbon steel as the material of construction and by applying the following equation:

$$t = \frac{PD}{2SE - 1.2P} + CA$$

where P is the design pressure of the vessel (in bar), D is the diameter of the vessel (m), S is the maximum allowable stress (940 bar for carbon steel), $E = 0.9$, and CA = corrosion allowance (assumed to be 0.00315 m here). Accordingly, the metal mass of the vessel is calculated. Two models of the flash vessel, one with the "constant duty" option and the other with the "LMTD" option, are set up in Aspen Plus. The simulation is exported to Aspen Plus Dynamics as a pressure-driven simulation. The pressure and the level of the vessel are maintained by PI controllers. The feed flow is decreased to 10 kmol/h. The corresponding transient response of the temperature is shown in Figure E17.3(b)(b). The temperature of the flash vessel with the "LMTD" option does not change appreciably. The initial increase in the temperature of the flash vessel with the "constant heat duty" option is slightly higher than the heat exchanger with the "LMTD" option. However, it is seen in Figure E17.3(b) that the level in the vessel with the "constant duty" option starts decreasing even with the liquid outlet valve completely closed. This is because the rate of vapor flow out is larger than the feed flowrate. Eventually, as the vessel becomes completely empty, the temperature steeply increases, as seen in Figure E17.3(b)(a). Note that the level of the flash vessel using the "LMTD" option is maintained at near its steady-state value after some negligible transient due to the steep change in feed flow. The reader is encouraged to verify that as the feed valve is completely closed, the temperature of the flash vessel with the "constant duty" option steeply increases to the maximum temperature allowed by the simulator (which is 1995°C in Aspen Plus Dynamics, by default). This example demonstrates that it is important to model the heat transfer option appropriately for jacketed flash vessels to obtain a representative transient response.

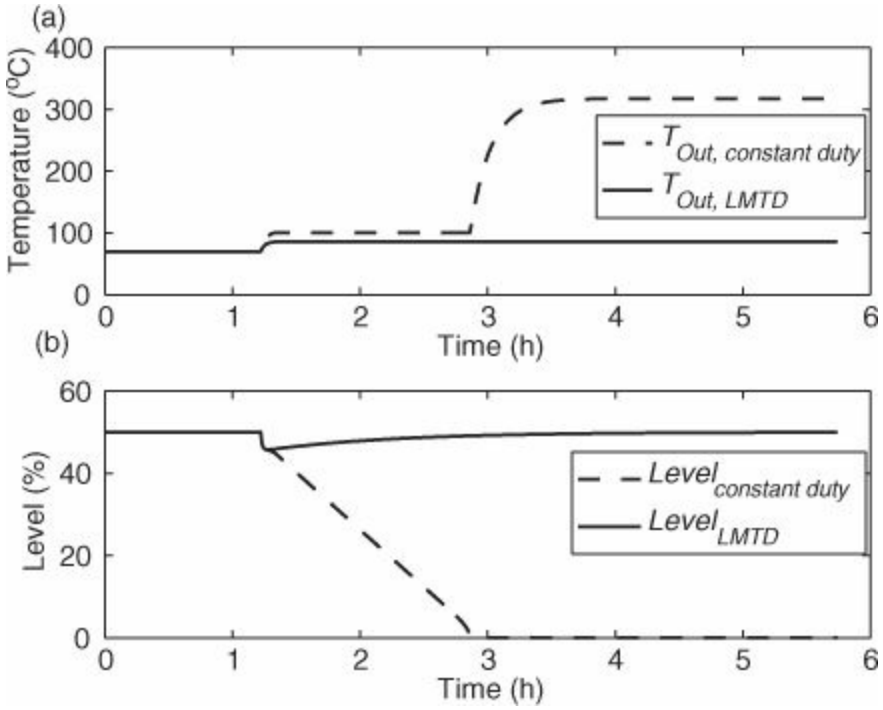


Figure E17.3(b). Transient Response of the Jacketed Flash Vessels with "Constant Duty" Option and "LMTD" Option: (a) Temperature Transient; (b) Level of the Flash Vessel

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Reactors. A number of excellent references discuss dynamic models for nonisothermal CSTR and PFR reactors [5, 6]. Interested readers should review the discussions provided in these books. In a process simulator environment, the user needs to provide the reactor orientation (note that this option matters only when a level is maintained or if the effect of gravity is considered for a liquid-phase reactor) and the reactor size. The reactor size (and therefore the residence time) not only affects the steady-state results but also has a significant effect on the transient response of the product composition and temperature. For dynamic simulation of jacketed reactors, the heat transfer options are similar to those discussed previously for utility heaters/coolers. The heat transfer option can strongly affect the transient response of the reactor. For packed-bed reactors, the catalyst temperature and its dynamics can be different from those of the process stream, especially when the heat transfer coefficient is low. To model such reactors, separate energy conservation equations for the process stream and the catalyst are considered in a process simulator. The model equations for a dynamic PFR consist of partial differential equations (PDEs). As the process simulators usually consider a one-dimensional model of a PFR, the steady-state model can be solved by an efficient ordinary differential equation (ODE) solver. For dynamic simulation, the usual approaches are as follows.

Method of Lines. In this method, the PDEs are discretized in the spatial dimension, leaving the time variable continuous, generating a system of ODEs. Coupled with the algebraic equations, this generates a system of differential algebraic equations (DAEs). The spatial discretization can be performed by several methods, such as finite-difference methods (backward or central finite difference), orthogonal polynomials (collocation methods), and others. The key point to note here is that the dynamic simulation can be initialized based on the steady-state results. However, there can be large errors (which may eventually lead to convergence failure) due to an insufficient number of grid points if there is a large change in the species concentration or temperature. If the number of grid points increases, so does the number of equations. Therefore, there is an optimum grid size that balances desired computational accuracy versus computation expense. A reasonable grid size for a

particular system is often established by a grid sensitivity study.

Series of CSTRs. A PFR can be replaced by a series of CSTRs. In this technique, the state variables again are initialized based on the steady-state results. Similar to the method of lines, the suitable number of CSTRs to replace a single PFR depends upon the system of interest and has to be determined on a case-by-case basis.

Distillation Columns. A number of excellent books are available that discuss the dynamic models and control of distillation columns [7, 8, 9]. The condenser of a distillation column is a special type of cooler in which phase change takes place. Therefore, the previous heat transfer options for utility heaters/coolers are applicable. The reflux drum in a distillation column with a partial condenser is similar to a flash vessel, and the discussions provided before are also applicable. The discussion of utility heaters is applicable to kettle- or thermosiphon-type reboilers. In the case of forced-circulation reboilers or fired heaters used as reboilers, pumps are usually used. Therefore, additional equations/unit operations will be required to capture the flow dynamics along with the appropriate heat transfer option. In the case of fired heaters, especially when they are large, a simple heater model is not representative. In large fired heaters, both radiative and convective heat transfer usually play a key role based on the spatial location. In addition, the dynamics of the fuel-oil/fuel-gas stream and the oxidant stream may have a large impact on the dynamics of the process streams. Therefore, appropriate process models should be chosen for these unit operations. The column sump and reflux drum volumes should be calculated mainly based on holdup requirements. For tray columns, the tray hydraulics should also be considered. A particular tray model is similar to a flash vessel. Therefore, the liquid and vapor holdup on a tray and the pressure drop (if important) should be modeled precisely. For these calculations, the tray type, spacing, configuration (single/double pass, etc.), the tower diameter, the weir height, the open area, downcomer details, and other characteristic parameters based on a type of tray should be specified. For packed columns, the packing type and packing void fraction, specific surface area, height of packing in a section, packing diameter, and other characteristic parameters based on packing type should be specified. Most steady-state process simulators offer sizing routines, and, therefore, these can be used to generate this information. In addition, the metal mass of the reflux vessel, the sump, all stages, and the column shell may be important, especially when a large variation in operating temperature is expected or for dynamic models intended for studying start-up/shutdown. In addition, heat loss to the environment can be modeled.

17.3. Dynamic Simulation Solution Methods

A dynamic model involves the solution of a system of DAEs. The differential equations relate the state variables to other state variables and the manipulated variables. The algebraic equations relate the output variables to the state variables and represent the constitutive relations, properties calculations, and any other closure equations. In addition, the algebraic equations relate the output variables to the state variables. Mathematically,

$$\frac{d\boldsymbol{x}}{dt} = \boldsymbol{f}(\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{u}, \boldsymbol{d}, \boldsymbol{\theta}) \qquad (17.31)$$

$$\boldsymbol{h}(\boldsymbol{x}, \boldsymbol{\theta}, \boldsymbol{y}) = 0 \qquad (17.32)$$

where $\boldsymbol{x}$, $\boldsymbol{u}$, $\boldsymbol{d}$, $\boldsymbol{\theta}$, and $\boldsymbol{y}$ denote state variables, manipulated inputs, disturbance inputs, parameter vector, and algebraic variables, respectively.

The index of a DAE system is defined as the minimum number of times the function $\boldsymbol{h}(\boldsymbol{x}, \boldsymbol{\theta}, \boldsymbol{y})$ must be differentiated to result in a DAE system. For problems that are of index higher than one, $\frac{\partial \boldsymbol{h}}{\partial \boldsymbol{y}}$ is singular, and consistent initial conditions must be specified. Most commercial process simulators handle only index-one problems, and, therefore, the discussion that follows pertains only to these types of problems. It should be noted that the stability of any numerical method can be markedly different in the case of higher-index problems, and certain sections of the following discussion are not applicable to problems of higher index. Solving a dynamic simulation involves two steps, namely, initialization and the solution of the DAE system. In the following paragraphs, these steps will be discussed in detail.

17.3.1. Initialization

Process simulators solve first-order ODEs as shown in Equation (17.31). In the initialization step, a consistent set of initial values is calculated by using Equations (17.31) and (17.32). If there are s state variables and w algebraic variables, then a total of $s + w$ equations is available. However, in the initialization steps, the unknowns are s number of $x(0)$, s number of $\frac{dx}{dt}|_{t=0}$, and w number of $y(0)$. Therefore, s number of variables among $2s$ unknown state variables and their derivatives should be specified. The variables that should be specified depend upon the problem being solved. When the initial state is steady state, then $\frac{dx}{dt}|_{t=0} = 0$. However, if the initial state is a cold start-up or shutdown of the system, or if the system is not at steady state, all or some of the initial values of $x(0)$ need to be specified. Additionally, some $\frac{dx}{dt}|_{t=0}$ values should be specified, if necessary, for making the system square. It should be noted that depending upon the values of the input and disturbance variables, steady-state solutions will vary.

17.3.2. Solution of the DAE System

As seen previously, it may be possible to convert the system of DAEs shown in Equation (17.31) to a system of ODEs by differentiating the algebraic equations and manipulating them. However, this procedure can be very tedious for many systems and is not always guaranteed to produce a system of ODEs in explicit form. Therefore, the popular approach is to carry out numerical integration of the differential equations in Equation (17.31) and then solve them along with the algebraic equations. Therefore, a linear/nonlinear algebraic system of equations is finally solved. However, the process dynamic simulators vary based on how the DAEs are solved. These are broadly divided into two methods: namely, modular and simultaneous.

Modular. The modular method is similar to the sequential modular (SM) method discussed in Chapter 16 for steady-state simulation. The idea is to solve the dynamic model of individual equipment separately and then iterate until a converged solution is reached. However, as discussed in Section 17.2.1, the flow into and out of a unit operation depends upon the upstream and downstream pressures of the corresponding blocks in a dynamic simulation. This necessitates an iterative approach even in the absence of a recycle. In the presence of recycle, tear streams are generated similar to the SM method. However, the initial guess for temporal variations of the tear stream is needed. This usually makes it much more computationally expensive, especially for large simulations and if a large number of recycles are present. The advantages are in using an efficient solution

approach for specific unit operations instead of using a general-purpose equation solver and easier troubleshooting in the case of convergence failure.

Simultaneous. In this method, all the equations for all the blocks are collected together and solved simultaneously. The simultaneous method again can take two different approaches. In one approach, a separate pressure-flow solver is used to solve only the pressure-flow network equations, while other equations can be solved at a different time interval (frequency). This approach has two advantages. First, an efficient solution approach for specific unit operations can be used. Second, time-consuming calculations such as flash calculations can be carried out at different frequencies. Another approach is to solve all the equations simultaneously, including the pressure-flow equations. This approach guarantees stability and accuracy of solution as long as an appropriate solver is chosen. These concepts will be made clear in the following discussions.

For solving the differential equations, an efficient integrator algorithm is required. As the integrator algorithm generates a set of linear/nonlinear equations, an efficient algebraic equation solver is also required for solving the coupled equations. A brief account of the integrator and linear/nonlinear algebraic equation solver algorithms will now be provided.

Dynamic Simulation Integrator Algorithms. Before further discussion of integrator algorithms, the definition of a stiff problem will be provided. Considering Equation (17.31). If $\boldsymbol{J} = \dfrac{\partial f}{\partial x}$ and the matrix $\boldsymbol{J}$ has eigenvalues λ_i for which $max|\lambda_i| >> min|\lambda_i|$, then the system is called stiff. Stiff problems are more difficult to solve and need special consideration when applying numerical methods. These points are discussed below.

Various numerical integration methods are usually taught as part of a numerical methods course. Therefore, only the salient points that are important from the point of view of dynamic simulation of a process model will be covered here.

Explicit Methods. In explicit methods, state variables at any time instant $\boldsymbol{n}+1$ are explicitly written in terms of the variables at the previous instant, that is, at time $\boldsymbol{n}$. For Equation (17.31), this takes the form

$$\boldsymbol{x}_{n+1} = \boldsymbol{g}(\boldsymbol{x}_n, \boldsymbol{y}_n, \boldsymbol{u}_n, \boldsymbol{d}_n, \boldsymbol{\theta}) \qquad (17.33)$$

This approach can be very advantageous for a system of ODEs, since the solution of a system of nonlinear equations is avoided. However, in the case of a DAE system, which usually is the case for a process simulation, a nonlinear system of equations still needs to be solved because of the coupled algebraic equations. The explicit Euler method is available in most dynamic simulators and will be discussed below.

Explicit Euler Method. This is probably the simplest first-order, explicit method based on a forward difference approximation of the derivative. Considering Equation (17.31), the numerical integration is written as

$$\boldsymbol{x}_{n+1} = \boldsymbol{x}_n + \Delta t_n \boldsymbol{f}(\boldsymbol{x}_n, \boldsymbol{y}_n, \boldsymbol{u}_n, \boldsymbol{d}_n, \boldsymbol{\theta}) \qquad (17.34)$$

This method is stable for a restrictive time step, beyond which it may be unstable; that is, $\boldsymbol{x}$ will eventually grow without limits and the integrator will fail to converge. The stiffer the system is, the smaller the time step must be to obtain a stable solution. On the other hand, the simulation should be run until the process with the smallest time constant has reached its new

steady state. In addition, a much smaller time step than is required for stability will make the approach computationally inefficient. This makes the Euler method difficult to use for large process simulations containing thousands of equations and where the time scales of different processes are widely different.

A few other explicit methods will also be discussed under "Multistep Methods."

Implicit Methods. In implicit methods, irrespective of whether an ODE or a DAE system is being solved, a system of algebraic equations needs to be solved. The biggest advantage of any implicit method is that it is stable for large step sizes, and some implicit algorithms are stable for any step size. However, a larger step size can cause errors in solution or convergence failure. Therefore, it makes sense to modify the step size adaptively: using a smaller step size when there is a significant change, and using a larger step size otherwise.

Implicit Euler Method. This is probably the simplest first-order implicit method based on a backward difference approximation of the derivative. Considering Equation (17.31), the numerical integration is written as

$$\boldsymbol{x}_{n+1} = \boldsymbol{x}_n + \Delta t_n \boldsymbol{f}(\boldsymbol{x}_{n+1}, \boldsymbol{y}_{n+1}, \boldsymbol{u}_{n+1}, \boldsymbol{d}_{n+1}, \boldsymbol{\theta}) \tag{17.35}$$

Trapezoidal Method. This is a very popular second-order, single-step method.

$$\boldsymbol{x}_{n+1} = \boldsymbol{x}_n + \frac{\Delta t_n}{2}(\boldsymbol{f}(\boldsymbol{x}_{n+1}, \boldsymbol{y}_{n+1}, \boldsymbol{u}_{n+1}, \boldsymbol{d}_{n+1}, \boldsymbol{\theta}) + \boldsymbol{f}(\boldsymbol{x}_n, \boldsymbol{y}_n, \boldsymbol{u}_n, \boldsymbol{d}_n, \boldsymbol{\theta})) \tag{17.36}$$

Multistep Methods. Multistep methods can be explicit or implicit. This family of methods is widely applicable for different types of process models. The generic formulation for the methods in this class is given by

$$\boldsymbol{x}_{n+1} = \sum_{i=0}^{q} a_i \boldsymbol{x}_{n-i} + \Delta t_n \sum_{j=0}^{q+1} b_j \boldsymbol{f}(\boldsymbol{x}_{n+1-j}, \boldsymbol{y}_{n+1-j}, \boldsymbol{u}_{n+1-j}, \boldsymbol{d}_{n+1-j}, \boldsymbol{\theta}) \tag{17.37}$$

Note that if b_0 is set to zero, this becomes an explicit method. Any multistep method can be used for different polynomial orders. Different multistep methods differ in how the index q varies based on the polynomial order and which coefficients are set to zero. Under this category, one of the most popular methods is Gear's method. In Gear's method,

$$q = k - 1$$

$$b_1 = b_2 = \ldots\ldots = b_k = 0 \tag{17.38}$$

A fourth-order Gear's formula is given by

$$\boldsymbol{x}_{n+1} = a_0 \boldsymbol{x}_n + a_1 \boldsymbol{x}_{n-1} + a_2 \boldsymbol{x}_{n-2} + a_3 \boldsymbol{x}_{n-3} + \Delta t_n b_0 \boldsymbol{f}(\boldsymbol{x}_{n+1}, \boldsymbol{y}_{n+1}, \boldsymbol{u}_{n+1}, \boldsymbol{d}_{n+1}, \boldsymbol{\theta}) \tag{17.39}$$

where $a_0 = \frac{48}{25}, a_1 = -\frac{36}{25}, a_2 = \frac{16}{25}, a_3 = -\frac{3}{25}, b_0 = \frac{12}{25}$.

Two other methods in this category are also popular. These are the Adams-Bashford and the Adams-Moulton methods. The Adams-Bashford method is explicit and the Adams-Moulton method is implicit.

If more points are used in a time interval, that leads to the popular Runge-Kutta family of methods. The Runge-Kutta family of methods can be explicit or implicit. An *s*th-order explicit Runge-Kutta method for a DAE system, such as Equations (17.31) and (17.32), is given by

$$\boldsymbol{x}_{n+1} = \boldsymbol{x}_n + \Delta t_n \sum_{i=1}^{s} b_i \boldsymbol{f}(\boldsymbol{X}_{n,i}, \boldsymbol{Y}_{n,i}, \boldsymbol{U}_{n,i}, \boldsymbol{D}_{n,i}, \boldsymbol{\theta})$$

$$\boldsymbol{X}_{n,i} = \boldsymbol{x}_n + \Delta t_n \sum_{j=1}^{s} a_{ij} \boldsymbol{f}(\boldsymbol{X}_{n,j}, \boldsymbol{Y}_{n,j}, \boldsymbol{U}_{n,j}, \boldsymbol{D}_{n,j}, \boldsymbol{\theta}) \qquad (17.40)$$

$$\boldsymbol{h}(\boldsymbol{X}_{n,i}, \boldsymbol{Y}_{n,i}, \boldsymbol{U}_{n,i}, \boldsymbol{D}_{n,i}, \boldsymbol{\theta}) = 0, i = 1..s$$

A very popular method in this family is the fourth-order, explicit Runge-Kutta method. Implicit Runge-Kutta methods are also known as the Gauss-Legendre method. They are computationally expensive but have very good stability properties.

Predictor-Corrector Methods. The implicit methods can be used effectively to solve stiff problems, and larger steps can be taken without sacrificing stability. However, due to convergence problems, quite often a larger step size cannot be taken. If a better initial guess can be generated, then a larger step can be taken without convergence failure. With this incentive, a family of predictor-corrector methods is used for solving dynamic simulations. In these methods, the initial guess is generated by an explicit method in the prediction step, which is followed by a correction step, where an implicit method is used. For example, an explicit Euler's algorithm can be used as the predictor algorithm while using an implicit Euler algorithm. The Adams-Bashford algorithm can be used for prediction while the Adams-Moulton algorithm can be used in the correction step.

Due to the numerical integration, an error, even though it may be very small, is unavoidable, due to the difference between the exact value of the variable and the calculated value of the variable. This error at each time step is known as the local truncation error (LTE). Various methods are used in process simulators to calculate the step size based on the LTE value.

In chemical processes, different unit operations vary widely in their time constants. For example, in a single reactor, there may be multiple reactions taking place, some of which are very fast (such as combustion reactions), while others are slow or very slow. Such systems lead to stiff processes that are very difficult to solve. Most explicit methods (including the explicit Runge-Kutta method) fail miserably or would require such a small step size that the computation would become very inefficient. Implicit methods are a natural choice for such systems. Even when using an implicit method, it is necessary to restrict the step size for convergence purposes. A larger step can be taken when the transients of the faster processes die out. Therefore, an adaptive method is particularly useful. It should be noted that a higher-order method does not necessarily lead to better stability, since only implicit methods of order less than or equal to 2 are A-stable. A-stable algorithms are stable for any $\Delta t > 0$, as long as $\mathrm{Re}(\lambda i) < 0$. A number of diagnostic methods can be used when the process equations are available to the user and are amenable to diagnosis. For example, for detecting the stiffness, the dominant eigenvalue of the Jacobian of the problem can be calculated. In process simulations, the number of differential equations can be in the tens of thousands and the number of algebraic equations can be in the hundreds of thousands. In addition, the model equations may not be extracted from the process simulator. Therefore, the user may have only those diagnostics that are provided by the simulator or that can be calculated with a reasonable effort. Considering all these issues, an implicit adaptive method of order between 2 and 4 is a very good choice for dynamic simulation in a process simulator environment.

Linear/Nonlinear Equation Solvers. Once the ODEs are discretized, a large set of equations that also includes the algebraic equations given by Equation (17.30) is formed. The number of equations in a set depends upon the solution approach (such as modular, simultaneous with pressure-flow network solved separately, simultaneous with all equations collected and solved together) as discussed previously. Nevertheless, a set of linear/nonlinear equations must be solved. The discussion in Section 16.3.2, for solving a set of linear/nonlinear equations in the EO approach, is also applicable here. This also includes the application of a block-decomposition algorithm for increasing the speed.

Example 17.4 demonstrates the effect of the choice of integrator algorithm.

Example 17.4.

Synthesis gas composed of CO, CO_2, H_2, and H_2O is sent to a plug-flow reactor, R-1101, through a feed valve for producing methanol as shown in Figure E17.4(a). The following reactions take place [10, 11]:

$$CO + 2H_2O = CH_3OH \quad \text{(E17.4a)}$$
$$CO + H_2O = CO_2 + H_2 \quad \text{(E17.4b)}$$
$$CH_3OH \rightarrow CH_2O + H_2 \quad \text{(E17.4c)}$$

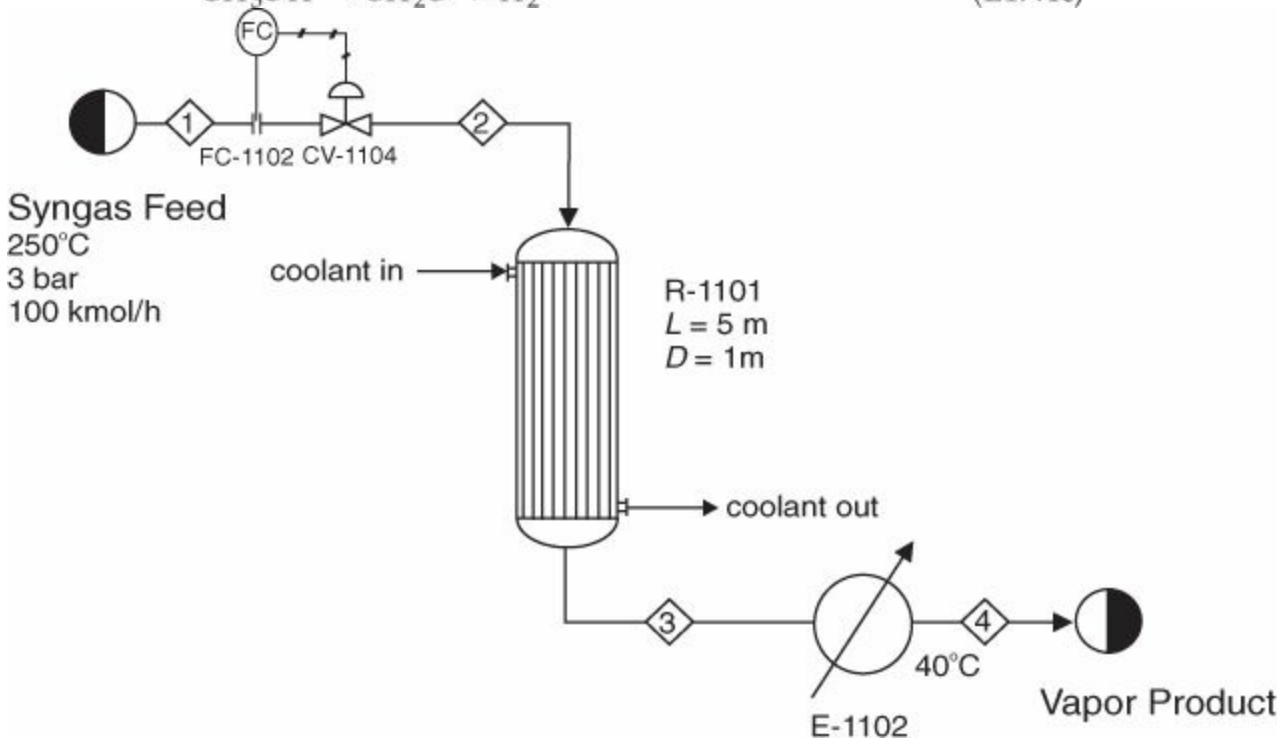


Figure E17.4(a). Configuration of the Reactor for Producing Methanol from Syngas

The corresponding rate laws for these reactions are [10, 11]

$$r_{CH_3OH} = 6.4278 \times 10^8 \exp\left(\frac{-105.5\,\frac{\text{kJ}}{\text{mol}}}{RT}\right)\left(C_{CO}C_{H_2}^2 - \frac{C_{CH_3OH}}{K_{eq,CH_3OH}}\right)\frac{\text{kmol}}{\text{kg cat s}}$$

$$-r_{CO} = 4.189 \times 10^{-8} \exp\left(\frac{-40\,\frac{\text{kJ}}{\text{mol}}}{RT}\right)\left(y_{CO}y_{H_2O} - \frac{y_{CO_2}y_{H_2}}{K_{eq,WGS}}\right)\frac{\text{kmol}}{\text{kg cat s}}$$

$$-r_{CH_3OH} = 6.314 \times 10^{-7} \exp\left(\frac{-58.65\,\frac{\text{kJ}}{\text{mol}}}{RT}\right)C_{CH_3OH}\frac{\text{kmol}}{\text{kg cat s}}$$

where C_i is the concentration of the species i in kmol/m^3.

A coolant with a constant temperature of 350°C and the overall heat transfer coefficient is 80 W/m^2°C. The reactor effluent is sent to E-1102 where it is cooled to 40°C at steady state. At steady state, the feed composition (mole fraction) and feed flowrate are

H_2	0.42
H_2O	0.16
CO	0.20
CO_2	0.22

Flowrate = 100 kmol/h

The catalyst particle density is 1800 kg/m^3, and the bed voidage is 0.45. The reactor length is 5 m, and the diameter is 1 m. At steady state, the feed valve is 50% open. The feed valve is closed to 25% in a single step. Compare the dynamic responses of the methanol and H_2 concentrations at the reactor outlet by using various explicit methods (such as the explicit Euler and Runge-Kutta methods) and implicit methods (such as the implicit Euler and Gear's method of various orders).

Solution

The problem is set up in Aspen Engineering Suite (AES) using Aspen Plus V7.2 and Aspen Plus Dynamics V7.2. The thermodynamics package used is PR EOS. The pressure drop in the reactor is calculated by the Ergun equation. It is assumed that the catalyst and the fluid are at the same temperature. The CuO/ZnO/Al_2O_3 catalyst used in this study contains about 63 wt% CuO, 25 wt% ZnO, and 12% Al_2O_3 [10]. The mass-weighted heat capacity of the catalyst is calculated to be 635 J/kg K. As the reactor model is solved in Aspen Plus Dynamics using the method of lines, the PFR is discretized into 100 grids and solved with the first-order, backward finite-difference method. Cooler E-1102 is set up using the "LMTD" option. In Aspen Plus Dynamics, when the explicit Euler's method is used, the dynamic simulation could be solved only with a minimum step size of 0.4×10^{-5} s. Such a small step is obviously unacceptable. Performance of the fourth-order explicit Runge-Kutta method is slightly better, but still unacceptable. The implicit Euler method, Gear's method of order two, and Gear's method of order five yield similar results. Figure E17.4(b) shows the methanol and H_2 concentrations at the reactor outlet. Considering the computational expense, the implicit Euler's method is the best choice for this system.

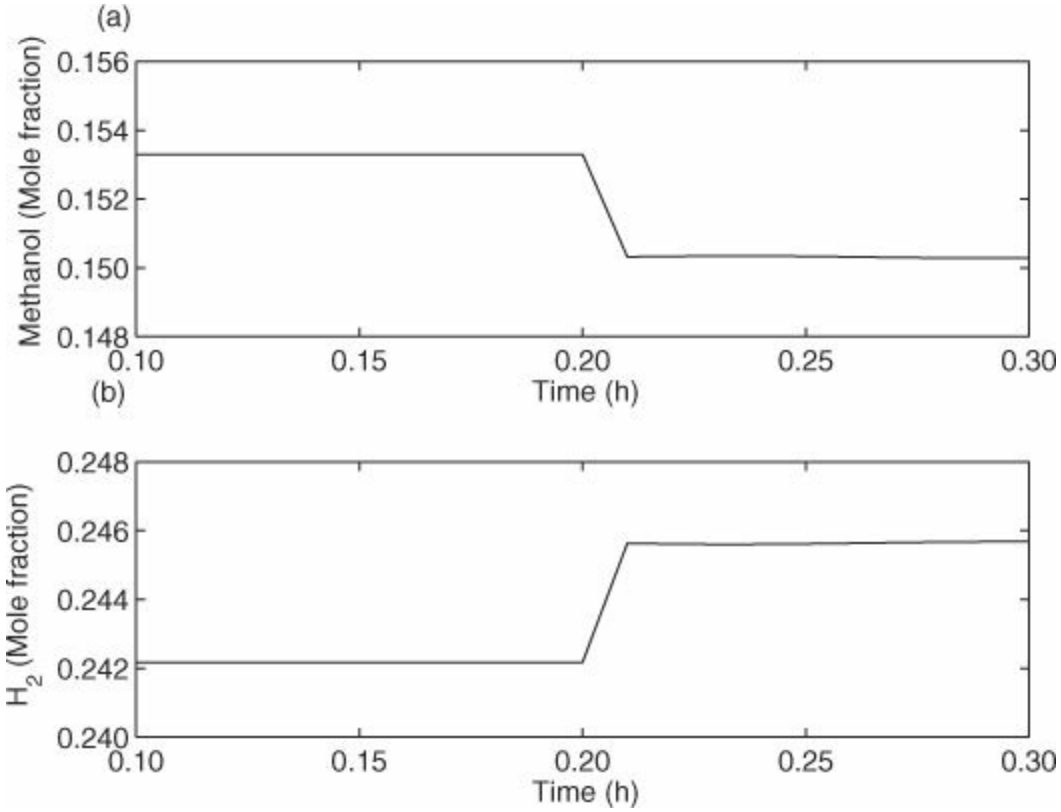


Figure E17.4(b). Transient Response at the Outlet of the Reactor (a) Methanol Concentration (Mole Fraction) (b) H_2 Concentration (Mole Fraction)

17.4. Process Control

When there is no controller present, the dynamic response is called the open-loop response. Open-loop dynamic simulation can be performed only for open-loop-stable processes. A process is open-loop stable if the state variables return to steady-state values when one or more input variables are perturbed. For the processes that are open-loop unstable, an appropriate regulatory control layer should be designed first. The dynamic response of a closed-loop process is not only due to the process itself but also due to the control configuration and controller design. This discussion will mainly focus on lower-level, control system design that is required both for a stable simulation and for satisfying the objectives of plant operation. Only the essentials of process control needed to obtain a stable dynamic simulation are discussed here, but the interested reader can find more details on process control from several excellent books in this area [12, 13, 14].

Lower-level controllers are usually single-input-single-output (SISO) controllers. These controllers maintain a single output, known as the controlled variable (CV), at its desired value, known as the set point (SP), by manipulating a single input, known as the manipulated variable (MV). There are two objectives for the lower-level control system design, namely, set point tracking or servo control, and regulatory control or disturbance rejection. In servo control, the objective is to track a reference trajectory in the SP, while in regulatory control, the objective is to maintain the CV at the SP in face of process disturbances.

If the lower-level control system design is not appropriate, the simulation may slowly drift from its nominal operating condition or reach an undesired operating region. In the worst case, it will lead to convergence failure. For stability of the dynamic simulation, both control structure design and controller design are important.

The most common control structure is feedback control used for both the servo and regulatory

functions. In feedback control, at every simulation time step, the CV is sampled and compared to the SP, and an error signal is generated. If the deviation variables (i.e., deviation from the steady-state values) for CV and SP are denoted by y_m and y_r, respectively, then the error is calculated as

$$\epsilon = y_r - y_m \tag{17.41}$$

The control action is almost always based on the error signal and depends upon the controller design. Most frequently a proportional-integral-derivative (PID), or a proportional-integral (PI), or a proportional-only (P-only) controller is used for calculating the control action. If the deviation variable of the control action is denoted by c and if a PID controller is used, then the control action can be written as

$$c(t) = K_c\left[\epsilon(t) + \frac{1}{\tau_I}\int_0^t \epsilon(t)dt + \tau_D\frac{d\epsilon(t)}{dt}\right] \tag{17.42}$$

In Equation (17.42), K_c is the proportional gain, τ_I is the integral time or reset time, and τ_D is the derivative time constant. While designing the controller, the direction of the control action must be provided by the user. If the steady-state gain of a system is positive, that is, an increase in the input variable causes the output variable to increase, the controller gain should be positive. This is known as direct action. In contrast, for a system with negative steady-state gain, the controller gain has to be negative. This is known as reverse action.

Controller type is chosen based on the process. P-only control results in a steady-state offset, except for processes with a natural integrator, such as level control of a vessel or pressure control of a gas drum. PI control is probably the most widely used type of controller, because it eliminates any offset between the steady-state value of CV and the SP. But care must be taken as the response can become oscillatory due to an aggressive integral action. PID controllers are most suitable for processes with some delay in their response. However, the CV value should be relatively noise free for the derivative action to be used effectively without generating a noisy MV. Details are again available in standard textbooks on process control.

To achieve the desired control performance with a PID controller, its parameters, K_c, τ_I, and τ_D, should be tuned. Controller tuning is a vast and complicated subject, and interested readers are again referred to any standard textbook on process control. The parameters can be tuned manually, but a trial-and-error method may not result in a satisfactory performance. For example, for a PID controller, there is a bound on the proportional gain, K_c, beyond which the process can become unstable. Therefore, various methods are available in dynamic simulators where approximate process model/information can be used for finding the appropriate tuning parameters. Two of these methods will be discussed here, mainly because these methods are easy to apply and are typically available in process simulators. The first method is based on the use of stability margins. The second method requires an approximate process model. The first method is based on determination of the ultimate controller gain (K_{cu}) that brings the closed-loop process to the verge of instability. The corresponding period of sustained oscillation is known as the ultimate period of oscillation (P_u). For determining K_{cu}, the proportional gain of the controller can be manually increased until the process reaches sustained oscillation in response to a step change in an input. Another popular method to determine K_{cu} and P_u is known as autotune variation (ATV). In this method, the controller is replaced by a relay that helps to determine K_{cu}. Once the ultimate controller gain and ultimate period of oscillation are established, the controller tuning parameters are decided by following rules such as

the Ziegler-Nichols stability margin controller tuning rule or the Tyreus-Luyben rule. In the second method, the control loop under consideration is opened, a step change in the input is introduced, and the transient response in the output is recorded. Then a simple process model, such as first-order, first-order plus time delay, or second-order plus time delay, is fitted to the process-response curve. Once the characteristic parameters of such models, such as time delay, process gain, time constant, and so forth, are extracted, there are various tuning rules, such as Cohen-Coon tuning rules or the Ziegler-Nichols tuning rule, that can be used. In summary, a stable dynamic simulation can usually be achieved by using an appropriate control structure and controller design even though the control system performance may not be satisfactory.

Example 17.5.

Consider Example 17.3, where a mixture of CO_2 and methanol is separated in a jacketed flash vessel. The inlet temperature of the heating medium is 90°C, and its specific heat is similar to that of water. There is no phase change of the heating medium in the jacket. The heat transfer option in the dynamic simulation is "LMTD," and the heating-medium flowrate is manipulated to maintain the vessel outlet temperature at 70°C, as shown in Figure E17.5(a). Figure E17.5(a) also shows that the flow dynamics of the heating medium are neglected, assuming perfect control. So there are four controllers: FC-1101, PC-1101, LC-1101, and TC-1101. Tune these controllers by using both methods mentioned before (i.e., by using stability margins and by using an approximate process model) and by applying the various rules discussed previously. Then decrease the feed flow to 50 kmol/h in a single step. Show the differences in the transient response of the outlet temperature with the controllers being tuned by different rules.

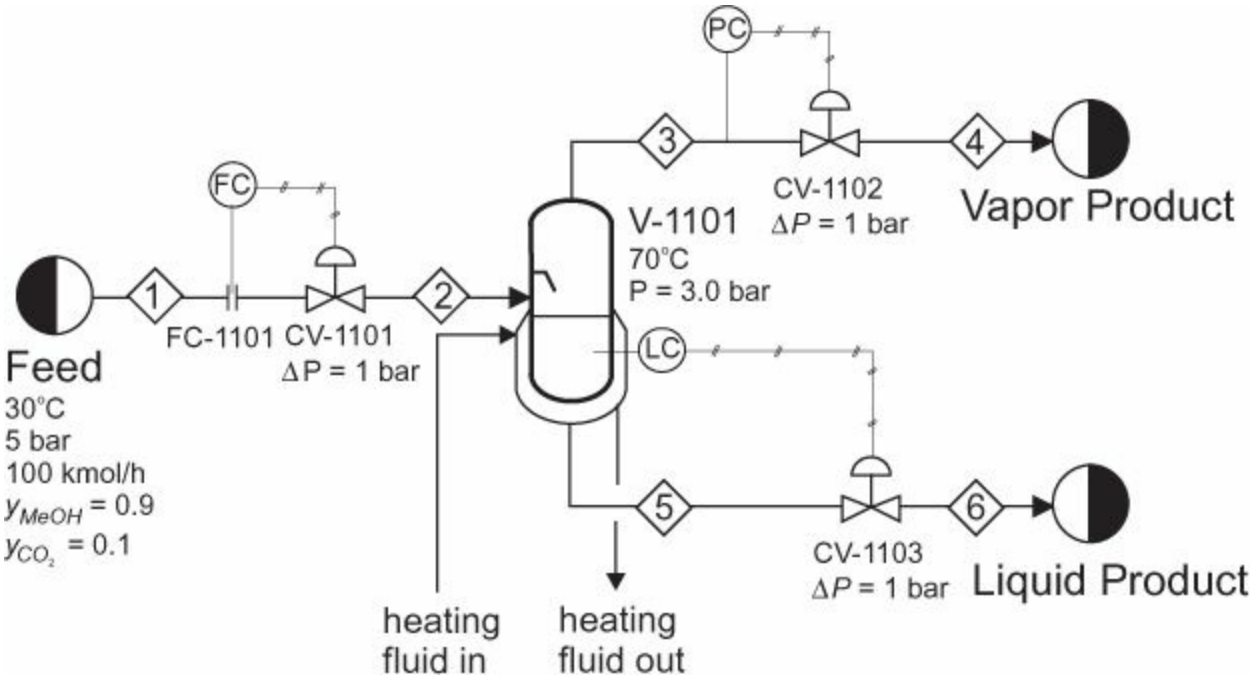


Figure E17.5(a). Configuration of the Jacketed Flash Vessel for Separating CO_2 and Methanol Where the Vessel Outlet Temperature Is Being Controlled by Manipulating the Flowrate of the Heating Fluid

Solution

As in previous problems, the problem is set up in Aspen Engineering Suite (AES) using Aspen Plus V7.2 and Aspen Plus Dynamics V7.2. The flow, pressure, and level controllers are considered to be

PI controllers, and the temperature controller is considered to be a PID controller. As seen later, the time delay of the temperature loop is small; thus the derivative action can be neglected. In Aspen Plus Dynamics V7.2, both methods for controller tuning are available under the "Tune" tab of individual controllers. For the first method that uses stability margin, the test method "Closed Loop (CL) ATV" is selected. The relay amplitude is specified to be 5% of the output range. At the end of this test, K_{cu} and P_u are calculated automatically. Then, under the "Tuning parameters" tab, the tuning parameters are calculated based on these values of K_{cu} and P_u and choice of tuning rule. Ziegler-Nichols (Z-N) and Tyreus-Luyben (T-L) tuning rules are used to obtain the tuning parameters shown in Table E17.5. For the second method that uses an approximate process model, the test method "open loop" (OL) is selected. A step up by 5% of the output range is selected to be the test specification. At the end of this test, Aspen Plus Dynamics automatically identifies the characteristic parameters, that is, open-loop gain, time constant, and time delay of a first-order-plus-time-delay process. Then, under the "Tuning parameters" tab, the tuning parameters are calculated based on these values of these characteristic parameters and choice of tuning rule. Ziegler-Nichols, Cohen-Coon (C-C), IMC, IAE, ISE, and ITAE tuning rules are used to obtain the tuning parameters shown in Table E17.5.

Table E17.5. Tuning Parameters Applying the Two Methods and Various Tuning Rules

		FC-1101		PC-1101		LC-1101		TC-1101		
Method	Tuning Rule	K_c (%/%)	τ_I (min)	K_c (%/%)	τ_I (min)	K_c (%/%)	τ_I (min)	K_c (%/%)	τ_I (min)	τ_η (min)
CL ATV	Z-N	1.71	0.09	50.61	0.11	306.34	0.09	1723.12	0.06	0.02
CL ATV	T-L	1.17	0.25	34.79	0.29	210.61	0.25	915.41	0.29	—
OL	C-C	46.18	0.01	401.88	0.01	134.44	0.13	3151.22	0.03	0.01
OL	Z-N	31.25	0.01	401.56	0.01	134.36	0.13	2838.31	0.03	0.01
OL	IMC	3.67	0.09	12.56	0.45	3.00	6.48	16.74	1.53	0.01
OL	IAE	15.22	0.01	410.63	0.03	136.75	0.29	2342.62	0.05	0.01
OL	ISE	22.73	0.01	478.67	0.03	157.98	0.30	2731.63	0.04	0.01
OL	ITAE	21.26	0.01	343.38	0.03	114.01	0.30	2502.84	0.06	0.01

For the IMC method, the tuning parameter, λ, is considered to be 0.3 times the process time constant. Table E17.5 shows that the tuning parameters calculated by the rules under the "closed-loop ATV" method are similar. On the other hand, all the rules for the "open-loop" method calculate similar tuning parameters except the IMC method. Also, note that the gain values calculated by all the rules under the "open-loop" method are much larger. As the feed flow is step decreased to 50 kmol/h, the differences in the transient response in the outlet temperature due to various tuning rules are shown in Figures E17.5(b) and E17.5(c), respectively. In Figure E17.5(b), the transient responses for all the tuning rules except the IMC rule are shown. Figure E17.5(b) shows that the performance of all the control loops is satisfactory. However, Figure E17.5(c) shows that the deviation is comparatively large when the IMC rule is used. It should be noted that the flash vessel is the only unit operation considered in this example. In case of other unit operations being present in the same process, significant interactions may take place and many of the controller gains calculated by the various rules under the "open-loop" method may have to be decreased ("detuned").

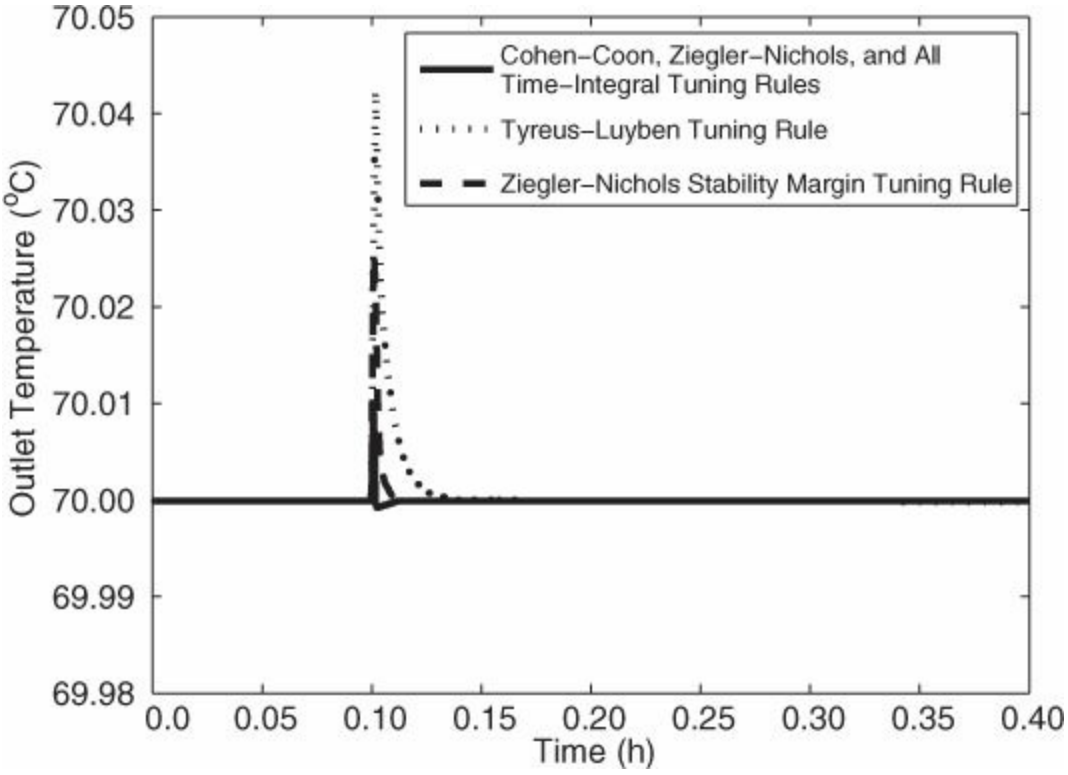


Figure E17.5(b). Transient Response of the Outlet Temperature Using Various Tuning Rules Except the IMC-Based Rule

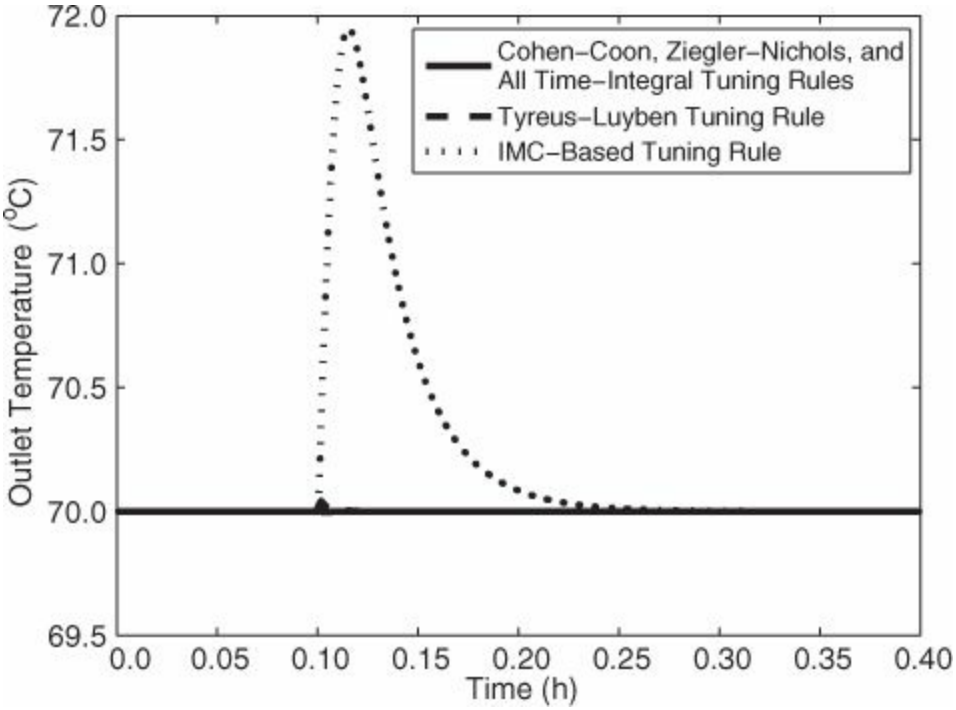


Figure E17.5(c). Transient Response of the Outlet Temperature Using Various Tuning Rules Including the IMC-Based Rule

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Example 17.6 demonstrates that a dynamic simulation can be used to study important changes in the transient response that may occur in the course of plant operations. Such studies can help to avoid potentially unsafe plant operations.

Example 17.6.

Figure E17.6(a) shows the schematic of a cooled tubular reactor in which maleic anhydride is being produced by oxidizing benzene [15]. This problem is similar to the problem in Appendix B.5.

However, there are some differences in the problem specification in this example compared to that in Appendix B.5. Ignoring the quinine formation reaction in Appendix B.5, the following reactions are considered:

$$C_6H_6 + 4.5O_2 \rightarrow C_4H_2O_3 + 2CO_2 + 2H_2O$$

$$C_4H_2O_3 + 3O_2 \rightarrow 4CO_2 + H_2O$$

$$C_6H_6 + 7.5O_2 \rightarrow 6CO_2 + 3H_2O$$

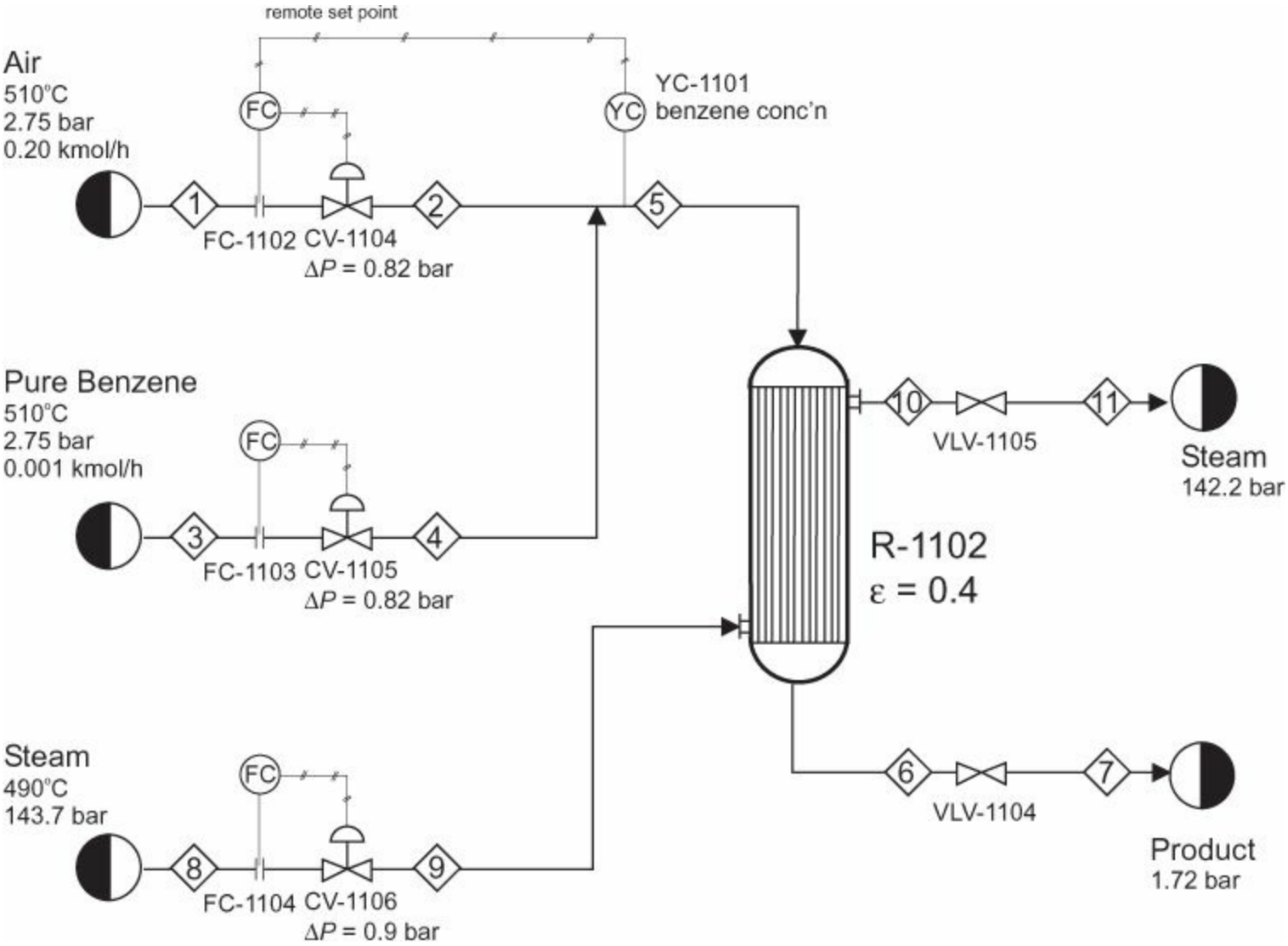


Figure E17.6(a). Configuration of the Cooled Tubular Reactor for Producing Maleic Anhydride from Benzene

These reactions are carried out using excess air to avoid runaway reactions. As a result, the reactions can be considered as pseudo-first-order reactions. The reaction rates can be written as [15]

$$k_1 = 4280 \exp\left[\frac{-12{,}660}{T(\mathrm{K})}\right] \frac{\mathrm{m}^3}{\mathrm{kg\ cat\ s}}$$

$$k_2 = 70{,}100 \exp\left[\frac{-15{,}000}{T(\mathrm{K})}\right] \frac{\mathrm{m}^3}{\mathrm{kg\ cat\ s}}$$

$$k_3 = 26 \exp\left[\frac{-10{,}800}{T(\mathrm{K})}\right] \frac{\mathrm{m}^3}{\mathrm{kg\ cat\ s}}$$

Since these reactions are highly exothermic, a molten, eutectic salt is circulated in a multitube reactor

to maintain the desired temperature. For simplicity, it can be assumed that an excess amount of steam is used to cool the reactor such that the change in the steam temperature during steady-state operation is not significant. This results in a nearly isothermal operation of the reactor. The reactor size is the same as recommended in the work of Westerink and Westerterp [15]. This gives the length and diameter of a single tube to be 12.8 m and 0.028 m, respectively. The pressure drop across the reactor on both the process and cooling-medium sides can be considered negligible. Catalyst density is 900 kg/m^3. Assume SS302 (stainless steel type 302) to be the material of construction. Heat loss to the ambient can be assumed to be negligible.

a. Develop a dynamic simulation of this cooled tubular reactor assuming that the dimensions of the reactor are that of a single tube. Implement the controllers as shown in Figure E17.6(a). Assume the overall heat transfer coefficient (U) to be 25 W/m^2°C. Then increase the flowrate of benzene to 0.0033 kmol/h while keeping the flowrate of air constant. Show the transient response of the temperature and the benzene and CO_2 concentrations at the exit of the reactor.

b. Now assume that the overall heat transfer coefficient (U) changes to 2 W/m^2°C due to fouling. Again, increase the flowrate of benzene to 0.0033 kmol/h, keeping the air flowrate constant as before. Compare the results with those obtained previously.

Solution

a. The simulation is set up in Dynsim 4.5.3 using the SRK EOS. In Dynsim, three "sink" blocks are used for the sources of air, benzene, and steam, respectively. In Dynsim, kinetic reactions can be simulated in a number of blocks; however, because of the presence of the cooling jacket and the catalyst in the reactor, a PFR block is chosen. The thickness of the reactor wall is calculated as in Example E17.3, considering SS302 as the material of construction. For specifying the pressure drop of a stream in a block, Dynsim provides the option to provide the flow conductance. The flow conductances of the flow and reaction passes of the PFR are provided as 150 kg/s/(kPa kg/m^3)$^{0.5}$. Three "reaction data sets" are created for modeling the kinetics of the reactions. The "reaction data sets" can be created in Dynsim 4.5.3 by clicking "RDS" under the "Process Equipment" tab of the "Icon Palette." These data sets are then associated with a reaction set. The reaction set block is known as "RD" in Dynsim and is available under the "Process Equipment" tab of the "Icon Palette." This reaction set is then enabled under the "Reactions" tab of the PFR. Three "PID" blocks available under the "Controls" tab of the "Icon Palette" are used for the controllers FC-1102, FC-1103, YC-1101, and FC-1104, respectively. Keeping the set point of FC-1102 constant, CV-1105 is manually opened to achieve a step change in the flowrate of the benzene feed. Figure E17.6(b) shows that the change in the temperature is negligible at the reactor outlet. The corresponding concentrations of benzene and CO_2 at the reactor outlet are shown in Figures E17.6(c)(a) and E17.6(c)(b), respectively. The benzene concentration increases at the reactor outlet while the change in the CO_2 concentration is negligible.

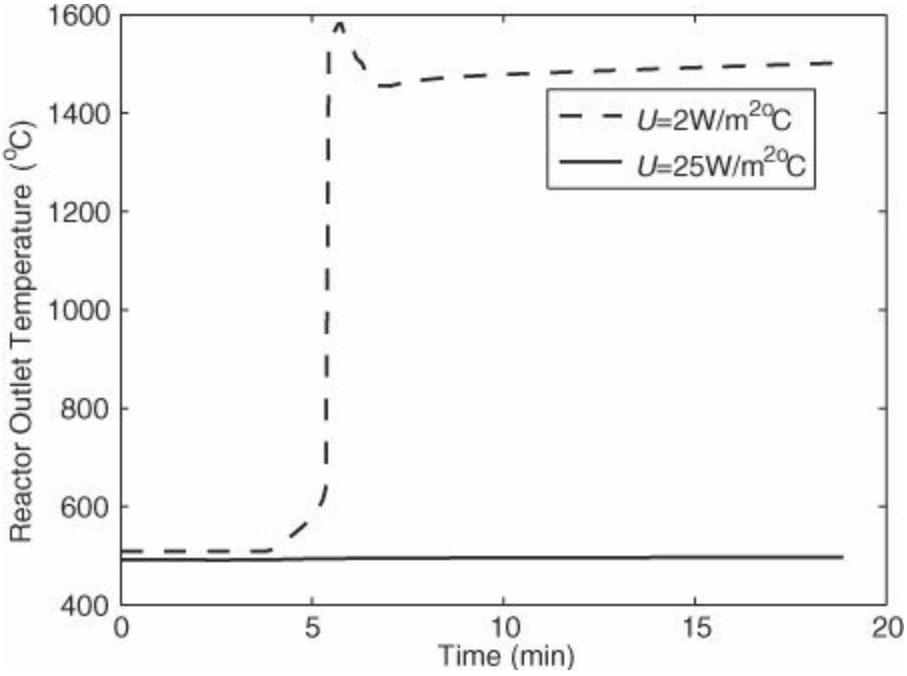


Figure E17.6(b). Transients in Reactor Outlet Temperature with Different Overall Heat Transfer Coefficients When the Benzene Concentration in the Feed Is Changed

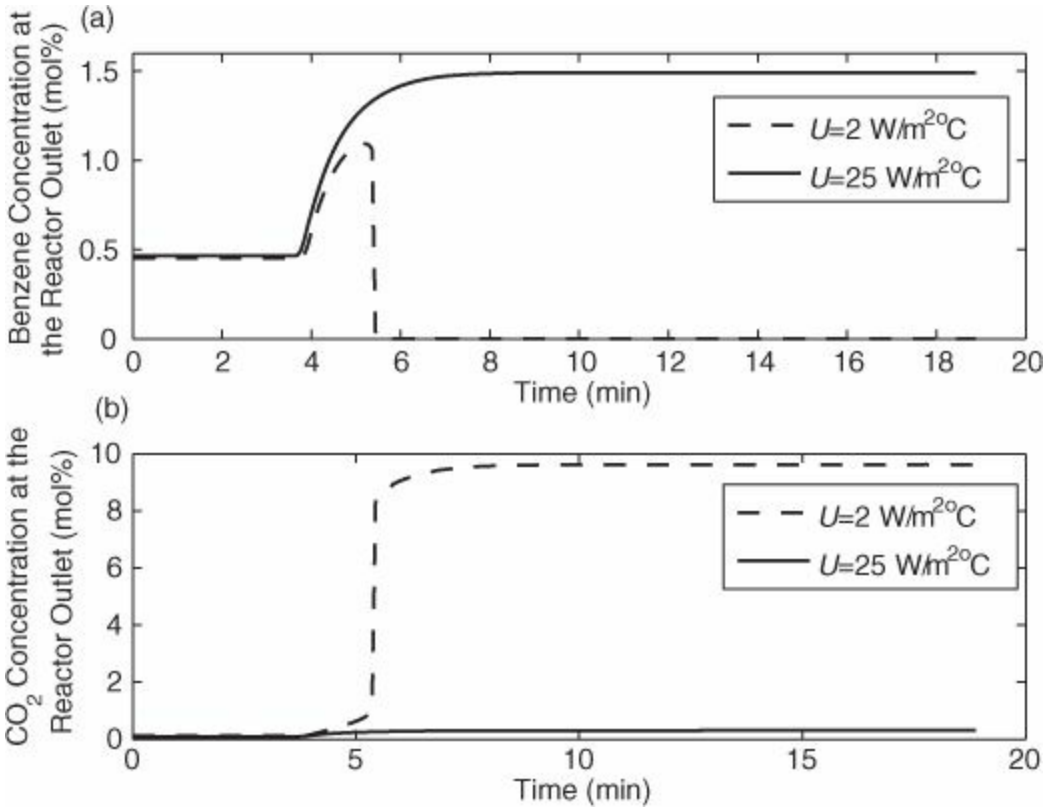


Figure E17.6(c). Concentration at the Reactor Outlet with Different Overall Heat Transfer Coefficients When the Benzene Concentration in the Feed Is Changed: (a) Benzene Concentration; (b) CO_2 Concentration

b. The overall heat transfer coefficient is now changed to 2 W/m^2°C. After making changes in an existing Dynsim simulation, the "LF" button must be clicked to load the simulation again. The simulation freezes at this point, and it can be restarted again. Once again, the previous steady-state snapshot is loaded by clicking the "IC" button and then selecting and loading the appropriate "IC" (initial condition) file. Due to the changed overall heat transfer coefficient, the exit temperature and composition will be different from before. The simulation is run for about 10 minutes, so that the process reaches its new steady state. It is noted in Figures

E17.6(b) and E17.6(c)(a) that these initial conditions are different from before. Now, as before, the set point of FC-1102 remains constant, and CV-1105 is manually opened to achieve a step change in the flow of benzene feed. The transient responses of the temperature and the benzene and CO_2 concentration are plotted in Figures E17.6(b), E17.6(c)(a), and E17.6(c)(b), respectively. Figure E17.6(b) shows that a temperature runaway has taken place. Figure E17.6(c)(a) shows that the benzene is almost entirely consumed due to Reaction 2, as reflected by a large increase in CO_2 shown in Figure E17.6(c)(b). In this process, Reaction 1 is dominant at lower temperatures while Reaction 2 is dominant at higher temperatures, causing a runaway oxidation reaction due to the presence of a large amount of excess air. According to the work of Westerink and Westerterp [15], a dimensionless group that is representative of the ratio between the heat withdrawal rate and the maximum heat generation rate must be larger than a desired value to avoid unsafe conditions for this reactor. As the feed rate is increased, the rate of heat generation becomes higher. However, when the overall heat transfer coefficient is 2 $W/m^2°C$, the heat removal rate is lower than the heat generation rate. Thus, the reactor temperature keeps increasing gradually, followed by a sharp rise in the temperature due to the fast oxidation reaction.

17.5. Summary

Dynamic simulations can provide information about the transient trajectory of a process that can be effectively used for a number of applications. In this chapter, various steps required for setting up dynamic simulations in a process simulator were discussed. Necessary data and specifications required for simulating realistic transient responses were covered. Troubleshooting stability issues and convergence failures of dynamic simulations are difficult and complicated. To this end, a number of issues were discussed with respect to both problem setup as well as choice of algorithms. A brief demonstration of process control shows how the performance of the control system varies based on the controller tuning parameters. Last, it should be noted, for a robust dynamic simulation such that it does not fail to converge in face of a wide range of disturbances of varying magnitudes, all three components—the problem setup and its specification, the control system design, and the solver algorithms—must be carefully addressed.

What You Should Have Learned

- The steps required for developing a stable dynamic simulation starting with a steady-state simulation involve
  - Topological changes in the steady-state simulation
  - Design of the equipment size and geometry
  - Additional dynamic specifications
  - Control systems design
  - Choice of appropriate solver algorithms
- Dynamic specifications should be carefully chosen from the options available in a simulator to avoid unrealistic transient responses.
- An implicit adaptive method of order between 2 and 4 is usually a very good choice for the integrator algorithm.

- A number of methods are available for calculating controller tuning parameters. However, the control system performance can vary widely based on the method chosen.

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Short Answer Questions

1. What information about a process can be obtained from a dynamic simulation that is not possible to obtain from a steady-state simulation?
2. For obtaining a valid pressure-flow network, why should the pressure nodes be connected through flow devices?

3. Two flash vessels have the same length (L) but different diameters (D). Both vessels contain the same material and have the same operating pressure and temperature. In both vessels, the liquid level is being maintained at 50% by manipulating a control valve at the bottom of the flash vessel. If both vessels are horizontal, at the inlet of which control valve will you expect the higher pressure? Why? What happens if the vessels are vertical?
4. In a process, it is desired to manipulate the refrigerant flowrate to a cooler to maintain the cooler outlet temperature. What heat transfer option would you choose for developing a dynamic model of this cooler?
5. In a reactor, it is known that a fast reaction takes place in the initial region combined with a slower reaction that occurs over the entire length of the reactor. What will be a computationally efficient way of modeling this reactor? (*Hint*: A single reactor or a combination of reactors?) For solving this problem, which integrator algorithm would you choose? Why?
6. When the fuel flow to a furnace is varied, in response the furnace outlet temperature changes after some time. The outlet temperature signal is noisy. Would you use a PID controller for this process? If yes, explain what other issues should be addressed and how.

Problems

7. Consider Example 17.5, where a mixture of CO_2 and methanol is being separated in a jacketed flash vessel. The heat content in the bottom product from the flash vessel is now recovered in heat exchanger E-1103, as shown in Figure P17.7. Note the difference in the inlet feed pressure compared to Example 17.5, which is included to take care of the pressure drop in the exchanger, E-1103. Also note the changed location of the control valve, CV-1103, used for level control of V-1102. The remainder of the specifications are the same as in Example 17.5. For this problem do the following:

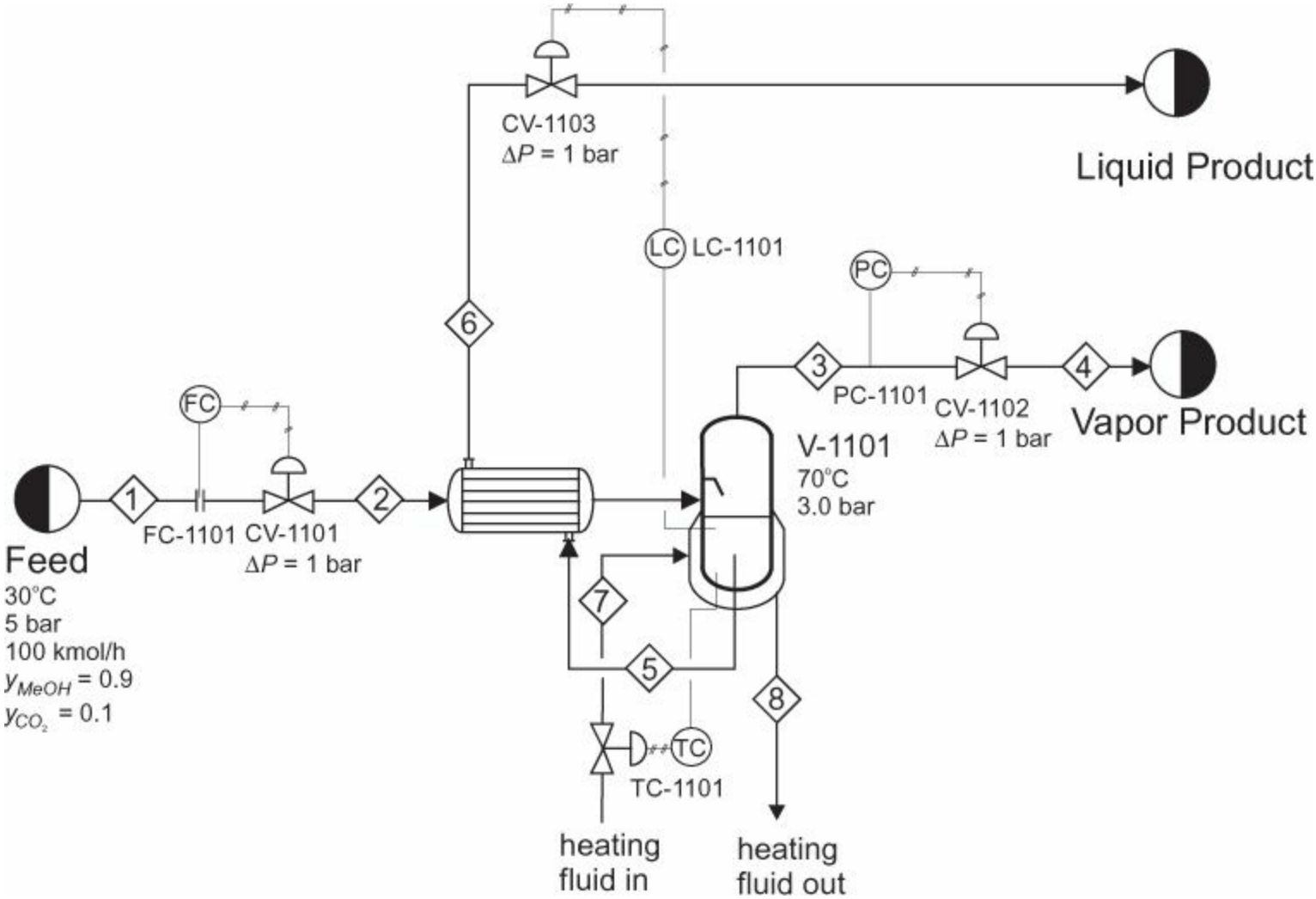


Figure P17.7. Configuration of the Jacketed Flash Vessel for Separating CO_2 and Methanol with a Bottom/Feed Heat Exchanger

a. Develop a "rigorous" design of the heat exchanger, E-1103, considering a maximum pressure drop of 0.1 bar in the shell and tube sides and a minimum temperature approach of 15°C.

b. Tune the four controllers, FC-1101, TC-1101, PC-1101, and LC-1101, by using both of the methods mentioned in Chapter 17 (i.e., by using stability margins and by using an approximate process model) and applying various rules similar to those used in Example 17.5. Did the tuning parameters differ from the ones in Example 17.5? If they did differ, explain why.

c. Step decrease the feed flow to 40 kmol/h. Show the differences in the transient response in the level controller with the controllers being tuned by different rules.

d. Use the tuning parameters for which you obtained the "best" performance in Part (c). The process is again at set at steady state with 100 kmol/h feed flowrate. Keep increasing the proportional gain of the level controller, LC-1101, each time by 30% up to 150% of the original gain. For each value of the proportional gain, step decrease the feed flow from 100 kmol/h to 40 kmol/h. Even though the tuning of the temperature controller, TC-1101, was not altered, did you notice any change in its performance? Why does this happen? Take corrective action such that the performance of the TC is similar to what it was before.

8. Consider Example 17.4, in which methanol is produced in a PFR. After being cooled, the reactor effluent is now sent to a flash vessel, V-1103, as shown in Figure P17.8. The overhead gas stream from V-1103 is sent to a compressor where it is compressed to 15 bar. The bottom liquid is pumped by P-1101. The control valve, CV-1105, is used for maintaining the level of V-

1103. The material of construction is carbon steel for all equipment. Assume the compressor to be isentropic with 80% efficiency. The efficiency of P-1101 is also 80%.

a. Develop a steady-state model of the process.

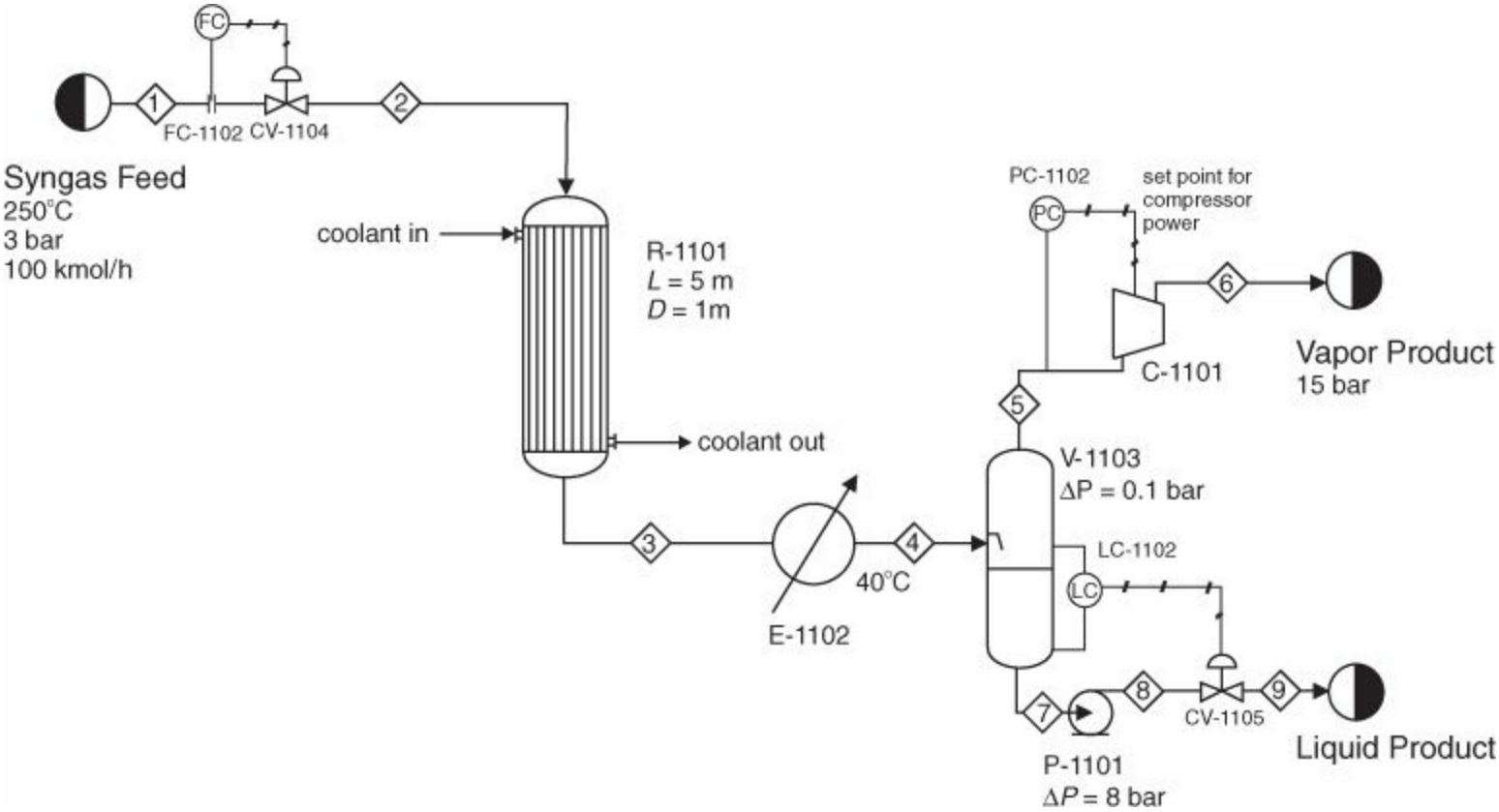


Figure P17.8. Configuration of a Section for Producing Methanol from Syngas

b. Develop a dynamic model. Size the required equipment following the heuristics provided in Chapter 11. Consider the metal mass of V-1103. Heat loss to the environment can be assumed to be negligible. Tune the controllers FC-1102, LC-1102, and PC-1102 one at a time. Now step decrease the syngas flow to 60 kmol/h. As you have tuned the controllers one at a time, does it perform satisfactorily when the controllers interact with each other? If not, what changes should you make to achieve satisfactory performance in case of loop interactions?

c. Now double the proportional gain of PC-1102. What happens to the performance of LC-1102? Why? Retune LC-1102 to achieve satisfactory performance.

9. Figure P17.9 shows a simplified configuration of a steam generation system. In combustor R-1102, the following reaction takes place:

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$

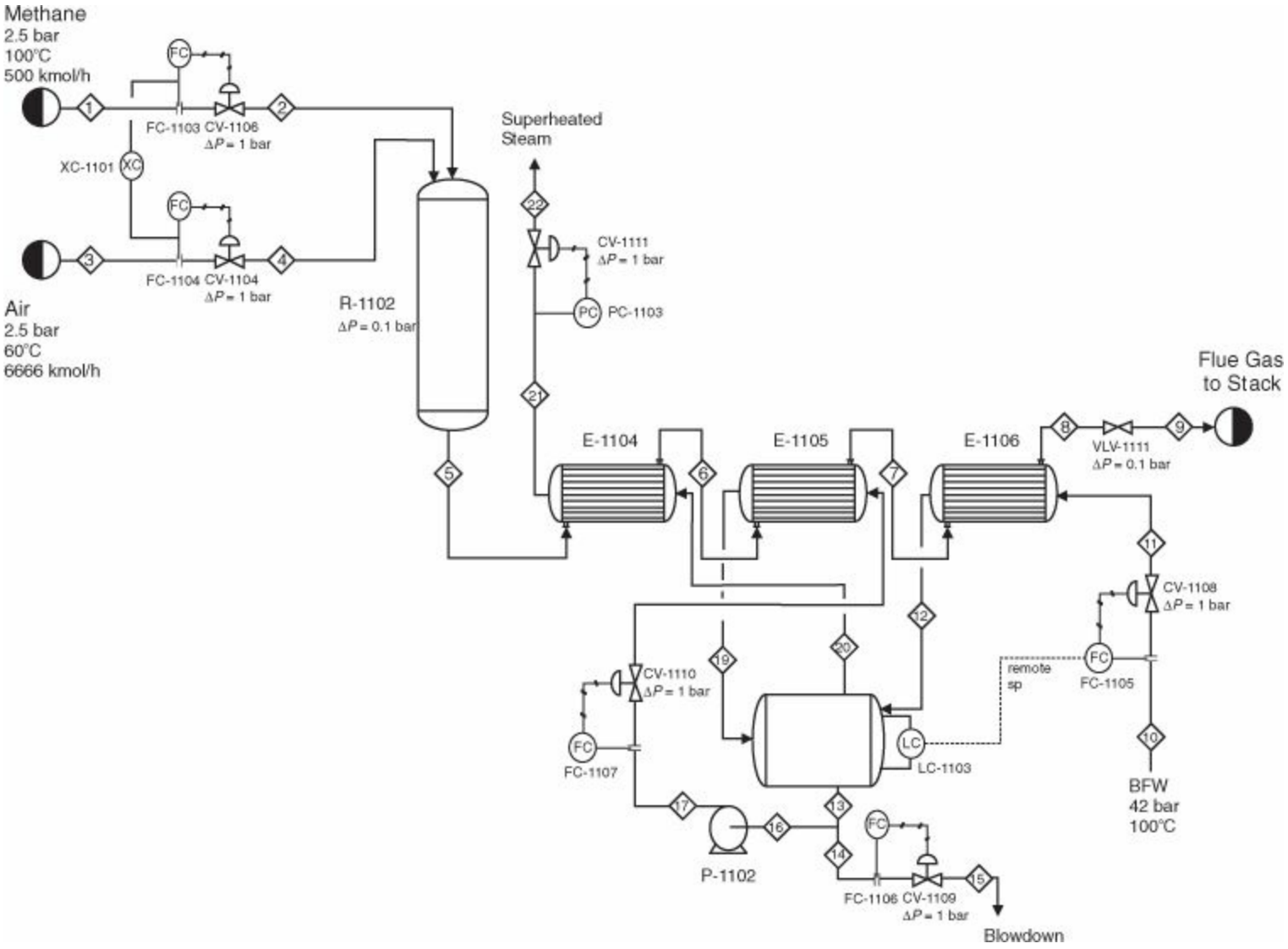


Figure P17.9. Configuration of a Simplified Steam Generation System

Complete conversion of the fuel gas in R-1102 can be assumed. Flue gas from the combustor goes to the superheater, E-1104, followed by the steam generator, E-1105. Finally, the flue gas flows through the economizer, E-1006, before going to the stack. The bfw flows through E-1006 before reaching the steam drum, V-1104. A portion of the bottom steam from the steam drum goes to the blowdown. The other portion goes to pump P-1102 and then to E-1105. The differential pressure across P-1102 should be equal to the pressure drop across CV-1110 and E-1105. The exit stream from E-1105 returns to V-1104. The pressure drop in V-1104 can be neglected. The generated steam gets superheated in E-1104 before leaving the unit. The degree of superheat in E-1104 is 100°C. Assume Stream 19 is 99% vapor. V-1104 may be considered to be adiabatic.

a. First, develop a steady-state model of this process. Simulate E-1104, E-1105, and E-1106 as "rigorous" heat exchangers. (Note that the pressure drop across the heat exchangers is not provided in the problem statement since it should be determined by the detailed design of these exchangers.) Implement two design specifications. The first design specification manipulates the flow of bfw, Stream 10, to ensure that the temperature of Stream 8 is 150°C to avoid "cold-end" corrosion. The other design specification manipulates the flowrate of the circulating water, Stream 16, so that the flowrate of the blowdown stream, Stream 14, is 1% of the bfw feed, Stream 10. (*Note:* Because of the recycle loop, the design specifications, and the rigorous heat exchangers and due to the strong interaction between the design

specifications, the steady-state simulation is difficult to converge unless appropriate convergence options are chosen. Refer to Section 16.3 for a discussion and approaches to solving such problems.)

b. Develop a dynamic model of this system. For E-1104, E-1105, and E-1106, provide the shell-side and tube-side volumes and the metal mass of each side. Heat loss to the environment for all equipment can be neglected. Size V-1104 following the heuristics in Chapter 11. Figure P17.3 shows that the air flowrate to R-1102 is regulated by a ratio controller, XC-1101, that maintains the molar ratio between fuel and air at the steady-state value. LC-1103 is cascaded with FC-1105 to maintain the level of V-1104. Information on cascaded loops and ratio controllers is available in Chapter 18. Tune the controllers with various methods and rules and compare their performance by simulating a 20% step increase in the fuel flowrate. Performance of all the controllers should be considered, especially that of LC-1103 and PC-1103.

c. Compare the performance of various integrator algorithms for this problem.

d. In Part (b), the performance of all the controllers has been considered for a 20% step increase in the fuel flowrate. Now consider simultaneously a 20% step decrease in the fuel flowrate as well as a step increase to the set point of PC-1103 by 0.5 bar. Did the same set(s) of controller tuning parameters that performed satisfactorily before again perform satisfactorily? If not, why? If the tuning parameters need to be changed, ensure that you are satisfied with the performance of the control system for both Part (b) of this problem and the current problem.

10. Consider Problem 17.9. Show the effect of the metal mass on the temperature transients during shutdown. To show this, ramp down the fuel flowrate to 20% of its steady-state value in 4 h and then completely close the fuel control valve, CV-1106. The air continues to flow with the flowrate being the same as when the fuel flowrate was 20%. Show the temperature transients of Streams 6 and 7. Now increase the metal mass of E-1104 and E-1105 by 50%. Carry out the same test again. Compare the temperature transients with what you obtained before.

11. Figure P17.11 shows the surge control loop of a compressor. The condensate in the feed and recycle stream is drained from V-1105. Then the feed gas is compressed to 25 bar in a compressor and sent to a knockout drum, V-1106. The condensate-free gas from the top of V-1106 is split into two portions. One portion goes out as product while the other portion is recycled to the compressor suction to prevent surge.

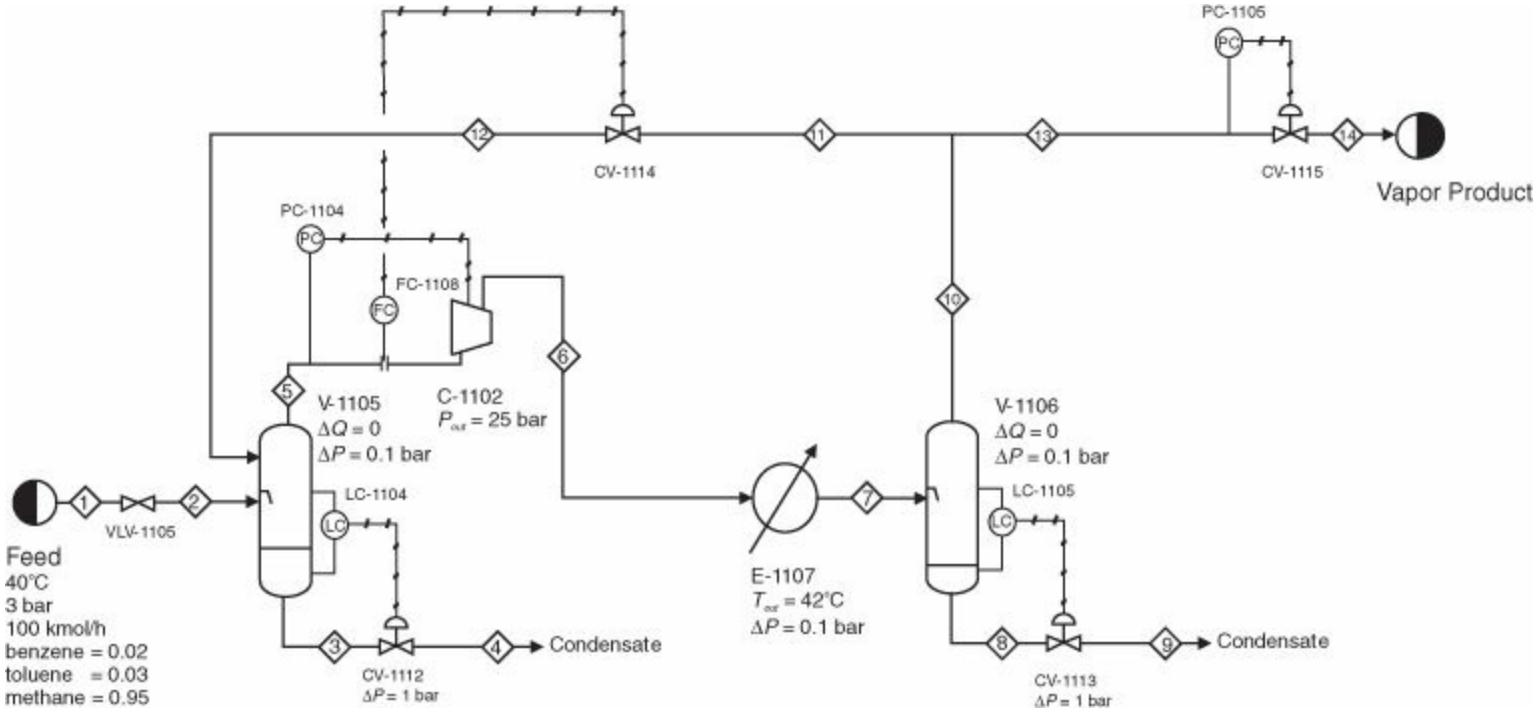


Figure P17.11. Surge Control Loop of a Compressor

a. Develop a steady-state model of this system. The suggested thermo-package is PR EOS. The isentropic efficiency of C-1102 is 80%. At steady state, there is no recycle flow; that is, flow of Stream 11 is zero.

b. Develop a dynamic model of this system. Heat loss to the environment for all equipment can be neglected. Size V-1105 and V-1106 following the heuristics in Chapter 11. In Figure P17.5, FC-1102 is the anti-surge controller. Compressor surge control algorithms, in general, can be very involved. For simplicity, it can be assumed that if the molar flowrate of Stream 5 can be maintained within 90% of its steady-state value, a surge can be prevented. Therefore, in case of a disturbance, FC-1102 should be able to maintain the flow of Stream 5 within 90% of its set point. When sizing CV-1114, it should be ensured that it can maintain the required flow of Stream 5 even if the flowrate of Stream 1 becomes zero. Determine the "best" set of tuning parameters that provides satisfactory performance when VLV-1105 is completely closed. To reiterate the control performance requirement, the flow of Stream 5 should be maintained within 90% of its steady-state value with no or negligible oscillation. This constraint should be satisfied along with satisfactory performance of PC-1104, PC-1105, and LC-1105.

c. In Part (b), if performance of any or some of these controllers is not satisfactory, what would you suggest for improvement? You may suggest hardware modification(s).

d. For this system, it is known that the pressure of Stream 1 may increase up to 3.2 bar under certain circumstances. To check the performance of the control system for this disturbance, again consider that the process is at steady state with the flow of Stream 1 being at 100 kmol/h. Now increase the pressure of Stream 1 from 3 bar to 3.2 bar. Do you get satisfactory performance with the previous tuning parameters, especially for LC-1105 and PC-1105? If not, why?

e. What would be your suggested overall improvement in the process design, including control system improvement and hardware modification, so that the control system performance is satisfactory for the disturbance considered in Part (b) and in this problem? Implement your

suggestions and compare the performance of the control system with the performance that you obtained before.

12. Consider Figure E17.6(a), in which the overall heat transfer coefficient (U) is assumed to be 25 W/m^2°C. It can be noted that in Figures E17.6(b) and E17.6(c)(b), the transients in exit temperature and CO_2 concentration appear to be negligible. Now increase the flowrate of benzene to 0.01 kmol/h, while keeping the flowrate of air constant. Simultaneously increase the temperature of air to 520°C. Did you notice any difference in the transient profile of temperature and benzene and CO_2 concentration at the exit of the reactor compared to what is obtained in Example 17.6? Why or why not?
13. Consider Problem P17.12. Now consider the overall heat transfer coefficient (U) to be 100 W/m^2°C, as suggested in Appendix B.5. Simulate the same changes as before. Did you notice any difference in the transient profiles in comparison to what you obtained before? Why or why not?

Chapter 18. Regulation and Control of Chemical Processes with Applications Using Commercial Software

What You Will Learn

- The basic methods used to control chemical processes
- How to regulate chemical processes
- What some typical control strategies for processes are
- What some typical regulation strategies for processes are
- What digital logic is and what its main components are
- What the benefits are of an operator training simulator (OTS)

Over the life of a plant, it is important for operating conditions to be regulated in order to obtain stable operations and to produce quality products efficiently and economically. In this chapter, regulation is considered; a subset of this is process control. Regulation establishes the strategy by which the process can be controlled. Regulation also involves the dynamic response (transient behavior) of the process to changes in operating variables. The latter will not be considered here as it is covered in the typical undergraduate process control course.

The regulation of process operations involves an understanding of two facts:

In most situations, processes are regulated, either directly or indirectly, by the manipulation of the flowrates of utility and process streams.

Changes in flowrates are achieved by opening or closing valves.

In order to decouple the effects of changes in process units, adjustments are most often made to the flow of the utility streams. Utility streams are generally supplied via large pipes called **headers**. Changes in flowrates from these headers have little effect on the other utility flows, and hence, they can be changed independently of each other. The one notable exception to this concept is when the flowrate of a process stream is to be controlled. In this case, the process stream clearly must be controlled or regulated directly by a valve placed in the process line.

In this chapter, it is assumed that utility streams are available in unlimited amounts at discrete temperatures and pressures. This is consistent with normal plant operations, and a typical (although not exhaustive) list of utilities is given in Table 8.3.

This chapter looks at several aspects of regulation that are important for the successful control of processes. The following topics are covered:

The characteristics of regulating valves

The regulation of flowrates and pressures

The measurement of process variables

Some common control strategies

Exchange of heat and work between process streams and utility streams

Case studies of a reactor and a distillation column

Before looking at these topics, however, a simple regulation problem from the overhead section of a distillation column is presented.

18.1. A Simple Regulation Problem

Consider the flow of liquid from an overhead condenser on a distillation column to a reflux drum, as illustrated in Figure 18.1(a). This is a section of the process flow diagram for the DME process shown in Appendix B. The liquid condensate flows from the heat exchanger, E-205, to the reflux drum, V-201. From the drum, the liquid flows to a pump, P-202, from which a portion (Stream 16) is returned to the distillation column, T-201, and the remainder (Stream 10) is sent to product storage. Assume that the amount returned to the column as reflux is set by a control valve, shown in the diagram. The amount of reflux is fixed in order to maintain the correct internal flows in the column and hence the product purity. Consider what happens if there is an upset and there is an increase in the amount of liquid being sent to the reflux drum. If no additional control strategy is employed, then the level of liquid in the reflux drum will start to increase, and at some point the drum may flood, causing liquid to back up into the overhead condenser and causing the condenser to malfunction. Clearly, this is an undesirable situation. The question is, How is the situation controlled? The answer is illustrated in Figure 18.1(b). A control valve is placed in the product line, and a level indicator and controller are placed on the reflux drum. As the level in the drum starts to increase, a signal is sent from the controller to open the control valve. This allows more flow through the valve and causes the level in the drum to drop. Although this may seem like a simple example, it illustrates an important principle of process control, namely, that a major objective of any control scheme is to maintain a steady-state material balance.

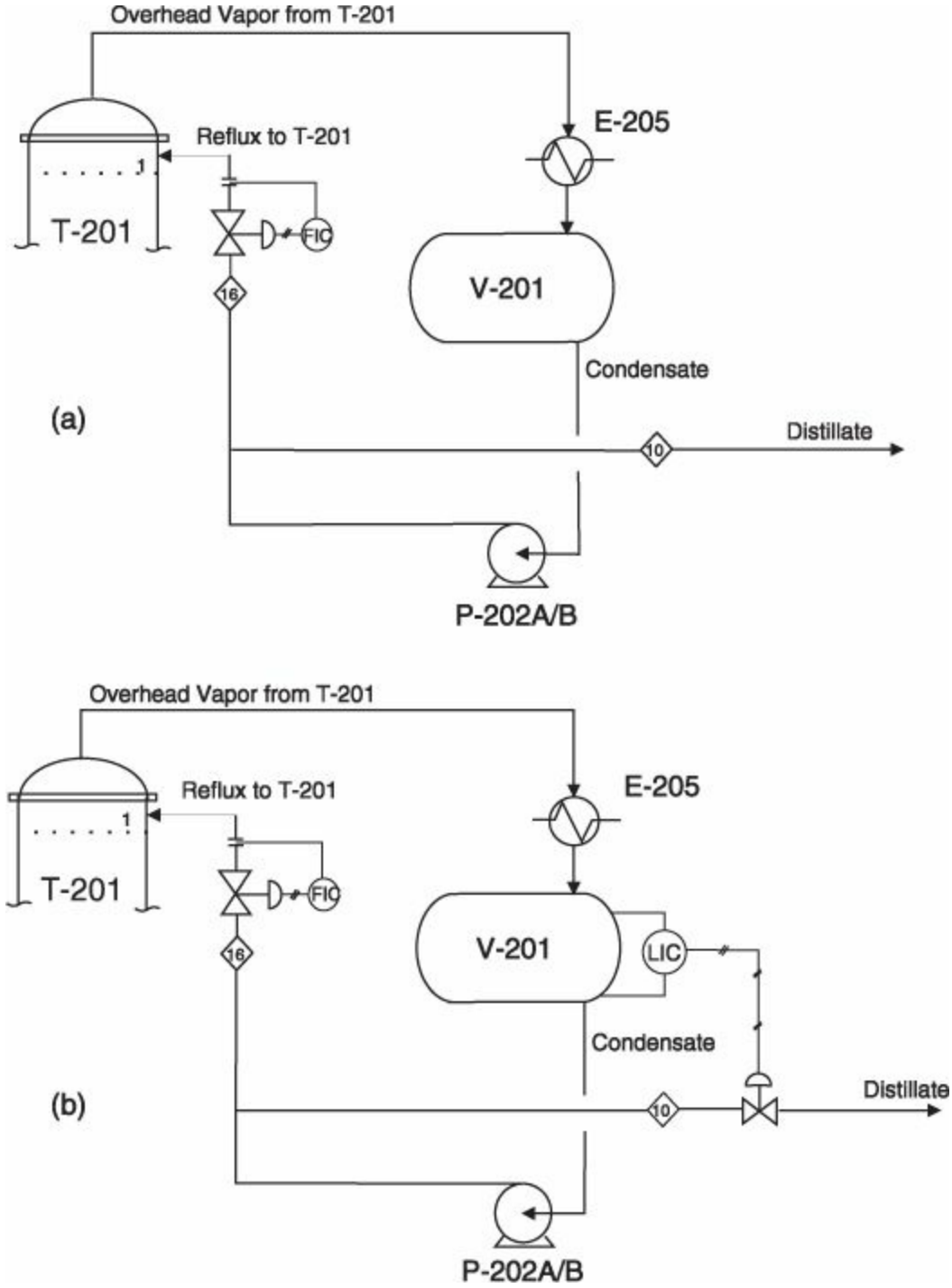


Figure 18.1. Basic Material Balance Control for DME Overhead Product

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When controlling a process, it is important to ensure that the steady-state material balance is maintained, that is, to avoid the accumulation (positive or negative) of material in the process.

In the following sections, the role and functions of valves in the control of processes and the types of control strategies commonly found in chemical processes will be investigated.

18.2. The Characteristics of Regulating Valves

Figure 18.2(a) is a crude representation of a regulating or control valve. Fluid enters on the left of the valve. It flows under the valve seat, where it changes direction and flows upward between the valve seat and the disk. It again changes direction and leaves the valve on the right. The disk is connected to a valve stem that can be adjusted (in the vertical direction) by turning the valve handle. The position

of the disk is given on the linear scale. The enlarged section shows the critical region involving the disk and the valve seat. The liquid flows through the annular space between the disk and the seat. As the disk is lowered, the area of this annulus decreases. The relationship between flowrate and valve position depends upon the shape of both the valve disk and the valve seat. It should be noted that the direction of flow through the valve could also be from the right to the left. In this case, the flow of the fluid pushes down on the disk and pushes it toward the seat. This configuration is preferred if the fluid is at a relatively high pressure or there is a large pressure drop across the valve.

Figure 18.2(b) shows the pressure drop versus flowrate characteristics of regulating valves. To make a specific change in pressure drop across the valve, the valve must be opened or closed, as appropriate. In order to evaluate the desired valve position, it is necessary to know the performance diagram or characteristic for the valve.

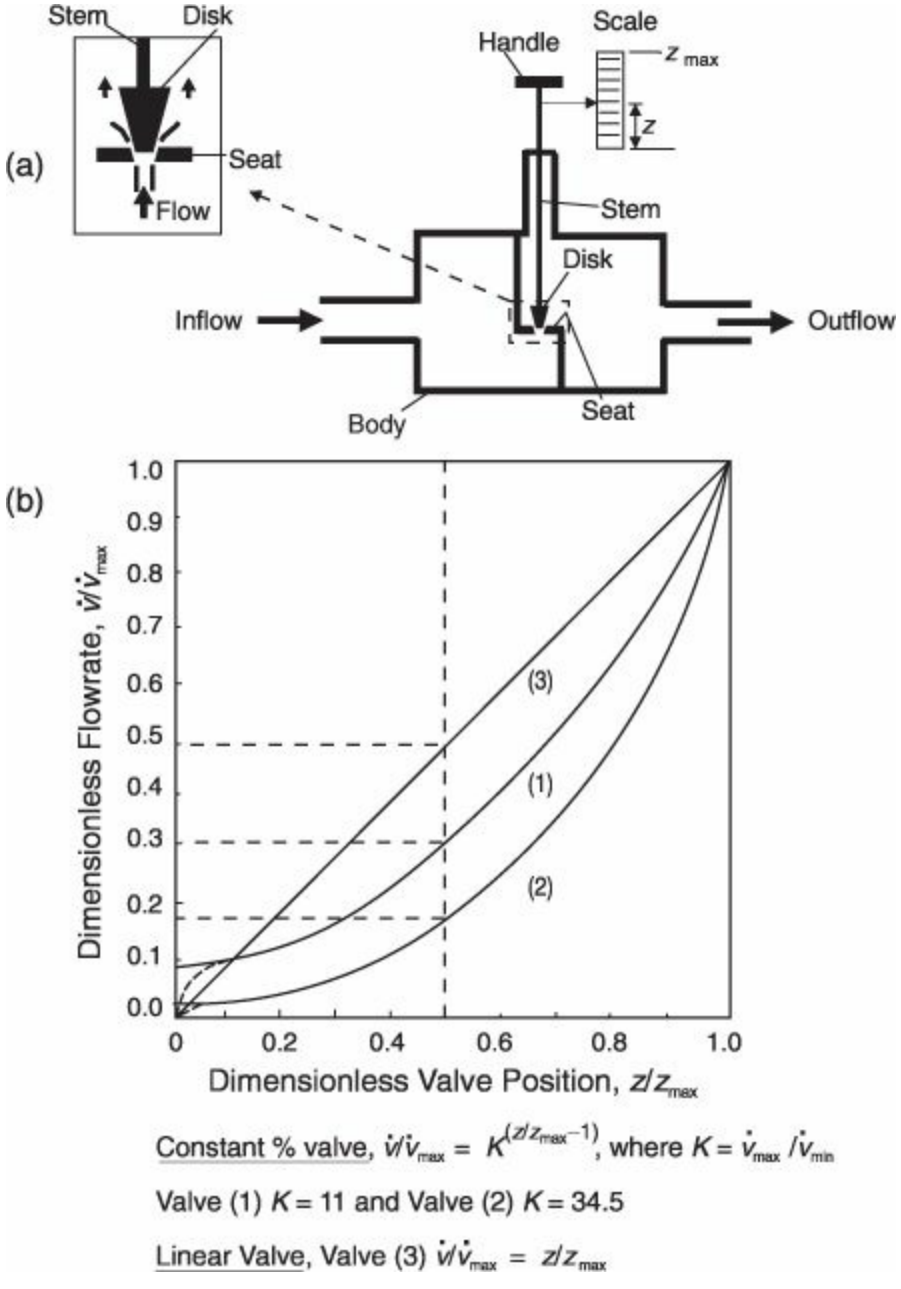


Figure 18.2. Characteristics of Regulating Valves

Figure 18.3 is a mechanical drawing of the cross section of a globe valve. Globe valves are often used for regulation purposes. There are two general valve types used for regulation:

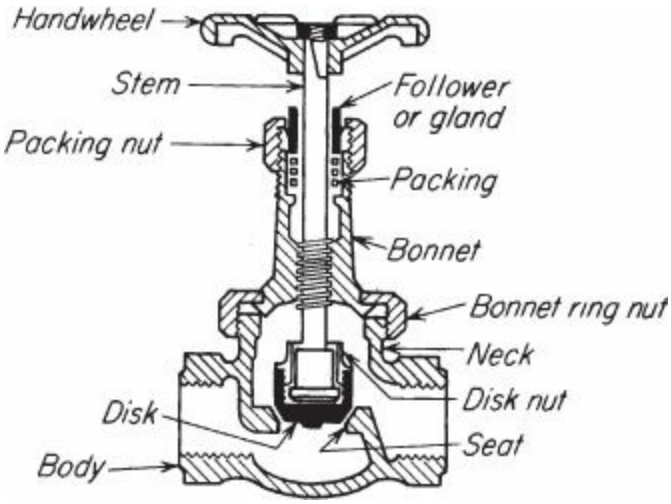


Figure 18.3. Cross Section of a Globe Valve (From W. L. McCabe, J. C. Smith, and P. Harriott, *Unit Operations of Chemical Engineering*, 5th ed. (New York: McGraw-Hill, 1993), copyright © 1993 by McGraw-Hill Companies, reproduced with permission of the McGraw-Hill Companies)

Linear Valves. In a **linear valve**, the flowrate is proportional to the valve position. This is given by the relationship $\dot{v} = kz$, where $\dot{v}$ is the volumetric flow and z is the vertical position of the disk or valve stem.

Constant or Equal Percentage Valves. For an **equal percentage valve**, an equal change in the valve position causes an equal percentage change in flowrate. The valve equation for the constant percentage valve is given by $\dot{v}/\dot{v}_{max} = K^{(z/z_{max}-1)}$. . Note that a true constant percentage valve does not completely stop the flow. However, in reality, the valve does stop the flow when fully closed, and the constant percentage characteristic does not apply to very low flowrates, as indicated by the dashed lines at the lower end of the curves in Figure 18.2(b).

Both of these valve characteristics are described by the equations shown on Figure 18.2(b). Note that these equations strictly apply only for a constant pressure drop across the regulating valve. Example 18.1 illustrates the effect of using different valves.

Example 18.1.

A valve on a coolant stream to a heat exchanger is operating with the valve stem position at 50% of full scale. You are asked to find what the maximum flowrate would be if the valve were opened all of the way (at the same pressure drop). What is an appropriate response given the information in Figure 18.2(b)?

The flow would increase by 100% or more. The exact increase depends upon the design of the valve.

From Figure 18.2(b) it is seen that a linear valve (Curve 3 on Figure 18.2[b]) has the smallest increase, from $\dot{v}/\dot{v}_{max} = 0.5$ to $\dot{v}/\dot{v}_{max} = 1$ (100% increase). For constant percent valve 1 (Curve 1), the increase is from $\dot{v}/\dot{v}_{max} = 0.3$ to $\dot{v}/\dot{v}_{max} = 1.0$ (233%), and for constant percent valve 2 (Curve 2), the increase is from $\dot{v}/\dot{v}_{max} = 0.17$ to $\dot{v}/\dot{v}_{max} = 1.0$ (488%). The flow increases in the range of 100% to 488%. The problem of predicting the flow from the valve position is even more complex because there usually exists some form of hysteresis. Thus, the pressure drop over the valve changes not only with flowrate of fluid through the valve but also with the direction of change, that is, whether the flow was

last increased or decreased.

Most valves installed are constant percentage valves, and there is no generally accepted standard design. Such valves offer fast response at high flowrates and fine control at low flowrates. The prediction of the disk position needed to give the required flowrate would be difficult using the performance diagram in Figure 18.2. In practice, the flowrate is controlled by observing a measured flowrate while changing the valve stem position. The valve position continues to be adjusted until the desired flowrate is achieved. This approach forms the basis of the **feedback control system** used for many automatic flow control schemes and discussed further in Section 18.5.

In practice, automatic control systems change valve positions to obtain a desired flowrate. The valve position is modified by installing a servomotor in place of the valve handle or by installing a pneumatic diaphragm on the valve stem.

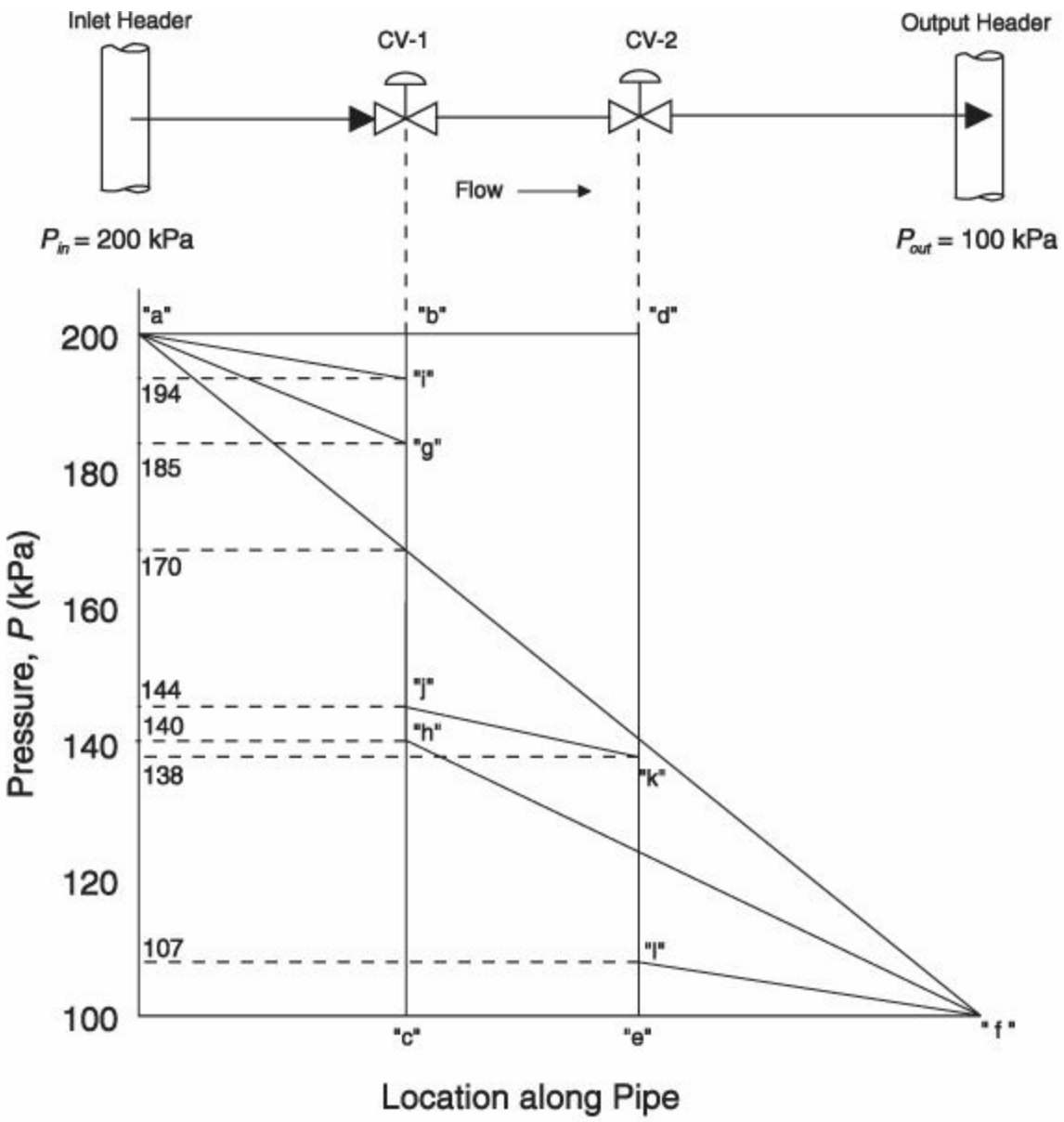
18.3. Regulating Flowrates and Pressures

The rate equation describing the flowrate of a stream is given by

$$\text{Flowrate} = \frac{\text{Driving force for flow}}{\text{Resistance to flow}} \qquad (18.1)$$

The driving force for flow is proportional to ΔP (pressure head), and the resistance to flow is proportional to friction. The resistance to flow can be varied by opening or closing valves placed in the flow path.

Figure 18.4 shows a pipe installed between a high-pressure header, containing a liquid, and a low-pressure header. The pressure difference, ΔP, between these two headers is the driving force for flow. Two valves are shown in the line, and when these valves are fully open, they offer little resistance to flow. The resistance in the transport line is due to frictional losses in the pipe. The flowrate is at a maximum value when the valves are fully open. When either valve in the line is fully closed, the resistance to flow is infinite, and the flowrate is zero. The valves may be adjusted to provide flows between these limits.



Profile	CV-1	CV-2	Flow (kmol/h)	ΔP (friction) (kPa)	P (before CV-1) (kPa)	ΔP over CV-1 (kPa)	ΔP over CV-2 (kPa)
1: a–f	open	open	100	100	170	0	0
2: a–b–c–f	closed	open	0	0	200	100	0
3: a–d–e–f	open	closed	0	0	200	0	100
4: a–g–h–f	partially open	open	74	55	185	45	0
5: a–i–j–k–l–f	partially open	partially open	44	19	194	50	31

Figure 18.4. Pressure Profiles in a Pipe Containing Two Valves

Plotted below the diagram in Figure 18.4 are pressure profiles for various valve settings. The pressure (in kPa) is plotted on the y-axis, and it is noted that for the example shown P_{in} = 200 kPa and P_{out} = 100 kPa. The x-axis indicates the relative location of the valves in the process. In addition, Figure 18.4 includes a table that provides information on the flowrate, pressure drop due to pipe friction, and the pressure before valve CV-1. The resistance in the pipe is proportional to the square of the flowrate, which is the case for fully developed turbulent flow (see Chapter 20).

Profile 1 (a–f) shows the pressure profile with both valves fully open. It gives the maximum flowrate, 100 kmol/h, possible for this system. Profile 2 (a–b–c–f) is for the case when CV-1 is fully closed and CV-2 is fully open. For this case, the flow is zero, and all the pressure drop occurs over CV-1.

The pressure upstream of CV-1 is P_{in} (200 kPa), and the downstream pressure is P_{out} (100 kPa). Profile 3 (a–d–e–f) is the case when CV-2 is fully closed and CV-1 is fully open. The pressure upstream of CV-2 is P_{in} (200 kPa), the downstream pressure is also equal to P_{in} (200 kPa), and the flowrate is zero.

For Profile 4 (a–g–h–f), valve CV-1 is partially open, providing a pressure drop of 45 kPa, and valve CV-2 is fully open. The pressure drop across CV-1 ($\Delta P_{g\text{-}h}$) can be varied by changing the valve position of CV-1. The greater the pressure drop across CV-1, the lower the pressure drop available to overcome friction and the lower the flowrate. In Profile 4, the flow is reduced to 74% of the maximum flow.

For every setting of CV-1 (with CV-2 fully open), a unique value for pressure and flowrate is obtained.

Either pressure or flowrate, but not both simultaneously, can be regulated by altering the setting of a single valve.

Two valves are required to regulate simultaneously both the pressure and flowrate of a stream. The total system resistance (pipe and valves) determines the flowrate. The ratio of valve resistances establishes the pressure profile through the process. This is shown in Profile 5 (a–i–j–k–l–f), where 50% of the available pressure drop is taken over CV-1 and 31% is taken over CV-2. The resistance ratio for the two valves is 31/50 = 1.61, the flow is 44% of the maximum flow, and the pressure upstream of CV-1 is 194 kPa. To illustrate this concept further, consider Example 18.2.

Example 18.2.

Consider the flow diagram in Figure 18.4. At design conditions, 70% of the total available pressure drop occurs across the two control valves, and the flowrate of fluid at these conditions is given as $100\ [30/100]^{0.5} = 54.8$ kmol/h. If a point "z" that is midway between the two valves is considered, over what range can the pressure at point "z" be varied at the design flowrate?

To solve this problem, two extreme cases are considered: (1) CV-1 regulates the flow and CV-2 is fully open, and (2) CV-2 regulates the flow and CV-1 is fully open. Both these situations are illustrated in Figure E18.2. From the diagram, it can be seen that the pressure at point "z" may vary between 185 kPa (CV-1 fully open) and 115 kPa (CV-2 fully open). Note that all possible combinations of partially open valves give pressures at point "z" between these two limits.

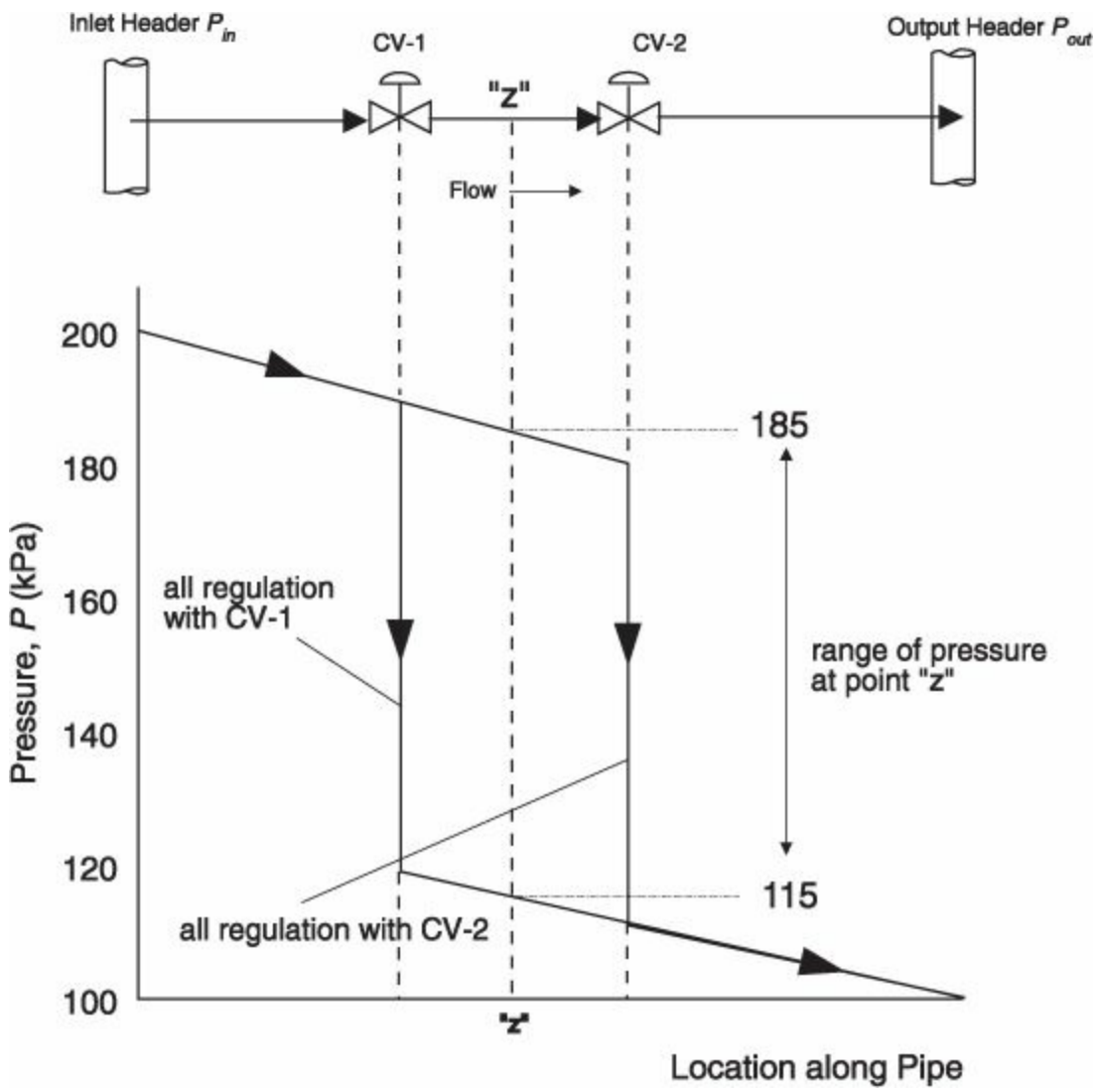


Figure E18.2. Range of Pressure at Point "z" for Design Flow

18.4. The Measurement of Process Variables

The process variables that are most commonly measured and used to regulate process performance are as follows:

- **Temperature:** Several instruments are available that provide continuous measurement of temperature—for example, thermocouples, thermometers, thermopiles, and resistance thermometric devices.
- **Pressure:** A variety of sensors are available to measure the pressure of a process stream. Many sensors use the deflection of a diaphragm, in contact with the process fluid, to infer the pressure of the stream. In addition, the direct measurement of process pressure by gauges—for example, Bourdon gauge—is still commonly used.
- **Flowrate:** Fluid flowrates, until recently, were most often measured using an orifice or venturi to generate a differential pressure. This differential pressure measurement was then used to infer the flowrate. More recently, several other instruments have gained acceptance in the area of flowrate measurement. These devices include vortex shedding, magnetic, ultrasonic, and turbine flowmeters.
- **Liquid Level:** Liquid levels are commonly used in the regulation of chemical processes. There are many types of level sensors available, and these vary from simple float-operated valves to

more sophisticated load cells and optical devices.

- **Composition and Physical Properties:** Many composition measurements are obtained indirectly. Physical properties such as temperature, viscosity, vapor pressure, electric conductivity, density, and refractive index are measured and used to infer the composition of a stream, in place of a direct measurement. A number of other measurement techniques have become commonplace for the on-line analysis of composition. These include gas chromatography and mass and infrared spectrometry. These instruments are very accurate but are expensive and often fail to provide the continuous measurements that are required for rapid regulation.

18.5. Common Control Strategies Used in Chemical Processes

There are many strategies used to control process variables in an operating plant. For more details, see Anderson [1] and Shinskey [2]. In this section, feedback, feed-forward, cascade, ratio, and split-range systems are considered.

18.5.1. Feedback Control and Regulation

The process variable to be controlled is measured and compared with its desired value (set-point value). If the process variable is not at the set-point value, then appropriate control action is taken.

Advantage. The cause of the change in the output variable need not be identified for corrective action to be taken. Corrections continue until the set-point value is achieved.

Disadvantage. No action is taken until after an error has propagated through the process and the error in the process variable has been measured. If there are large process lag times, then significant control problems may occur.

Example 18.3 illustrates the use of feedback control in a chemical process.

Example 18.3.

Identify all the feedback control loops in the process flow diagram for the production of DME, Figure B.1.1, and explain the control action of each. *Note:* There are other control valves on the utility streams, but these are shown only on the P&ID and not considered here.

All the control loops associated with the control valves shown on the PFD exhibit feedback control strategies. These are shown individually in Figure E18.3. Each control action is explained below.

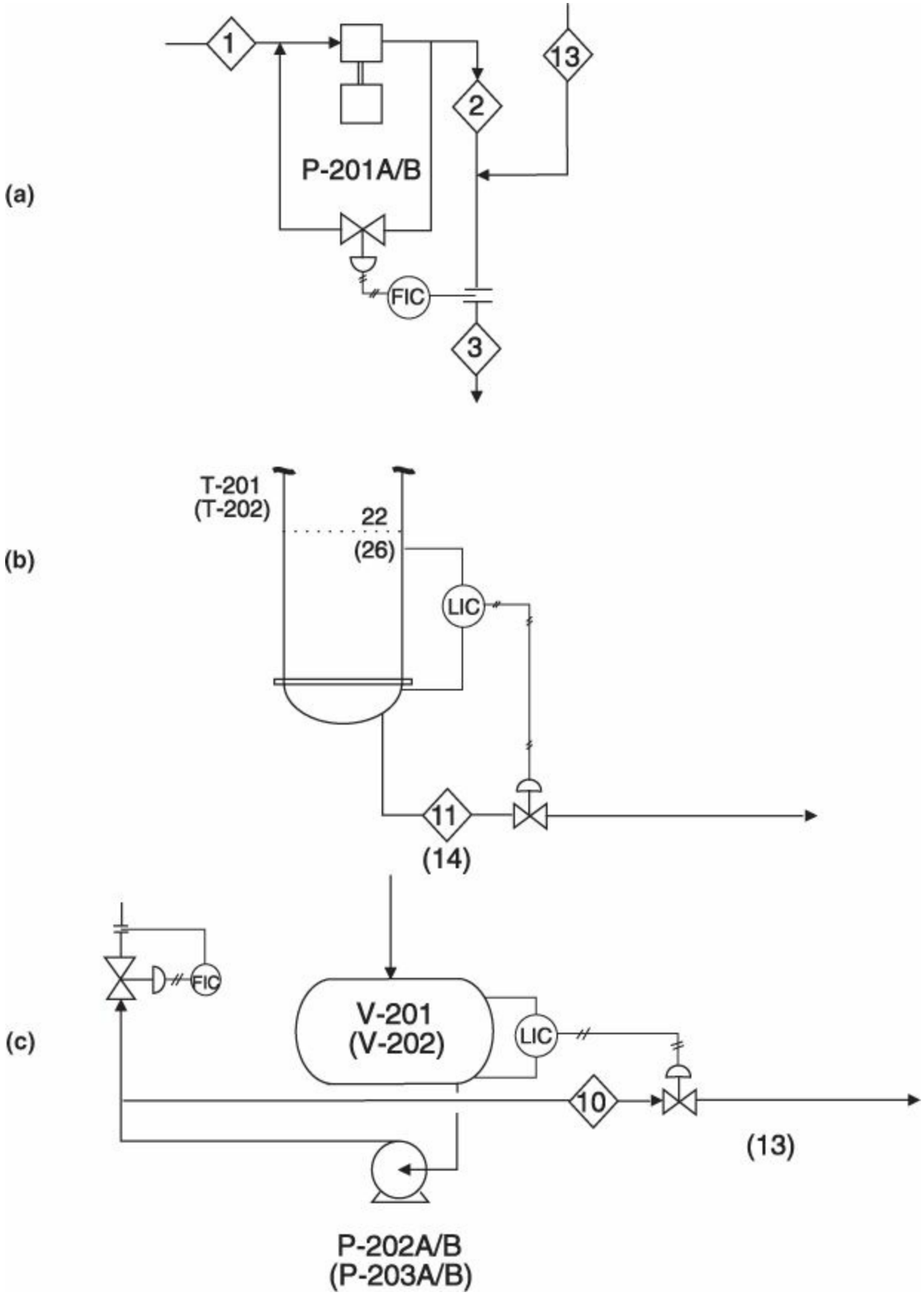


Figure E18.3. Feedback Control Loops on DME Flowsheet

Figure E18.3(a): In this figure, the object of the controller is to control the flowrate of Stream 4, which is sent through two heat exchangers and then into reactor R-201. Because P-201 is a positive displacement pump, the flow is controlled by varying the amount of liquid bypassed from the exit to the inlet of the pump (see Section 21.2.3). The signal to adjust the setting of the valve in the bypass line is obtained from an orifice placed in Stream 3. Thus, if the flow sensed by the pressure cell (not shown) across the orifice is below the set-point value, a signal is sent to the bypass valve to close the

valve slightly. This has the effect of reducing the amount of liquid bypassed around the pump, and that increases the flow of Stream 2 and hence increases the flow of Stream 3. If the flow of Stream 3 lies above the set point, then the opposite control action is initiated.

Figure E18.3(b): The flowrate of the bottoms product in both distillation columns is adjusted to maintain a constant level of liquid in the bottom of the tower. The control strategies for the bottoms of both T-201 and T-202 are identical. Assume that the level in the bottom of the column drops below its set point. A signal from the level sensor would be sent to close slightly the valve on the bottoms product stream. This would reduce the flow of bottoms product and result in an increase in liquid inventory at the bottom of the column, causing the liquid level to rise. If the liquid level were to increase above the set-point value, then the opposite control action would be initiated.

Figure E18.3(c): The control strategy at the top of both columns (T-201 and T-202) is illustrated in Figure E18.3(c). The control action was explained previously in Example 18.1, where the reflux stream is held constant by a control valve and the liquid level in the reflux drum is held constant by adjusting the flow of the overhead product.

It should be noted that at present there is no product quality (purity) control on either column. This is addressed under cascade control below.

18.5.2. Feed-Forward Control and Regulation

Process input variables are measured and used to provide the appropriate control action.

Advantages. Changes in the output process variable are predicted, and adjustments are made before any deviation from the desired output takes place. This is useful, especially when there are large lag times in the process.

Disadvantages. It is necessary to identify all factors likely to cause a change in the output variable and to describe the process by a model. The regulator must perform the calculations needed to predict the response of the output variable. The output variable being regulated is not used directly in the control algorithm. If the control algorithm is not accurate and/or the cause of the deviation is not identified, then the process output variable will not be at the desired value. The accuracy and effectiveness of the control scheme are directly linked to the accuracy of the model used to describe the process.

Example 18.4 illustrates how feedback control, feed-forward control, or a combination of both can be used to control a process unit.

Example 18.4.

Consider the process illustrated in Figure E18.4. The object is to cool, in a heat exchanger, a process stream (Stream 1) to a desired temperature (Stream 2) using cooling water supplied from a utility header. In Figure E18.4(a), a feedback control scheme is illustrated. The control strategy is to measure the temperature of the process stream leaving the heat exchanger (Stream 2) and to adjust the flow of cooling water to obtain the desired temperature. Thus, if the temperature of Stream 2 were to be greater than the desired set-point value, then the control action would be to increase the flow of cooling water and vice versa.

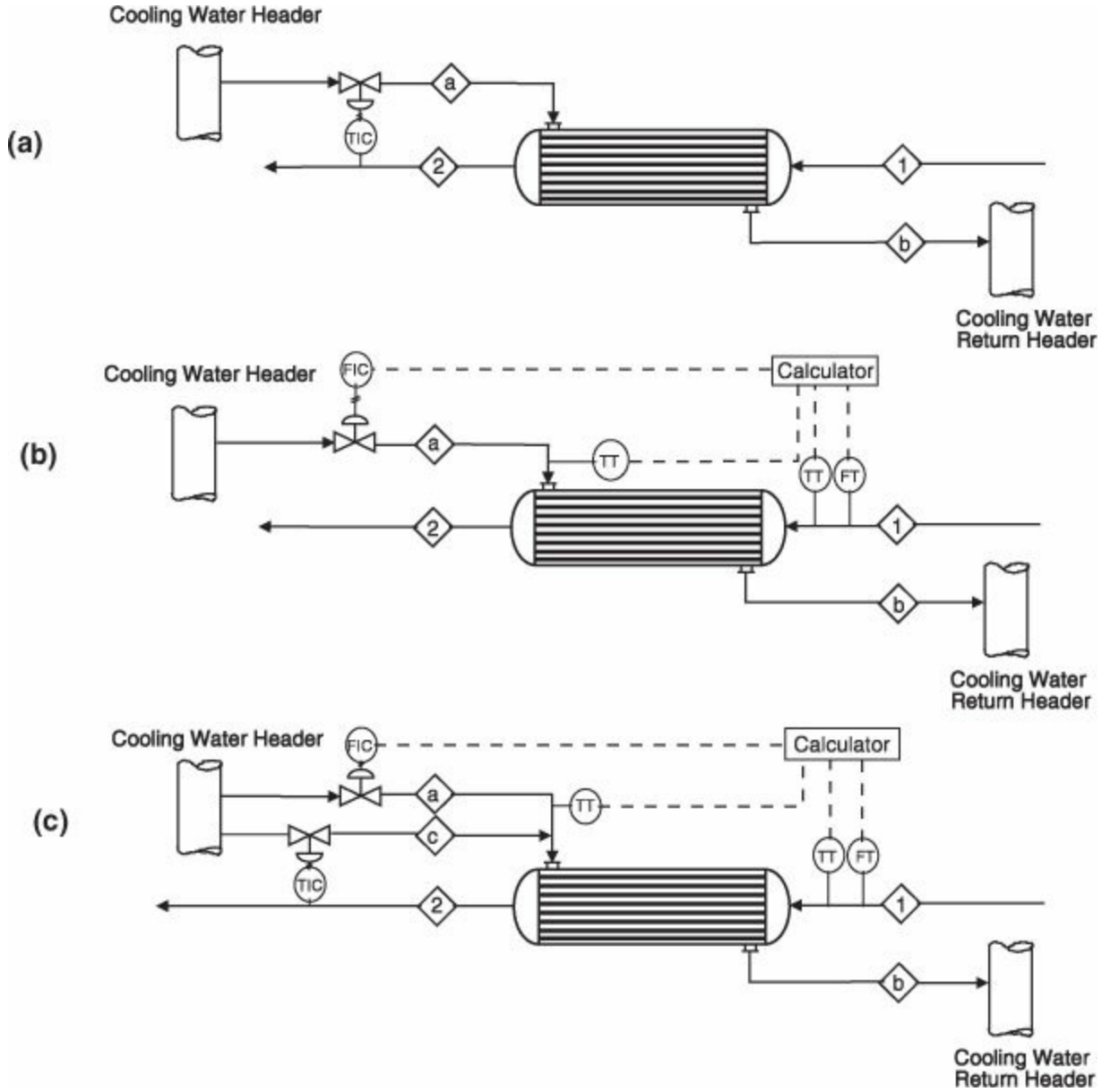


Figure E18.4. Control Strategies for Cooling a Process Stream

A feed-forward control scheme for this process is illustrated in Figure E18.4(b). Here, both the flowrate and temperature of the input process stream and the inlet cooling water temperature are measured. A calculation is then made that predicts the flowrate of cooling water needed to satisfy the energy balance and the exchanger performance equations as given in Chapter 21. Using the subscripts *c* and *p* to refer to the cooling water and process streams, respectively,

$$Q = \dot{m}_c C_{p,c}(T_b - T_a) \qquad \text{(E18.4a)}$$

$$Q = \dot{m}_p C_{p,p}(T_1 - T_2) \qquad \text{(E18.4b)}$$

$$Q = UA \frac{(T_1 - T_b) - (T_2 - T_a)}{\ln \dfrac{(T_1 - T_b)}{(T_2 - T_a)}} \qquad \text{(E18.4c)}$$

From Equations (E18.4a) through (E18.4c), the variables can be categorized as unknown, measured, known, and specified according to Table E18.4.

Table E18.4. Variables in Example 18.4

Unknown	Measured	Known	Specified
$Q, \dot{m}_c, T_b$	$\dot{m}_p, T_a, T_1$	$C_{p,c}, C_{p,p}, U, A$	T_2

Therefore, for a given value of the exit process temperature (T_2), Equations (E18.4a), (E18.4b), and (E18.4c) can be solved to give the unknowns in the table. Thus, by measuring the inlet process stream flow and temperature and the inlet cooling water temperature, the model given by Equations (E18.4a) through (E18.4c) can be solved to yield the desired value of the cooling water flowrate. The valve on the cooling water inlet can then be adjusted to give this value. There are some assumptions associated with this model that will affect the performance of this control scheme. The first assumption is that both streams flow countercurrently, and hence the exchanger effectiveness factor, F, is assumed to be equal to 1. If the value of F is not close to unity, then the model given above will not be accurate. However, the model can be modified by including another equation to calculate F based on the process variables. A more serious assumption is that the overall heat transfer coefficient, U, has a constant value. In real processes, this is seldom the case, either because of flowrate changes or due to fouling of heat-exchange surfaces occurring throughout the life of the process. As the heat transfer surfaces foul or flowrates change, the value of U changes and the predictions of the above model will deviate increasingly from the true value of T_2. This illustrates one of the major disadvantages of feed-forward control strategies, in that the efficacy of the control strategy is only as good as the predictions of the equations used to model the process.

An alternative scheme to pure feed-forward control is to use a combination of feedback and feed-forward control strategies. This is illustrated in Figure E18.4(c) and discussed below.

In feed-forward control, the process must be modeled using material and energy balances and the performance equations for the equipment.

The effectiveness of feed-forward control is strongly influenced by the accuracy of the process model used.

18.5.3. Combination Feedback and Feed-Forward Control

By correctly combining these two control strategies, the advantages of both methods can be realized. The feed-forward strategy uses measured input variables to predict changes necessary to regulate the output. The feedback regulator then measures the regulated output variable and makes additional changes to ensure that the process output is at the set point.

Advantages. The advantages of both feedback and feed-forward regulation are achieved. The feed-forward regulator makes the major corrections before any deviation in process output takes place. The feedback regulator ensures that the final set-point value is achieved.

Disadvantages. The control algorithm and hardware to achieve this form of control are somewhat more complicated than either individual strategy.

Example 18.5 considers the operation of the combination of feedback and feed-forward control.

Example 18.5.

Returning to Example 18.4 and looking at the operation of the combined control strategy illustrated in Figure E18.4(c), it can be seen that this system is essentially a combination of Figures E18.4(a) and E18.4(b). The feed-forward scheme of Figure E18.4(b) has been retained but is used to regulate only

a fraction of the cooling water required, say, 80%. In addition, a feedback control loop has been added. This feedback loop consists of a second parallel cooling water feed stream that will be adjusted so as to maintain the desired set-point value for the temperature of Stream 2. The amount of cooling water regulated by the feedback loop is the remaining 20% required to satisfy the regulation. This combined system will respond quickly to changes in process flowrate or inlet temperatures via the feed-forward control loop. In addition, a second cooling water stream is adjusted, based on the feedback control loop, to control exactly the process outlet temperature.

18.5.4. Cascade Regulation

The **cascade** system uses controllers connected in series. The first control element in the system measures a process variable and alters the set point of the next control loop.

Advantages. This system reduces lags and allows finer control.

Disadvantages. It is more complicated than single-loop designs.

Example 18.6 illustrates cascade regulation.

Example 18.6.

Consider the control of the top-product purity in distillation column T-201 in the DME process. As shown in Example 18.3, the material balance control is achieved by a flow controller on the reflux stream and a level controller on the top product stream. From previous operating experience, it has been found that the top-product purity can be measured accurately by monitoring the refractive index (RI) of the liquid product from the top of the column, Stream 10. Using a cascade control system, indicate how the control scheme at the top of T-201 should be modified to include the regulation of the top-product composition.

The solution to the problem is illustrated in Figure E18.6. An additional control loop has been added to the top of the column that consists of a refractive index measuring element that sends a signal to the flow controller placed on the reflux stream (Stream 16). The purpose of this signal is to change the set point of the flow controller. Consider a situation where the purity of the top product has fallen below its desired value. This change may be due to a number of reasons; for example, the flowrate or purity of the feed to the column may have changed. However, the reason for the change is not important at this stage. The decrease in purity will be detected by the change in refractive index of the liquid product, Stream 10, and a signal will be sent from the RI sensor to increase the reflux flowrate of Stream 16. The flow of Stream 16 will increase, which will result in an improved separation in the column and an increase in purity of the top product. For an increase in product purity, the reverse control action will occur.

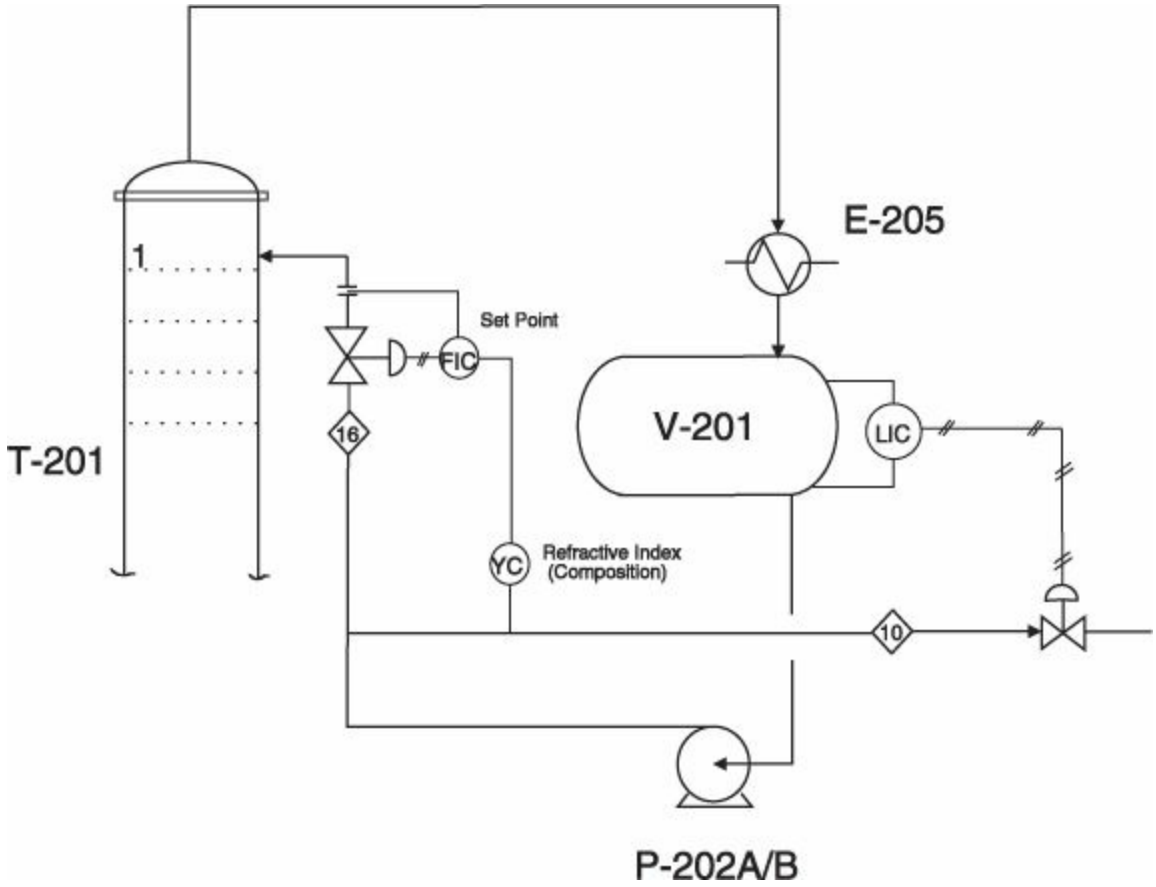


Figure E18.6. Cascade Control for DME Overhead Product Purity

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18.5.5. Ratio Control

In a number of process systems, it is desired to maintain the ratio between two concentrations or between two flowrates entering a system to satisfy some desired objective. Ratio control has been applied to both reacting and nonreacting systems. Examples of reacting systems include the water-gas shift (WGS) reactors where the H_2O/CO ratio is maintained at some optimum value, the Claus unit where a desired H_2S/SO_2 ratio is maintained at the Claus reactor inlet, and combustors where a desired $(C + H_2)/O_2$ ratio is maintained to ensure very low levels of CO in the combustion product stream. Examples of nonreacting systems include slurry-fed systems where the ratio of the flowrate of the liquid to the flowrate of the solids must be maintained at some value to ensure the flowability of the slurry, steam atomization of burners where the steam-to-fuel flowrate is maintained for desired atomization, and systems where two streams are mixed to modify the physical properties of one of the streams such as its surface tension, viscosity, density, and so forth.

Advantages. Ratio control is a special type of feed-forward control system in which a ratio is maintained to achieve a desired control objective. Therefore, this strategy has all the advantages of a feed-forward control system but without the need of a process model, which is a requirement for feed-forward control.

Disadvantages. The main assumption used in ratio control is that the controlled ratio is the key variable, so that if it is maintained at a desired set point, the control objective will be satisfied. However, there may be other variables that play a significant role in a given operating region. For example, for a water-gas shift (WGS) reactor, the H_2O/CO ratio might be maintained at the inlet to obtain a desired conversion of CO in the system. However, the actual conversion of CO depends

upon many other variables such as residence time, catalyst activity, presence of other impurities, and so on. Thus, the actual control objective may not be satisfied by ratio control alone. The advantages and disadvantages of ratio controllers are investigated further in Example 18.7.

Example 18.7.

Consider the first water-gas shift (WGS) reactor shown in Figure B.12.1. It is desired to maintain the H_2O/CO ratio at the inlet of the first WGS reactor at a given value. The flowrate of the steam, Stream 4, can be manipulated to achieve the desired ratio. However, the pressure of Stream 4 is known to vary. Develop two control configurations to control the H_2O/CO ratio (R_{SP}). What are the advantages and disadvantages of each of the control configurations?

Solution

Figures E18.7(a) and E18.7(b) show two possible control strategies. In Figure E18.7(a), the flow of the syngas and its composition (CO and H_2O) are measured. Then the desired flowrate of Stream 4 required to achieve the desired ratio is calculated. If the molar flowrates of Streams 3 and 4 are F_3 and F_4, respectively, and the concentrations of CO_2 and H_2O in Stream 3 are y_{CO2} and y_{H_2O}, respectively, then the set point for the steam flow controller, F_{SP}, can be calculated to achieve R_{SP}, the desired H_2O/CO ratio.

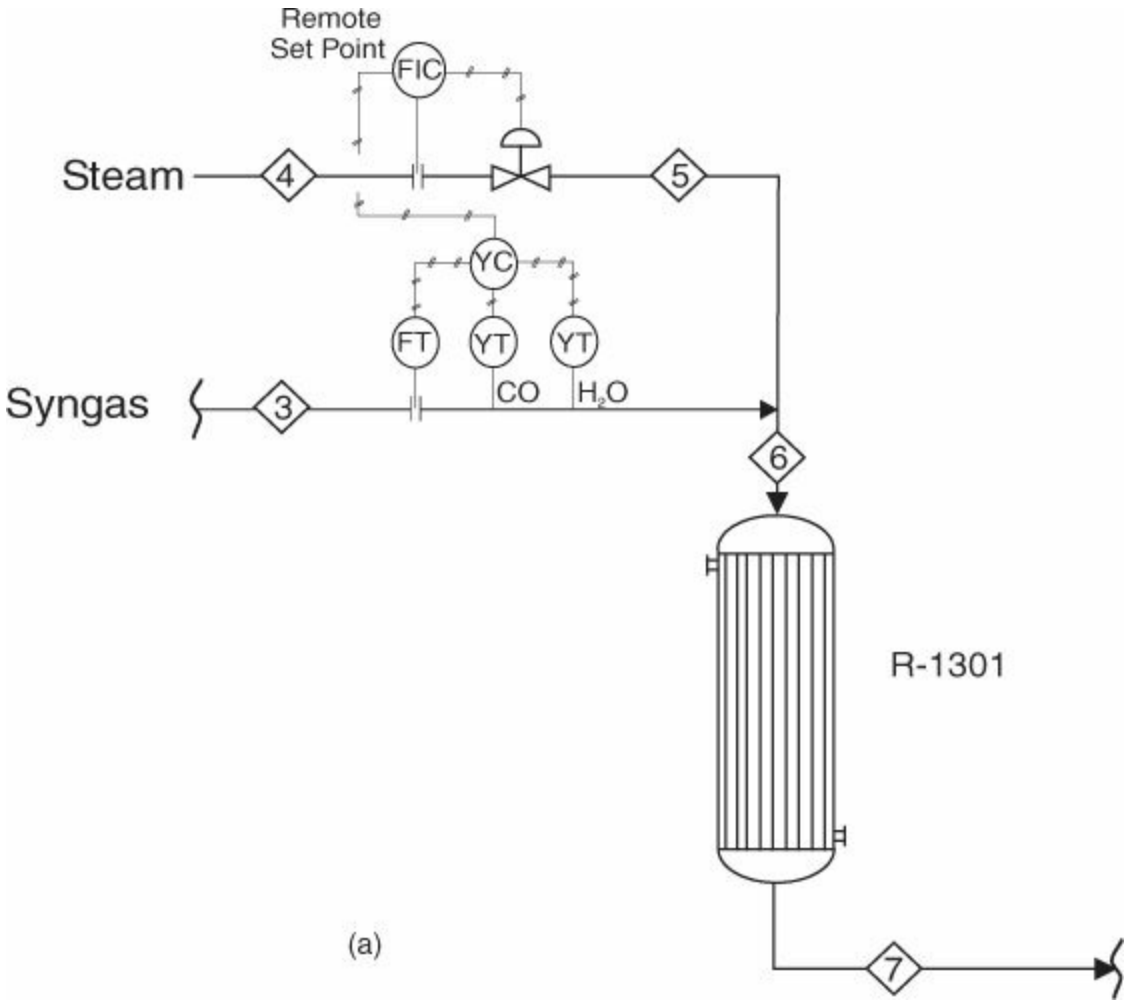


Figure E18.7. (a) Ratio Control Strategy of a WGS Reactor System Where the Inlet Flowrate to the System Is Measured

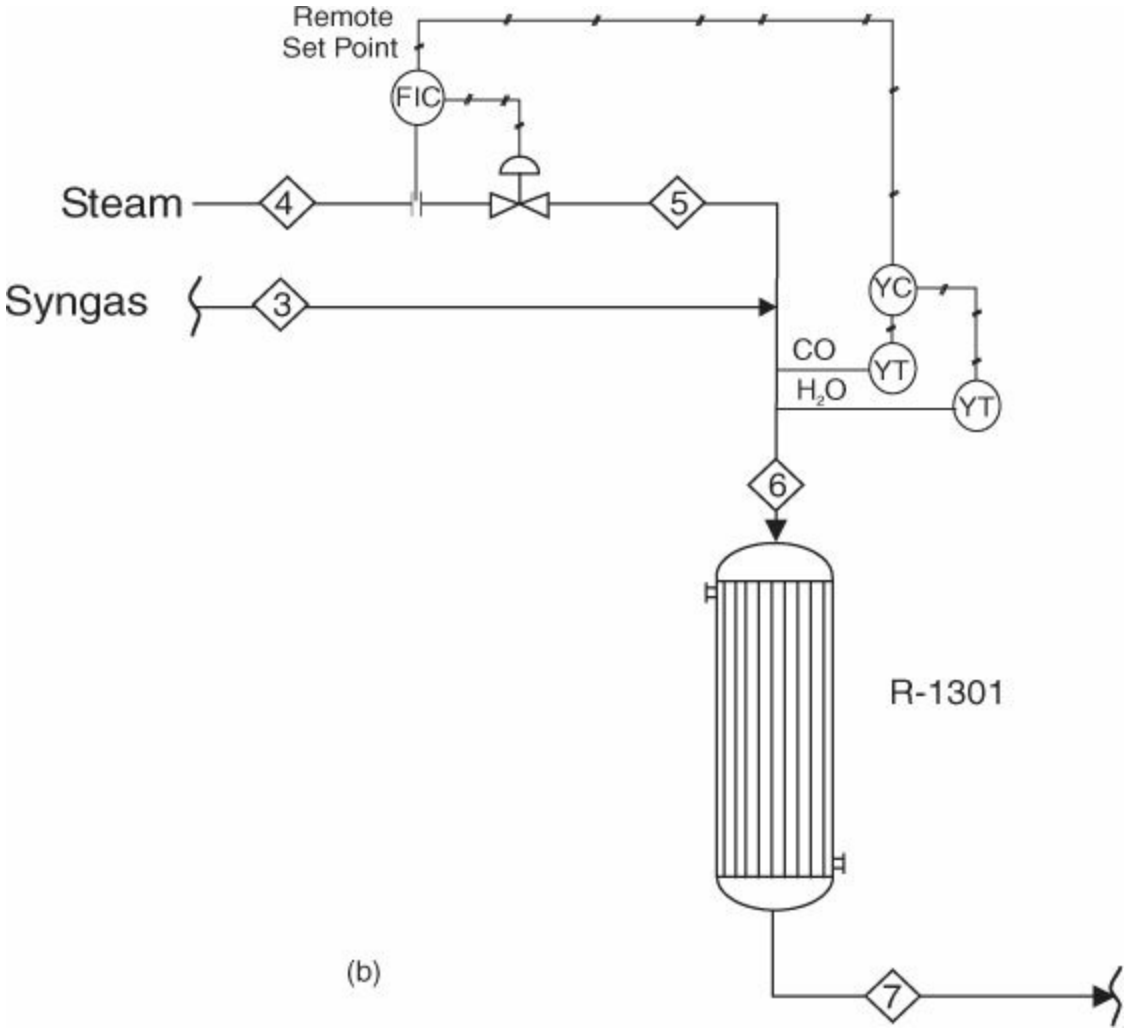


Figure E18.7. (b) Ratio Control Strategy of a WGS Reactor System Where the Inlet Flowrate Is Not Measured

$$F_{SP} = F_3(y_{CO}R_{sp} - y_{H_2O})$$

Since the steam pressure is known to vary, a cascade control strategy is considered so as to reject the disturbances in the steam flow caused by the varying steam header pressure. The advantage of this ratio control strategy is that the desired flowrate of the steam can be exactly calculated. The disadvantage is that the flowrate of the syngas has to be measured.

In the second strategy, shown in Figure E18.7(b), the flow of the steam is again set by a flow indicator controller (FIC). However, in this case, the set point of the FIC is adjusted so as to maintain the desired H_2O/CO measured at the reactor inlet. Therefore, in the control strategy shown in Figure E18.7(b), the composition (CO and H_2O) at the inlet of the reactor is measured and the flowrate of the steam is manipulated by a feedback mechanism. The performance of this control strategy depends upon the tuning of the ratio controller as the exact set point FSP cannot be calculated.

18.5.6. Split-Range Control

A split-range control strategy is used when a single manipulated variable (MV) is not sufficient to maintain the controlled variable (CV) at its set point. Split-range control can be used for both servo and regulatory controls. In the case of servo control, split-range control is used when the set point varies over a wide range such that it cannot be maintained with a single MV. A split-range control strategy is also used for regulatory control, where a single MV fails to reject the entire range of disturbances. Split-range control strategies vary based on how the control valves open and close in

response to the split-range controller. For example, if there are two control valves, A and B, then the following strategies may be considered:

Split-Range Strategy 1: At 0% output of the split-range controller, control valve A is 100% open and B is closed. As the split-range controller output increases from 0% to 100%, control valve A closes and control valve B opens. At 100% output of the split-range controller, control valve B is 100% open and A is fully closed.

Split-Range Strategy 2: At 0% output of the split-range controller, control valve A is 100% open and B is closed. As the split-range controller output increases from 0% to x% ($x < 100$; the value of x is often chosen to be 50), control valve A closes whereas control valve B remains closed. At x% output of the controller, both control valves are completely closed. As the controller output increases from x% to 100%, control valve B opens and reaches 100% open at 100% of the controller output. During this time, control valve A remains closed.

Split-Range Strategy 3: At 0% output of the split-range controller, both control valves are fully closed. As the controller output increases from 0% to x% (x < 100; the value of x is often 50), control valve A opens and becomes fully open when the controller output reaches x%. On the other hand, during this time, control valve B remains closed. As the controller output increases from x% to 100%, control valve B opens and becomes 100% open at 100% of the controller output. During this time, control valve A remains fully open.

Advantages. A split-range controller is required to avoid input saturation or to achieve satisfactory control over a wide operating region.

Disadvantages. Controller tuning can be very difficult as the process gain and transients for each of the inputs can be very different.

Example 18.8 shows the use of a split-range controller for servo control using split-range Strategy 1.

Example 18.8.

A tempered-water system is used for maintaining the temperature of a batch reactor. The set point for the tempered water varies between 45°C and 90°C. Feed water is available at 40°C, and steam is available at 120°C. Develop a split-range control configuration to maintain the temperature of this tempered-water system.

Figure E18.8 shows the split-range control configuration. When the set point is 45°C, the steam control valve is open a small amount. As the set point increases, the water control valve keeps closing while the steam control valve starts to open. When the set point is 90°C, the steam control valve is fully open, while the water control valve will be at some minimum open value. In this example, a modified split-range Strategy 1 is being used. In this strategy, the water and steam valves are clamped so that a minimum flow of each stream will occur at the extreme limits of the controller to maintain the correct energy balance.

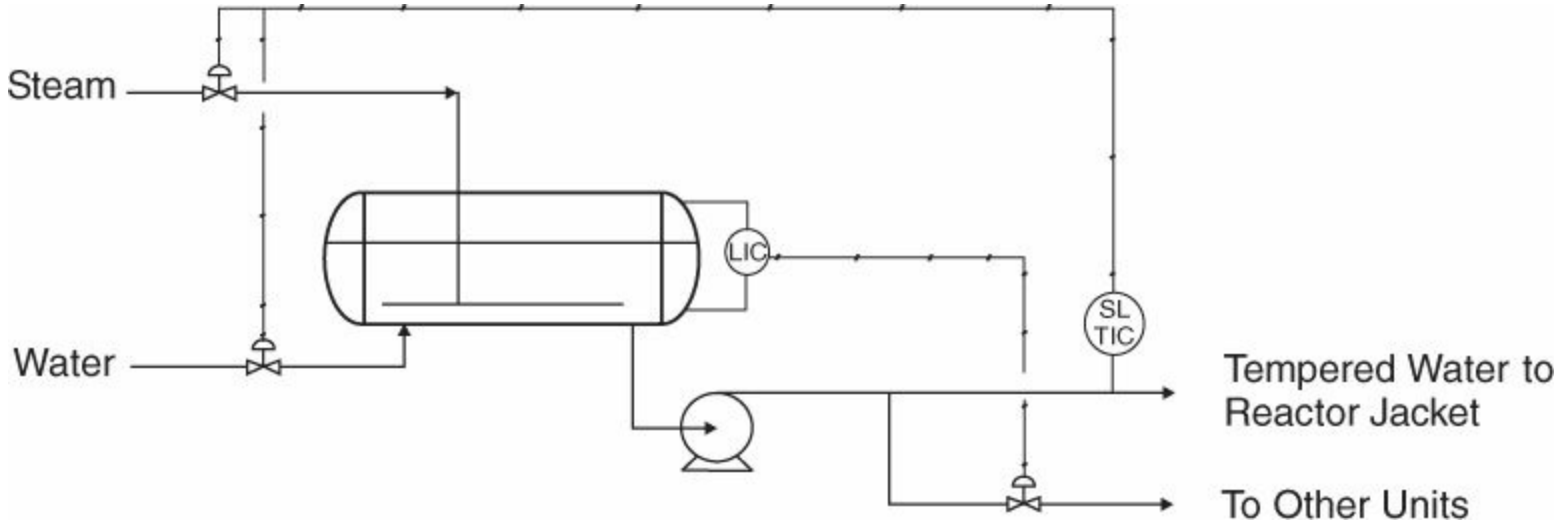


Figure E18.8. Temperature Control of a Tempered-Water System Using Split-Range Control

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Example 18.9 shows a split-range control strategy for regulatory control using split-range Strategy 2.

Example 18.9.

Figure B.6.1 shows the process for ethylene oxide production. Noncondensable light gases are vented from V-701. The amount of this gas at steady-state design conditions is very low. During plant operation, it is known that the amount of noncondensable gas in V-701 varies. Devise a split-range control strategy where the pressure of V-701 can be maintained at its steady-state design value even though the amount of noncondensable gas becomes negligible or higher than the design value.

The split-range control strategy is shown in Figure E18.9, where split-range Strategy 2 is used. Under the design condition, light gases are vented from V-701; consequently, only the vent valve (in Stream 34) remains open. If the pressure keeps decreasing, then its set point, the split-range controller output, keeps decreasing. This causes the vent valve to close gradually, being fully closed at 50% of the controller output. If the pressure decreases further, the split-range controller output decreases further. As a result, the control valve for makeup gas starts opening and becomes fully open at 0% of the controller output. The vent and makeup control valves should be designed considering the extremes of the flow of noncondensable gases in the system.

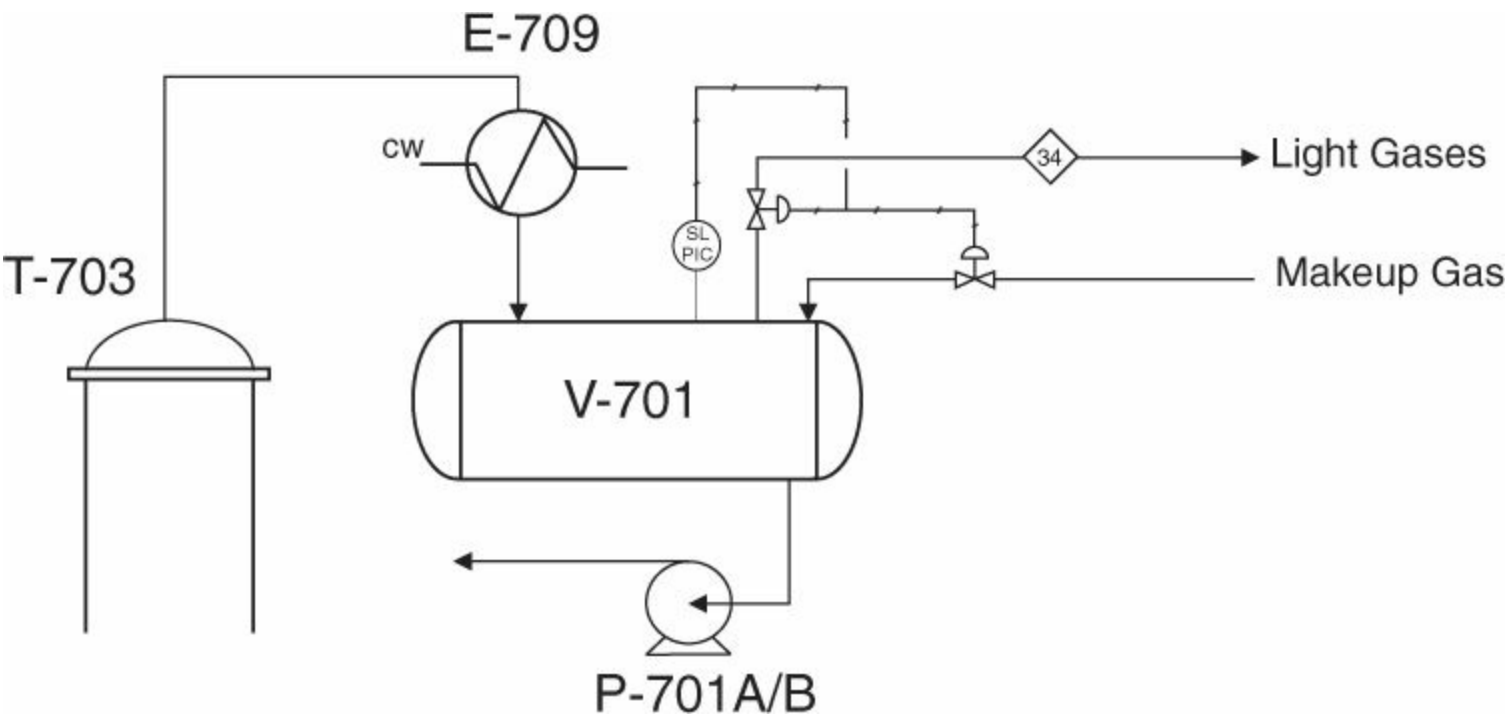


Figure E18.9. Split-Range Pressure Control of the EO Column Reflux Drum in Ethylene Oxide Production

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These control strategies do not represent a comprehensive list of possibilities. The range of strategies is very large. This is due, in part, to the flexibility that software has added to the control field by allowing sophisticated process models to be used in simulating processes, as well as the use of more complicated control algorithms.

No mention has been made of the types of controller (proportional, differential, integral, etc.) and strategies to tune these controllers. Such information is covered in traditional process control texts, such as Stephanopolous [3], Coughanowr [4], Smith and Corripio [5], Seborg et al. [6], and Marlin [7].

18.6. Exchanging Heat and Work Between Process and Utility Streams

In order to obtain the correct temperatures and pressures for process streams, it is often necessary to exchange energy, in the forms of heat and work, with utility streams. In order to increase the pressure of a process stream, work is done on the process stream. The conversion of energy (usually electrical) into the pressure head is provided by pumps (for liquid streams) or compressors (for gas streams) that are inserted directly into the process stream. For a process gas stream undergoing a significant reduction in pressure, the recovery of work using a gas turbine may have a significant impact (favorable) on process economics. In order to change the temperature of a process stream, heat is usually transferred to or from a process by exchange with a heat transfer medium—for example, steam and cooling water. As shown in Chapter 15, it may also be beneficial for heat to be exchanged between process streams using heat integration techniques.

18.6.1. Increasing the Pressure of a Process Stream and Regulating Its Flowrate

In the preceding examples, streams were available at constant pressure. This is normally true for utility streams. However, for a process stream, the pressure may change throughout the process. When higher pressures are needed, pumps or compressors are installed directly into a process stream. These units convert electrical energy into the required pressure head for the stream.

It should be noted that when a pump or compressor is required in a process, it is necessary to specify the type of fluid and fluid conditions, the design flowrate of fluid, the inlet (suction) and outlet (discharge) pressures at the design conditions, and an overdesign (safety) factor. The pump or compressor conforming to these specifications must be able to operate at and somewhat above the design conditions. However, in order to regulate the flow of the process streams, as will be required throughout the life of the process, it is necessary to implement a control or regulation system. Some typical methods of regulating the flow of process streams are outlined below and shown in Figure 18.5.

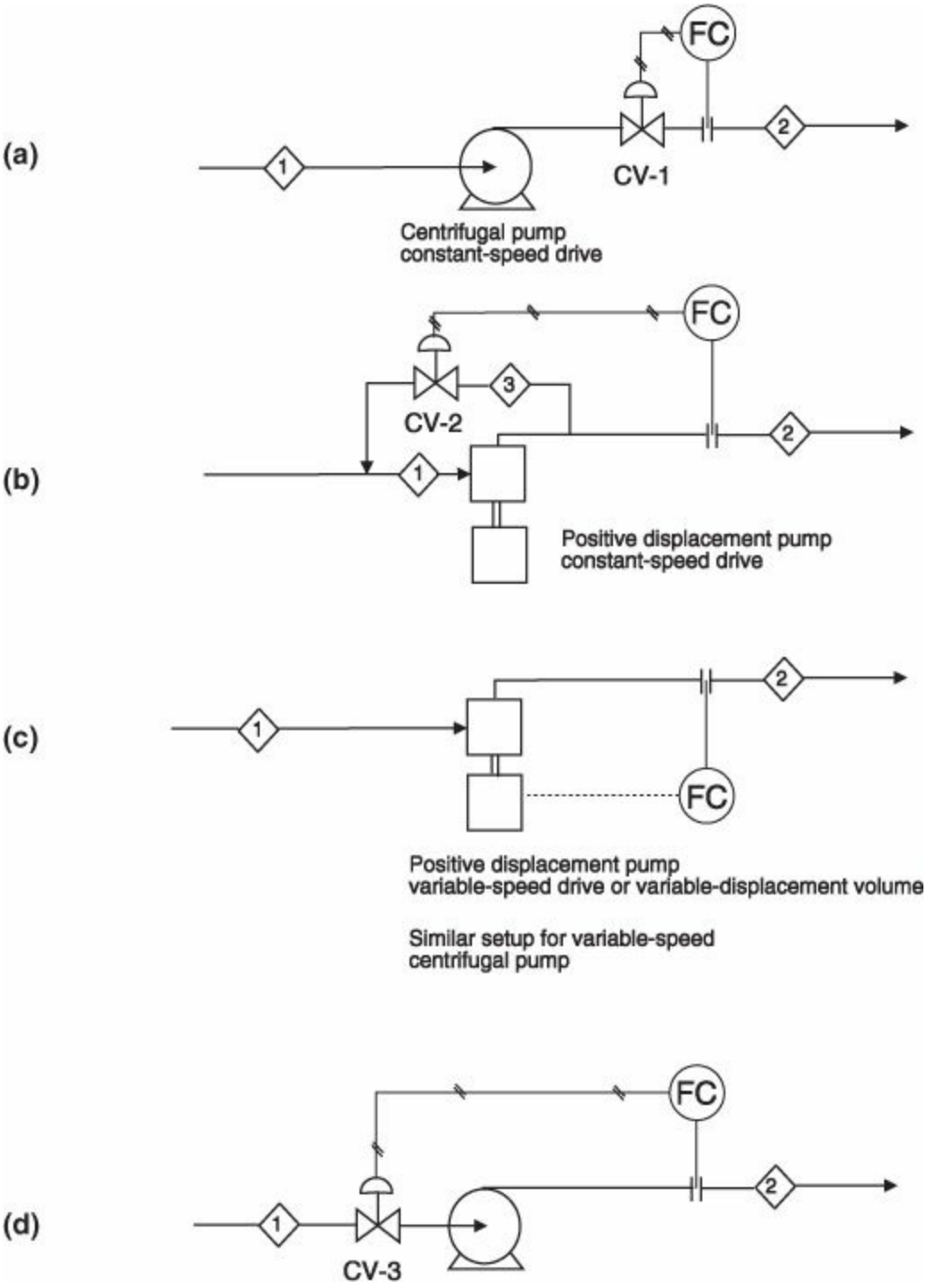


Figure 18.5. Flowrate Feedback Control Schemes for Pumping Liquids

Figure 18.5(a) shows a centrifugal pump system that increases the pressure of a process stream. The position of the control valve, CV-1, is at the discharge side of the pump. The flowrate of Stream 2 is changed in order to regulate the flow of the stream passing through the pump. The operation of the pump and the interaction of the pump curve, the system curve, and the control valve will be discussed

in the presentation of pump performance curves in Chapter 21. In reviewing this material, it is important to remember that the maximum flowrate of the fluid is determined by the intersection of the pump and system curves. Regulation of flowrate is possible only for flows less than this maximum value, that is, to the left of the intersection of the pump and system curves, point "a" in Figure 21.6.

Figure 18.5(b) shows a positive displacement pump increasing the pressure of a process stream. The positive displacement pump can be considered to be a constant-flow, variable-head device; that is, it will deliver the same flowrate of fluid at a wide range of discharge pressures. Thus

$$\dot{v}_2 + \dot{v}_3 = \dot{v}_1 = \text{a constant} \qquad (18.2)$$

For this reason, in order to regulate the flow of the process stream, Stream 2, a portion of the output stream from the pump must be recycled. In Figure 18.5(b) this is accomplished by returning Stream 3 to the suction side of the pump. By altering the position of valve CV-2, the recycle stream flowrate is altered, and because the flow of liquid through the pump is almost constant, this also provides flow regulation for the main process stream, Stream 2. It should be noted that one should never throttle the output stream of a positive displacement pump because the pump curve is almost vertical and the flow will change little with throttling, although the discharge pressure will increase drastically (see Section 21.2.3, Figure 21.8).

Figure 18.5(c) uses a variable-speed drive—or variable displacement volume, for a positive displacement pump—to regulate the flow of the process stream. For a centrifugal pump, the impeller speed is regulated to provide the required flow, at the desired pressure, for the process stream. The advantage of using this type of control strategy is that there is no wasted energy due to throttling across a control valve. However, variable-speed controls and motors are expensive and less efficient. Therefore, this type of control scheme is usually cost effective only for gas blowers, compressors, and large liquid pumps, because a large savings in utilities is required to offset the large capital investment for the variable-speed drives and controls.

Figure 18.5(d) regulates the input flow with a valve, CV-3, installed in the suction line to the pump. The position of CV-3 is altered to provide the desired flowrate of fluid. This may work well for gases but is seldom used for liquid pumps. For liquid streams, the reduction in pressure at the pump inlet increases the possibility of cavitation; that is, $NPSH_A$ is reduced drastically. The causes of cavitation and NPSH calculations will be covered in Section 21.2.4. On the other hand, for the case of gas compression using centrifugal machines, the throttling of the inlet stream is essential for start-up purposes. Thus, this method is often the preferred control strategy for flow regulation in centrifugal blowers and compressors.

All the control systems shown in Figure 18.5 for the regulation of liquid process streams can be applied to compressor systems to regulate the flow of gaseous process streams.

18.6.2. Exchanging Heat between Process Streams and Utilities

The amount of heat added to or removed from a process stream is usually altered by changing the flow or pressure of utility streams. The primary utility streams in a chemical plant are as follows:

1. Cooling water is used to remove heat from a process stream. The heat transferred to the coolant adds to the sensible heat (enthalpy) of the coolant stream (temperature increases).
2. Air can be used to remove heat from a process stream and is often used in product coolers and overhead condensers. The heat transferred to the coolant adds to the sensible heat (enthalpy) of the coolant stream (temperature increases).

3. Steam condensation is used to add heat to a process stream. The heat transferred from the steam decreases the enthalpy of the steam (steam condenses).
4. Boiler feed water (bfw) is used to remove heat from a process stream to make steam that can be used elsewhere in the process. The heat transferred to the bfw increases the enthalpy of the bfw stream (bfw vaporizes).

When using cooling water or air in which there is no change of phase of the utility stream, regulation is generally performed by changing the flowrate of the cooling stream. For example, see Figure E18.4 and Example 18.4. In this section, the focus is on systems in which the utility stream undergoes a change of phase. The focus is on boiler feed water and steam. However, the results apply equally well to other heat transfer media that undergo a phase change. It is further assumed that utility streams are taken from and returned to headers and that the process streams are a single phase. The control of reboilers and condensers in a distillation column is covered in the case study on distillation given in the following section.

There are many ways to regulate systems using steam. No effort is made here to try to present an exhaustive list of possible schemes, but the focus is on several of the more common techniques. Figures 18.6 and 18.7 show several systems used to control the transfer of heat between a utility stream and a process stream. The systems on the left-hand side of the figures add heat to the process stream by condensing steam. Systems on the right-hand side remove heat from the process stream by vaporizing bfw. In either case, there are two phases present in equilibrium on the utility side of the exchanger. The temperature and pressure are related by the vapor-pressure relationship for water. If steam from the header is significantly superheated, it may be passed through a desuperheater prior to being fed to the heat exchanger. The desuperheater adds just enough condensate to saturate the steam. The reason for using a desuperheater is that highly superheated steam acts like a gas with a correspondingly low film heat transfer coefficient. Thus, a significant amount of heat-exchanger area may be taken up in desuperheating the steam. In such situations, it is more cost effective to saturate the steam before entering the heat exchanger, reducing significantly the heat exchange area required.

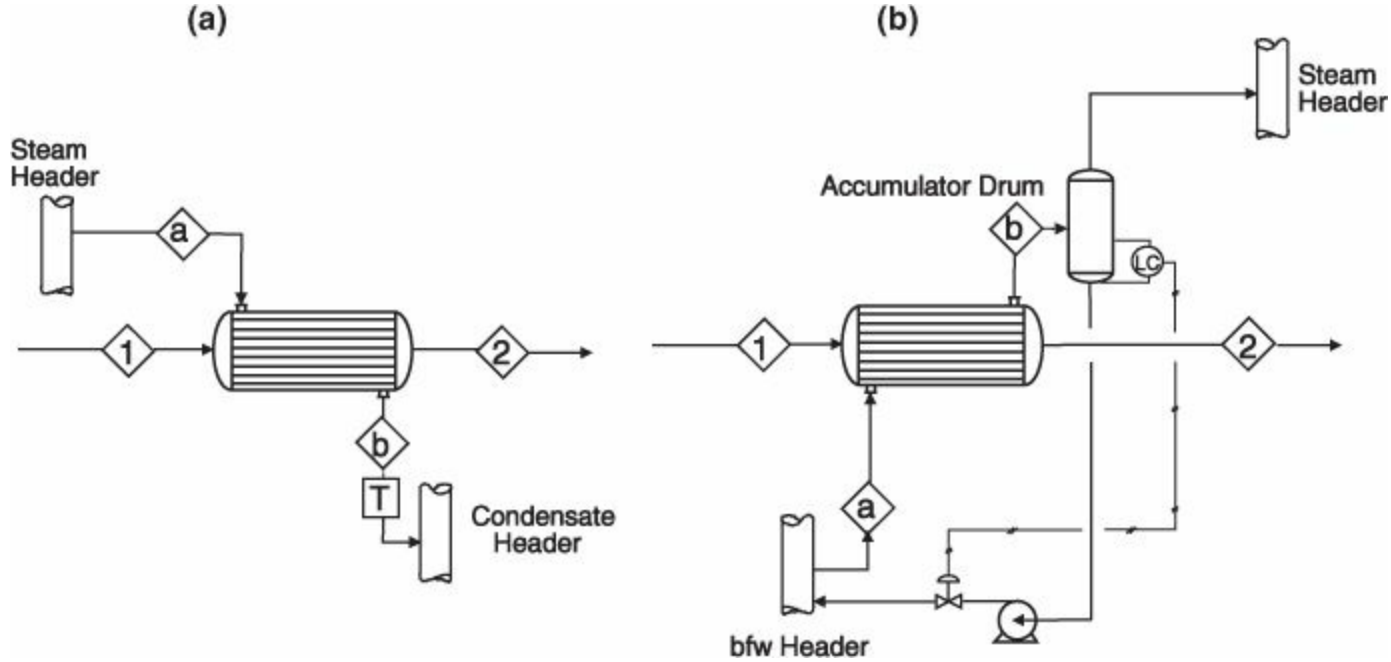


Figure 18.6. Unregulated Heat Exchanger Using Utility Streams with a Phase Change: (a) Process Heater and (b) Process Cooler

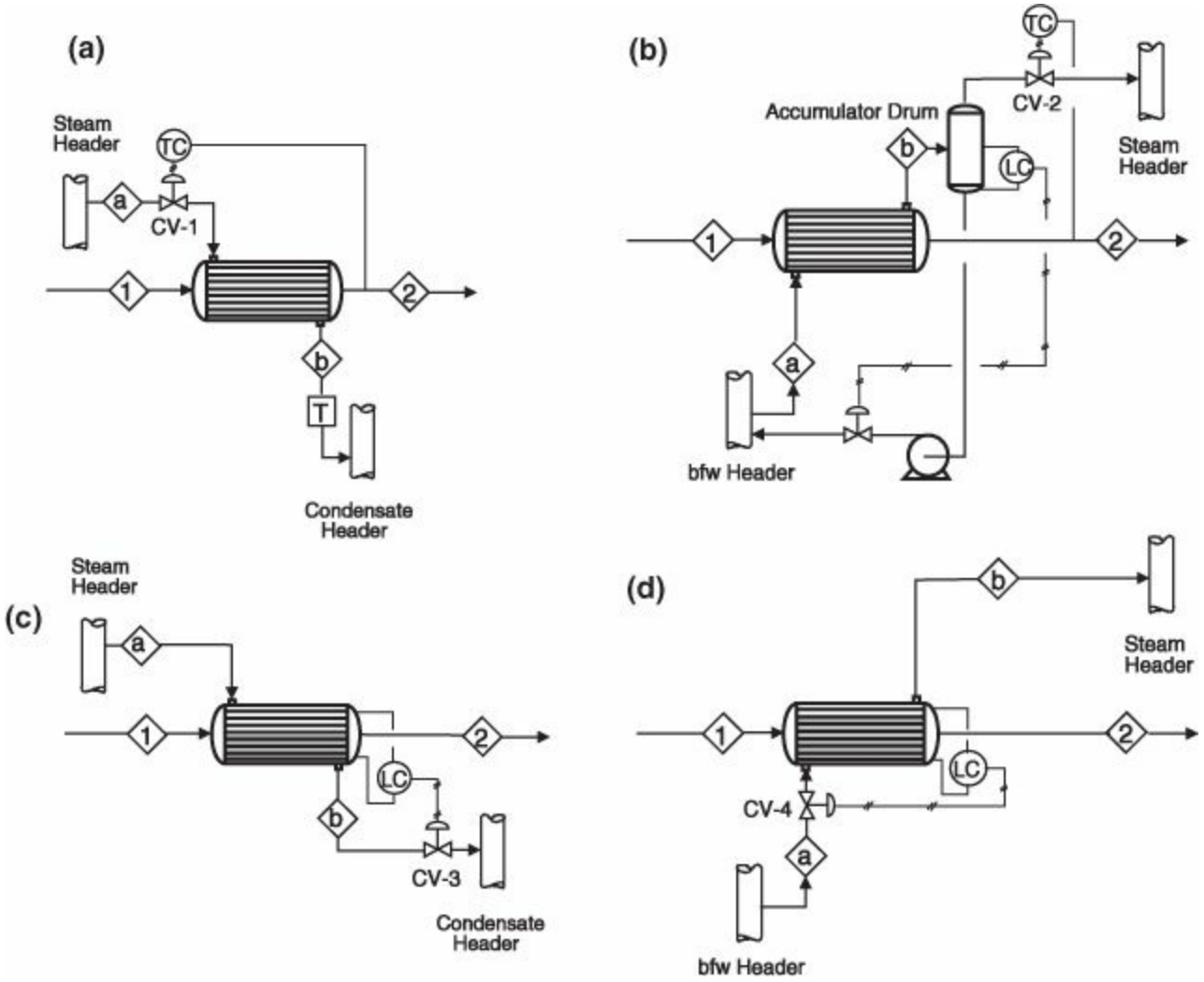


Figure 18.7. Regulation Schemes for a Heat Exchanger Using Utility Streams with a Phase Change

Figures 18.6(a) and 18.6(b) show a process heater (steam condenser) and a process cooler (bfw vaporizer) without control valves. The heater shown in Figure 18.6(a) includes a **steam trap** (shown as a box with a *T* in the middle) on the utility line. This steam trap separates the condensate formed from the vapor. The condensate is collected by the trap in the bottom of the exchanger and discharged intermittently to the condensate header. The steam flowrate, Stream a, is established by the rate at which heat is exchanged. This is different from normal utility flow regulation. As the steam condenses, there is a large decrease in the specific volume of the utility stream. Thus, steam is continually "sucked" from the header into the heat exchanger. For this system, no regulation of process temperature is attempted.

The process cooler shown in Figure 18.6(b) vaporizes bfw. In this case, the flow of bfw is more than sufficient to provide for the vaporization taking place. The exit stream is a two-phase mixture of steam and bfw. The bfw is separated from the vapor in an accumulation drum (phase separator) and recycled back to the inlet of the exchanger. Again, for this system, no regulation of process temperature is attempted.

Although no control schemes are implemented in the systems in Figures 18.6(a) and 18.6(b), to some extent, both systems are self-regulating. The reason for this self-regulating property is that the major resistance to heat transfer is on the process side (film heat transfer coefficients for condensing steam and vaporizing bfw are very high). Consider an increase in the flowrate of the process stream in Figure 18.6(a). As the flow increases, so does the process-side heat transfer coefficient, and this

increase is proportional to the (process flowrate)$^{0.8–0.6}$. See Table 20.1 for an explanation of the range of exponents. Because the major resistance to heat transfer is on the process side, this suggests that the overall heat transfer coefficient changes by the same amount. Thus, for a 10% increase in process flowrate, the overall heat transfer coefficient increases by 6% to 8%. Because the change in the overall heat transfer coefficient does not quite match the change in process flowrate, the exit temperature of the process stream, Stream 2, must drop slightly. Although the temperature of the exit stream drops, it does not drop by much due to the partial regulation provided by the increase in heat transfer coefficient.

In discussing the operation of this heat exchanger, no mention was made of the change in flowrate of the steam that would be required to provide the increase in heat-exchanger duty caused by the increased process flowrate. As the exchanger duty increases, more steam will condense, and this increased demand for steam does have an effect on the operation. It should be noted that steam is supplied from the header to the exchanger in the quantity that is required; that is, it is determined by the energy balance. As the steam flowrate increases, the frictional pressure losses in the supply pipe from the header to the exchanger increase. This causes the pressure on the steam side of the heat exchanger to decrease. Thus, the utility side of the heat exchanger essentially "floats" on the header pressure, with an appropriate pressure loss to account for flow through the supply line. As the pressure of the steam side of the exchanger drops, this causes the temperature at which the steam condenses to drop slightly, thus reducing the temperature driving force for heat exchange. However, compared with the change in heat transfer coefficient, this change is minor.

In order to regulate the temperature of the process stream leaving the heat exchanger, it is necessary to control the heat duty. In order to do this, a variable on the right-hand side of the heat-exchanger performance equation must be able to be regulated:

$$Q = UA\Delta T_{lm} \qquad (18.3)$$

This can be achieved by doing one or more of the following:

1. Regulate the temperature driving force (ΔT_{lm}) between the process fluid and the utility.
2. Adjust the overall heat transfer coefficient (U) for the heat exchanger.
3. Change the area (A) for heat exchange.

Two alternatives are considered for regulating the temperature of the process exit stream.

Regulate the Temperature Driving Force between the Process Fluid and the Utility. The systems shown in Figures 18.7(a) and 18.7(b) include a valve on the utility line. This valve is used to change the pressure of the utility stream in the exchanger. Because there are two phases present, the pressure establishes the temperature at which the phase change takes place. Reducing pressure reduces temperature according to the vapor-pressure-temperature relationship for water, for example, from Antoine's equation.

To increase the heat duty for the process heater, Figure 18.7(a), the temperature driving force is increased by increasing the pressure. This is achieved by opening CV-1 to decrease the frictional resistance to flow. Because CV-1 is located on the input side of the heat exchanger, opening the valve increases the pressure of the steam in the exchanger, and the temperature at which condensation occurs will also increase. To increase the process cooler heat duty, Figure 18.7(b), the temperature driving force is increased by opening CV-2, which decreases the resistance to flow. CV-2 is located on the discharge side of the utility, that is, between the exchanger and the steam header. In this case,

the exchanger once again floats on the steam header pressure. As CV-2 is opened, the pressure on the utility side of the exchanger decreases, and this reduces the temperature at which the bfw boils and increases the temperature driving force for heat transfer.

Adjust the Overall Heat Transfer Coefficient for the Heat Exchanger by Adjusting the Area Exposed to Each Phase. The systems shown in Figures 18.7(c) and 18.7(d) operate such that the interface between the liquid and vapor on the utility side of the exchanger covers some of the tubes. For this situation, a fraction of the heat-exchange area is immersed in the liquid region, with the remaining fraction in the vapor-phase region. The heat transfer coefficients and the temperature driving forces for these two regions differ significantly. Thus, by adjusting the level of the liquid-vapor interface in the exchanger, it is possible to regulate the duty.

For the process heater, Figure 18.7(c), decreasing the level increases the heat duty. The reason for this is that in the vapor-phase region the utility-side film coefficient and temperature driving force are large because steam is condensing. For the liquid-phase region, both the film coefficient and temperature driving force are low because the condensate is being subcooled. Therefore, as the liquid level decreases, more heat transfer area is exposed to condensing steam, the overall average value of UA increases, and the duty increases.

For the process cooler, Figure 18.7(d), increasing the liquid level increases the heat duty. The reason for this is that in the vapor-phase region, the utility-side film coefficient and temperature driving force are low because steam is being superheated. For the liquid-phase region, both the film coefficient and temperature driving force are high because the bfw is boiling. Therefore, as the liquid level increases, more heat transfer area is exposed to boiling water, the overall average value of UA increases, and the duty increases.

18.6.3. Exchanging Heat between Process Streams

The integration of heat between process streams is often economically advantageous, and a strategy to do this is explained in Chapter 15. When heat integration is implemented in a process, it is likely that heat exchange will occur between two process streams. The regulation of the flow of these process streams cannot effectively be used to control the heat transfer, because the flow of the two streams will be directly coupled. One method to control the exit temperature in such an exchanger is to bypass some portion of one or both of the process streams around the exchanger. By altering the amount of the stream that bypasses the equipment, temperature regulation is possible. This concept is considered further in Problem 18.4.

18.7. Logic Control

Logic control, often neglected in traditional undergraduate curricula, is an inseparable part of the overall control system design of a modern plant. Logic control executes logical steps and implements its decisions. Logic controllers are used in batch, continuous, and semi-batch processes. In Chapter 3, a number of examples were given that show the various steps involved in a typical batch process. A logic controller carries out this sequence of steps in a batch process and repeats them based on some preprogrammed condition(s). In continuous processes, logic controllers are used for plant/equipment safety and for avoiding interruption in plant operation in the case of failure of an equipment/section of a plant. Logic controllers ensure that the start-up conditions for an equipment/plant section (known as start permissives) are satisfied before an equipment/plant section is permitted to start. Moreover,

logic controllers continuously monitor various equipment/plant sections to avoid unsafe or dangerous situations and implement a series of preprogrammed steps in case of a shutdown. In a semibatch process, logic controllers usually execute a series of steps for smooth switching between two or more reactors/beds/process equipment at a regular interval. The platform in which the logic control system is usually implemented in industry is known as a programmable logic controller (PLC). The programming language for a PLC varies depending on the manufacturer. Examples of programming languages include Ladder Diagram (LD), Structured Text (ST), Sequential Function Chart (SFC), Function Block Diagram (FBD), and Instruction List (IL). LD is the most widely used language. Most of these programming languages follow the IEC-61131 standard. A single PLC can be used for implementing logic control of a number of equipment/process sections. Some manufacturers of special equipment such as turbines, compressors, and furnaces have dedicated PLCs for their equipment. Otherwise, even for large process plants, a single or a few PLCs may be sufficient. A brief discussion of LD will be provided, because of its popularity in the process industries.

Components of LD. An LD looks like a ladder—hence the name—where some logical processing is carried out at each "rung." An LD can span several thousands of rungs. The components of an LD are of three types: input devices or contacts, internal devices, and output devices or coils. Each rung usually starts with one or more contacts and terminates in one or more coils directly or through one or more internal devices. Based on the state of the input devices (true or false) and the mathematical/logical operation carried out in the internal devices, the state of the output device becomes true (i.e., energized) or false (i.e., deenergized). The state of the input devices can be altered (i.e., true or false) by field instruments (such as start/stop switches, level switches, etc.) or by internal flags that are generated by the output device(s). When the output device becomes energized or deenergized, it can operate some field equipment (such as start/stop a motor, open/close valves, etc.), or it can change the status of some internal flags. Contacts can be used as internal devices as well. A few basic components of an LD are shown in Figure 18.8. Figure 18.8(a) represents a contact that is normally open (NO). Its state can be altered by a flag such as a motor start switch, a limit switch, or any internal flag. For example, if a motor start switch changes the state of an NO contact, then initially the output of this contact is false or 0. As the motor start button is pressed, the contact becomes closed, changing its state to true or 1. Figure 18.8(b) represents a contact that is normally closed (NC), that is, normally true. Its status can be changed to false by a flag as before. Figure 18.8(c) represents an internal device known as one-shot rising (OSR) that can be used to trigger a one-time event. When the input to the OSR becomes true, its output becomes true for one cycle, then becomes false in subsequent scans unless its input changes to true again. Figure 18.8(d) shows a coil that becomes true when its input flag is true. Figure 18.8(e) shows an output latch that becomes true when its input becomes true. It then remains true even when its input turns false. The output is triggered false when it is unlatched by an "output unlatch," shown in Figure 18.8(f). Many other components are used in an LD. Examples include timer on/off delay, various comparators, function blocks, and various mathematical operations that can be used to turn a signal on or off. For a detailed discussion of these topics, refer to one of the many good books in this area [9-11].

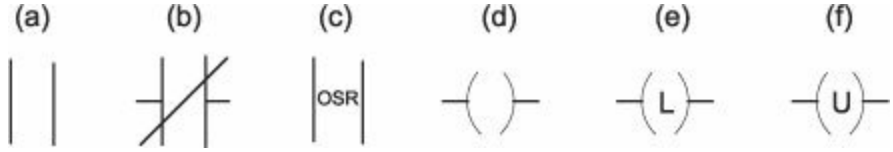


Figure 18.8. Basic Components of an LD: (a) Normally Open (NO) Contact; (b) Normally

Example 18.10.

Figure E18.10(a) shows the schematic of a storage vessel, V-101. Pump P-101 has two start and stop switches (one in the plant and the other in the control room). Assume that the pump start switch is a momentary signal, that is, is true as long as the start button is pushed. The pump can be started or stopped by either of the start/stop switches. Pump P-101 should stop if the level of the vessel becomes low as detected by the level switch, LSL-101. Develop a ladder diagram for the pump.

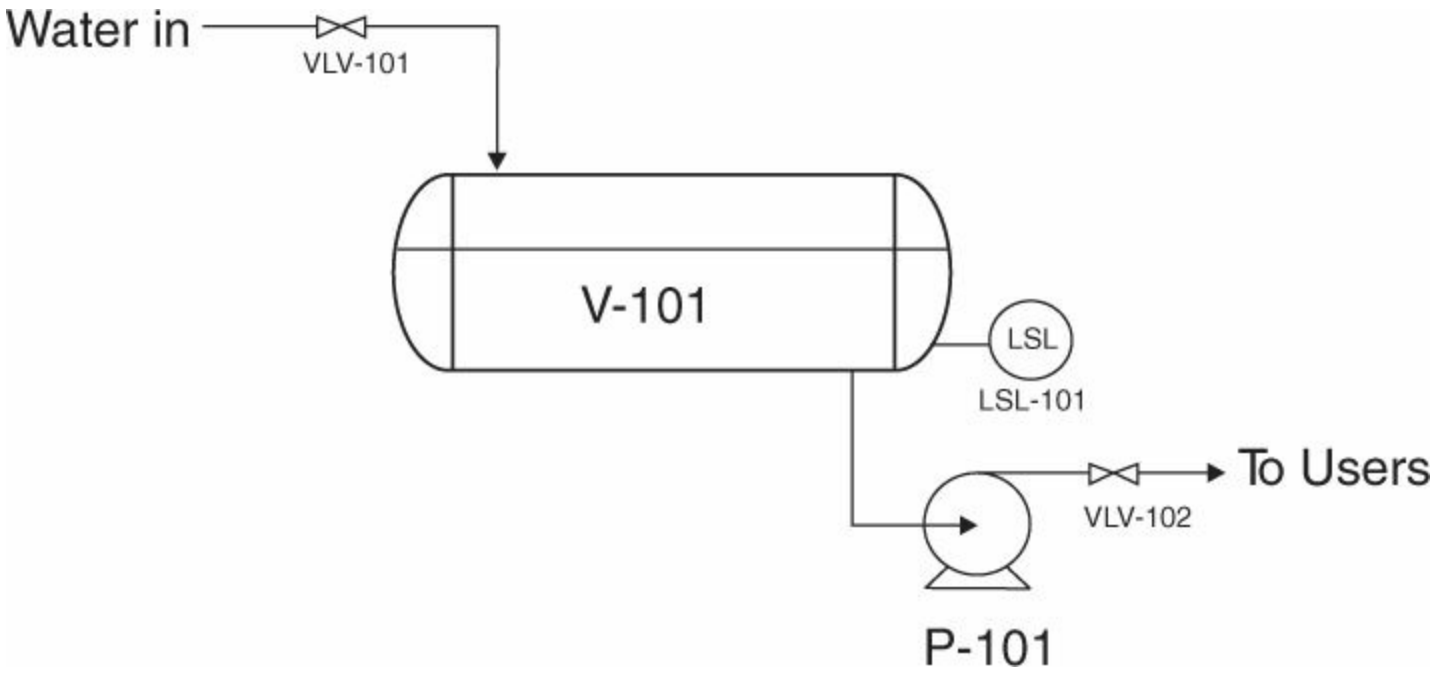


Figure E18.10(a). Schematic of a Storage Vessel

The ladder diagram is shown in Figure E18.10(b). In Rung 0, if any one of the pump start switches is pressed, it generates a true flag, making the OSR output to be true for only one cycle. This makes the output of ONM1 true. If any of the stop switches and LSL-101 are not true, then when ONM1 is true, a pump start signal, Start P-101, is generated in Rung 1. This start signal is usually sent to a motor control center (MCC) located in an electrical substation to start the pump. As the OSR output is true only once when any of the pump start switches is true, ONM1 will be false at the next scan and the pump will turn off. To prevent this, the Start P-101 signal is used in parallel to ONM1. While the pump is running, if any of the stop switches is pressed or the LSL-101 is activated due to low level, the input to the Start P-101 contact becomes false and trips the pump.

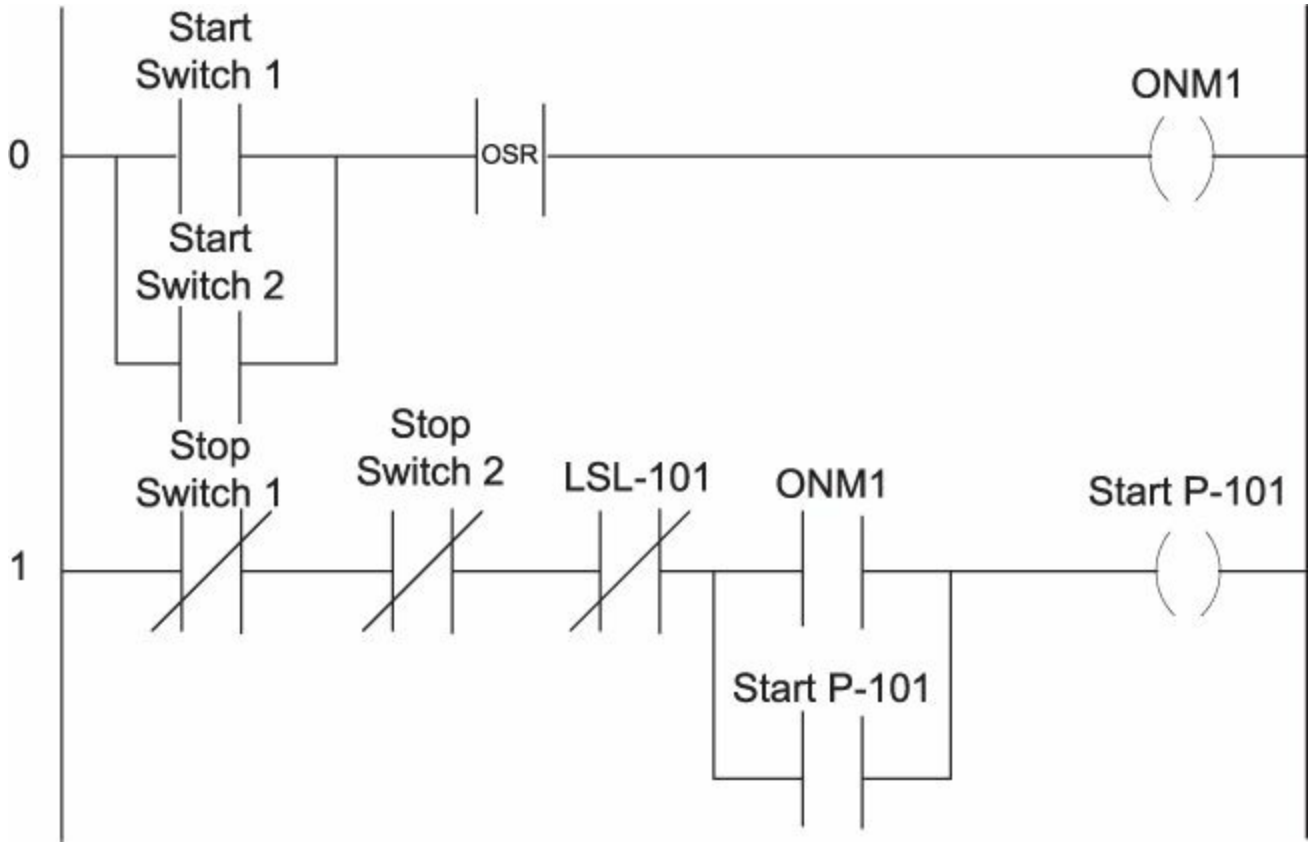


Figure E18.10(b). Ladder Diagram for Pump Start/Stop

18.8. Advanced Process Control

Advanced process control (APC) involves many tools from process control theory. This term broadly covers advanced techniques employed for process control applications. APC is very effective for process systems under the following circumstances:

- When multivariable interactions prohibit satisfactory control performance with a single-loop control
- When the process dynamics are so complex that a traditional control fails to give acceptable performance
- When the control system must satisfy some desired dynamic behavior
- When there are process constraints that cannot be violated under any circumstances
- When the control objective is to optimize some function, such as maximize profit, minimize auxiliary power consumption, and so forth, that involves multivariable interactions and (often) explicit process constraints
- When consistent product specifications cannot be met with traditional control
- When the plant operation is desired to be highly flexible

Nonetheless, APC is an umbrella term for a number of process control techniques. Based on their popularity, two such techniques will be briefly discussed here.

18.8.1. Statistical Process Control (SPC)

In this category, statistical methods are applied for process control. Quality control is one of the main focuses of SPC, ensuring that the product qualities are satisfied consistently in the face of inherent variability. In SPC, the process is monitored by using a quality control chart such as the Shewart

chart, CUSUM (Cumulative Sum) chart, or other similar technique. In the case of undesired deviation of a process variable from its desired value, an objective analysis is carried out to determine the root cause by using techniques such as Ishikawa diagrams, Pareto charts, and other such tools. A control action is then taken to eliminate the root cause. SPC is primarily used in the manufacturing industry where the costs of making such adjustments are large and the process is not subject to persistent disturbances. In the process industry, usually the cost of making adjustments is minimal and the disturbances are not only persistent but significant. Therefore, SPC has fewer applications in the process industry.

18.8.2. Model-Based Control

In model-based control, a process model is used to decide the appropriate control action. Two approaches are very popular in this category. In the first approach, known as the direct synthesis approach, the controller is designed to follow a desired trajectory. Two common techniques are internal model control and generic model control. The other approach is known as optimal control, where the controller is designed to optimize some objective function, quite often subject to some constraints. Model Predictive Control (MPC) is probably the most popular control scheme in this category. In linear MPC, a linear process model is used to predict the future process trajectory over a time horizon known as the prediction horizon. The control action is then calculated over a time horizon known as the control horizon by carrying out an optimization. Popular methods under this category are linear quadratic control (LQC), dynamic matrix control (DMC), and model algorithmic control (MAC). For systems that cannot be well represented by a linear model, a nonlinear process model is necessary, leading to nonlinear MPC. The optimization problem in a linear MPC can be solved by very efficient algorithms available for solving quadratic programming (QP) problems. However, nonlinear MPC leads to a nonlinear programming (NLP) problem that can be computationally expensive for large and complicated process systems. Another issue with any model-based control is to obtain a representative process model. When a representative first-principles process model is available, it can be used. When such models are not available, the actual process is excited by an appropriately designed input signal, and a process model is identified using the process response. The performance of an MPC application can significantly deteriorate if the actual process deviates considerably from the model over the course of time. In such cases, the identification of an updated process model is required. To obtain satisfactory control performance in the face of model and process mismatch is the focus of robust process control, which is an active field of research. Another problem for any APC application is its maintenance because complicated process control theory is usually involved.

Many other APC techniques are available in the existing literature. Readers interested in these techniques and the theory and applications of APC techniques are referred to a number of good references in this area [12–14].

18.9. Case Studies

In this section two operations that require more complex control schemes are studied in detail. Again, it is emphasized that these are not the only ways to control these units but are typical schemes that might be employed. Many alternatives exist, and in the course of a career in process engineering, you will encounter a wide variety of regulation systems.

18.9.1. The Cumene Reactor, R-801

Consider the reactor system for the production of cumene shown in Appendix C, Figure C.8, and redrawn in Figure 18.9. The reactor feed, Stream 7, comes from a fired heater, where it is heated to the temperature required in the catalytic reactor. The reaction takes place in a bank of parallel catalyst-filled tubes and is mildly exothermic. In order to regulate the temperature of the reacting mixture and catalyst, the tubes are immersed in boiler feed water. The heat is removed by vaporizing the water to make high-pressure steam, which is then sent to the high-pressure steam header.

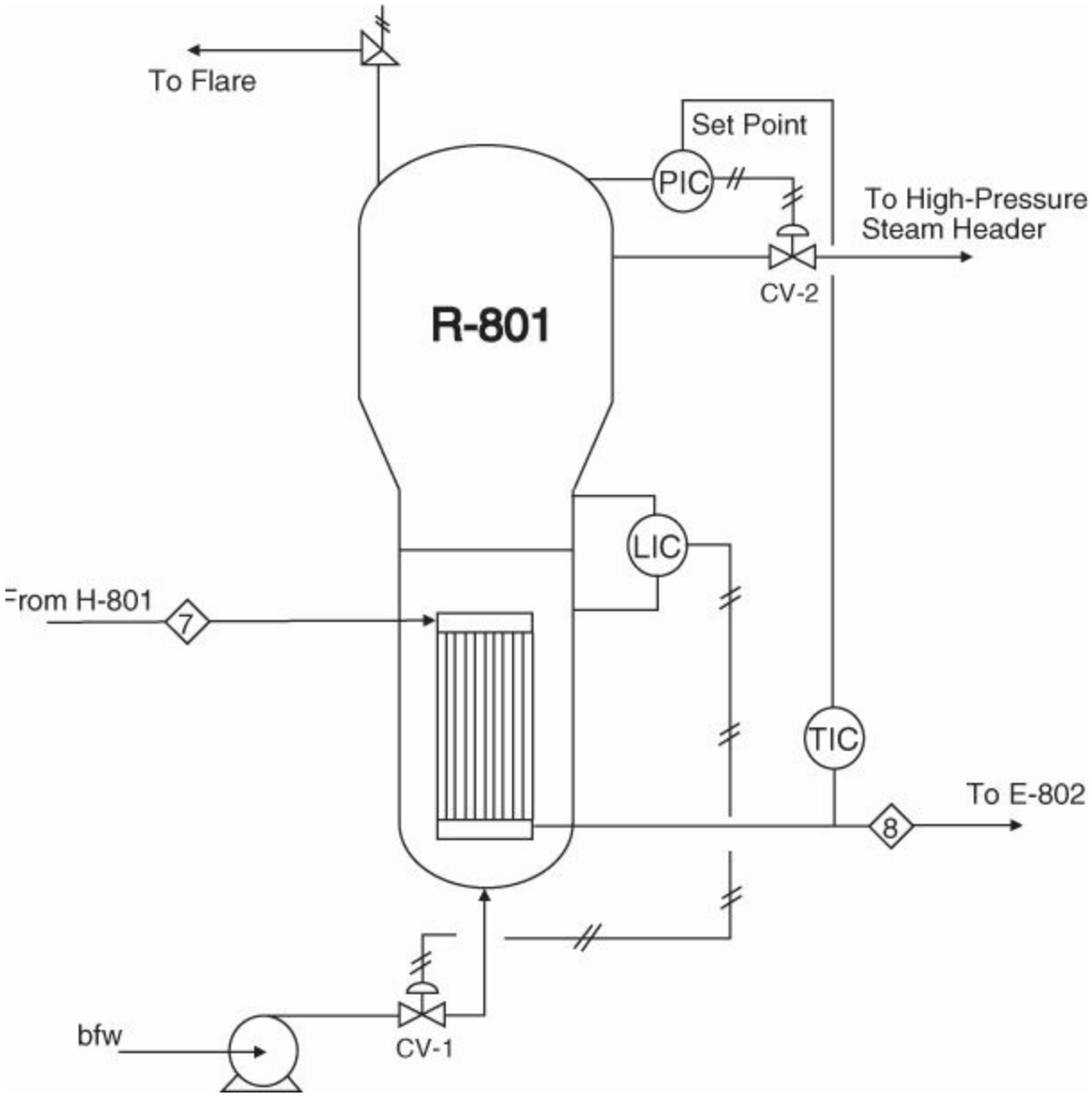


Figure 18.9. Basic Regulation Scheme for Cumene Reactor, R-801

The first issue is what should be controlled in the reactor and why. This is not a simple question to answer because many things must be considered. Some of the important considerations for exothermic catalytic reactions are discussed in Chapter 23. Here, it is assumed that the exit temperature from the reactor, Stream 8, is the variable that must be controlled. If the reactor is designed such that the temperature increases monotonically from the inlet to the outlet, then the exit stream is the hottest point in the reactor. More commonly, there will be a temperature bump or warm (hot) spot somewhere within the reactor, and the exit temperature will be cooler than at the temperature bump. In this case, a series of in-bed thermocouples could be used to measure the temperature profile within the catalyst tubes and use the maximum temperature as the controlled variable. In either case, it is important to control the reactor temperature, because the reaction rate and catalyst activity are both affected strongly by temperature.

The first part of the control scheme is a feedback material balance control on the boiler feed water. Control valve CV-1 is adjusted using a signal from the level controller mounted on the side of the reactor. This scheme ensures that the bank of catalyst tubes is always totally immersed in the bfw. Regulation of the bfw level below the top of the tubes, as discussed in Section 18.6.2, is inadvisable for this reactor, because the poor heat transfer coefficient for the portion of the tubes above the liquid level might cause a hot spot to occur at the entrance of the reactor. The second part of the control scheme uses cascade control to regulate the reactor exit temperature. The temperature at which the bfw boils in the reactor is regulated by the setting of CV-2. The logic is the same as described for the situation in Figure 18.7(b): that the pressure of the steam in the reactor is set by the steam header pressure (fixed) and the pressure drop across CV-2 (adjustable). The temperature of Stream 8 is monitored and used to adjust the set point on CV-2 as required.

Consider a situation in which the reactor exit temperature is seen to drop slowly. This situation may be caused by a number of reasons—for example, the catalyst slowly loses its activity and has the undesirable effect of reducing the conversion in the reactor with the possibility of a reduction in cumene production. With the control scheme shown in Figure 18.8, the system would respond in the following manner. As the temperature of Stream 8 drops, the set point on CV-2 would be adjusted to close the valve and increase the pressure of the steam in the reactor. This would have the effect of increasing the temperature at which the bfw boiled and would reduce the temperature driving force for heat transfer. The net effect would be to reduce the amount of heat removed from the reactor, causing the exit stream temperature (and reactor temperature profile) to increase and also causing the amount of reaction to increase. If the reactor exit temperature were to increase for some reason, then the control strategy would be the opposite of that described above. The increase in temperature of Stream 8 would be sensed by the temperature controller, which would then adjust downward the set-point pressure for the reactor. This would cause CV-2 to open, reducing the pressure and temperature of the steam in the reactor. This, in turn, would increase the temperature driving force for heat transfer and increase the amount of heat removed from the reactor, causing the exit stream temperature to decrease and also causing the amount of reaction to decrease. Clearly, for exothermic reactions, the control of temperature is essential to safe reactor operation. For such equipment, several safety features would be incorporated into the overall control scheme. These safety features are extremely important and are treated separately in Chapter 26.

18.9.2. A Basic Control System for a Binary Distillation Column

The purpose of a control system for a distillation column is to provide stable operation and to produce products with the desired purity. Figure 18.9 shows a control scheme typically used to regulate a binary distillation system. Flowrates, pressure, stream composition, and liquid levels are regulated. The five control variables to be regulated are shown (column pressure, composition of distillate, composition of bottoms product, liquid level in the bottom of the column, and the liquid level in the reflux drum).

Shown in Figure 18.10 are five feedback control loops and one cascade control loop used to regulate the five control variables.

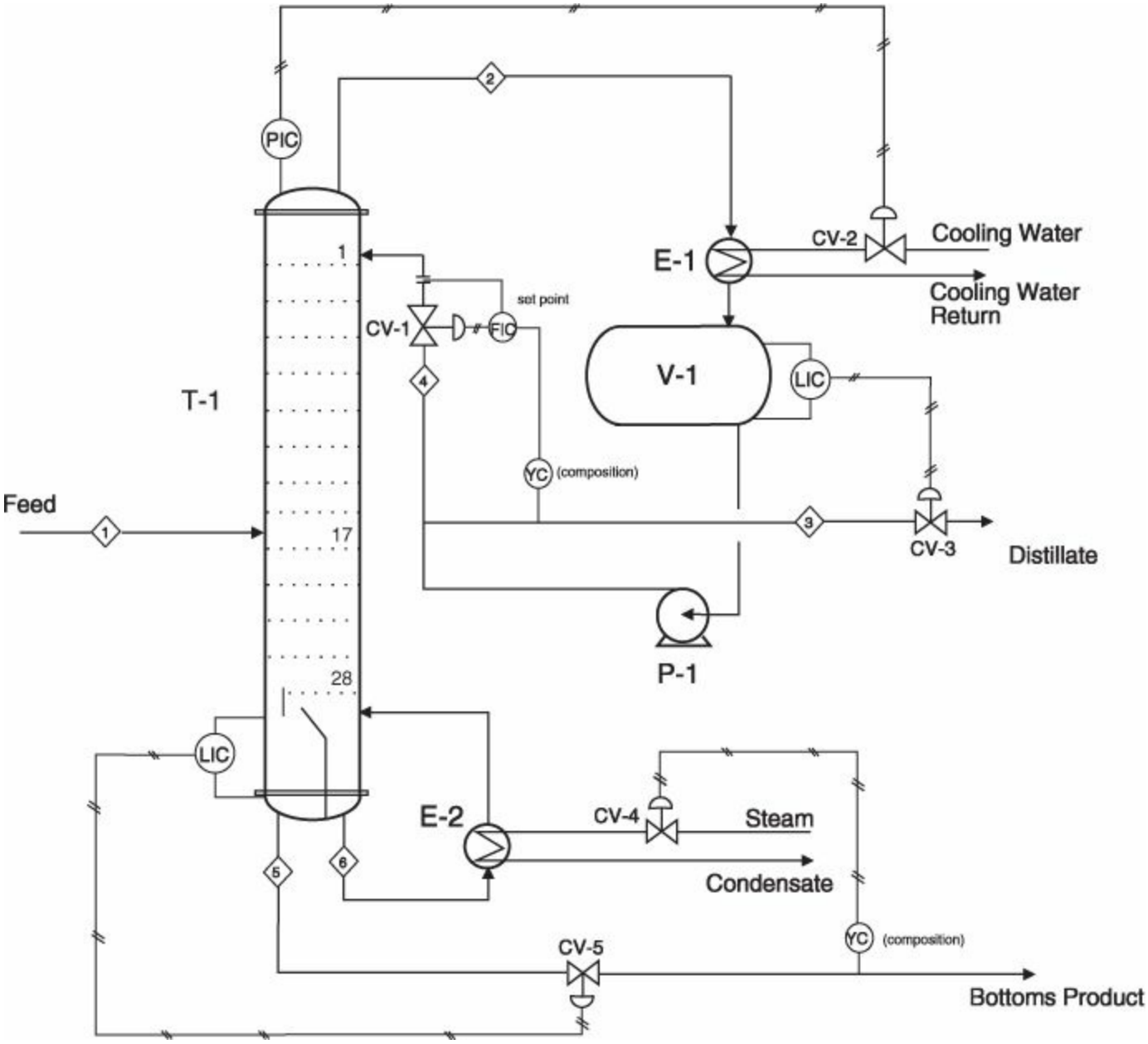


Figure 18.10. Typical Basic Control Scheme for a Binary Distillation Column

- Valve CV-1 regulates the liquid reflux, Stream 4, in order to maintain the desired distillate composition. In addition, a composition measurement is made on the overhead product stream, Stream 3, and this is used to change the set point of CV-1.
- Valve CV-2 regulates the condenser heat duty (by changing the flowrate of cooling water) in order to maintain a constant column pressure.
- Valve CV-3 regulates the distillate flowrate, Stream 3, in order to maintain a constant liquid level in the reflux drum, V-1.
- Valve CV-4 regulates the reboiler heat duty (by changing the pressure of the stream flowing into E-2) in order to maintain a constant distillate bottoms composition.
- Valve CV-5 regulates the bottoms product flowrate, Stream 5, in order to maintain a constant liquid level in the bottom of the column.

Consider the changes that result from a decrease in the concentration of the light component in the feed—assuming the feed flowrate remains unchanged—and the regulation that the control system provides. It is observed for this system that as a lower amount of light material is fed to the column, the purity of the distillate and amount of overhead vapor begin to drop. The concentration detector

located on Stream 3 will detect this change and will send a signal to change the set point of CV-1. Valve CV-1 will begin to open in order to increase the reflux rate. Simultaneously, the level of liquid in V-1 will start to drop. The level control will sense this change and start to close CV-3, thus reducing the flow of overhead product, Stream 3. In addition, as the amount of overhead vapor, Stream 2, flowing to E-1 also drops, the column pressure will start to decrease slightly and the cooling water flowrate, regulated via CV-2, will be reduced. At the bottom of the column, the heavier material will start to accumulate. For this system, it is observed that this will result in an increase in the liquid level in the bottom of the column and an increase in the purity of the bottoms product. The level controller at the bottom of the column will sense the increase in liquid level and open valve CV-5, increasing the bottoms product flowrate. Finally, as the composition detector on Stream 5 senses the increase in purity of the bottoms product, it will send a signal to CV-4 to close, reducing the boil-up.

The action of the control scheme to the change in feed composition essentially regulated five streams in the following manner:

1. Stream 3↓
2. Stream 5↑
3. Stream 4↑
4. Cooling water to condenser (E-1)↓
5. Steam to reboiler (E-2)↓

Actions 1, 2, 4, and 5 are consistent with satisfying the material and energy balances for the distillation system. Action 3 is required to adjust the purity of the products.

The regulation scheme shown in Figure 18.10 is only one of many possible systems that can be used to regulate a binary distillation column. If there is a sudden change in a process variable, this system may become unstable, and careful tuning of the controllers is necessary to avoid such problems. It should also be pointed out that the material balance for the column is automatically satisfied by using the liquid levels in the column and reflux drum to control the product flowrates. The same is not true for the energy balance. For example, if valve CV-2 opens rapidly while valve CV-4 opens slowly, then a disparity in the energy balance will occur. Less vapor is produced in the reboiler than is condensed in the condenser, and the pressure drops. Fortunately, the distillation column tends to be self-regulating in response to pressure. If pressure decreases, the temperature decreases because of saturation conditions in the column. This increases the driving force for heat transfer in the reboiler and decreases the driving force for heat transfer in the condenser. This increases the boil-up and decreases the condensation of overhead vapor. Therefore, this results in an increase in the system pressure that tends to correct for the disparity in the energy balance.

For distillation columns with side products, the control strategy is more complicated. In general, for each additional variable that is to be regulated or controlled, an additional control loop must be added.

It is worth noting that most major column upsets arise from a change in the conditions of the feed stream to the column. These changes are most often caused by process upsets occurring upstream of the distillation column. The effects of sudden changes in column feed conditions can be significantly reduced by installing a surge tank upstream of the column. This tank acts as a buffer or capacitor by storing and mixing feed of differing composition. The overall effect is to dampen the amplitude of concentration fluctuations and reduce the impact of sudden changes on the column operation. The use

of surge tanks is not restricted to distillation columns only. In fact, any place where a significant inventory of liquid is stored acts to dampen changes in feed conditions to the downstream units.

A surge tank reduces the effects of sudden changes in feed conditions.

18.9.3. A More Sophisticated Control System for a Binary Distillation Column

Figure 18.11 shows a control system for a binary distillation process, adapted from Skrokov [8]. The distillation unit is similar to the one shown in Figure 18.10. Valves CV-1, CV-2, CV-3, CV-4, and CV-5 are in the same location and perform the same function in both systems.

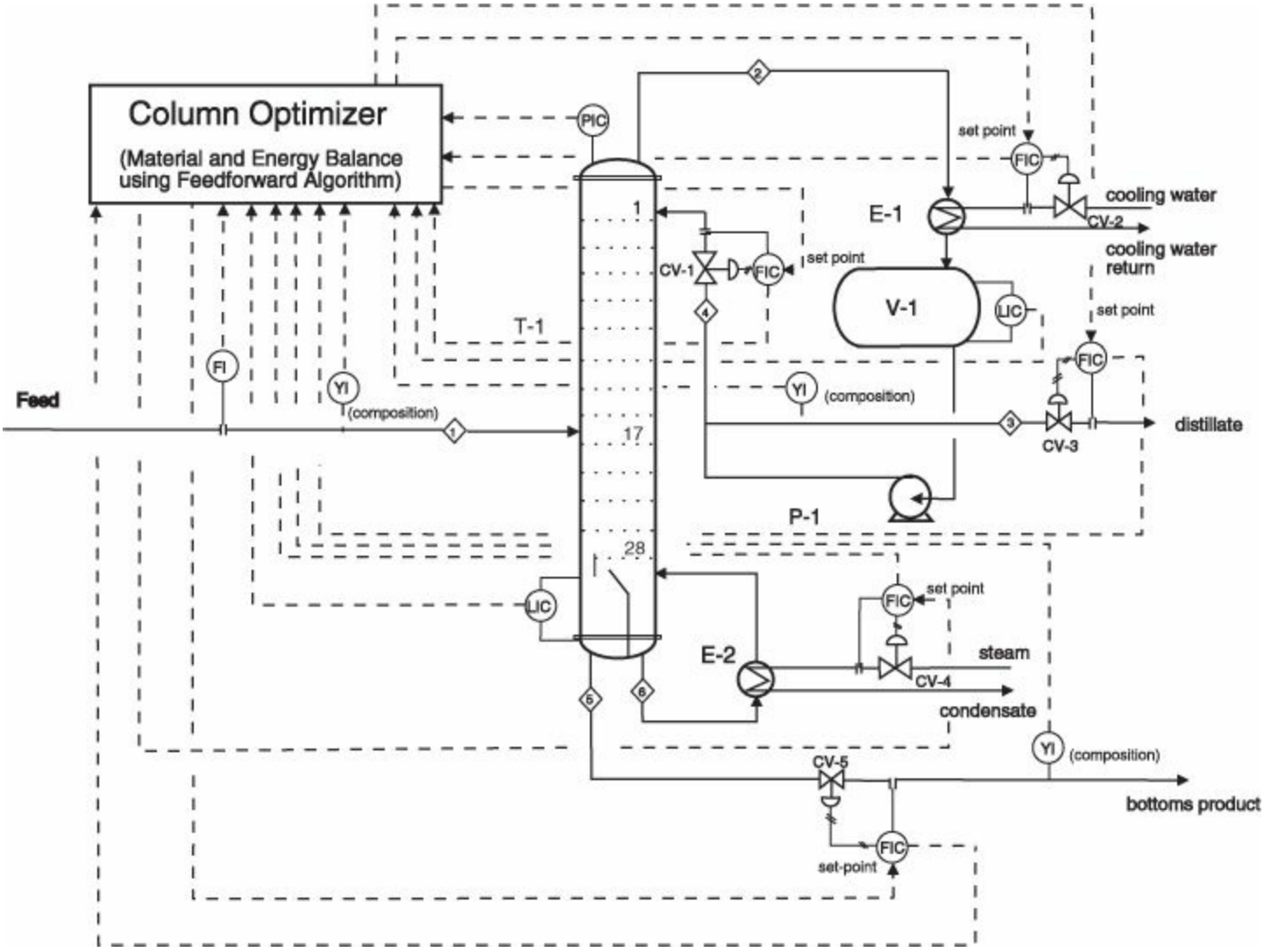


Figure 18.11. An Advanced Control Scheme for a Binary Distillation Column (Adapted from M. R. Skrokov, *Mini- and Microcomputer Control in Industrial Processes: Handbook of Systems and Application Strategies* [New York: Van Nostrand Reinhold, 1980]. Reproduced by permission.)

However, for the system shown in Figure 18.11, the concentrations and flows of the input stream, exit streams, and reflux stream are measured and sent to the monitor/analyzer. This unit performs energy and material balances and uses performance relationships to evaluate new set points for the recycle, distillate, and bottom streams. It is a feed-forward system that predicts and makes changes in operations based on the predictions of a detailed process model.

Modern control capabilities involving sophisticated computer hardware and software also require a high degree of chemical engineering expertise in order to develop a system that optimizes the

performance of process units.

18.10. Putting it all Together: The Operator Training Simulator (OTS)

An OTS can be very effectively used to train control room operators even before a chemical plant is operated for the first time. This is particularly important when new technologies are employed in a process plant or a less experienced workforce takes the place of an experienced workforce. This book includes discussions of all the components required for development of an OTS. In Chapters 13 and 16, various aspects of steady-state design of a process plant were discussed. This steady-state design is then used to develop a dynamic model of a system, as discussed in Chapter 17. One of the key requirements of a stable dynamic simulation is the appropriate design of the control system. Brief discussions on basic as well as advanced control system design were provided in Chapter 17 and in this chapter. After that, the logic control system is designed and implemented. Finally, an APC layer can be designed to satisfy objectives that cannot be satisfied with traditional control strategies. The APC layer is optional, and barring a few exceptions, in general, its absence will not impede developing an OTS but may result in unsatisfactory control performance. The steps mentioned above can be very involved and complicated for large, complex, and highly interacting process systems. The graphical interface of a dynamic simulator is usually not suitable for mimicking a "virtual control room" for control room engineers. Therefore, a user-friendly human machine interface (HMI) similar to the distributed control system (DCS) screen is used for easy interfacing to the dynamic simulator (see Chapter 1, Figure 1.16). By putting all these components together, an OTS can be developed. The benefits of an OTS include the following:

- The control room operators can be trained far ahead of running the actual plant. Other than normal plant operation, the OTS can be used to train operators to handle abnormal and emergency situations, which may happen only rarely in a plant, but if such situations do occur and they are not handled appropriately, they might result in serious conditions that would jeopardize equipment and personnel safety. This is similar to a flight simulator used for commercial pilots.
- The plant control system design and the DCS can be checked well in advance before connecting to the actual field equipment and instruments.
- Not only normal running of the plant, but also plant start-up and planned and emergency shutdowns can be simulated and valuable experience can be gained in terms of understanding the dynamics of the process during these transients. This can save valuable time and result in accident avoidance. As most of the equipment damage takes place during these transients, better equipment life can also be attained.

One of the key requirements of an OTS is the real-time execution of the dynamic simulation. This is hard to achieve for large process plants, especially when start-up, shutdown, or abnormal situations are simulated. Multiple processors must be used to work together to satisfy this requirement. Another challenge is to solve the process model in face of large changes in the process. A robust solver is a primary requirement of an OTS. Nonetheless, modern OTS systems can solve hundreds of thousands of equations robustly and in real time.

18.11. Summary

In controlling any chemical process, the final control element is almost always a valve that regulates the flow of a process or, more commonly, a utility stream. The basic construction and operation of a

control valve were reviewed. The way in which valves regulate flow and the pressure profiles in a pipe system were illustrated with several examples.

In this chapter, the basic regulation systems commonly used in simple process control schemes were reviewed. These systems were feedback, feed-forward, cascade, combinations of feedback and feed-forward control, ratio, and split-range control. The logic behind each of these control strategies was explained, and examples illustrating this logic were given. Methods of controlling the temperature of process streams using heat transfer media that undergo phase changes were discussed. Several strategies for controlling the temperature of process streams exchanging energy with these heat transfer media were given. Elements of logic control were discussed with a simple example. A brief discussion on APC was given. Two case studies were presented in which several control schemes were used to regulate variables in an exothermic reactor and a simple binary distillation column. Finally, the essential components of an OTS were provided.

What You Should Have Learned

- Most of what can be controlled in a chemical process involves opening or closing a valve.
- Typical control strategies include feedback, feed-forward, cascade, ratio, and split-range control. These strategies are normally taught in another class in the curriculum.
- It is important to consider the regulation strategies (what is measured and what is controlled) of typical process equipment such as heat exchangers, reactors, and distillation columns.
- Logic control is a key component of the control system of a plant.
- A number of components are needed to build an operator training simulator (OTS).

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Problems

1. Consider an alternative reactor configuration for the cumene reactor, R-801, discussed in Section 18.9.1. The alternative is shown in Figure P18.1 and consists of a series of adiabatic catalytic packed beds through which the reactants pass. As the reactants and products pass through each bed, they are cooled by a cold shot of inert diluent—in this case, propane—before entering the next bed. The catalyst must be protected from excessive temperatures that cause it to sinter and to lose activity rapidly. For each of the control strategies given below, sketch the control loops that must be added to the system and discuss how the regulation is achieved—for example, "that is, as x increases, valve y opens, causing…"
   a. Use the exit temperature from a given bed to adjust the amount of diluent fed to that bed.
   b. Use the exit temperature from the previous bed to adjust the amount of diluent fed to the next bed.
   c. To what types of control strategy do Parts (a) and (b) conform? Which scheme do you think is better for this type of reactor? Explain your reasoning.
   d. Devise a control strategy that incorporates both the ideas used in Parts (a) and (b).

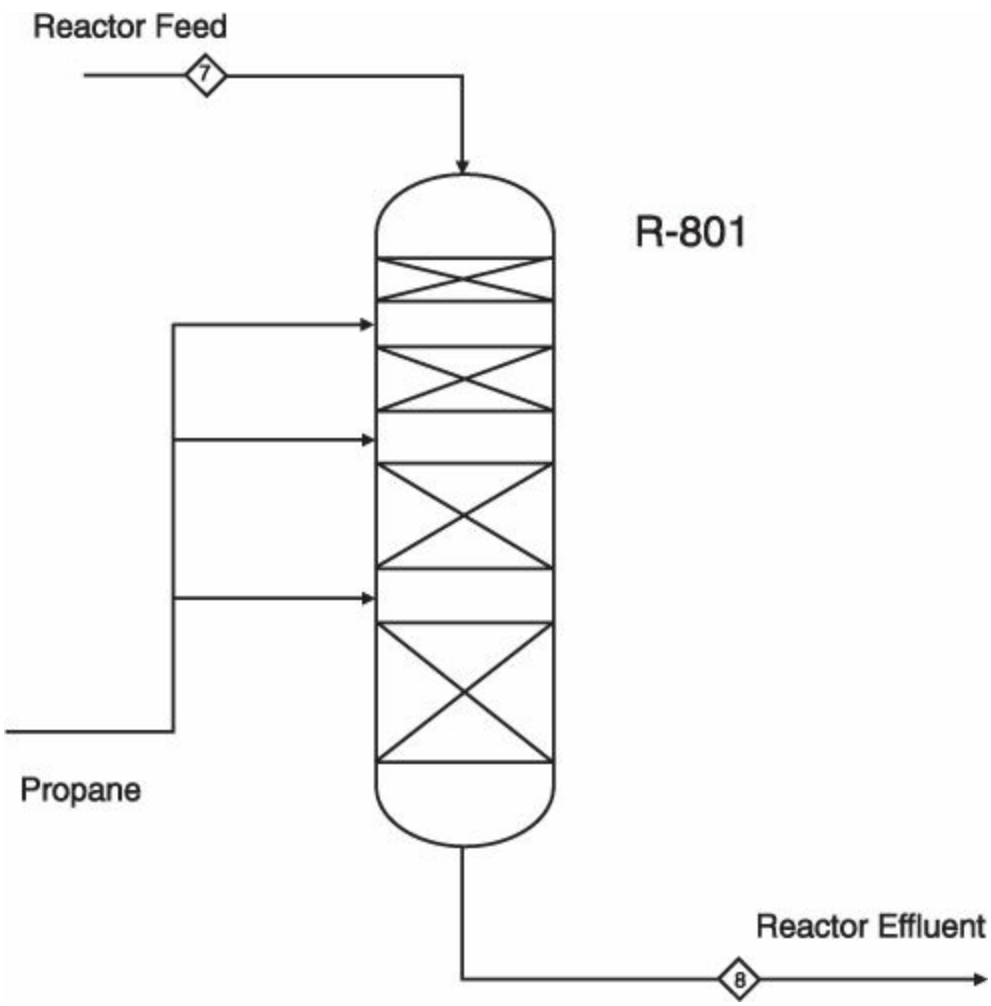


Figure P18.1. Alternative Configuration for Cumene Reactor from Problem 18.1

2. Consider the benzene purification column, T-101, in Figure 1.5 for the toluene hydrodealkylation process. The column feed contains noncondensables, mainly methane and a small amount of hydrogen, that must be vented from the system. The vent is taken off the top of the reflux drum, V-104. Sketch a control system in which the valve on this vent line is used to control the pressure of the column.

   Explain what happens when

   a. The column pressure begins to drop

   b. The amount of noncondensables fed to the column suddenly increases

3. It has been proposed that the feed toluene to the process shown in Figure 1.5 be vaporized prior to mixing with the hydrogen. It is believed that this scheme will allow more flexibility in the operation of the plant. You have been asked to devise a conceptual design for this vaporizer. The source of heat is the condensation of high-pressure steam. The system designed should be capable of controlling the amount of toluene vaporized and the pressure at which the toluene leaves the vaporizer. Sketch a diagram showing the major pieces of equipment and major control loops.

4. In the DME process shown in Figure B.1.1, the reactor feed exchanges heat with the reactor effluent stream in exchanger E-202. From the diagram, it is evident that the temperature of the stream entering the reactor is controlled by regulating the amount of reactor effluent that is bypassed around the heat exchanger. For this system, answer the following questions:

   a. Explain how this system works. For example, explain what happens if the temperature of the feed into E-202 (Stream 4) were to increase or decrease.

b. How would this system respond to fouling in the heat exchanger or a loss of activity of catalyst in the reactor?

c. What type of control strategy is used in this example—feedback, feed-forward, and so on?

d. Design a control system that would regulate the exit temperature of the reactor (Stream 6) rather than the inlet stream temperature.

5. For the benzene column (T-101) in Figure 1.5, do the following:

a. Implement a control scheme that will regulate the purity of the benzene product (Stream 15). You may assume that the purity of this stream can be evaluated by an on-line refractive index monitor placed on Stream 15.

b. What is the type of control system that you have designed in Part (a) called?

6. Consider the feed section of the phthalic anhydride process in Appendix C, Figure C.5. A single control valve is used to control the flow of the combined vaporized naphthalene and air streams, Stream 7. In this process it is important to regulate both the flowrate of Stream 7 and the relative amounts of air and naphthalene in Stream 7. Does the current control scheme allow this type of regulation to occur? If not, devise a control scheme that will allow both these variables to be controlled independently.

7. Describe which form of control strategy (feed-forward, feedback, cascade, or a combination of these) best describes how a responsible person drives an automobile.

What would be the consequence of using a feedback control strategy alone?

8. Figure P18.8 shows a CSTR, R-901, carrying out a liquid-phase exothermic reaction. The feed, Stream 1, comes from an upstream unit, and its flowrate is known to vary. The heat of reaction is removed by circulating a portion of the contents of the reactor through an external heat exchanger. Cooling water is used as the cooling utility in E-901.

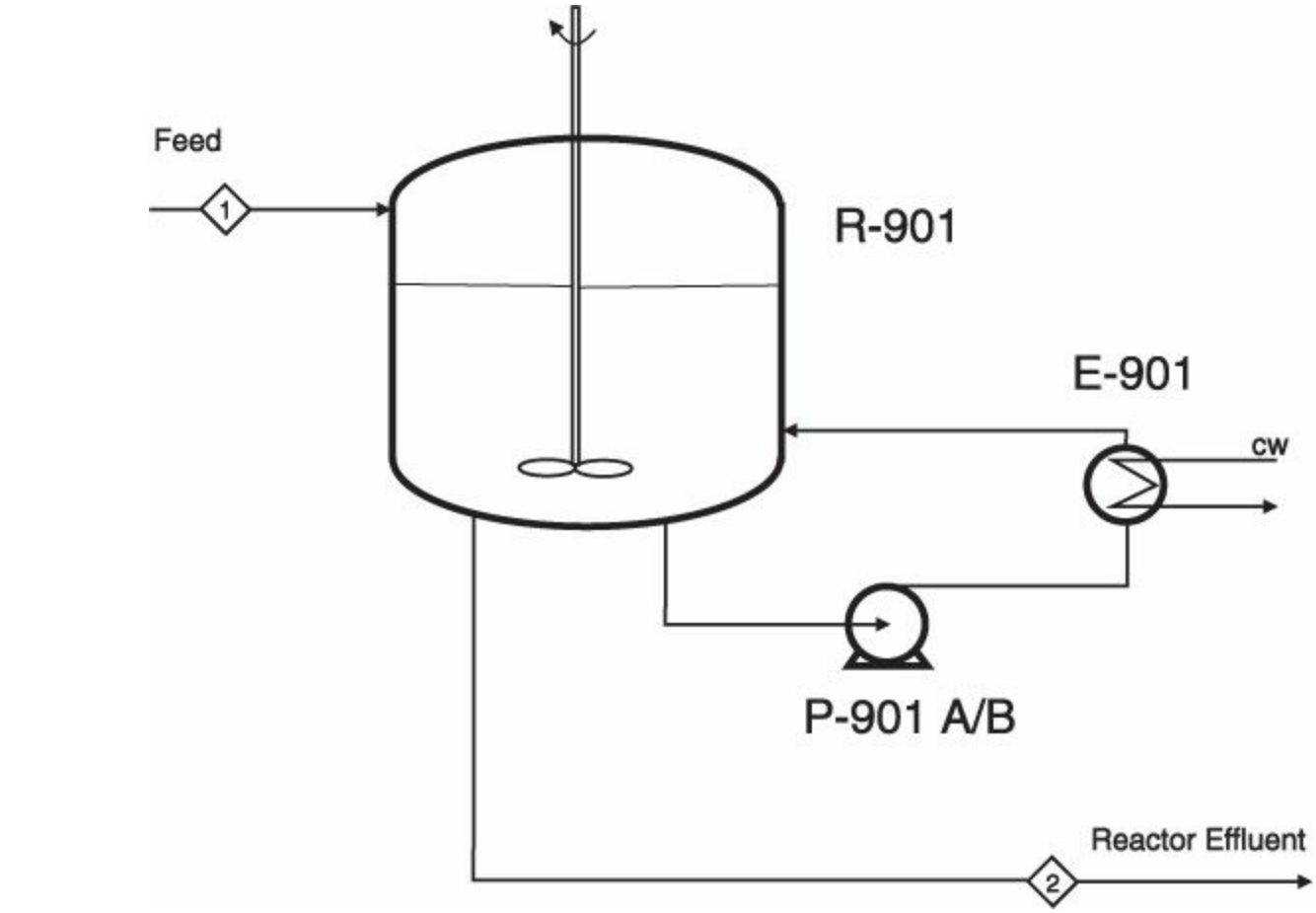


Figure P18.8. CSTR Configuration for Problem 18.8

For this reactor scheme, devise a system to implement the following control actions:

a. Regulate the temperature of the reactor

b. Regulate the inventory of the reactor, that is, keep a constant liquid level Explain how your control system would compensate for a change in the flowrate of Stream 1.

What additional control scheme would be needed to maintain a constant conversion in the reactor, assuming that constant conversion can be achieved by ensuring constant residence time in the reactor?

9. Figure P18.9 shows a CSTR carrying out a liquid-phase, exothermic reaction. The heat released partially vaporizes the contents of the reactor. This vapor is condensed in an external condenser, and the condensate is returned to the reactor. The reactor operates at the boiling point (T and P) of the mixture in the CSTR. The vapor formed consists of reactants and products.

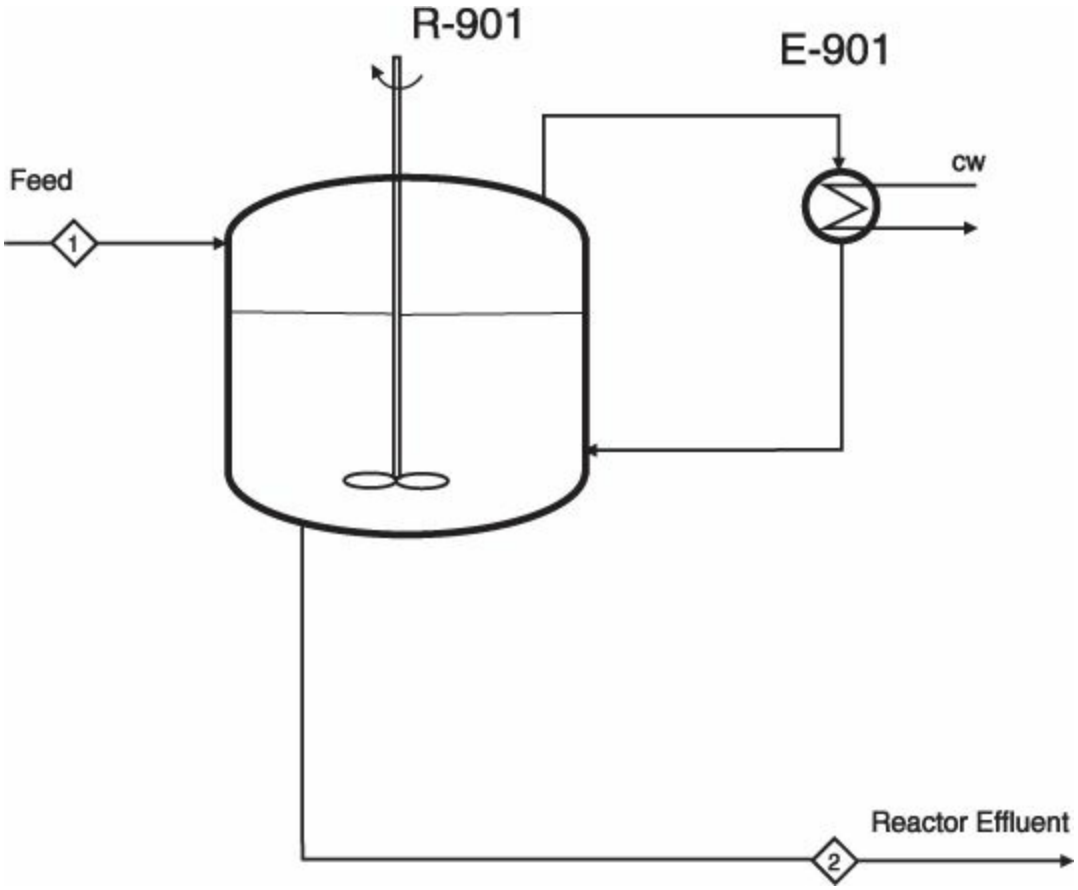


Figure P18.9. CSTR Configuration for Problem 18.9

For this system, devise a system to regulate the following variables:

a. Temperature in reactor

b. Residence time in the reactor

Explain how your system would respond to the following changes:

c. Increase in flowrate of feed

d. Fouling of the tubes (on cw side) of the condenser.

10. Consider the feed section of the toluene process given in Figure 1.5. The flow of fresh toluene, Stream 1, is regulated by monitoring the level in the toluene storage tank, V-101. If the level is seen to drop, then the valve on Stream 1 opens and vice versa. This is an example of a feedback material balance control loop. For this system, implement a feed-forward control scheme in

which the flow of the recycle, Stream 11, is measured and used to control the flow of Stream 1. Do you foresee any potential problems with this control strategy?

11. In the feed section of the maleic anhydride process shown in Figure B.5.1, consider that the air flowrate must be regulated so that a desired ratio between benzene and air is maintained. However, as the air flow changes, the discharge pressure of C-601 should also be maintained at a desired set point. Devise a control scheme to achieve the desired regulation. What type of control system did you design? Why?
12. In the maleic anhydride process shown in Figure B.5.1, the temperature of Stream 6 at the outlet of the feed heater, H-601, needs to be maintained. For this system, do the following:
    a. Devise a control scheme for maintaining the temperature of Stream 6 by manipulating the flowrate of the natural gas to the furnace (i.e., firing rate of H-601). The flowrate of combustion air must be maintained at a desired ratio to the flowrate of the natural gas.
    b. In an alternative scenario, it is decided that, for maintaining the furnace temperature, fuel oil will be used to minimize the consumption of natural gas. When the fuel oil alone is not sufficient to maintain the temperature, natural gas will be fired along with the fuel oil. The flowrate of combustion air should be regulated such that the desired ratios with respect to the flowrate of the natural gas and the fuel oil are both maintained. Devise a control scheme to achieve this control objective. What type of control system(s) did you design? As the fuel oil and the natural gas have very different heating values, what challenge would you expect in achieving a satisfactory performance with this control scheme?
13. In Example 18.10, there are two switches to start the pump. In addition, consider that the pump can be automatically started by a newly installed high-level switch as long as the stop switches are not pressed. Modify the ladder diagram shown in Figure E18.10(b) accordingly.
14. Consider Problem 18.13. The control logic is now modified such that the pump can be automatically started by the high-level switch even though the stop switches are pressed. Modify the ladder diagram you developed in Problem 18.13 accordingly.

Section IV: Analysis of Process Performance

The previous three sections focused on problems associated with the design, synthesis, and economics of a new chemical process, where there was freedom to select equipment. This section explores problems associated with an existing chemical process. Two important factors must be understood in dealing with existing equipment:

1. Changes are limited by the performance of the existing equipment.
2. Any changes in operation of the process cannot be considered in isolation. The impact on the total process must always be considered.

Over the 10 to 30 years or more a plant is expected to operate, process operations may vary. A plant seldom operates at the original process conditions provided on the design PFD. This is due to the following:

- **Design/Construction:** Installed equipment is often oversized. This reduces risks resulting from inaccuracies in design correlations, uncertainties in material properties, and so on.
- **External Effects:** Feed materials, product specifications and flowrates, environmental regulations, and costs of raw materials and utilities all are likely to change during the life of the process.
- **Replacement of Equipment:** New and improved equipment (or catalysts) may replace existing units in the plant.
- **Changes in Equipment Performance:** In general, equipment effectiveness degrades with age. For example, heat transfer surfaces foul, packed towers develop channels, catalysts lose activity, and bearings on pumps and compressors become worn. Plants are shut down periodically for maintenance to restore equipment performance.

To remain competitive, it is necessary to be able to alter process operations in response to changing conditions. Therefore, it is necessary to understand how equipment performs over its complete operating range to quantify the effects of changing process conditions on process performance.

The material provided in this section involves several categories of performance problems:

1. **Predictive Problems:** An examination of the changes that take place for a change in process or equipment input and/or a change in equipment effectiveness.
2. **Diagnostic/Troubleshooting Problems:** If a change in process output (process disturbance or upset) is observed, the cause (change in process input, change in equipment performance) must be identified.
3. **Control Systems Problems:** If a change in process output is undesirable or a change in process input or equipment performance is anticipated, compensating action that can be taken to maintain process output must be identified.
4. **Debottlenecking Problems:** Often, a process change is necessary or desired, such as scale-up (increasing production capacity) or allowance for a change in product or raw material specifications. Identification of the equipment that limits the ability to make the desired change or constrains the change is necessary.

This section introduces the basic principles by which existing equipment and processes can be evaluated, operated, controlled, and subjected to changes in operating conditions. This material is

treated in the following chapters.

Chapter 19: Process Input/Output Models

The basic structure of performance problems is considered in the context of an input, an output, and a system.

Chapter 20: Tools for Evaluating Process Performance

Tools needed to analyze performance problems, such as ratios, limiting resistances, and base cases, are presented.

Chapter 21: Performance Curves for Individual Unit Operations

The performance of single pieces of equipment is analyzed for changes in process conditions, flowrates, utility flowrates, and degradation of equipment. It is assumed that the equipment has been designed and built and that the physical parameters of the equipment cannot change.

Chapter 22: Performance of Multiple Unit Operations

The performance of multiple pieces of equipment is analyzed. It is shown how a change in one unit affects the performance of another unit.

Chapter 23: Reactor Performance

Evaluation of the performance of different types of reactors is illustrated. The choice of process conditions to change selectivity is addressed.

Chapter 24: Process Troubleshooting and Debottlenecking

Case studies are presented to introduce the philosophy and methodology for process troubleshooting and debottlenecking.

Chapter 19. Process Input/Output Models

What You Will Learn

- All chemical processes have an input-output structure.

Imagine you are in charge of operations for a portion of a chemical plant when you are informed that the pressure of a distillation column has begun to rise slowly. You know that if the pressure continues to rise, the structural integrity of the column may be in jeopardy, or that a relief valve will open and release valuable product to the stack. Both of these scenarios have serious negative consequences. In order to solve the problem without shutting down the plant, which might be very costly, it is necessary to understand how the distillation column performs in order to diagnose the problem and determine a remedy.

Dealing with the day-to-day performance of a chemical process differs from design of a new process. When designing a new process, there is freedom to choose equipment specifications as long as it produces the desired performance. However, once a piece of equipment has been designed and constructed, it performs in a unique manner. The specific performance of a piece of equipment must be considered when operating such equipment.

When designing equipment, alternative specifications can yield the same operating results. When dealing with existing equipment, day-to-day operation is constrained by the fixed equipment characteristics.

Although it may be tempting to proceed immediately to the analysis of performance of individual pieces of equipment, it is important to develop an intuitive understanding of how equipment performs. This chapter introduces a framework by which individual equipment and complete process performance may be understood. The following chapters develop and use tools for analysis of system performance. Having an intuitive understanding of process and equipment performance is a necessary complement to the ability to do numerous, repetitive, high-speed calculations.

To determine the outputs of a unit operation or chemical process, the process inputs must be known and the performance for each unit of equipment involved in the process must be understood. The relationship between input and output can be described as

$$\text{Output} = f(\text{Input},\ \text{Unit Performance}) \qquad (19.1)$$

Input changes are the driving force for change.

Unit performance defines the characteristics of fixed equipment by which inputs are changed to outputs.

To change process output, the process input and/or equipment performance must be altered. Conversely, the cause of a process output disturbance is a change in process input, equipment performance, or both.

Changes in process output result from changes in process inputs and/or equipment performance.

19.1. Representation of Process Inputs and Outputs

Figure 19.1 illustrates how outputs are connected to inputs through the process system. The process system may consist of a single piece of equipment or several unit operations, with the output from one unit becoming the input to another unit. As a result, a change of input to one unit operation affects all of the downstream units. For systems containing recycle streams, the output from a unit operation returns to affect its input.

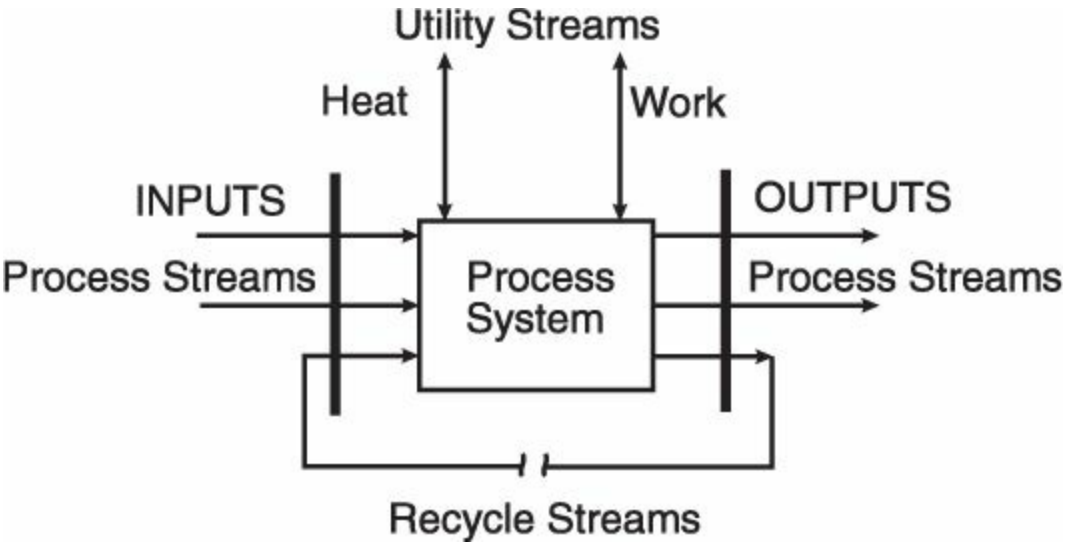


Figure 19.1. Input/Output Diagram for Chemical Process

Figure 19.1 provides the input/output representation of a chemical process. It shows

a. Process System (shown in the center box): This may consist of a single process unit, or a collection of process units (such as a distillation system), that, taken together, performs a specific function or a complete chemical process.

b. Process Flow Streams: These are divided into two types:

i. Input Streams (shown on the left): They consist of process flow streams entering a unit operation or process.

ii. Output Streams (shown on the right): They consist of process flow streams exiting a unit operation or process.

c. Utility Streams: Utility streams provide for the transfer of energy to or from process streams or process units. They are used to regulate temperatures and pressures required in the process. Utility stream inputs and outputs are shown at the top of Figure 19.1.

i. Heat: Heat is most often provided by the flow of a heating or cooling medium but can be provided by other sources such as electrical energy.

ii. Work: This represents shaft work for a pump or compressor doing work on the fluid.

d. Recycle Streams: These streams are internal to the process. They are critical to the operation of the process system. Recycle streams must be identified and their impact on the process understood. A recycle stream is illustrated by **cutting** or **tearing** the recycle stream (see Chapter 13). The **cut ends** create a set of pseudo-input and pseudo-output streams. They are shown along the bottom of the process system block, connected by a broken line. The pseudo-output stream is fed back to the process as a pseudo-input stream.

Recycle streams fall into two categories:

i. Process recycle streams recover raw materials and/or energy to reduce the cost of raw materials, waste disposal, and energy.

ii. Equipment recycle streams affect equipment performance. As an example, increasing reflux to a distillation tower improves separations.

Example 19.1 illustrates how to represent process inputs and outputs for individual pieces of equipment.

Example 19.1.

Draw an input/output model for

a. A pump

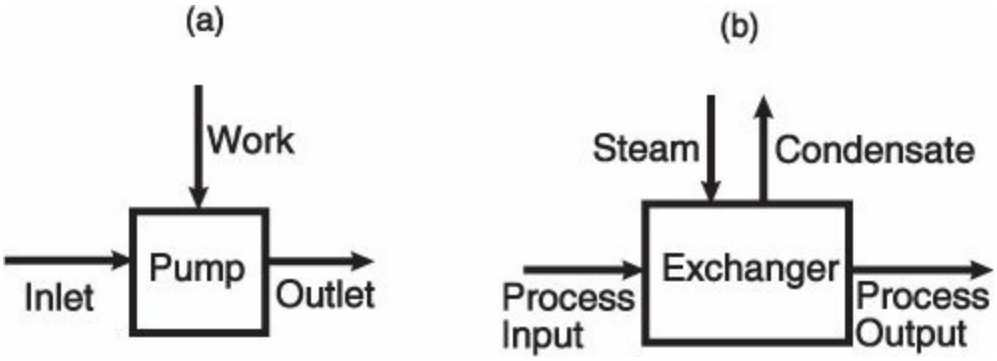
b. A heat exchanger in which a process stream is heated using condensing steam

c. A distillation column

Solution

a. The result is shown in Figure E19.1(a). The mass balance on a pump has one input and one output, as shown. The energy balance on a pump (or one's intuitive understanding of how a pump works) indicates that there is energy input to the process stream, as shown.

b. The result is shown in Figure E19.1(b). A heat exchanger using a utility has one process stream input and one process stream output. The utility also flows in (steam) and out (condensate) of the heat exchanger.



Figures E19.1(a) and (b). Solutions to Example 19.1

c. The result is shown in Figure E19.1(c). The process streams are the feed, bottoms, and distillate. The utility streams are steam for the reboiler and cooling water for the condenser. Finally, the reflux from the condenser and the boil-up from the reboiler are represented as recycle streams, which both leave and enter across system boundaries.

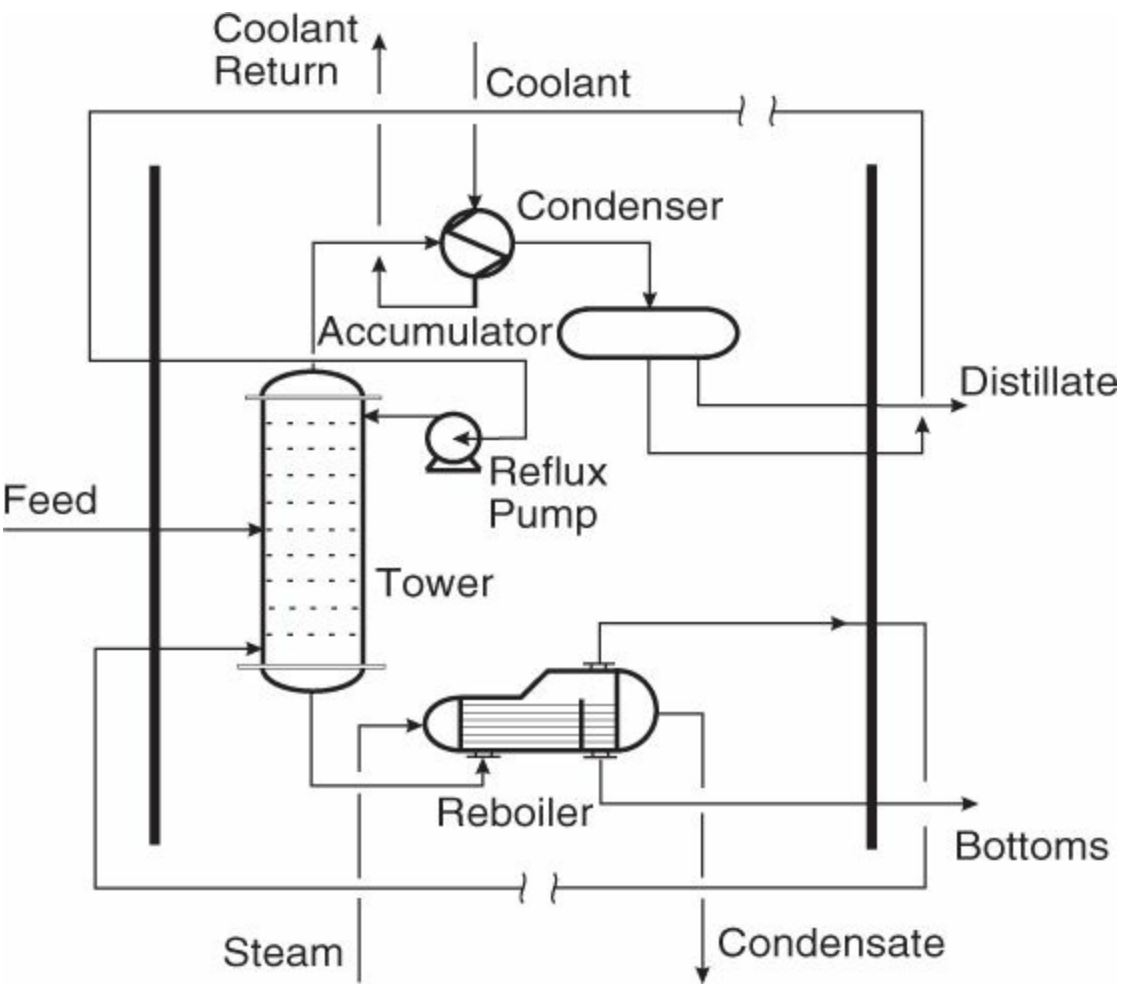


Figure E19.1(c). Solution to Example 19.1(c)

Using the input/output diagram in Figure 19.1, two classifications are identified for process analysis problems encountered in this text:

1. **Process Design Analysis:** Input and output streams are fixed. A process system is designed to transform the input into the output.
2. **Process Performance Analysis:** Input and equipment are fixed. The outputs are determined by the process system.

19.2. Analysis of the Effect of Process Inputs on Process Outputs

An intuitive understanding of the effect of process inputs on process outputs can be obtained by categorizing the relationships used to analyze equipment. These relationships are broken down into two groups:

1. **Equipment-Independent Relationships:** These relationships are independent of equipment specifications. Material balance, energy balance, kinetics, and equilibrium relationships are examples of equipment-independent relationships.
2. **Equipment-Dependent Relationships:** These are often called **design equations** and involve equipment specifications. The heat transfer equation (contains area, A) and the frictional pressure relationship (contains pipe size, D_p, and the equivalent length, L_{eq}) are examples of equipment-dependent relationships.

Unless equipment-dependent relationships are known and used, the impact of a

change of process input on the output cannot be determined correctly.

Example 19.2. illustrates equipment-independent and equipment-dependent relationships.

Example 19.2.

What relationships are used to analyze the following pieces of equipment? Classify these as equipment independent and equipment dependent.

a. Heat exchanger

b. Adiabatic reactor

c. Multistage extraction

Solution

a. The energy balance—which for a temperature change without phase change is $Q = \dot{m}\, C_p \Delta T$, and for a phase change is $Q = \dot{m}\, \lambda$—is an equipment-independent relationship. The design (or performance) equation for a heat exchanger is $Q = UA\Delta T_{lm}F$. It is observed that only the equipment-dependent relationship contains equipment specifications—in this case, the area for heat transfer, A.

b. In a reactor, equipment-independent relationships may include kinetics and/or the definition of equilibrium. If there are no equilibrium limitations, the kinetics may take the form $r = kC_AC_B$, where A and B are the reactants. All kinetic expressions are equipment independent and are only functions of temperature, pressure, and concentration. The energy balance, which is necessary to determine the outlet temperature of the adiabatic reactor, is another relevant equipment-independent relationship. One equipment-dependent relationship is the design equation for the reactor, and it depends upon the type of reactor. For example, for a CSTR, this relationship is $V/F_{Ao} = X/(-r_A)$. It is observed that this relationship contains an equipment specification—in this case, the reactor volume, V. Another equipment-dependent relationship is for the pressure drop through the reactor, which is important in analyzing changes in flowrates.

c. In any multistage separation involving a mass separating agent, the mass balance is the key equipment-independent relationship. For example, it is understood that increasing the solvent rate results in a better separation. Another equipment-independent relationship is the statement of phase equilibrium. An equipment-dependent relationship does not exist as a simple, closed-form equation, except in certain limiting cases. However, an intuitive understanding of the equipmentdependent relationship is possible. For example, it is understood that increasing the number of stages will (usually) improve the separation. For the limiting case of dilute solutions, all the above relationships can be expressed as a single, closed-form equation, the Kremser equation. This will be discussed in Chapter 21. Another equipmentdependent relationship is the efficiency of the equipment, which is dependent on the liquid and vapor flowrates.

19.3. A Process Example

It is assumed that both the equipment-independent and equipment-dependent relationships are understood, and attention is focused on integrating these relationships to analyze a complete

processes. In a chemical process, a change in input to one piece of equipment or a change in performance of that piece of equipment affects more than just the output from that piece of equipment. Because the output from the piece of equipment in question usually becomes the input to another piece of equipment, the disturbance caused by the change in the original piece of equipment can propagate through the process.

This is important in two types of problems that are discussed in later chapters. In one type of problem, the effect of a planned disturbance, such as a 10% scale-up in production, can be quantified only by considering the effect of a changed output from one unit on the subsequent unit. Similarly, in a second type of problem, an observed disturbance in the output of a particular unit may trace back to a disturbance in a unit far removed from the observed disturbance.

In order to analyze these problems, the input/output model for an entire process must be understood, as must the equipment-independent and equipment-dependent relationships for each piece of equipment in the process. This is illustrated in Example 19.3.

Example 19.3.

Consider the toluene hydrodealkylation process illustrated in Figure 1.5. Draw and label an input/output diagram, similar to Figure 19.1, for this process. Label all process inputs and outputs, all utility streams, and all recycles. Then pick any two adjacent units and draw their input/output diagrams together, showing how the output from one unit affects the adjacent unit.

Figure E19.3(a) is the input/output diagram for the entire process. It is observed that there are two recycles: one for hydrogen and one for toluene, both unreacted reactants. This is a particularly useful representation because all of the inputs and outputs also represent cash flows. By showing all of the utilities, it is less likely that one could be omitted from a cash flow analysis.

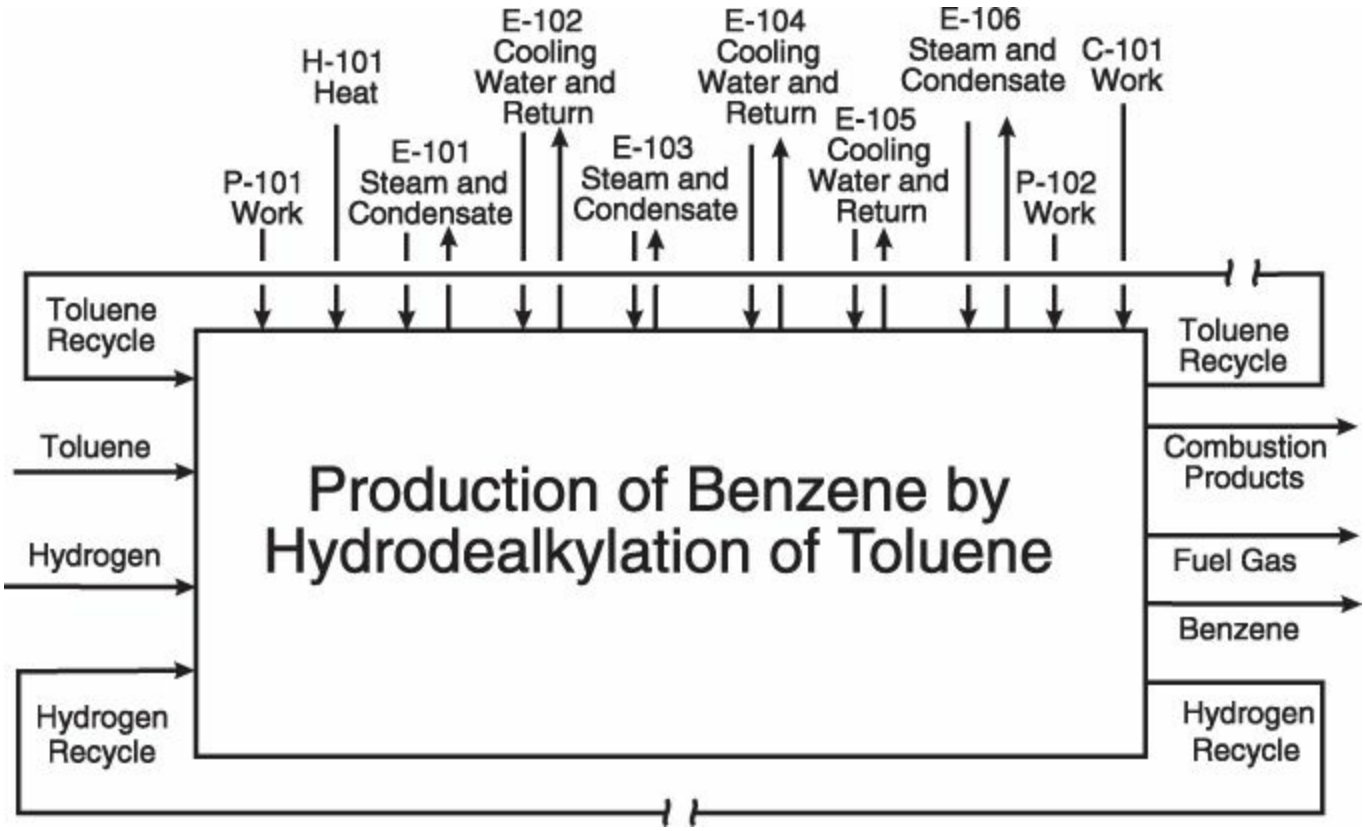


Figure E19.3(a). Solution to Example 19.3

Figure E19.3(b) is an input/output diagram for the toluene feed pump (P-101) and the heat exchanger

(E-101). This diagram makes it evident that any disturbance in the feed to or the operation of the pump not only affects the pump output but also affects the heat-exchanger output. Clearly, this disturbance would also propagate to other downstream equipment.

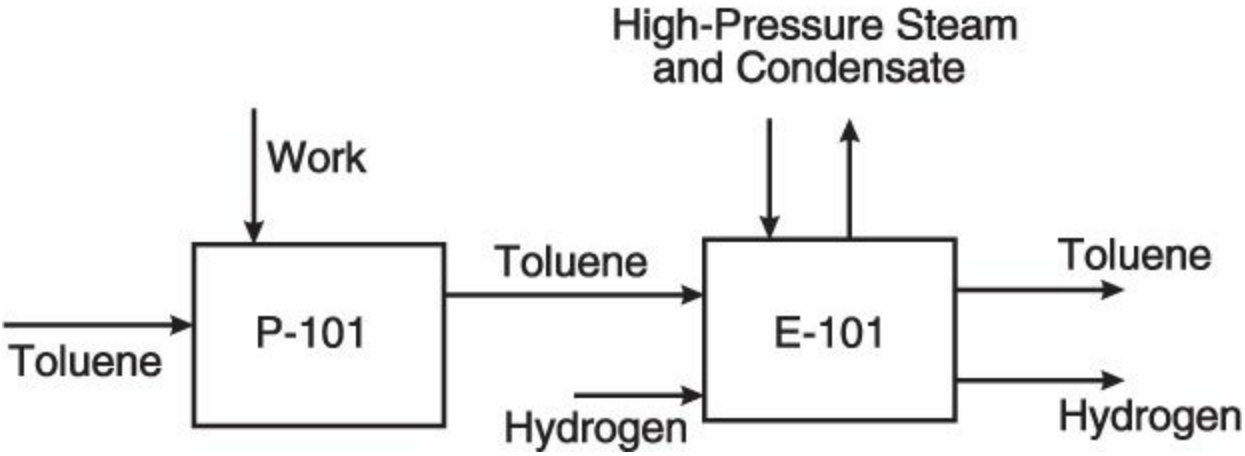


Figure E19.3(b). One Possible Solution to Example 19.3

19.4. Summary

This chapter introduced and demonstrated the importance of the input/output characteristics of chemical processes. In the input/output structure, process inputs are the driving force for change and the unit operations are the mechanism for change.

Recycle streams are of special importance and create pseudo-input/output streams that are critical to analysis of process changes. Utility streams act as "servants" of the process units and streams and provide the desired temperature and pressure for the process units. They exchange energy with the process stream and process units.

As a consequence of the linkage between process units, a change in a single input or unit affects the total system. The impact on the process cannot be evaluated solely from analysis of isolated units.

What You Should Have Learned

- How to represent and understand the input-output structure of a chemical process

Problems

1. Draw input/output diagrams for the following pieces of equipment:
   a. A fluidized bed
   b. A turbine
   c. A pump
   d. A stripper
   e. An adiabatic batch reactor
   f. A semibatch reactor with heat removal
   g. A heat exchanger between two process streams (no utilities)
2. Write down the equipment-independent and equipment-dependent relationships for each piece of equipment listed in Problem 19.1.

3. Write down the equipment-independent and equipment-dependent relationships for a distillation column.
4. Draw input/output diagrams for the following processes. Pick any two adjacent pieces of equipment, and draw input/output diagrams for these, clearly showing how the output from one affects the input to the other.
   a. Ethylbenzene, described in Appendix B, Project B.2
   b. Styrene, described in Appendix B, Project B.3
   c. Drying oil, described in Appendix B, Project B.4
   d. Maleic anhydride, described in Appendix B, Project B.5
   e. Ethylene oxide, described in Appendix B, Project B.6
   f. Formalin, described in Appendix B, Project B.7

Chapter 20. Tools for Evaluating Process Performance

What You Will Learn

- There are important relationships, probably taught in earlier classes, that are used to evaluate process performance.

Several important computational and graphical tools used to analyze plant operations and changes in process design are developed and demonstrated in this chapter. Many of these tools are keyed to actual system performance. Tools presented are used extensively in future chapters.

Intuitive understanding is emphasized over computational complexity. All problems can be solved using a calculator without special functions. Graphical representations are also emphasized. They illustrate the characteristic behavior of a unit or process over a wide range of operations. Graphical presentations reveal critical operating regions that demand careful assessment.

20.1. Key Relationships

In analyzing equipment performance, there are certain key relationships that are used over and over again. These are shown in Table 20.1. Although these should be familiar to the reader, they are important enough to be reviewed here.

Table 20.1. Typical Key Performance Relationships

Situation	Equation	Trends	Comments
Frictional loss for fluid flow	$\Delta P = \frac{2\rho f L_{eq} u^2}{D}$	$\lvert\Delta P\rvert \propto u^2$ $\lvert\Delta P\rvert \propto D^{-5}$ $\lvert\Delta P\rvert \propto L$	Assumes fully developed turbulent flow, i.e., constant friction factor; for laminar flow $\Delta P \propto D^{-4}$.
Heat transfer	Of form $\left(\frac{hD}{k}\right) = c\left(\frac{Du\rho}{\mu}\right)^a\left(\frac{\mu C_p}{k}\right)^b$	$h_i \propto v^{0.8}$ inside closed channels $h_o \propto v^{0.6}$ cross flow outside pipes	Equations given are for no phase change; if phase change, weak flow dependence, but some ΔT dependence.
Kinetics	$r = k\Pi c_i^{a_i}$ $k = k_o e^{-\left(\frac{E}{RT}\right)}$	ln k vs $1/T$ is linear	As $T \uparrow, k \uparrow$ for ideal gases $P \uparrow, c_i \uparrow$, so $r \uparrow$.
Reactor	Mixed flow: $\frac{V}{F_{A0}} = \frac{\tau}{C_{A0}} = \frac{X}{-r_A}$ Plug flow: $\frac{V}{F_{A0}} = \frac{\tau}{C_{A0}} = \int_0^X \frac{dX}{-r_A}$	$\tau \propto V$ as $\tau \uparrow$ or $V \uparrow, X \uparrow$	τ is space time, V is reactor volume, X is conversion of limiting reactant, A assumes one reaction and constant volumetric flowrate.
Separator using mass separating agent	Not necessarily described by a single equation	As flow of mass separating agent $\uparrow$, or as number stages or height of packed tower $\uparrow$, degree of separation $\uparrow$	For certain cases, there are limitations to the effect of increasing number of stages or packed tower height.
Distillation	Not necessarily described by a single equation	As reflux ratio $\uparrow$, degree of separation $\uparrow$	Complicated analysis; see Chapter 21.

The first entry deals with the pressure drop due to frictional losses in a pipe. The key relationship is the proportionality between pressure drop and the square of the velocity, and the proportionality between pressure drop and length (or equivalent length) of pipe. Although it is intuitive that the pressure drop should increase with length of pipe and with increasing velocity, the quantitative relationship reveals the square dependence on velocity. Similarly, although it is intuitive that a larger pipe diameter should reduce frictional losses, the negative fifth-power dependence is revealed only by the equation describing the actual physical situation. Similarly, the general trends for heat transfer coefficients and for rate constants may be intuitive, but the equation describing the actual physical situation shows that quantitative dependence. For reactors and separators, only the intuitive trends can be shown because the exact, quantitative dependence is either situation specific or not easily quantifiable using a closed-form equation.

The relationships in Table 20.1 will be used extensively in Chapters 21, 22, and 23.

20.2. Thinking with Equations

It is possible to quantify equipment performance without resorting to extensive, detailed calculations. This involves using equations to understand trends. The first step is to identify the equations necessary to quantify a given situation. Wales and Stager [1] have termed this "thinking with

equations" and have used the acronym GENI to describe the associated problem-solving strategy. The second step involves predicting trends from equations. These methods are described and then illustrated in an example.

20.2.1. GENI

GENI is a method for solving quantitative problems. The name GENI is an acronym for the four steps in the method.

1. **Goal:** Identify the goal. This is usually the unknown that needs to be calculated.
2. **Equation:** Identify the equation that relates the unknown to known values or properties.
3. **Need:** Identify additional relationships that are needed to solve the equation in Step 2.
4. **Information:** List additional information that is available to determine whether what is needed in Step 3 is known. If the correct information is not known, the need becomes the new goal and the process is repeated.

20.2.2. Predicting Trends

The following method can be used to predict trends from equations known to apply to a given physical situation. In this method, there are four possible modifiers to a term in an equation:

1. ¢: value remains constant.
2. ↑: value increases.
3. ↓: value decreases.
4. ?: value change not known.

Each variable in an expression has one of these identifiers appended. If x is a constant, then $x \rightarrow x(¢)$. The symbol in parentheses identifies the effect the variable has on the term; that is, reducing a value in the denominator of a term increases the term.

The application of the techniques described in Sections 20.2.1 and 20.2.2 is illustrated in Example 20.1.

Example 20.1.

For a bimolecular, elementary, gas-phase reaction, the rate expression is known to be $-r_A = kC_AC_B$.

a. What is the effect on the reaction rate of increasing the reaction pressure by 10% while maintaining constant temperature?

b. What is the effect on the reaction rate of increasing the reaction temperature by 10% while maintaining constant pressure?

The **goal** is to determine the effect of increasing pressure on the reaction rate. The **equation** containing the unknown value, which is the reaction rate, r_A, is given. A relationship is needed between pressure and at least one variable in the equation. The ideal gas law states that $C_i = P_i/RT$, where i is A or B.

Now that the necessary relationships are known, an intuitive understanding can be obtained by predicting trends.

a. First, examine the ideal gas relationship. If the pressure increases with the temperature remaining constant, then the ideal gas relationship can be written as

$$C_i(\uparrow) = y_i(\not\epsilon)P(\uparrow)/R(\not\epsilon)T(\not\epsilon) = P_i(\uparrow)/R(\not\epsilon)T(\not\epsilon)$$

Therefore, the concentration increases because the pressure increases while the temperature and the gas constant remain constant. Intuitively, if the pressure increases by 10%, the concentration must increase by 10%.

Moving to the rate expression, because the rate constant is not affected by pressure, the resulting trend is predicted by

$$r_A(\uparrow) = k(\not\epsilon)C_A(\uparrow)C_B(\uparrow)$$

which means that the reaction rate increases. Intuitively, because each concentration increases by 10%, then the reaction rate changes by a factor of $(1.1)^2 = 1.21$, an increase of 21%.

b. In this case, from the ideal gas relationship,

$$C_i(\downarrow) = y_i(\not\epsilon)P(\not\epsilon)/R(\not\epsilon)T(\uparrow) = P_i(\not\epsilon)/R(\not\epsilon)T(\uparrow)$$

From the rate expression, because the rate constant is a function of temperature,

$$r_A(?) = k(\uparrow)C_A(\downarrow)C_B(\downarrow)$$

Because the concentrations decrease and the rate constant increases, it cannot be determined, a priori, whether the rate increases or decreases. If the activation energy in the rate constant were known, a quantitative evaluation could be made.

20.3. Base-Case Ratios

The calculation tool provided in this section combines use of fundamental relationships with plant operating data to form a basis for predicting changes in system behavior.

The ability to predict changes in a process design or in plant operations is improved by anchoring an analysis to a base case. For design changes, it is desirable to identify a design proven in practice as the base case. For operating plants, actual data are available and are chosen as the base case. It is important to put this base case into perspective. Assuming that there are no instrument malfunctions and the operating data are correct, then these data represent a real operating point at the time the data were taken. As the plant ages, the effectiveness of process units changes and operations is altered to account for these changes. As a consequence, recent data on plant operations should be used in setting up the base case.

Establish predictions of process changes on known operating data, not on design data.

The base-case ratio integrates the "best available" information from the operating plant with design relationships to predict process changes. It is an important and powerful technique with wide application. The base-case ratio, X, is defined as the ratio of a newcase system characteristic, x_2, to the base-case system characteristic, x_1.

$$X \equiv x_2/x_1 \qquad (20.1)$$

Using a base-case ratio often reduces the need for knowing actual values of physical and transport properties (physical properties refer to thermodynamic and transport properties of fluids), equipment, and equipment characteristics. The values identified in the ratios fall into three major groups. They are defined below and applied in Example 20.2.

1. **Ratios Related to Equipment Sizes** (L_{eq}, equivalent length; diameter, D; surface area, A): Assuming that the equipment is not modified, these values are constant, the ratios are unity, and these terms cancel out.
2. **Ratios Related to Physical Properties** (such as density, ρ; viscosity, μ): These values can be functions of material composition, temperature, and pressure. Absolute values are not needed, only the functional relationships. Quite often, for small changes in composition, temperature, or pressure, the properties are unchanged, and the ratio is unity and cancels out. An exception to this is gas-phase density.
3. **Ratios Related to Stream Properties:** These usually involve velocity, flowrate, concentration, temperature, and pressure.

Using the base-case ratio eliminates the need to know equipment characteristics and reduces the amount of physical property data needed to predict changes in operating systems.

The base-case ratio is a powerful and straightforward tool to analyze and predict process changes. This is illustrated in Example 20.2.

Example 20.2.

It is necessary to scale up production in an existing chemical plant by 25%. It is your job to determine whether a particular pump has sufficient capacity to handle the scale-up. The pump's function is to provide enough pressure to overcome frictional losses between the pump and a reactor.

The relationship for frictional pressure drop is given in Table 20.1. This relationship is now written as the ratio of two base cases as follows:

$$\frac{\Delta P_2}{\Delta P_1} = \frac{2\rho_2 f_2 L_{eq2} u_2^2 D_1}{2\rho_1 f_1 L_{eq1} u_1^2 D_2}$$

Because the pipe has not been changed, the ratios of diameters (D_2/D_1) and lengths (L_{eq2}/L_{eq1}) are unity. Because a pump is used only for liquids, and liquids are (practically) incompressible, the ratio of densities is unity. If the flow is assumed to be fully turbulent, which is usually true for process applications, the friction factor is not a function of Reynolds number. (This fact should be checked for a particular application.) Therefore, the friction factor is constant, and the ratio of friction factors is unity. The above ratio reduces to

$$\frac{\Delta P_2}{\Delta P_1} = \frac{u_2^2}{u_1^2} = \frac{\dot{m}_2^2/A_2^2\rho_2^2}{\dot{m}_1^2/A_1^2\rho_1^2} = \frac{\dot{m}_2^2}{\dot{m}_1^2}$$

where the second equality is obtained by substituting for u_i in numerator and denominator using the mass balance $\dot{m}_i = \rho_i A_i u_i$, canceling the ratio of densities for the same reason as above, and canceling the ratio of cross-sectional areas because the pipe has remained unchanged. Therefore, by assigning the base-case mass flow to have a value of 1, for a 25% scale-up, the new case has a mass flow of 1.25, and the ratio of pressure drops becomes

$$\frac{\Delta P_2}{\Delta P_1} = \left(\frac{\dot{m}_2}{\dot{m}_1}\right)^2 = \left(\frac{1.25}{1}\right)^2 = 1.56$$

Thus, the pump must be able to deliver enough head to overcome 56% additional frictional pressure

drop while pumping 25% more material.

It is important to observe that Example 20.2 was solved without knowing any details of the system. The pipe diameter, length, and number of valves and fittings were not known. The liquid being pumped, its temperature, and its density were not known. Yet the use of base-case ratios along with simple assumptions permitted a solution to be obtained. This illustrates the power and simplicity of base-case ratios.

20.4. Analysis of Systems Using Controlling Resistances

Design relationships for many operations such as fluid flow, heat transfer, mass transfer, and chemical reactors all involve rate equations of the general form

$$\text{Rate} = \text{Driving Force/Resistance.} \tag{20.2}$$

For resistances in series,

$$R_T\,(\text{Total Resistance}) = R_1 + R_2 + R_3 + \cdots + R_N \tag{20.3}$$

For certain situations, one resistance dominates all other resistances. For example, if resistance R_1 dominates, then

$$R_1 >> R_2 + R_3 + \cdots + R_N \tag{20.4}$$

and

$$R_T \approx R_1 \tag{20.5}$$

where R_1 represents the "controlling resistance." Other resistances have little impact on the rate. Only those factors that impact R_1 have a significant impact on the rate.

As an example, an overall heat transfer coefficient for a clean (nonfouling) service, U_o, can be expressed as

$$\frac{1}{U_o} = \frac{1}{h_o} + \frac{D_o \ln\left(\frac{D_o}{D_i}\right)}{2k} + \frac{D_o}{D_i h_i} \tag{20.6}$$

where D_o and D_i are the outer and inner tube diameters, respectively, k is the thermal conductivity of the tube material, and h_o and h_i are the outer and inner heat transfer coefficients. It is assumed that Equation (20.6) can be simplified by assuming $D_o \approx D_i$, and that the conduction resistance is negligible, so that

$$\frac{1}{U_o} = \frac{1}{h_o} + \frac{1}{h_i} \tag{20.7}$$

Suppose that it is desired to use a base-case ratio of a new overall heat transfer coefficient, U_{o2}, to an original overall heat transfer coefficient, U_{o1}. For a situation when no phase change is occurring on either side of a shell-and-tube heat exchanger, from Equation (20.7), this ratio would be

$$\frac{\left(\frac{1}{U_{o1}}\right)}{\left(\frac{1}{U_{o2}}\right)} = \frac{U_{o2}}{U_{o1}} = \frac{\frac{1}{\alpha u_{i1}^{0.8}} + \frac{1}{\beta u_{o1}^{0.6}}}{\frac{1}{\alpha u_{i2}^{0.8}} + \frac{1}{\beta u_{o2}^{0.6}}} \tag{20.8}$$

where the individual heat transfer coefficients have been expressed as indicated in Table 20.1, and the proportionality factors α and β contain the lead constant and all of the properties contained in the dimensionless groups other than the heat transfer coefficient and the velocity. From Equation (20.8), it would not be possible, as it was in Example 20.2, to determine quantitatively how the overall heat transfer coefficient changes with changing velocity (i.e., mass flowrate) without knowing values for all of the physical properties. However, if it could be assumed that one resistance were dominant, the problem would be greatly simplified. For example, assume that a heat transfer fluid in the shell is heating a gas in the tubes. It is likely that the resistance in the tubes would dominate, given the low film heat transfer coefficient for gases. Therefore, the base-case ratio would reduce to

$$\frac{U_{o2}}{U_{o1}} = \frac{h_{i2}}{h_{i1}} = \left(\frac{u_{i2}}{u_{i1}}\right)^{0.8} \qquad (20.9)$$

and it would be possible to predict a new heat transfer coefficient without having values for the physical properties.

The reduction of the heat transfer coefficient ratio using a limiting resistance described above is very powerful but must be used with care. It is not valid for all situations. It is most likely valid when one resistance is for a boiling liquid or condensing steam and the other resistance is for a liquid or gas without phase change. In other situations, the base-case ratio can be determined from Equation (20.8) only if the relative magnitude for each resistance is known for the base case, as is illustrated in Example 20.4. It is also important to understand that Equations (20.8) and (20.9) do not represent all possible base-case ratios arising in heat transfer. Each situation must be analyzed individually to ensure that a correct solution is obtained. Problems of this type are given at the end of the chapter.

Situations in which the simplifications leading to Equation (20.9) are valid, along with situations that require a form for the base-case ratio similar to Equation (20.8), will be applied to heat-exchanger performance in Chapter 21. Examples of how Equations (20.8) and (20.9) can be applied are presented in Examples 20.3 and 20.4.

Example 20.3.

It is desired to scale down process capacity by 25%. In a particular heat exchanger, process gas in the tubes is heated by condensing steam in the shell. By how much will the overall heat transfer coefficient for the heat exchanger change after scale-down?

Using the subscript 2 for the new, scaled-down operation and the subscript 1 for the original conditions, a scale-down of the mass flowrate of the process stream by 25% means that $u_{i2} = 0.75u_{i1}$.

For a process gas heated by condensing steam, it is certain that the heat transfer coefficient for condensing steam will be at least 100 times as large as that for the process gas. Although Equation (20.9) is applicable, it is not derived from Equation (20.8) because of the phase change. The correct derivation is assigned in Problem 20.5 at the end of the chapter. The result is $U_{o2}/U_{o1} = (u_{i2}/u_{i1})^{0.8} = (0.75)^{0.8} = 0.79$, and the overall heat transfer coefficient is reduced by 21%.

Example 20.4.

In a similar process as in Example 20.3, there is a heat exchanger between two process streams, neither of which involves a phase change. It is known that the resistances on the shell-and-tube sides are approximately equal before scale-down. By how much will the overall heat transfer coefficient

for the heat exchanger change after scale-down by 25%?

Here, Equation (20.7) is required. Because both original resistances are equal, both original heat transfer coefficients will be denoted h_1. In the tubes, $h_{i2}/h_1 = (u_{i2}/u_{i1})^{0.8}$, and in the shell $h_{o2}/h_1 = (u_{o2}/u_{o1})^{0.6}$. Both velocity ratios are 0.75. Therefore, Equation (20.7) reduces to

$$\frac{U_2}{U_1} = \frac{\frac{1}{h_1} + \frac{1}{h_1}}{\frac{1}{h_1\left(\frac{u_{i2}}{u_{i1}}\right)^{0.8}} + \frac{1}{h_1\left(\frac{u_{o2}}{u_{o1}}\right)^{0.6}}} = \frac{2}{\frac{1}{(0.75)^{0.8}} + \frac{1}{(0.75)^{0.6}}} = 0.82$$

and the new heat transfer coefficient is reduced by 18%.

20.5. Graphical Representations

At times, graphical representations are useful descriptions of physical situations. They provide a means to an intuitive understanding of a problem rather than a computational tool. Probably the best-known example of this is the McCabe-Thiele diagram for distillation. Even though no one would design a distillation column nowadays using this method, the McCabe-Thiele diagram provides a means for an intuitive understanding of distillation. Another example is the reactor profiles illustrated in Chapter 23.

In this section, three graphical representations that will be used to analyze performance problems are discussed.

20.5.1. The Moody Diagram for Friction Factors

An example of a graphical representation commonly used for illustrative and for computational purposes is the Moody diagram, which gives the friction factor as a function of Reynolds number for varying roughness factors. It is illustrated in Figure 20.1. Although this diagram is often used for numerical calculations, it also provides an intuitive understanding of frictional losses. For example, it is observed that the friction factor increases as the pipe roughness increases. It is also observed that the friction factor becomes constant at high Reynolds numbers, and the dashed line represents the boundary between variable and constant friction factor.

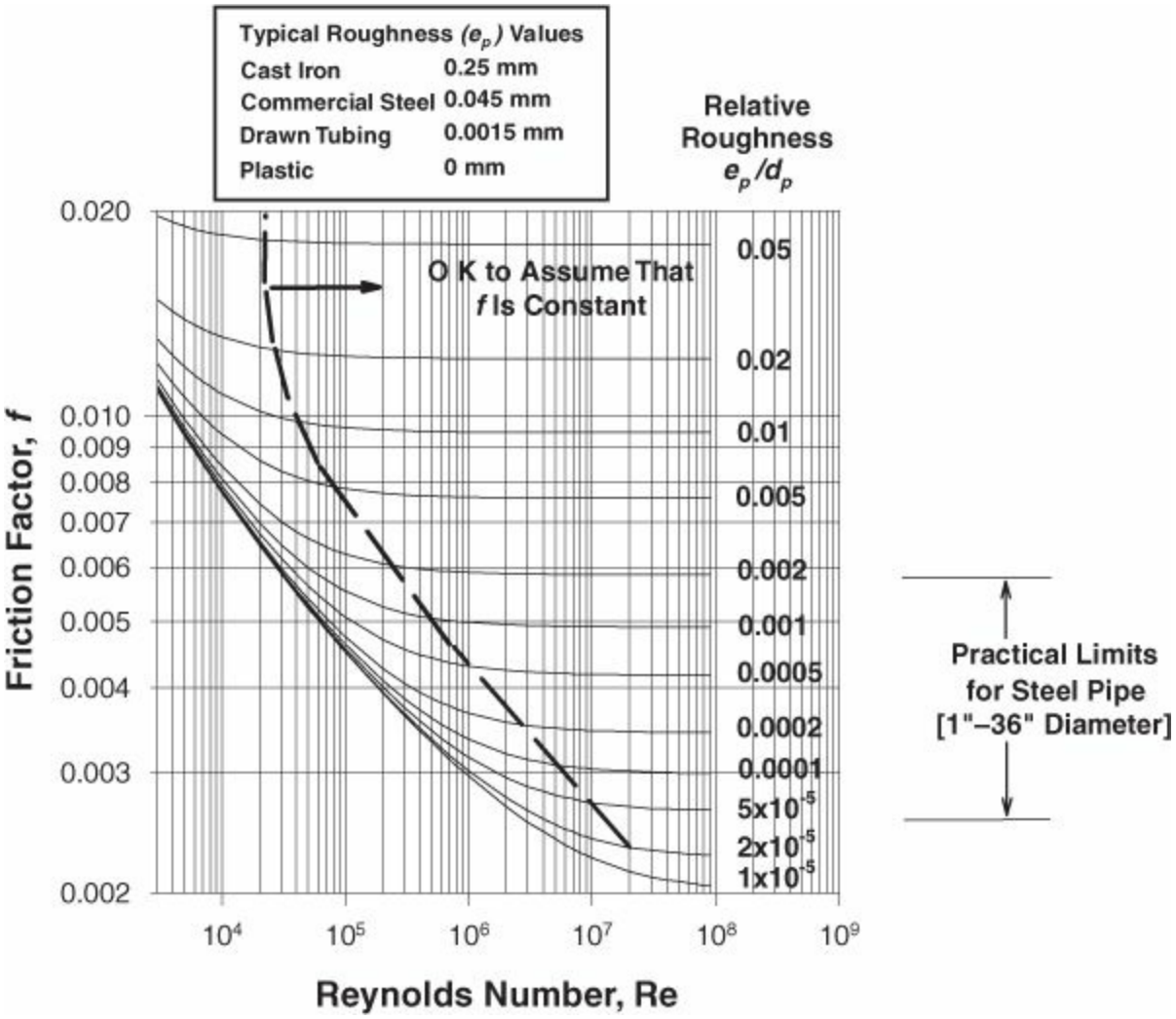


Figure 20.1. Moody Plot for Turbulent Flow in Pipes

20.5.2. The System Curve for Frictional Losses

In Table 20.1, an equation was given for frictional losses in a pipe. This equation is derived from the mechanical energy balance for constant density.

$$\frac{\Delta P}{\rho g} + \Delta z + \Delta\frac{u^2}{2g} - \frac{W_s}{g} + \frac{F_d}{g} = 0 \qquad (20.10)$$

In Equation (20.10), Δ means out – in, and the specific energy dissipation due to drag, F_d, is a positive number. For a constant diameter length of pipe with no pump at constant elevation, $\Delta z = 0$, there is no work, the kinetic energy term is zero, and, using the expression for frictional losses, the result is

$$\Delta P = -\rho F_d = -\frac{2\rho f L_{eq} u^2}{D} \qquad (20.11)$$

If fully developed turbulent flow is assumed, the friction factor, f, is constant. For process changes involving the same fluid, the density remains constant, and if the pipe is unchanged, the equivalent length and diameter are unchanged. Therefore, Equation (20.11) describes how the pressure drop in a length of pipe changes with flowrate or velocity. This can be plotted as ΔP versus velocity, and the result is a parabola passing through the origin. This is called the **system curve** and will be shown in Chapter 21 to be a useful tool in evaluating pump performance.

If, for example, there were an elevation change over the length of pipe in question, there would be an additional term in Equation (20.11), and the result would be a parabola with a nonzero intercept.

Examples 20.5 and 20.6 illustrate how a system curve is obtained.

Example 20.5.

Develop the system curve for flow of water at approximately 10 kg/s through 100 m of 2-in schedule-40 commercial steel pipe oriented horizontally.

The density of water will be taken as 1000 kg/m^3, and the viscosity of water will be taken as 1 mPa s (0.001 kg/m s). The inside diameter of the pipe is 0.0525 m. The Reynolds number can be determined to be 2.42 $\times 10^5$. For a roughness factor of 0.001, $f = 0.005$. Equation (20.11) reduces to

$$\Delta P = -19u^2$$

with ΔP in kPa and u in m/s. This is the equation of a parabola, and it is plotted in Figure E20.5. Therefore, from either the equation or the graph, the pressure drop is known for any velocity.

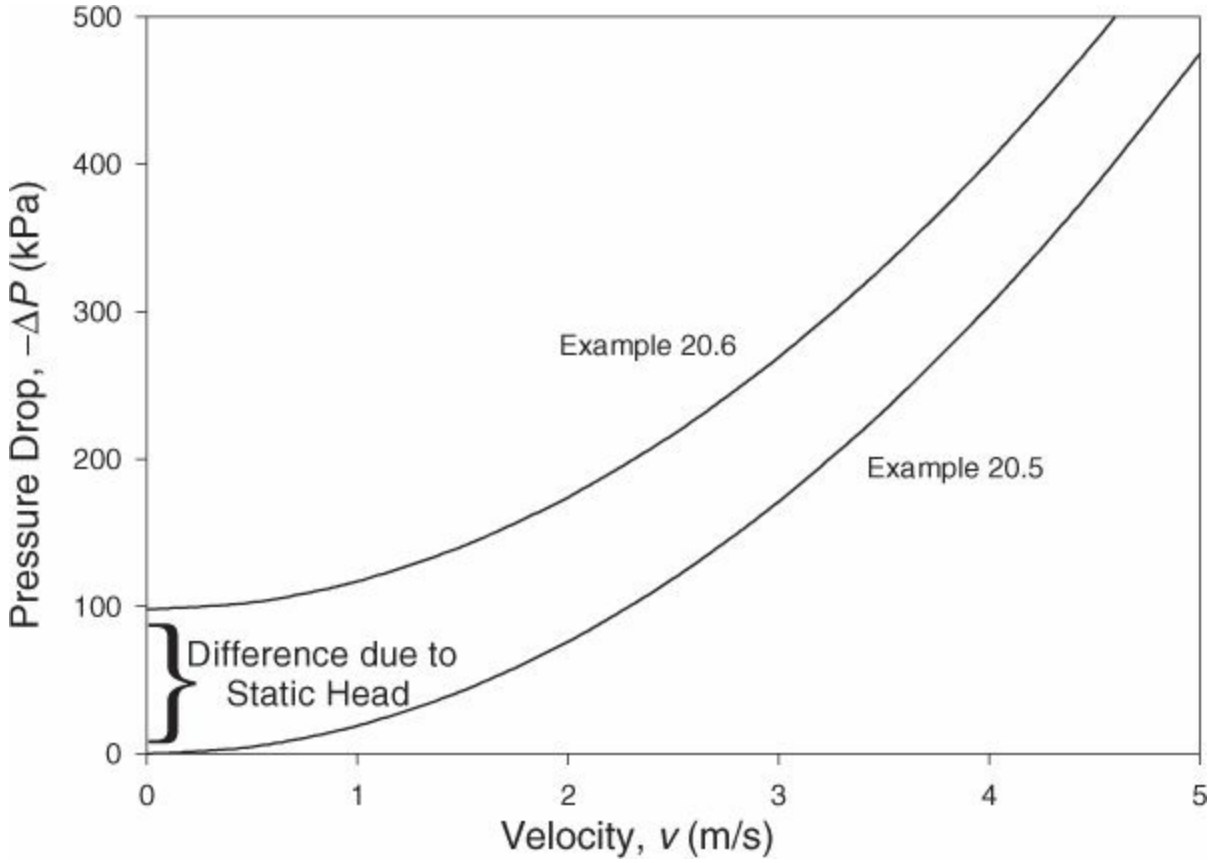


Figure E20.5. System Curves for Examples 20.5 and 20.6

Example 20.6.

Repeat Example 20.5 for pipe with a 10 m vertical elevation change, with the flow from lower to higher elevation.

Here, the potential energy term from the mechanical energy balance must be included. The magnitude of this term is 10 m of water, so $\rho g \Delta z = 98$ kPa. Equation (20.10) reduces to

$$\Delta P = -(98 + 19u^2)$$

with ΔP in kPa and u in m/s. This equation is also plotted in Figure E20.5. It is observed that the system curve has the same shape as that in Example 20.5. This means that the frictional component is unchanged. The difference is that the entire curve is shifted up by the constant, static pressure difference.

20.5.3. The *T-Q* Diagram for Heat Exchangers

Another example of a useful diagram that illustrates the behavior of a piece of equipment is the *T-Q* diagram for a heat exchanger. Figure 20.2 illustrates a *T-Q* diagram for the countercurrent heat exchanger with no phase change shown in the figure.

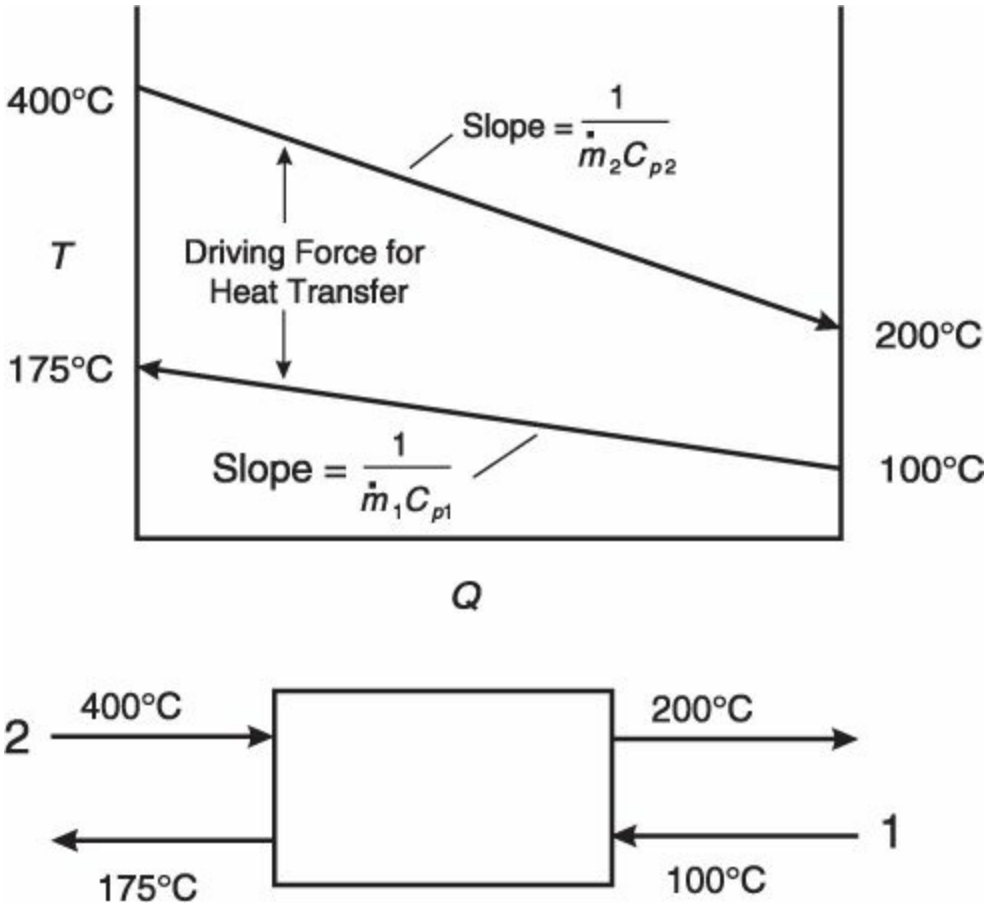


Figure 20.2. Example of *T-Q* Diagram

A *T-Q* diagram is a visual representation of the energy balance equation for each stream. Because, for single-phase streams with constant C_p and no pressure effect on the enthalpy,

$$Q = \dot{m} C_p \Delta T \qquad (20.12)$$

process streams that undergo no phase change are represented by a line with a slope of $1/(\dot{m}C_p)$. Because, for pure component streams undergoing a phase change process streams that involve constant temperature phase changes (pure component vaporizers and condensers) are represented by a horizontal line.

$$Q = \dot{m}\lambda \qquad (20.13)$$

The temperature differences between the two streams shown on the *T-Q* diagram provide the actual temperature driving force throughout the exchanger. The greater the temperature separation, the larger the driving force (ΔT_{lm}), and the greater the heat transferred.

The representations described above are for simple situations commonly encountered. However, more complex cases exist. If the heat capacity is not constant, then the line for heat transfer without phase change is a curve. For phase changes involving multicomponent systems, because the bubble and dew points are at different temperatures, the line representing the phase change is not horizontal. For partial condensers and vaporizers, the representation on a *T-Q* diagram is a curve rather than a straight line.

The *T-Q* diagram reveals two important truths regarding heat transfer:

1. **Temperature Lines Cannot Cross:** This is an impossible situation. Temperature lines will never cross when dealing with operating equipment. If a temperature cross is encountered in doing a calculation, an error has been made.
2. **Temperature Lines Should Not Approach Each Other Too Closely:** As temperature lines approach each other, the area required for a heat exchanger approaches infinity. The point of closest approach is called the pinch point. When dealing with multiple heat exchangers, the pinch point is a key to heat-exchanger network integration, that is, determining the configuration for most efficient heat transfer between hot and cold streams. This concept was discussed in Chapter 15.

Example 20.7 illustrates the construction of *T-Q* diagrams.

Example 20.7.

Sketch a *T-Q* diagram for the following situations:

a. A single-phase process stream is heated from 100°C to 200°C by condensation of saturated steam to saturated liquid at 250°C in a countercurrent heat exchanger.

b. A single-phase process stream is heated from 120°C to 220°C by condensation of saturated steam at 250°C and subcooling of the condensate to 225°C in a countercurrent heat exchanger.

The solution to Part (a) is shown in Figure E20.7(a). The horizontal line at 250°C is for the steam condensing at constant temperature. The sloped line is for heating of the process stream. The arrow on the sloped line indicates the direction of flow of the process stream, because it is being heated. The arrow on the condensing steam line is opposite because of countercurrent flow.

The solution to Part (b) is shown in Figure E20.7(b). The difference from Part (a) is the subcooling zone. It is important to understand that when there is a pure-component phase change, there must be a horizontal portion of the line. It is incorrect to draw a single straight line between the two end temperatures. In fact, due to the amount of heat associated with phase changes relative to the heat in temperature changes, the horizontal portion associated with the phase change will almost always be the longer segment.

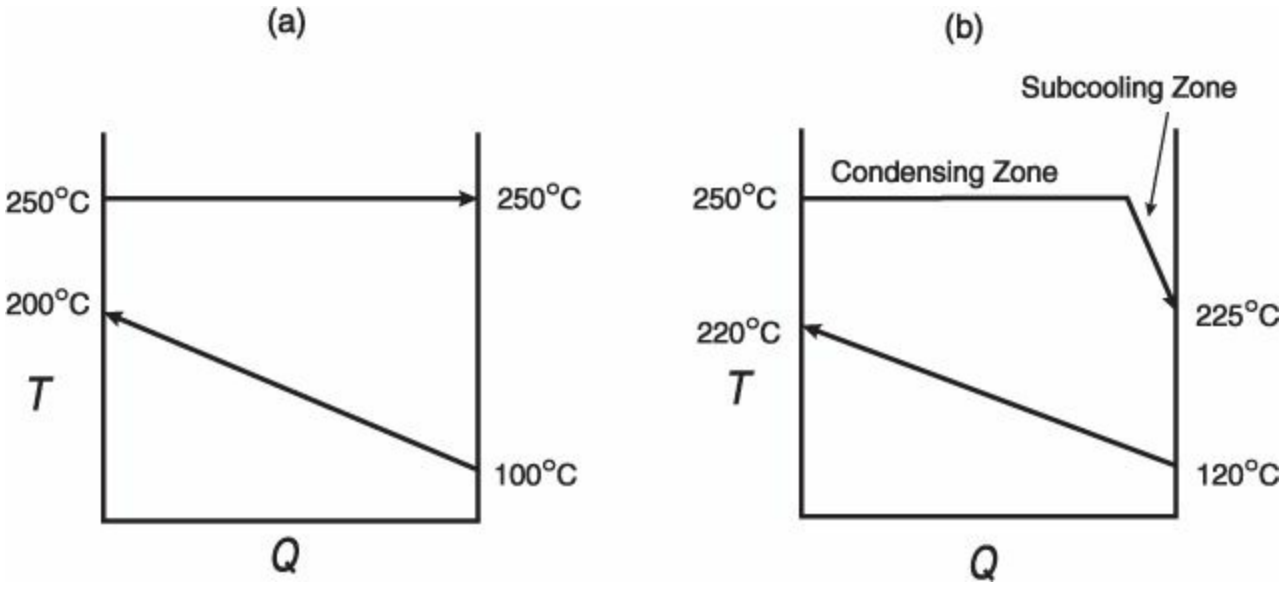


Figure E20.7. Solutions to Example 20.7

20.6. Summary

In this chapter, several important tools were introduced that are essential in analyzing equipment performance problems. Base-case ratios are the most important tool. They permit comparison of two cases, usually without complex calculations, and often without the need to know physical and transport properties. Under the circumstances for which it is valid, using a limiting resistance simplifies the base-case ratio. Finally, graphical representation of equipment performance is a useful tool in understanding the physical situation. All these techniques require a minimum of calculations. However, they do provide an intuitive understanding of equipment performance that is very rarely achieved from merely doing repetitive, complex computations.

What You Should Have Learned

- There are important relationships, probably taught in earlier classes, that are used to evaluate process performance.
- For small variations in process parameters and physical properties, ratios are a powerful tool for analyzing chemical process performance.

Reference

1. Wales, C. E., and R. A. Stager, *Thinking with Equations* (Morgantown, WV: West Virginia University, 1990).

Problems

1. It is known that for a certain second-order, elementary, gas-phase reaction, the rate of reaction doubles when the temperature goes from 220°C to 250°C. If the rate of reaction is 5 mole/m^3s at the base conditions, which are 10 atm pressure and 225°C, and the feed is pure reactant (no inerts), answer the following questions:
   a. Compared to the base case, by how much does the rate of reaction (at inlet conditions) change if the temperature is increased to 245°C at constant pressure?
   b. Compared to the base case, by how much does the rate of reaction (at inlet conditions) change if the pressure is increased by 10%?
2. A storage tank is connected to a pond (at atmospheric pressure!) by a length of 3-in pipe and two gate valves. From previous operating experience, it has been found that when the tank is at a pressure of 3 atm, the flow through the pipe is 12.5 m^3/h, when both gate valves are fully open. If the pressure in the tank increases to 5 atm, what will be the maximum discharge rate from the tank?
3. In a single-pass shell-and-tube heat exchanger, cooling water is used to condense an organic vapor. Under present operating conditions, the heat transfer coefficients are h_o = 2000 W/m^2K (turbulent flow of cooling water), h_i = 700 W/m^2K. Fouling is negligible, and the tubes are 1.25-in 16-BWG carbon steel. Water flows in the shell. If the cooling water rate were to rise suddenly by 15%, estimate the change in overall heat transfer coefficient. Clearly state all assumptions made.
4. In a shell-and-tube heat exchanger, the overall and individual heat transfer coefficients are U =

300 W/m^{2}K, h_i = 1000 W/m^{2}K, and h_o = 500 W/m^{2}K. Both the shell-side and the tube-side fluids are liquids, and no change of phase occurs. The flow of both fluids is turbulent.

a. Estimate the new value of U if the flowrate of the shell-side fluid is decreased by 20%.

b. Estimate the new value of U if the flowrate of the tube-side fluid is decreased by 20%.

c. Estimate the new value of U when both situations in Parts (a) and (b) exist.

5. Derive the relationship, identical to Equation (20.9), for the situation described in Example 20.3.

6. You are considering two pipes to connect liquid leaving a pump to the entrance to a reactor. For a given mass flowrate of liquid, how much operating cost would you save (or lose) by using 2.5-in schedule-40 pipe rather than 3-in schedule-40 pipe? The pump runs on electricity, and electricity costs \$0.06/kWh. The pump efficiency is 80%.

7. For laminar flow of a Newtonian liquid in a pipe, determine the effect on flowrate of the following changes:

a. The pressure drop triples (everything else remains constant).

b. The pipe is changed from 1.25-in schedule-40 to 2-in schedule-40 (everything else remains constant).

c. The viscosity of the fluid is increased by 50% (everything else remains constant).

d. The equivalent length of pipe is decreased by an order of magnitude (everything else remains constant).

e. (a) and (b)

f. (a) and (c)

g. (b) and (d)

8. Sketch T-Q diagrams for the following situations:

a. The condenser on a distillation column; vapor condenses at 160°C and is sub-cooled to 130°C, cooling water enters at 30°C and exits at 40°C.

b. The reboiler on the same distillation column; vapor is reboiled at 240°C, and saturated, high-pressure steam is condensing to saturated water.

c. Methanol, initially at 30°C and atmospheric pressure, is vaporized to 150°C and atmospheric pressure, and saturated, medium-pressure steam is condensed to saturated water.

9. Air at approximately STP and 15 kg/s flows through 100 m of 8-in commercial steel schedule-40 pipe. Derive an expression for the system curve and sketch the system curve for this situation.

10. In a batch reactor, a first-order, irreversible, liquid-phase reaction, A → B, occurs. The initial concentration is C_{Ao}.

a. By what percentage must the reaction time be increased to raise the conversion of A from 0.9 to 0.95?

b. If the initial conversion is 0.8, what will the final conversion be if the reaction time is increased by 50%?

11. Repeat Problem 20.10 for a catalytic/enzymatic reaction with a rate expression of the form

$$-r_A = \frac{K_1 C_A}{1 + K_2 C_A}$$

Chapter 21. Performance Curves for Individual Unit Operations

What You Will Learn

- The relationship between input and output when equipment is fixed (already exists) for
  - Fluid flow/pumps/compressors
  - Heat exchangers
  - Tray columns
  - Packed columns
- How to evaluate the performance of the above equipment
- How to represent the performance of the above equipment graphically
- Equipment limitations

As pointed out in the introduction to Section 4, the way in which a process operates will vary significantly throughout its lifetime. Plant operations do not correspond to the conditions specified in the design. This is *not* necessarily a reflection of a poor design. It is a consequence of changes in the process during the life of the plant. There are numerous reasons why a process might not be operated at design conditions. As stated previously, some examples are the following:

- **Design/Construction:** Installed equipment is often oversized. This reduces risks resulting from inaccuracies in design correlations, uncertainties in material properties, and so on.
- **External Effects:** Feed materials, product specifications and flowrates, environmental regulations, and costs of raw materials and utilities all are likely to change during the life of the process.
- **Replacement of Equipment:** New and improved equipment (or catalysts) may replace existing units in the plant.
- **Changes in Equipment Performance:** In general, equipment effectiveness degrades with age. For example, heat transfer surfaces foul, packed towers develop channels, catalysts lose activity, and bearings on pumps and compressors become worn. Plants are shut down periodically for maintenance to restore equipment performance.

With these factors in mind, a good design is one in which operating conditions and equipment performance can be changed throughout the life of the process and plant. This is known as process flexibility. For a company or operation to remain competitive in the marketplace, it must respond to these changes. Therefore, it is essential to understand how equipment performs over its entire operating range and to be able to evaluate the effects of changing process conditions on the overall process performance.

Several techniques for evaluating operating systems are presented in Chapters 19 and 20. The purpose of this chapter is to apply these techniques to obtain a solution to a performance problem for a specific piece of equipment. This solution may be a single answer. However, a much more useful solution is a curve or a family of curves that represents the way an existing piece of equipment or system responds to changes in input or equipment variables. These curves are referred to as **performance curves**. They are the basis for predicting the behavior of existing equipment.

Performance curves present a range of possible solutions rather than merely a single answer. In principle, performance equations could be used instead of performance curves. However, by representing equipment performance in graphical form, the performance characteristics are easier to visualize, providing a better intuitive understanding. For example, in Figure 20.1, the boundary for fully developed turbulent flow, above which the friction factor is constant, is more effectively represented by the dotted curve on the graph than by the equation of that curve.

Performance curves represent the relationship between process outputs and process inputs.

By plotting the response variables as a function of the input variables, the sensitivity of one to the other becomes immediately obvious. Such sensitivity cannot be inferred from a single (numerical) solution. With the wide availability of spreadsheets and process simulators, the effort expended generating performance curves may be justified.

In order to construct performance and system curves, material and energy balance equations must be used along with the (design) equations relating equipment parameters. However, other constraints may also have to be considered, such as the maximum or minimum system temperature and pressure allowed for the equipment, the maximum velocity of fluid through the equipment to avoid excessive erosion, the maximum or minimum velocity to avoid flooding in packed towers and tray columns, the minimum velocity through a reactor to avoid defluidization, the maximum residence time in a reactor to avoid coking/cracking reactions or by-product formation, the minimum flow through a compressor to avoid surging, or the minimum approach temperature to avoid the condensation of acidic gases inside heat exchangers.

It is possible to construct performance curves for essentially any piece of equipment. In this chapter, performance curves are developed for several specific equipment types. This case-study approach is used to help you develop your own methods for generating performance and system curves for equipment not covered in this text.

21.1. Application to Heat Transfer

In this section, the steam generator shown in Figure 21.1(a) is analyzed to illustrate the preparation and value of a performance diagram for predicting the response of a heat exchanger to changing conditions. The data shown were obtained from an actual operating system. A steam generator is similar to a shell-and-tube heat exchanger. Figure 21.2 contains drawings of portions of shell-and-tube heat exchangers.

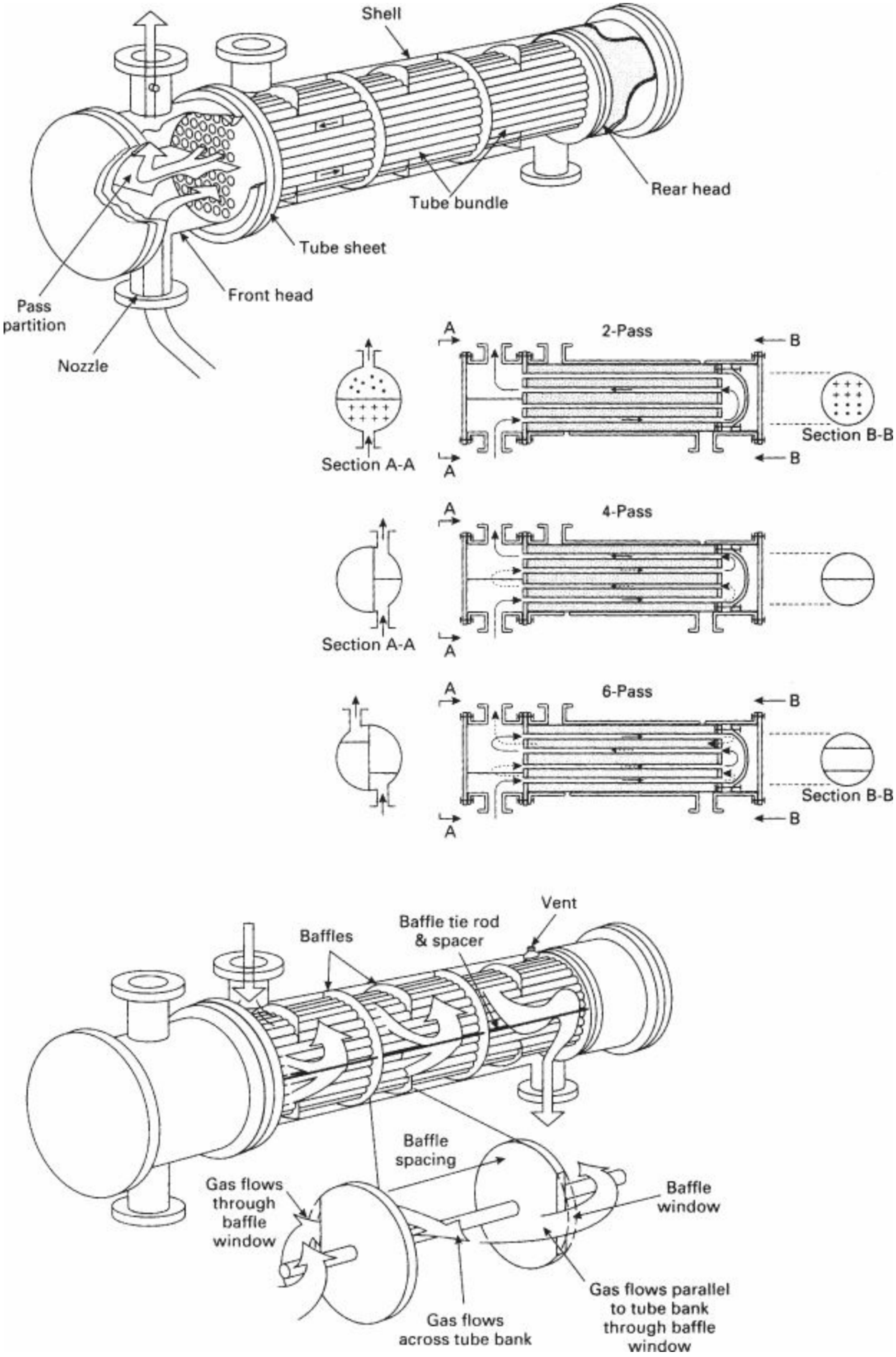
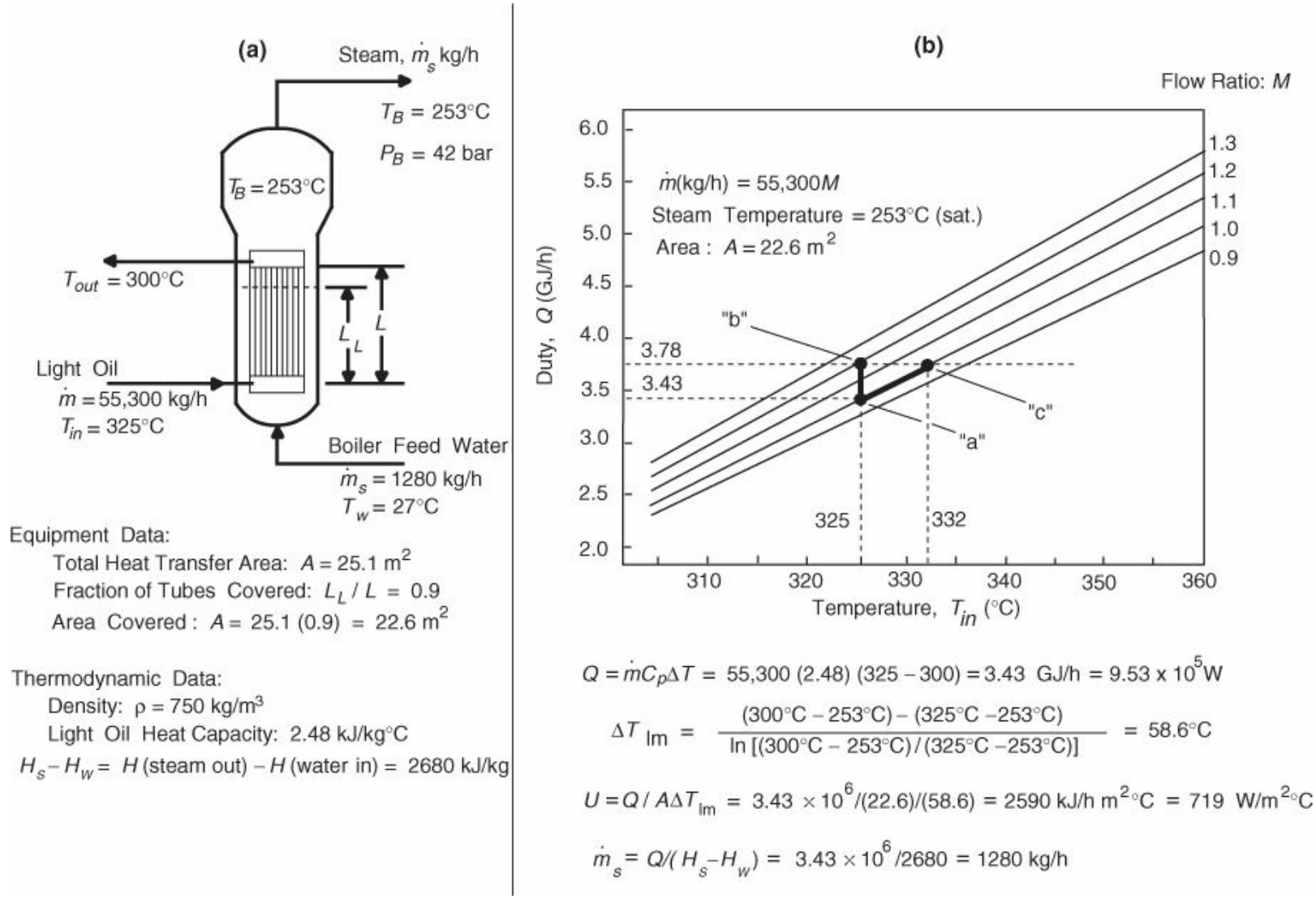


Figure 21.2. Details of a Shell-and-Tube Heat Exchanger (From D. R. Woods, *Process Design and Engineering Practice*, Englewood Cliffs, NJ: Prentice Hall, 1995)

Saturated steam is produced in a kettle-type vaporizer containing long vertical tubes.

Heat is provided from a hot light oil stream that enters at 325°C and leaves at 300°C. The effective area for heat transfer is adjusted by changing the level of the boiling liquid in the exchanger. Figure 21.1a provides the current operating conditions, some limited thermodynamic data, data on the vaporizer, and a sketch of the equipment.



$$Q = \dot{m}C_p\Delta T = 55{,}300\ (2.48)\ (325 - 300) = 3.43\ \text{GJ/h} = 9.53 \times 10^5 \text{W}$$

$$\Delta T_{lm} = \frac{(300°\text{C} - 253°\text{C}) - (325°\text{C} - 253°\text{C})}{\ln[(300°\text{C} - 253°\text{C})/(325°\text{C} - 253°\text{C})]} = 58.6°\text{C}$$

$$U = Q / A\Delta T_{lm} = 3.43 \times 10^6/(22.6)/(58.6) = 2590\ \text{kJ/h m}^2\text{°C} = 719\ \text{W/m}^2\text{°C}$$

$$\dot{m}_s = Q/(H_s - H_w) = 3.43 \times 10^6/2680 = 1280\ \text{kg/h}$$

Figure 21.1. Performance Diagram for a Heat-Exchange System

The conditions given in Figure 21.1(a) designate the base case. Development of performance curves involves solving the following three equations simultaneously:

$$\text{Heat lost by light oil, } Q = \dot{m}(H_1 - H_2) = \dot{m}C_{p,\,oil}(T_{in} - T_{out}) \qquad (21.1)$$

$$\text{Heat gained by water stream, } Q = \dot{m}_s(H_s - H_w) = \dot{m}_s[C_p(T_B - T_w) + \lambda_s] \qquad (21.2)$$

$$\text{Heat transferred, } Q = UA\Delta T_{lm} \qquad (21.3)$$

In these equations,

H_1 and H_2 refer to the specific enthalpy, kJ/kg, for the light oil, with the subscripts 1 for inlet and 2 for outlet conditions.

H_s and H_w refer to the specific enthalpy, kJ/kg for the steam and water, respectively.

$\dot{m}$ and $\dot{m}_s$ refer to the stream flowrate, kg/h, for the light oil and water/steam stream, respectively.

λ_s is the latent heat of the steam.

The heat transfer equation, Equation (21.3), contains the characteristic factors specific to the heat

transfer equipment.

Figure 21.1(b) shows the calculations used for the base case. They include the heat transfer rate, Q, the steam generation rate, $\dot{m}_S$, the overall heat transfer coefficient, U, and the log-mean temperature difference, ΔT_{lm}.

Figure 21.1(b) is the performance diagram for this boiler system subject to the following constraints:

1. The temperature of the boiling water, $T_B = 253°C$, which is set by the pressure of the water in contact with the tubes
2. The liquid level, which is $0.9L$ (where L = tube height)
3. Total heat transfer area, $A_T = 25.1\ m^2$
4. The time at which the operating data were obtained

The heat transfer rate or vaporization duty, Q, is plotted in Figure 21.1(b) as a function of the inlet light oil coolant temperature, T_{in}, with flowrate ratio of light oil, M, as a parameter. M is the ratio of the current oil flowrate (subscript 2) to the base-case oil flowrate (subscript 1).

$$M = \dot{m}_2/\dot{m}_1 \qquad (21.4)$$

where $\dot{m}_1 = 55{,}300\ kg/h$.

Before discussing how these curves were developed, Example 21.1 illustrates how the performance curves can be used to predict the effects of changing operating conditions.

Example 21.1.

An increase in steam production of 10% is needed. You are to provide the operator with the new input stream conditions for two cases by completing the following table:

	Light Oil Flow (Mg/h)	T_{in}(°C)	T_{out} (°C)
Current Values	55.3	325	300
Case (a)	55.3	?	?
Case (b)	?	325	?

These problems can be solved by the methods developed in Chapter 20. If only a single answer is desired, this method is faster than preparation of a complete performance curve, which is described later.

If the steam production must increase by 10%, then the ratio of the new case (2) to the base case (1) from Equation (21.2) is

$$\frac{Q_2}{Q_1} = \frac{\dot{m}_{s2}(H_s - H_w)_2}{\dot{m}_{s1}(H_s - H_w)_1} = 1.1 \qquad (E21.1a)$$

Because the enthalpy difference is unchanged for the phase change of water to steam, the ratio $Q_2/Q_1 = 1.1$. Now, the ratio of Q_2/Q_1 must be written for the remaining two equations, (21.1) and (21.3). For Case (a), these are

$$\frac{Q_2}{Q_1} = 1.1 = \frac{\dot{m}_2 C_{p2}(T_{in} - T_{out})_2}{\dot{m}_1 C_{p1}(T_{in} - T_{out})_1} = \frac{(T_{in} - T_{out})_2}{25} \qquad (E21.1b)$$

$$\frac{Q_2}{Q_1} = 1.1 = \frac{U_2 A_2 \Delta T_{lm2}}{U_1 A_1 \Delta T_{lm1}} = \frac{(T_{out} - T_{in})_2}{58.6 \ln\left(\frac{T_{out2} - 253}{T_{in2} - 253}\right)} \frac{U_2}{U_1} \qquad (E21.1c)$$

Because the mass flowrate of the oil does not change, its heat transfer coefficient remains constant. Because a boiling heat transfer coefficient does not change with flowrate, the overall heat transfer coefficient is unchanged. Therefore, $U_1 = U_2$. These assumptions were used in obtaining Equation (E21.1[c]). Solving Equations (E21.1[b]) and (E21.1[c]) simultaneously yields

$$T_{in2} = 332°C$$

$$T_{out2} = 304.5°C$$

For Case (b), it is necessary to know more detail about the heat transfer coefficient, because the mass flowrate of the oil changes. For this system, it is known that the boiling heat transfer coefficient (h_o) is two times the oil heat transfer coefficient (h_i). Because only the oil heat transfer coefficient changes with flowrate, assuming negligible fouling and wall resistances, the overall heat transfer coefficient is expressed in terms of the oil heat transfer coefficient as

$$\frac{1}{U_1} = \frac{1}{h_{i1}} + \frac{1}{h_{o1}} = \frac{3}{2h_{i1}} \qquad \text{(E21.1d)}$$

$$\frac{1}{U_2} = \frac{1}{h_{i1}M^{0.8}} + \frac{1}{h_{o2}} = \frac{1}{h_{i1}}\left(\frac{1}{M^{0.8}} + 0.5\right) \qquad \text{(E21.1e)}$$

where $M = \dot{m}_2/\dot{m}_1$. The base-case ratios now become

$$1.1 = \frac{M(325 - T_{out2})}{25} \qquad \text{(E21.1f)}$$

$$1.1 = \frac{3(T_{out2} - 325)}{2(58.6)\left(\frac{1}{M^{0.8}} + 0.5\right)\ln\left(\frac{T_{out2} - 253}{72}\right)} \qquad \text{(E21.1g)}$$

Solving these two equations simultaneously yields $T_{out2} = 301.5°C$ and $M = 1.17$, which means that the flowrate of oil must be increased by 17% to obtain a 10% increase in steam production, and the resulting outlet oil temperature rises slightly.

The same results can be obtained from the performance graph in Figure 21.1(b).

New Steam Production, $\dot{m}_s = 1.1(1280) = 1410$ kg/h

New Exchanger Duty, $Q = \dot{m}_s\,(H_s - H_w) = 1410(2680) = 3.78 \times 10^6$ kJ/h

Case (a): On Figure 21.1(b), the base-case operating condition is point "a." From point "a," follow the constant flow line, $M = 1.0$, to a vaporizer duty, $Q = 3.78 \times 10^6$ kJ/h. This is line segment "a"–"c," and, from this, the inlet oil temperature, $T_{in2} = 332°C$.

From Equation (21.1)

$$T_{out2} = T_{in2} - Q/(\dot{m}_2 C_{p,oil}) = 332 - 3.78 \times 10^6/[55{,}300(2.48)] = 305°C$$

Case (b): On Figure 21.1(b) follow the constant temperature line for $T_{in2} = 325°C$ to the new vaporizer duty, $Q = 3.78 \times 10^6$ kJ/h. This is shown as line segment "a"–"b." From this, the value of $M = 1.17$.

$$\dot{m} = 1.17(55{,}300) = 64{,}700 \text{ kg/h (17\% increase in flow)}$$

From Equation (21.1)

$$T_{out2} = T_{in2} - Q/(\dot{m}_2 C_{p,oil}) = 332 - 3.78 \times 10^6/[64{,}700(2.48)] = 301.5°C$$

In Example 21.1, two sets of operating conditions were calculated that would provide the required

increase in steam production. The input oil flowrate, $\dot{m}$, could be increased with the temperature, T_{in}, held constant, or the oil flowrate, $\dot{m}$, could be held constant while the input oil temperature, T_{in}, is increased. These two solutions, along with an infinite number of other solutions, lie on a line of constant heat duty, Q = 3.78 GJ/h.

The curves for constant flow ($\dot{m}$ = 55,300M) in Figure 21.1(b) are straight lines. Equating and rearranging Equations (21.1) and (21.3) produces

$$(T_{in} - T_B)/(T_{out} - T_B) = K \qquad (21.5)$$

$$\text{where } K = \exp[UA/(\dot{m}/C_{p,oil})] \qquad (21.6)$$

By solving Equation (21.5) for T_{out} and substituting it into Equation (21.1),

$$Q = \dot{m}C_{p,oil}(T_{in} - T_B)[1 - (1/K)] \qquad (21.7)$$

The overall heat transfer coefficient, U, varies with the light oil flowrate, $\dot{m}$. The performance for a constant value of oil flowrate is obtained once the value of K is known.

Equation (21.7) was used to obtain the curves given in Figure 21.1(b). The small amount of heat transferred above the liquid level (where the heat transfer coefficient for the gas phase will be small) was ignored. In addition, it was assumed that the incoming feed water mixes rapidly with the large volume of boiling liquid water in the vaporizer. Thus, the water outside the tubes is essentially constant and equal to the saturation temperature. The simple form of Equation (21.7) is a consequence of this constant temperature. When neither stream involves a phase change, the evaluation is more complicated. One reason is the need to consider the log-mean temperature correction factor for these types of shell-and-tube heat exchangers.

In reality, fouling will affect heat-exchanger performance over time. **Fouling** is a buildup of material on tube surfaces, and it occurs to some extent in all heat exchangers. When a heat exchanger is started up, there will be no fouling; however, with time, trace impurities in the fluids deposit on the heat exchanger tubes. This is usually more significant for liquids, and among the possible impurities are inorganic salts or microorganisms. The fouling layer provides an additional resistance to heat transfer. For a heat exchanger constructed from material with high thermal conductivity operating with fluids having high heat transfer coefficients, fouling may provide a greater resistance than the convective film resistance. The influence of fouling on heat-exchanger performance is the subject of problems at the end of the chapter.

Which of the two heat transfer surfaces provides the major fouling resistance in the steam generator? The water outside the tubes is designated as boiler feed water. This stream is an expensive source of water. It has been treated extensively to remove trace minerals and hence reduces significantly the fouling of heat transfer surfaces. This suggests that fouling on the outside of the tubes will remain low and the oil stream is the major contributor to fouling.

Example 21.2 suggests ideas for alternative performance of the steam generator. Some of these are the subject of problems at the end of the chapter.

Example 21.2.

Assume that neither the oil stream flowrate, $\dot{m}$, nor the inlet temperature, T_{in}, can be changed. What can be done to increase steam production, $\dot{m}_s$?

The heat transfer equation, $Q = UA\Delta T_{lm}$, shows that Q can be increased by

a. Increasing U: Clean the tubes.

b. Increasing A: Increase the liquid level in the boiler.

c. Increasing ΔT_{lm}: Decrease the boiler temperature by lowering the pressure.

d. Combinations of (a), (b), and (c).

21.2. Application to Fluid Flow

In this section, performance curves for centrifugal pumps, reciprocating pumps, and piping networks are discussed. The use of pump and system curves is introduced and the concepts of net positive suction head are discussed.

21.2.1. Pump and System Curves

In this section, performance curves for a centrifugal pump and the flow of a liquid through a pipe network connecting a storage tank to a chemical reactor are presented. Centrifugal pumps are very common in the chemical industry. Figure 21.3 shows the inner workings of a centrifugal pump. It is important to understand that the performance curves presented here are unique to centrifugal pumps. Positive displacement pumps, the other common type of pump used in the chemical industry, have a completely different performance curve and are discussed briefly in Section 21.2.3.

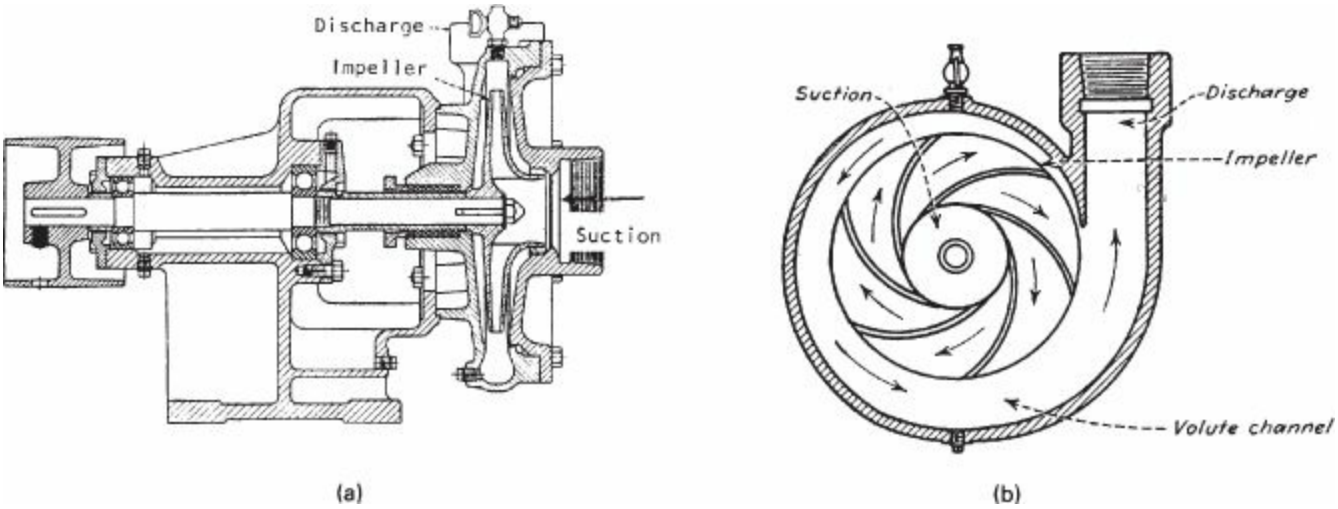


Figure 21.3. Inner Workings of a Centrifugal Pump (From S. Walas, *Chemical Process Equipment: Selection and Design.* Stoneham, MA: Butterworth, 1988. Reproduced with permission.)

In situations involving the flow of fluid, the equation used to relate pressure changes and flowrate is the mechanical energy balance (or the extended Bernoulli equation):

$$\frac{\Delta P}{\rho g} + \frac{\Delta u^2}{2g} + \Delta z = \frac{W_s}{g} - \frac{F_d}{g} \qquad (21.8)$$

The terms shown on the left-hand side of Equation (21.8) are point properties. They are independent of the path taken by the fluid. The Δ in Equation (21.8) represents the difference between outlet and inlet conditions on the control volume. In contrast, the terms on the right-hand side of the equation are **path properties** that depend on the path followed by the fluid. Work is defined as positive when done on the system. The terms related to the path taken by the fluid are specific to the operating system and form the basis for the performance curves.

Equation (21.8) is written in terms of fluid head. Each term has units of length. (The equation could

be written so that each term has units of pressure by multiplying each term by ρg.) **Fluid head** is a way of expressing pressure as an equivalent static pressure of a stationary body of fluid. For example, one atmosphere of pressure is equivalent to about 34 feet of water, because the pressure difference between the top and bottom of a column of 34 feet of water is one atmosphere. Equation (21.8), with each term defined as fluid head, is

$$\Delta h_p + \Delta h_v + \Delta h_z = h_s - h_f \qquad (21.9)$$

A centrifugal pump is shown in Figure 21.4 along with its performance diagram. In the performance diagram, the ordinate is in units of pressure head, which is how all of the curves discussed in this section are usually represented. However, it is also possible to represent these curves in pressure units. In this book, examples and problems using both pressure units and head units are included. For this analysis, the change in the velocity head and elevation head between points "1" and "2" is either zero or small, and Equation (21.9) reduces to

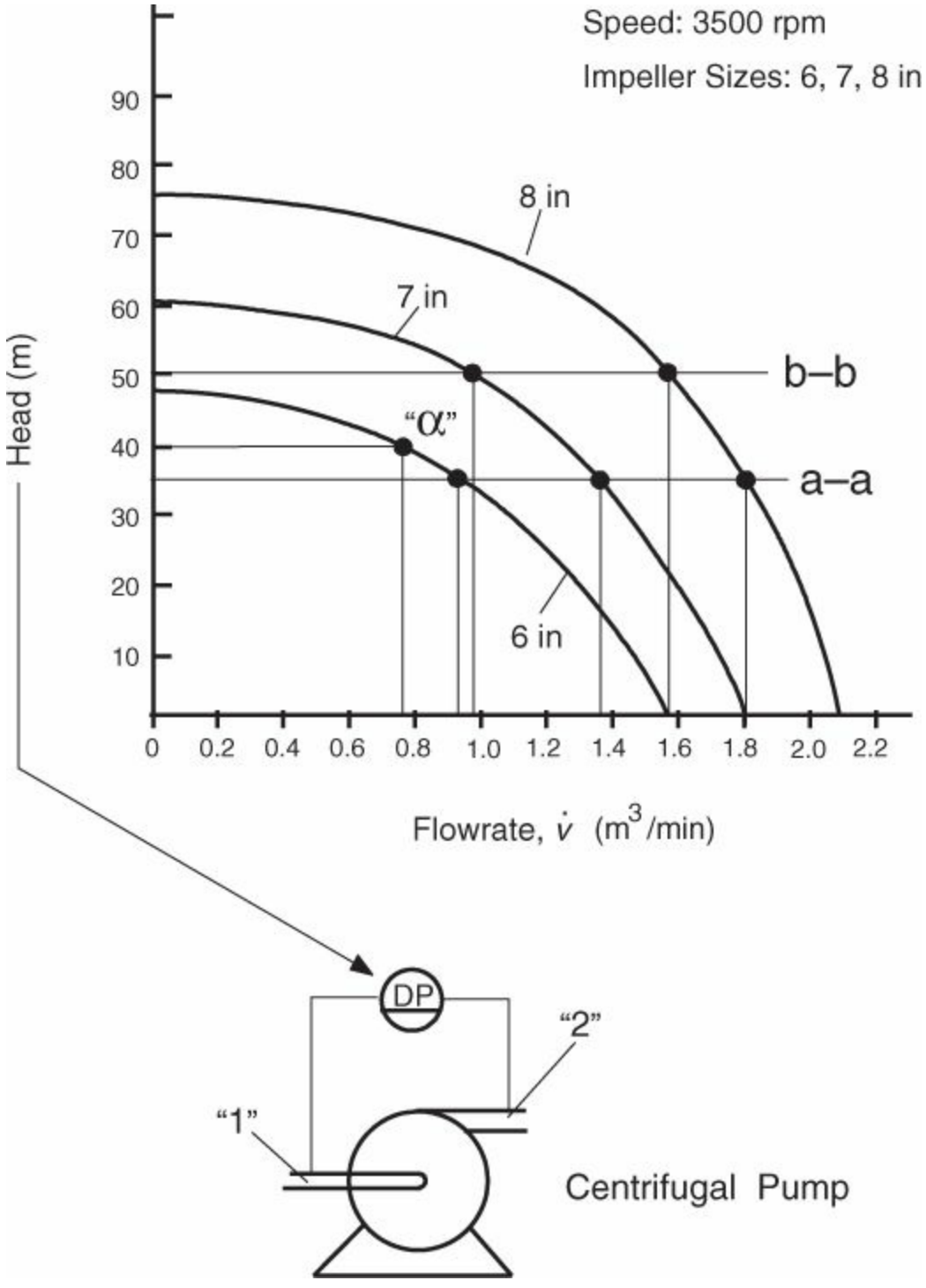


Figure 21.4. Performance Diagram for a Centrifugal Pump

$$\Delta h_p = h_s - h_f \qquad (21.10)$$

Centrifugal pumps are used in a variety of applications and are available from many manufacturers. Pump impellers may have forward or backward vanes, may have enclosed or open configurations, and may operate at different speeds. Their performance characteristics depend on their mechanical design. As a result, experimentally determined performance curves are supplied routinely by the pump manufacturer.

The performance curve, or pump curve, shown in Figure 21.4 is typical of a centrifugal pump handling normal (Newtonian) liquids. It relates the fluid flow-rate to the head, h_s. To understand this relationship, consider point "α" shown on the performance curve in Figure 21.4. This point lies on the curve for a 6-in impeller. It shows that the pump delivers 0.76 m^3/min of liquid when the pressure differential between the suction and discharge side of the pump is equivalent to a column of liquid 40 m in height.

Figure 21.4 contains three curves, each depicting the pump performance with a different impeller diameter. The pump casing can accept any of these three impellers, and each impeller has a unique pump curve. Pump curves often display efficiency and horsepower curves in addition to the curves shown in Figure 21.4.

From the pump curves in Figure 21.4, the following trends can be seen for each impeller:

1. The head produced at a given flowrate varies (increases) with the impeller diameter.
2. The pump provides low flowrates at high head and high flowrates at low head.
3. The head produced is sensitive to flowrate at high flowrates; that is, the curve drops off sharply at high flowrates.
4. The head produced is relatively insensitive to flowrate at low flowrates; that is, the curve is relatively flat at low flowrates.

Example 21.3 demonstrates how to read a pump curve.

Example 21.3.

The centrifugal pump shown in Figure 21.4 is used to supply water to a storage tank. The pump inlet is at atmospheric pressure and water is pumped up to the storage tank, which is open to atmosphere, via large-diameter pipes. Because the pipe diameters are large, the frictional losses in the pipes and any change in fluid velocity can be safely ignored.

a. If the storage tank is located at an elevation of 35 m above the pump, predict the flow using each impeller.

b. If the storage tank is located at an elevation of 50 m above the pump, predict the flow using each impeller.

Solution

a. From Figure 21.4, at Δh_p = 35 m (see line "a–a")

6-in Impeller: Flow = 0.93 m^3/min

7-in Impeller: Flow = 1.38 m^3/min

8-in Impeller: Flow = 1.81 m^3/min

b. From Figure 21.4, at $\Delta h_p = 50$ m (see line "b–b")

6-in Impeller: Flow = 0 m^3/min

7-in Impeller: Flow = 0.99 m^3/min

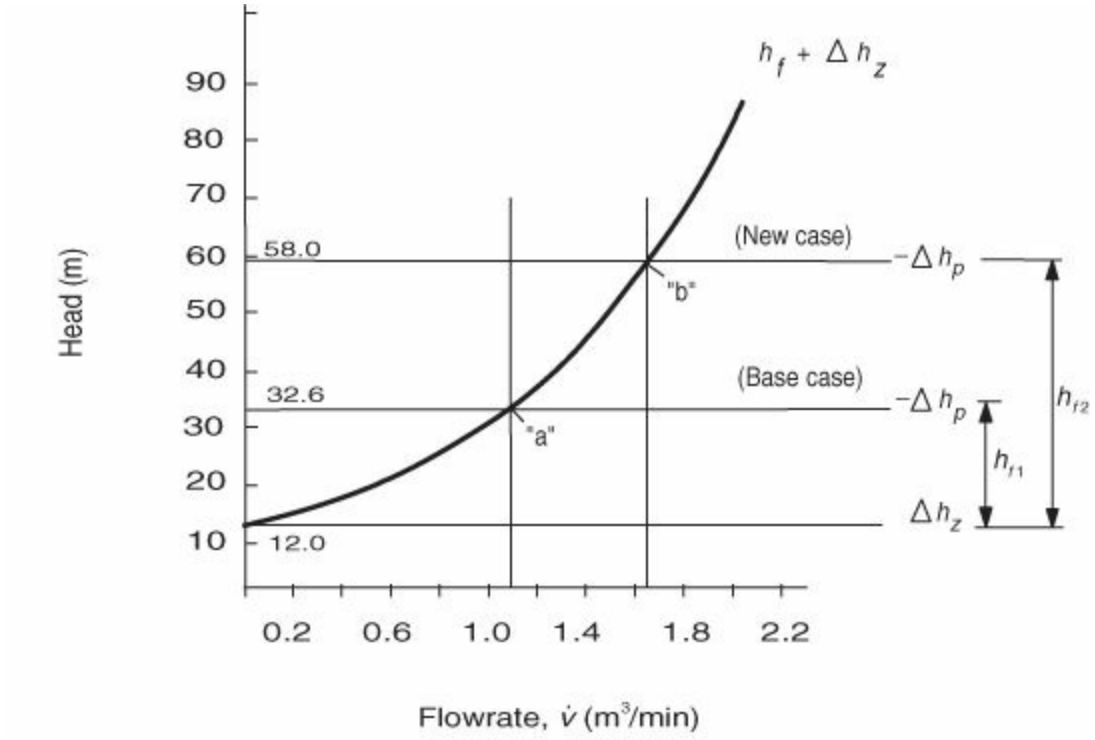
8-in Impeller: Flow = 1.58 m^3/min

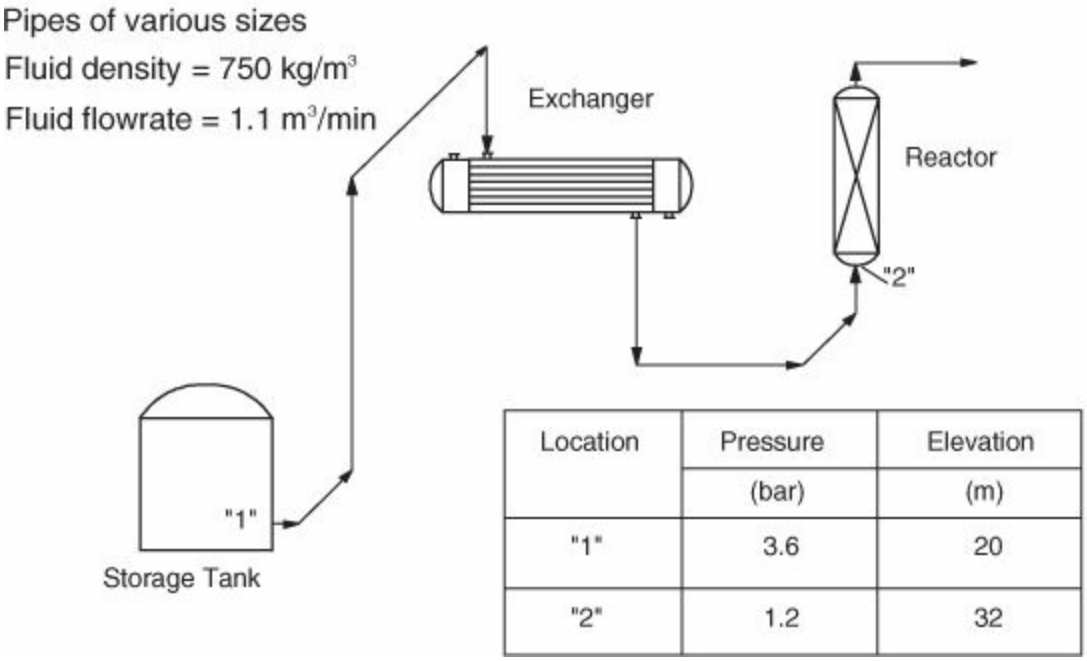
In Example 21.3, the flowrate into the tank is restricted to one of three discrete values (depending on the impeller installed in the pump housing). For the system described, once the elevation of the tank and the impeller diameter are chosen, a single unique flowrate is obtained. Other flowrates cannot be obtained for this system.

Example 21.3 demonstrates the need to know the characteristic shape of the performance curve at the current operating point to predict the effect of any change in tank elevation. In Example 21.3, because the 8-in impeller is operating in a region where the flow is not greatly affected by an increase in head, the flowrate was reduced by less than 15%. In contrast, for the 6-in impeller, where a change in head has a large effect, the flowrate is reduced by 100% (no fluid flows).

It is essential to understand the system performance before making predictions or recommendations.

Consider the flow situation shown in Figure 21.5. The figure illustrates a pipe network through which feed material is transported from a storage tank through a heat exchanger to a chemical reactor. From the information provided on Figure 21.5, it is possible to construct the performance curve shown, which is called the **system curve**.





Location	Pressure (bar)	Elevation (m)
"1"	3.6	20
"2"	1.2	32

Figure 21.5. Sketch and Performance Diagram for an Operating Flow System

Because the fluid is a liquid, it can be assumed that the change in velocity head, Δh_v, is small. In addition, the work head $\Delta h_s = 0$, and Equation (21.9) written between points "1" and "2" reduces to

$$\Delta h_p = -h_f - \Delta h_z \qquad (21.11)$$

The pressure head term, Δh_p, and the elevation head term, $-\Delta h_z$, are constant and independent of the flowrate. The friction term, $-h_f$, in Equation (21.11) depends upon

1. The specific system configuration
2. The flowrate of fluid

For this system, for fully developed turbulent flow, the relationship needed to predict the friction term, h_f, as a function of fluid velocity is known. The relationship is given in Table 20.1 and in Example 20.2. This relationship in terms of fluid head is

$$h_{f2} = h_{f1}(u_2/u_1)^2 = h_{f1}(\dot{v}_2/\dot{v}_1)^2 \qquad (21.12)$$

where $\dot{v}$ is the volumetric flowrate, the subscript 2 refers to the new case, and the subscript 1 refers to the base case. Equation (21.12) represents a parabola, which is the shape of the system curve in Figure 21.5. In terms of pressure, Equation (21.12) becomes

$$\Delta P_2 = \Delta P_1(\dot{v}_2/\dot{v}_1)^2 \qquad (21.13)$$

and it is also possible to plot the system curve in terms of pressure, as is done later in Figure 21.6.

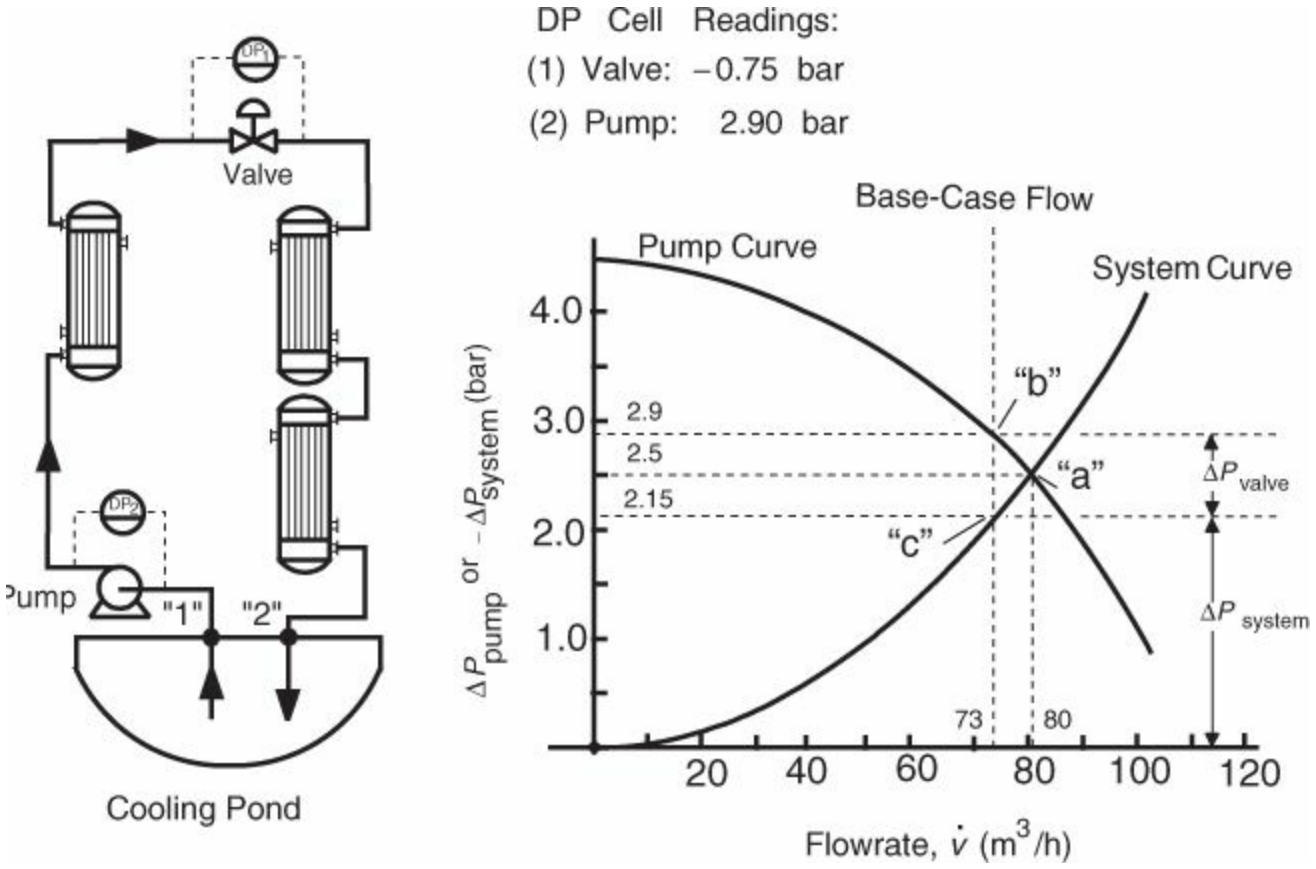


Figure 21.6. Performance Curves for Coolant System

The operating conditions given in Figure 21.5 serve as the base case in Examples 21.4 and 21.5, which illusrate the ratio method discussed previously.

Example 21.4.

The fluid flowrate measured for the conditions shown in Figure 21.5 is 1.1 m^3/min.

a. Using the information given on the flow diagram (see Figure 21.5) for the base case, determine the value of h_f.

b. Develop the equation for h_f as a function of the flowrate, $\dot{v}$.

Solution

a. From Equation 21.11,

$$h_f = \Delta - h_z - \Delta h_p$$

$$\Delta h_z = z_2 - z_1 = 32\text{ m} - 20\text{ m} = 12\text{ m}\ (\Delta h_z \text{ is drawn as a horizontal line in Figure 21.5})$$

$$\Delta h_p = (P_2 - P_1)/\rho g = (1.2 - 3.6) \times 10^5/[750(9.81)] = -32.6\text{ m}$$

$$h_f = -12\text{ m} + 32.6\text{ m} = 20.6\text{ m}$$

b. $h_{f2} = h_{f1}(\dot{v}_2/\dot{v}_1)^2 = (20.6\text{ m})(\dot{v}_2/1.1)^2 = 17.02\dot{v}_2^2$

Example 21.5.

The flow to the reactor in Example 21.4 is increased by 50%. The pressure of the reactor is held constant. Determine the pressure required at the exit of the storage tank.

For a 50% increase, $\dot{v}_2 = 1.5\ \dot{v}_1 = 1.1(1.5) = 1.65\ \text{m}^3/\text{min}$.

The line of constant flow, $\dot{v} = 1.65\ \text{m}^3/\text{min}$, is shown as the vertical line through point "b" in Figure 21.5. It intersects the performance line, $h_f + \Delta h_z = 58$ m (point "b").

$$-\Delta h_p = 58\text{ m} = (P_1 - P_2)/\rho g = P_1/\rho g - 1.2 \times 10^5/[750(9.81)] = P_1/\rho g - 16.3\text{ m}$$

$$P_1 = (58 + 16.3)\rho g = 74.3(750)(9.81) = 5 \times 10^5\text{ Pa} = 5.47\text{ bar}$$

In this section, two representative types of performance curves were considered. For the pump, the information needed for developing a performance diagram was obtained experimentally and supplied by the manufacturer. In the flow network, a base case was established using actual operating data and the performance diagram, known as the system curve, calculated using the mechanical energy balance.

21.2.2. Regulating Flowrates

In all systems presented in this chapter, input flowrates are the primary variables that are used to change the performance of a system. In fact, in a chemical plant, process regulation is achieved most often by manipulating flowrates, which is accomplished by altering valve settings. If it is necessary to change a temperature, the flow of a heating or cooling medium is adjusted. If it is necessary to change a reflux ratio, a valve is adjusted. In this section how to regulate these input flows to give desired values is considered.

Process conditions are usually regulated or modified by adjusting valve settings in the plant.

Although valves are relatively simple and inexpensive pieces of equipment, they are nevertheless indispensable in any chemical plant that handles liquids or gases.

Figure 21.6 illustrates a fluid system containing three components:

1. A flow system, including piping and three heat exchangers
2. A pump
3. A regulating valve

The process shown in Figure 21.6 is described briefly as follows:

> *A liquid process stream is pumped at a rate of $\dot{v}$ m^3/min from a cooling pond, through a heat exchanger, through a regulating valve and two more heat exchangers connected in series, and returned to the cooling pond. The intake and discharge pipes are at the same elevation. Differential pressure gauges are installed across the pump and the regulating valve. The pump used here has the same characteristics as that shown in Figure 21.4, with a 7-in impeller.*

Conditions shown in Figure 21.6 represent a base case. The mechanical energy balance equation, Equation (21.8), written between points "1" and "2" in Figure 21.6, gives

$$-(\Delta P_{valve} + \Delta P_{pipes} + \Delta P_{exchangers}) = \Delta P_{pump} \qquad (21.14)$$

In Equation (21.14),

ΔP_{valve} represents the pressure drop across the control valve.

ΔP_{pipe} represents the pressure drop due to friction in the piping and pipe fittings between points "1" and "2."

$\Delta P_{exchangers}$ represents the pressure drop due to friction in the three heat exchangers.

ΔP_{pump} represents the pressure increase produced by the pump.

The frictional drop in pressure through the pipe system and the heat exchangers is given by

$$\Delta P_{system} = \Delta P_{pipes} + \Delta P_{exchangers} \qquad (21.15)$$

ΔP_{system} is called the system pressure drop, and Equation (21.14) can be written as

$$-(\Delta P_{valve} + \Delta P_{system}) = \Delta P_{pump} \qquad (21.16)$$

The performance curve for this system, shown in Figure 21.6, consists of a plot of pressure against the liquid flowrate, as was done in Figures 21.4 and 21.5. (In this section pressure units are used instead of units of liquid head.)

The system pressure drop is estimated relative to the base case by Equation (21.13).

$$\Delta P_{2,system} = \Delta P_{1,system}(\dot{v}_2/\dot{v}_1)^2 \qquad (21.17)$$

$$\Delta P_{2,system}(\text{bar}) = 2.15\ (\dot{v}_2/73)^2 \qquad (21.18)$$

This curve has been plotted and labeled as the system curve.

Sufficient information is available to prepare a full performance diagram. In Figure 21.6, for this system, each side of Equation (21.16) is plotted. The pressure produced by the pump, ΔP_{pump}, depends on the volumetric flowrate, $\dot{V}$, as was shown earlier in Figure 21.4. Only the units used to express the pressure and flowrate terms have been changed.

Example 21.6 illustrates how the component terms of the system curve are related to performance parameters.

Example 21.6.

Using the pump curve and the differential pressures provided on Figure 21.6, find for the base case

a. The system pressure drop, ΔP_{system}

b. The volumetric flowrate, $\dot{v}$

Solution

a. For the system pressure drop, ΔP_{system}, from Equation (21.16),

$$-\Delta P_{system} = \Delta P_{pump} + \Delta P_{valve} = 2.9 \text{ bar} - 0.75 \text{ bar} = 2.15 \text{ bar}$$

b. For the volumetric flowrate, $\dot{v}$, see point "b" on Figure 21.6.

$$\text{for } \Delta P_{pump} = 2.9 \text{ bar}, \ \dot{v} = 73 \text{ m}^3/\text{h}$$

Base-case conditions have been added to Figure 21.6. All pressures for the base case lie along the constant flow line, $\dot{v} = 73$ m^3/h. Point "c" gives the value for the system pressure drop, ΔP_{system}, and point "b" gives the pressure increase provided by the pump. The difference between these points is the pressure drop over the regulating valve, ΔP_{valve}.

If there were no valve in the line, $\Delta P_{valve} = 0$, the system would operate at point "a," where the pump curve and the system curve cross. It can be seen from Figure 21.6 that as the pressure across the valve increases, the move is toward the left and lower flowrates. The flow becomes zero when the valve is fully closed. Thus, by manipulating the valve setting, the flow of fluid through the system can be altered.

Example 21.7 illustrates obtaining information from a pump and system curve.

Example 21.7.

For the base-case condition shown in Figure 21.6, do the following:

a. Check the pressure drop over the valve against the guideline for control valves (Table 11.8).

b. Determine the percent increase in flow by fully opening the valve.

Solution

a. From guideline, $\Delta P \geq 0.69$ bar (see Table 11.8).
$\Delta P = 0.75$ bar, and therefore the guideline in Table 11.8 is satisfied.

b. With no valve resistance, $\dot{v} = 80$ m^3/h.
The percent increase in flow = [(80 – 73)/73]100 = 9.6%

The increase in flowrate is limited (less than 10% of the base case) by the pump and system, and only modest increases of flowrate are possible for this system.

21.2.3. Reciprocating or Positive Displacement Pumps

Positive displacement pumps perform differently from centrifugal pumps. They are used to achieve higher pressure increases than centrifugal pumps. Figure 21.7 is a drawing of the inner workings of a positive displacement pump. The performance characteristics are represented on Figure 21.8(a). It can be observed that the flowrate through the pump is almost constant over a wide range of pressure increases. One method for regulating the flow through a positive displacement pump is illustrated in Figure 21.8(b). By carefully regulating the flow of the recycle stream, the pressure rise in the pump is controlled. The details were presented in Chapter 18.

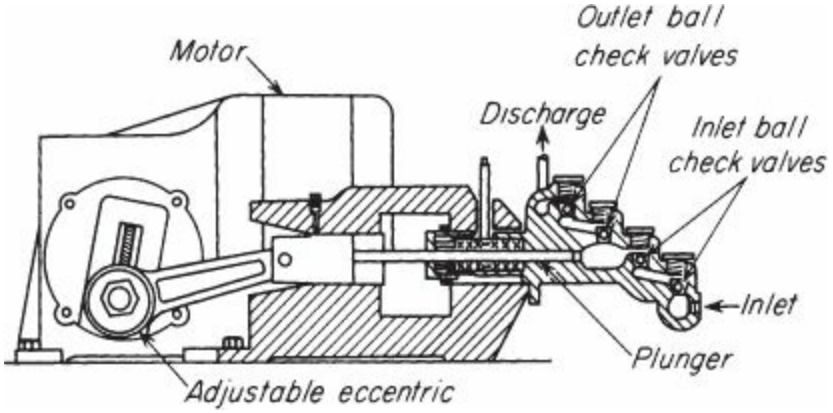


Figure 21.7. Inner Workings of a Positive Displacement Pump (From W. L. McCabe, J. C. Smith, and P. Harriott, *Unit Operations of Chemical Engineering*, 5th ed. New York: McGraw-Hill, 1993. Copyright © 1993 by New York: McGraw-Hill Companies, reproduced with permission of the McGraw-Hill Companies.)

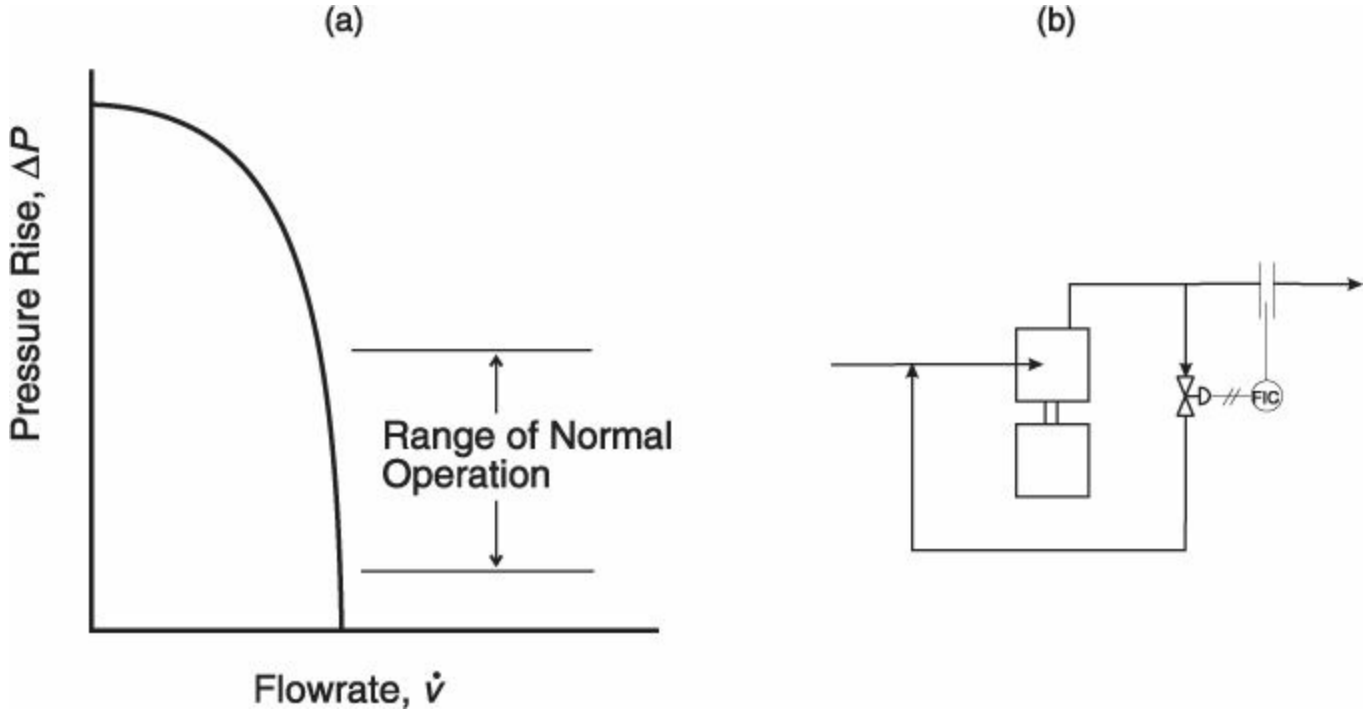


Figure 21.8. Typical Pump Curve for Positive Displacement Pump and Method for Flowrate Regulation

21.2.4. Net Positive Suction Head

There is a significant limitation on pump operation called Net Positive Suction Head (NPSH). Its origin is as follows. Although the effect of a pump is to raise the pressure of a liquid, frictional losses at the entrance to the pump, between the feed (suction) pipe and the internal pump mechanism, cause the liquid pressure to drop upon entering the pump. This means that a minimum pressure exists somewhere within the pump. If the feed liquid is saturated or nearly saturated, the liquid can vaporize upon entering due to the pressure drop. This results in formation of vapor bubbles called **cavitation**. These bubbles rapidly collapse when exposed to the forces created by the pump mechanism. This process usually results in noisy pump operation and, if it occurs for a period of time, will damage the pump. As a consequence, regulating valves are not normally placed in the suction line to a pump.

Pump manufacturers supply NPSH data with a pump. The required NPSH, denoted $NPSH_R$, is a function of the square of velocity, because it is a frictional loss. Figure 21.9 shows an $NPSH_R$ curve, which defines a region of acceptable pump operation. This is specific to a given liquid. Typical $NPSH_R$ values are in the range of 15–30 kPa (2–4 psi) for small pumps and can reach 150 kPa (22 psi) for larger pumps. On Figure 21.9, there are also curves for $NPSH_A$, the available NPSH. The available $NPSH_A$ is defined as

$$NPSH_A = P_{inlet} - P^* \qquad (21.19)$$

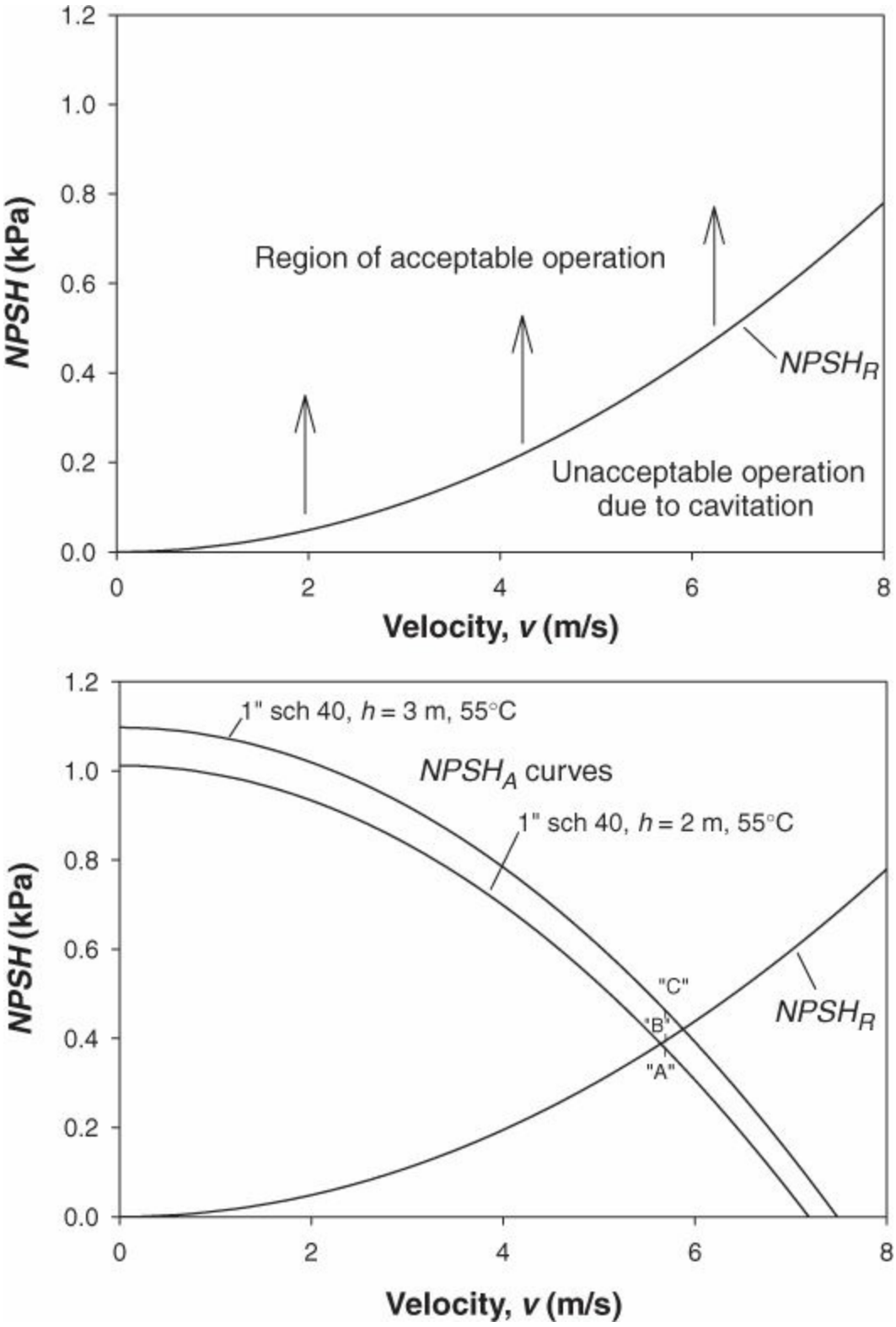


Figure 21.9. $NPSH_A$ and $NPSH_R$ Curves

Equation (21.19) means that the available NPSH ($NPSH_A$) is the difference between the inlet pressure, P_{inlet}, and P^*, which is the vapor pressure (bubble point pressure for a mixture). It is a system curve for the suction side of a pump. It is required that $NPSH_A \geq NPSH_R$ to avoid cavitation. All that remains is to calculate or know the pump inlet conditions in order to determine whether there is enough available NPSH ($NPSH_A$) to equal or exceed the required NPSH ($NPSH_R$).

For example, consider the exit from a distillation column reboiler, which is saturated liquid. If it is necessary to pump this liquid, cavitation could be a problem. A common solution to this problem is to elevate the column above the pump so that the static pressure increase minus any frictional losses

between the column and the pump provides the necessary NPSH. This can be done either by elevating the column above ground level using a metal skirt or by placing the pump in a pit below ground level, although pump pits are usually avoided due to safety concerns arising from accumulation of heavy gases in the pit.

In order to quantify NPSH, consider Figure 21.10, in which material in a storage tank is pumped downstream in a chemical process. This scenario is a very common application of the NPSH concept. From the mechanical energy balance, the pressure at the pump inlet can be calculated to be

$$P_{inlet} = P_{tank} + \rho g h - \frac{2\rho f L_{eq} u^2}{D} \qquad (21.20)$$

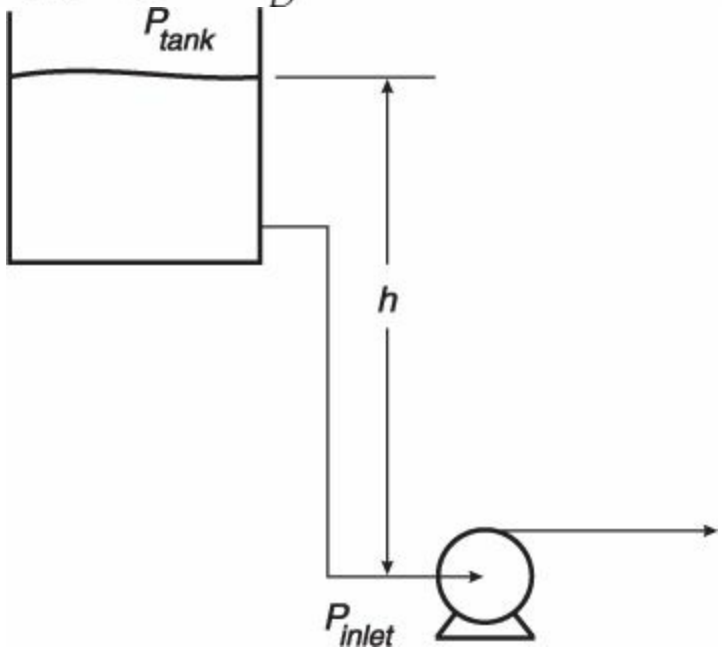


Figure 21.10. Illustration of NPSH for Pumping from Storage Tank

which means that the pump inlet pressure is the tank pressure plus the static pressure minus the frictional losses. Therefore, by substituting Equation (21.20) into Equation (21.19), the resulting expression for $NPSH_A$ is

$$NPSH_A = P_{tank} + \rho g h - \frac{2\rho f L_{eq} u^2}{D} - P^* \qquad (21.21)$$

which is the equation of a concave downward parabola, as illustrated in Figure 21.9.

If there is insufficient $NPSH_A$ for a particular situation, Equation (21.21) suggests methods to increase the $NPSH_A$:

1. Decrease the temperature of the liquid at the pump inlet. This decreases the value of the vapor pressure, P^*, thereby increasing $NPSH_A$.
2. Increase the static head. This is accomplished by increasing the value of h in Equation (21.21), thereby increasing $NPSH_A$. As was said earlier, pumps are most often found at lower elevations than the source of the material they are pumping.
3. Increase the diameter of the suction line (feed pipe to pump). This reduces the velocity and the frictional loss term, thereby increasing $NPSH_A$. It is standard practice to have larger-diameter pipes on the suction side of a pump than on the discharge side.

Example 21.8 illustrates how to do NPSH calculations and one of the methods listed above for

increasing $NPSH_A$. The other methods are illustrated in a problem at the end of the chapter.

Example 21.8.

The feed pump (P-101) on Figure 1.5 pumps toluene from a feed tank (V-101) maintained at atmospheric pressure and 55°C. The pump is located 2 m below the liquid level in the tank, and there is 6 m of equivalent pipe length between the tank and the pump. It has been suggested that 1-in schedule-40 commercial steel pipe be used for the suction line. Determine whether this is a suitable choice. If not, suggest methods to avoid pump cavitation.

The following data can be found for toluene: $\ln P^*(\text{bar}) = 10.97 - 4203.06/T(\text{K})$, $\mu = 4.1 \times 10^{-4}$ kg/m s, $\rho = 870$ kg/m^3. For 1-in schedule-40 commercial steel pipe, the roughness factor is about 0.001 and the inside diameter is 0.02664 m. From Table 1.5, the flow of toluene is 10,000 kg/h. Therefore, the velocity of toluene in the pipe can be found to be 5.73 m/s. The Reynolds number is 426,000, and, from a friction factor chart, $f = 0.005$. At 55°C, the vapor pressure is found to be 0.172 bar.

From Equation 21.21,

$$NPSH_A = 1.01325 \text{ bar} + 870(9.81)(2)(10^{-5}) \text{ bar}$$
$$- 2(870)(0.005)(6)(5.73)^2(10^{-5})/(0.02664) \text{ bar} - 0.172 \text{ bar}$$
$$NPSH_A = 0.37 \text{ bar}$$

This is shown as point "A" on Figure 21.9. At the calculated velocity, Figure 21.9 shows that $NPSH_R$ is 0.40 bar, point "B." Therefore, there is insufficient $NPSH_A$.

One method for increasing $NPSH_A$ is to increase the height of liquid in the tank. If the height of liquid in the tank is 3 m, with the original 1-in schedule-40 pipe at the original temperature, $NPSH_A = 0.445$ bar. This is shown as point "C" on Figure 21.9.

21.2.5. Compressors

The performance of centrifugal compressors is somewhat analogous to that of centrifugal pumps. There is a characteristic performance curve, supplied by the manufacturer, that defines how the outlet pressure varies with flowrate. However, compressor behavior is far more complex than that for pumps because the fluid is compressible.

Figure 21.11 shows the performance curve for a centrifugal compressor. It is immediately observed that the y-axis is the ratio of the outlet pressure to inlet pressure. This is in contrast to pump curves, which have the difference between these two values. Curves for two different rotation speeds are shown. As with pump curves, curves for power and efficiency are often included but are not shown here. Unlike most pumps, the speed is often varied continuously to control the flowrate. This is because the higher power required in a compressor makes it economical to avoid throttling the outlet as in a centrifugal pump.

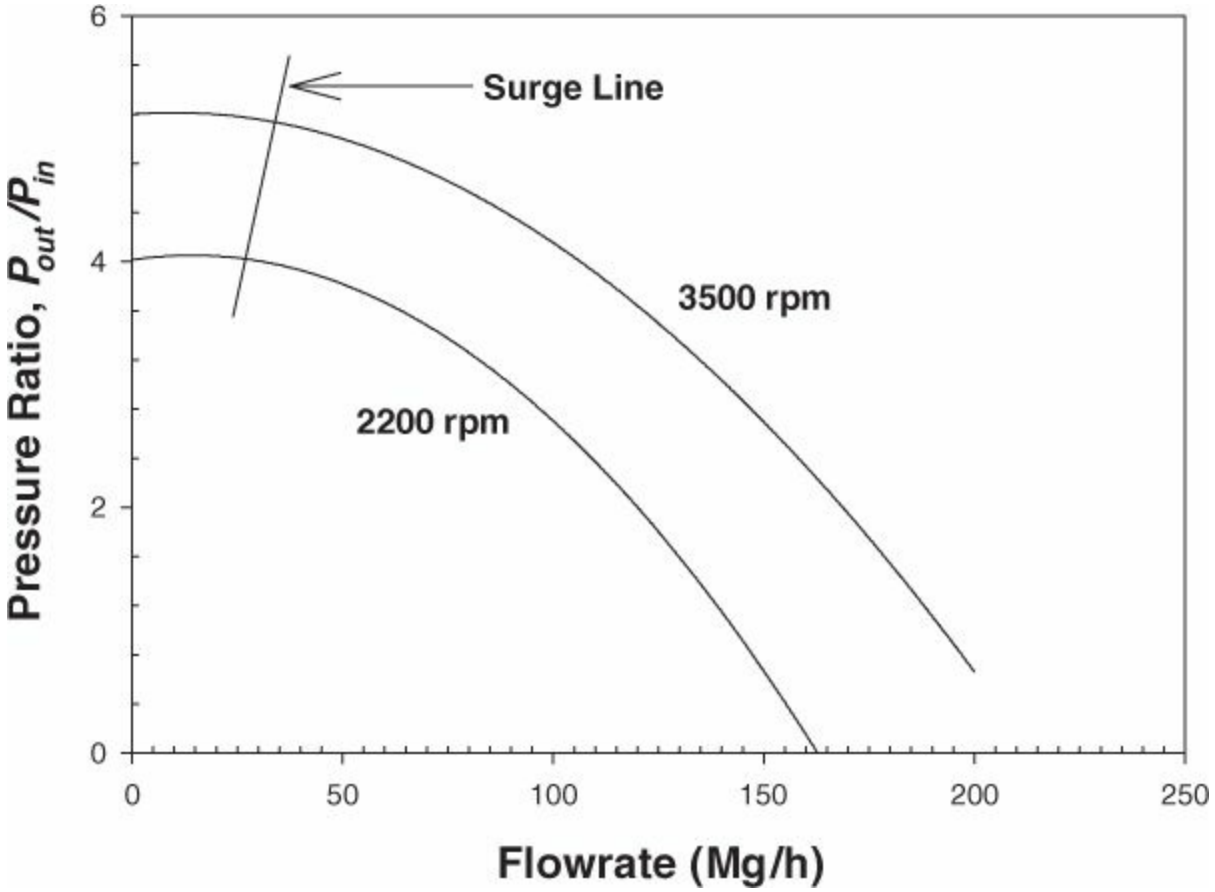


Figure 21.11. Centrifugal Compressor Curves

Centrifugal compressor curves are read just like pump curves. At a given flowrate and rpm there is one pressure ratio. The pressure ratio decreases as flowrate increases. A unique feature of compressor behavior occurs at low flowrates. It is observed that the pressure ratio increases with decreasing flowrate, reaches a maximum, and then decreases with decreasing flowrate. The locus of maxima is called the surge line. For safety reasons, compressors are operated to the right of the **surge line**. The surge line is significant for the following reason. Imagine that starting at a high flowrate and the flowrate is lowered continuously, causing a higher outlet pressure. At some point, the surge line is crossed, lowering the pressure ratio. This means that downstream fluid is at a higher pressure than upstream fluid, causing a backflow. These flow irregularities can severely damage the compressor mechanism, even causing the compressor to vibrate or surge (hence the origin of the term). Severe surging has been known to cause compressors to become detached from the supports keeping them stationary and literally to fly apart, causing great damage. Therefore, the surge line is considered a limiting operating condition, below which operation is prohibited.

Positive displacement compressors also exist and are used to compress low volumes to high pressures. **Centrifugal compressors** are used to compress higher volumes to moderate pressures and are often staged in order to obtain higher pressures. Figure 21.12 illustrates the inner workings of a compressor.

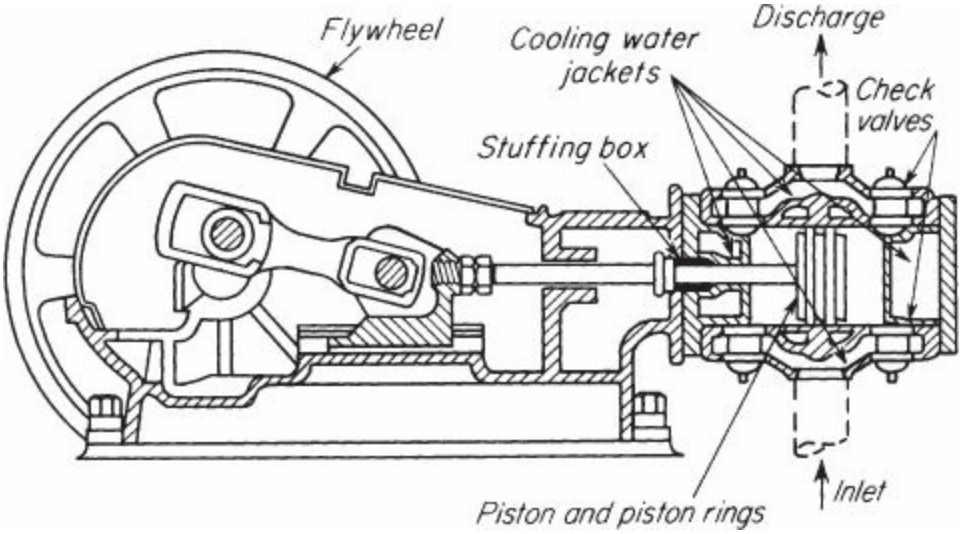


Figure 21.12. Inner Workings of a Positive Displacement Compressor (From W. L. McCabe, J. C. Smith, and P. Harriott, *Unit Operations of Chemical Engineering*, 5th ed. New York: McGraw-Hill, 1993. Copyright © 1993 by the McGraw-Hill Companies, reproduced with permission.)

Problems requiring reading compressor curves are given at the end of the chapter.

21.3. Application to Separation Problems

21.3.1. Separations with Mass Separating Agents

Multistage equilibrium separations involve simultaneous solution of material balances and equilibrium relationships for each equilibrium stage. Therefore, there is no simple, closed-form relationship that describes the behavior of these systems for all situations. There are qualitative relationships that are applicable to almost all situations, and these were included in Table 20.1. The key relationships are that a better separation is usually achieved by increasing the number of stages or by increasing solvent flowrate.

Similarly, continuous differential equilibrium separations, which involve simultaneous solution of material balances and mass transfer relationships, do not yield a closed-form solution either. The key qualitative relationships are that better separation is usually achieved by increasing column height or by increasing flowrate.

For the specific assumptions of dilute solutions and a linear equilibrium relationship that results in approximately constant stream flows, an analytical solution is possible for the above situations. For staged separations, the situation is shown in Figure 21.13(a). The result is

$$\frac{y_{A,out} - y^*_{A,out}}{y_{A,in} - y^*_{A,out}} = \frac{1 - A}{1 - A^{N+1}} \qquad (21.22)$$

where $A = (L/mG)$ is called the absorption factor, N is the number of equilibrium stages, y_A is the mole fraction of the solute in the gas phase, L and G are the molar flowrates of each stream, m is the equilibrium relationship ($y = mx$), and $y^*_{A,out} = mx_{A,in}$. Equation (21.22) is known as the Kremser equation and is a key relationship for multistage equilibrium separations obeying the assumptions listed above. It describes transport of solute, A, from the G phase to the L phase. For the reverse situation, a similar equation is derived in which the left side of Equation (21.22) involves x_A, the mole fraction in the liquid phase, and the right side involves $S = (mG/L)$. The term $y^*_{A,out} = mx_{A,in}$ is

replaced by $x^*_{A,out} = {}_{A,in}/m$. If the separation involves phases that are not gas or liquid, Equation (21.22) may still be used by defining L and G appropriately. Figure 21.14 is a plot of Equation (21.22) and contains the performance relationship between key variables for multistage equilibrium separations following the assumptions listed above. Performance curves for a specific staged separation can be generated from the information in Figure 21.14. This is illustrated in Example 21.10. It should be noted that tray performance issues such as flooding, which are specific to a particular column design, are not predicted by the Kremser relationship.

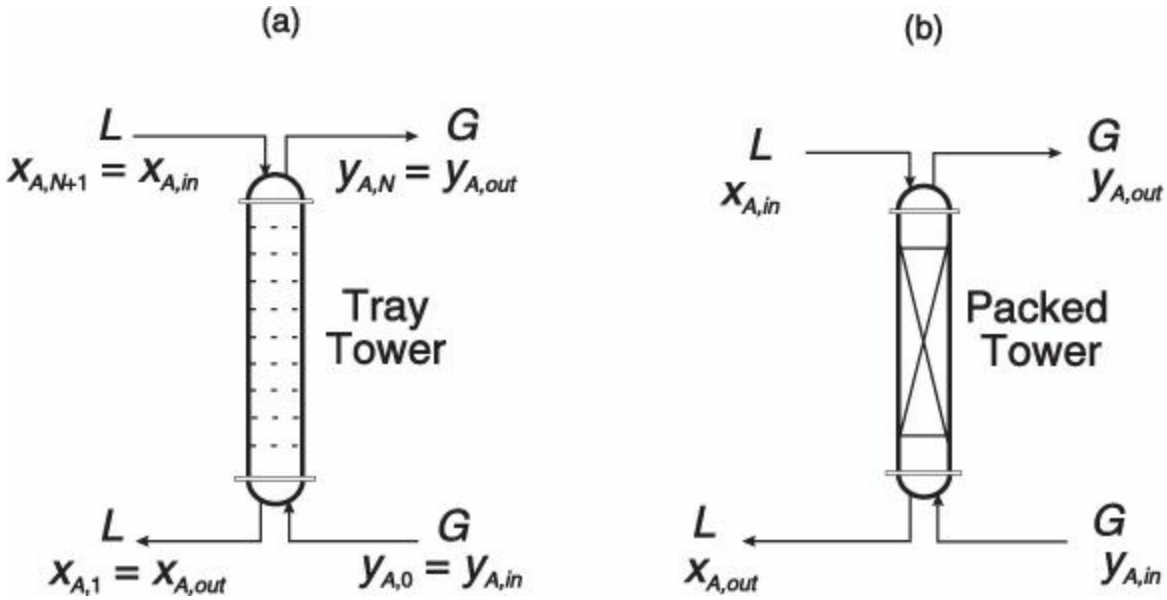


Figure 21.13. Tray and Packed Absorbers

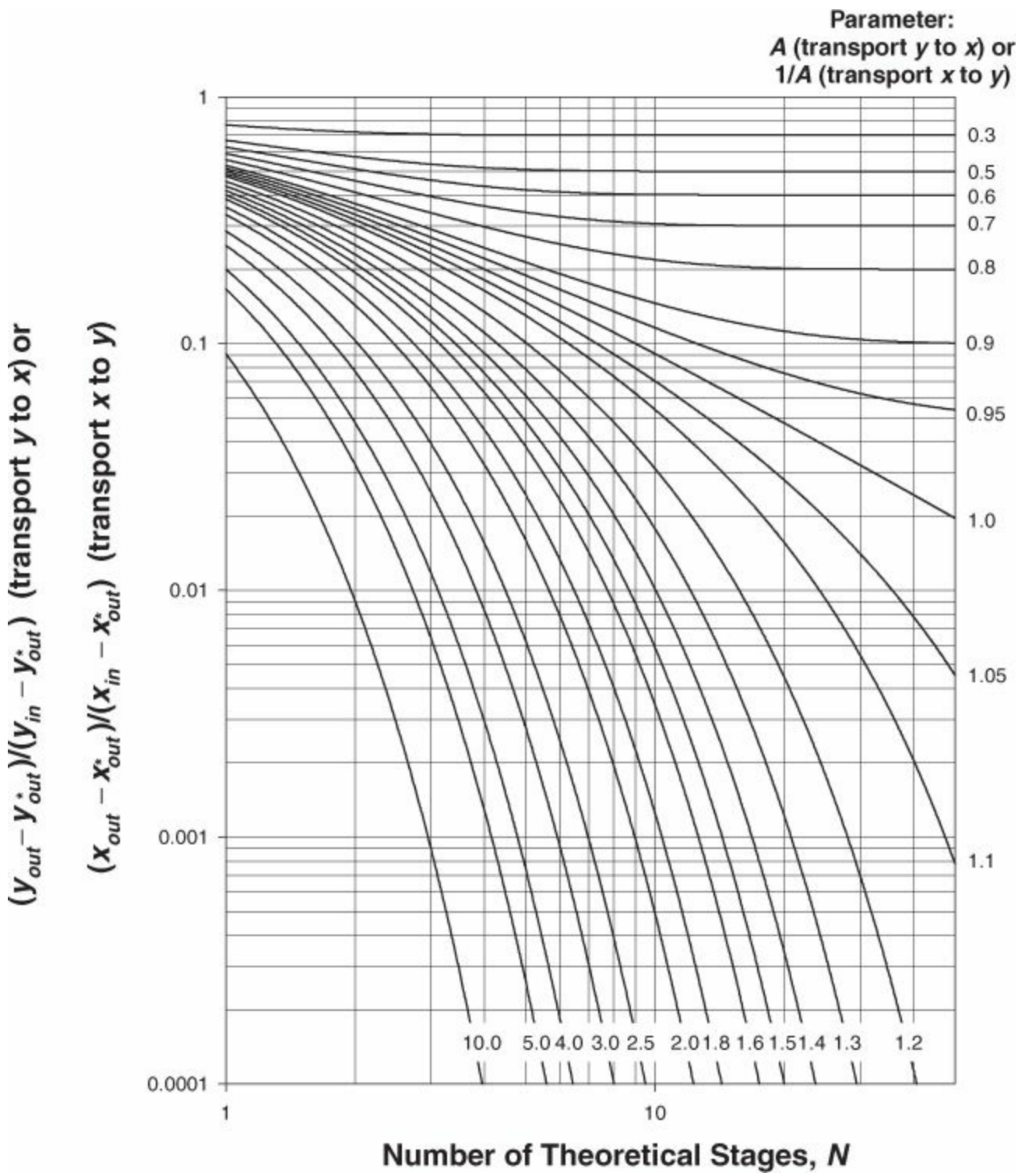


Figure 21.14. Plot of Kremser Equation, Number of Theoretical Stages for Countercurrent Operation, Henry's Law Equilibrium, and Constant A or $1/A$

Even though Equation (21.22) and Figure 21.14 are only valid subject to the assumptions listed above, the qualitative performance of all staged separations can be understood from these relationships. For example, as illustrated in Figure 21.14, if a line of constant A (if $A > 1$) is followed for an increasing number of stages, N, it is seen that the separation continues to improve (lower value of y-axis). For $A < 1$, a best separation is approached asymptotically. If a vertical line of constant N is followed, it is seen that as the separation improves, the value of A increases. A increases if L increases or if G decreases, meaning a larger solvent to feed ratio, or if m decreases, meaning equilibrium more in favor of the L phase.

A similar relationship to the Kremser equation exists for continuous differential separations (packed beds), subject to the same assumptions. The physical situation is illustrated in Figure 21.13(b). This

relationship, known as the Colburn equation, is

$$\frac{y_{A,in} - y^*_{A,out}}{y_{A,out} - y^*_{A,out}} = \frac{e^{N_{tOG}[1-(1/A)]} - (1/A)}{1 - (1/A)} \qquad (21.23)$$

where N_{tOG} is the number of overall gas-phase transfer units. Equation (21.23) is for absorption, that is, transfer into the L phase. For the reverse direction of transport, the same changes are made as in the Kremser equation, with N_{tOL}, the number of overall liquid-phase transfer units, replacing N_{tOG}. Equation (21.23) is plotted in Figure 21.15. Performance curves for a specific staged separation can be generated from the information in Figure 21.15. This is the subject of a problem at the end of the chapter. Because increasing the number of transfer units increases column height, the same qualitative understanding applicable to all systems is gleaned from Figure 21.15 as was described above. For increasing N_{tOG} (which means increased column height) at constant A, a better separation is observed (for $A > 1$). For $A < 1$, a best separation is approached asymptotically. Similarly, at constant column height (constant N_{tOG}), increasing A results in better separation.

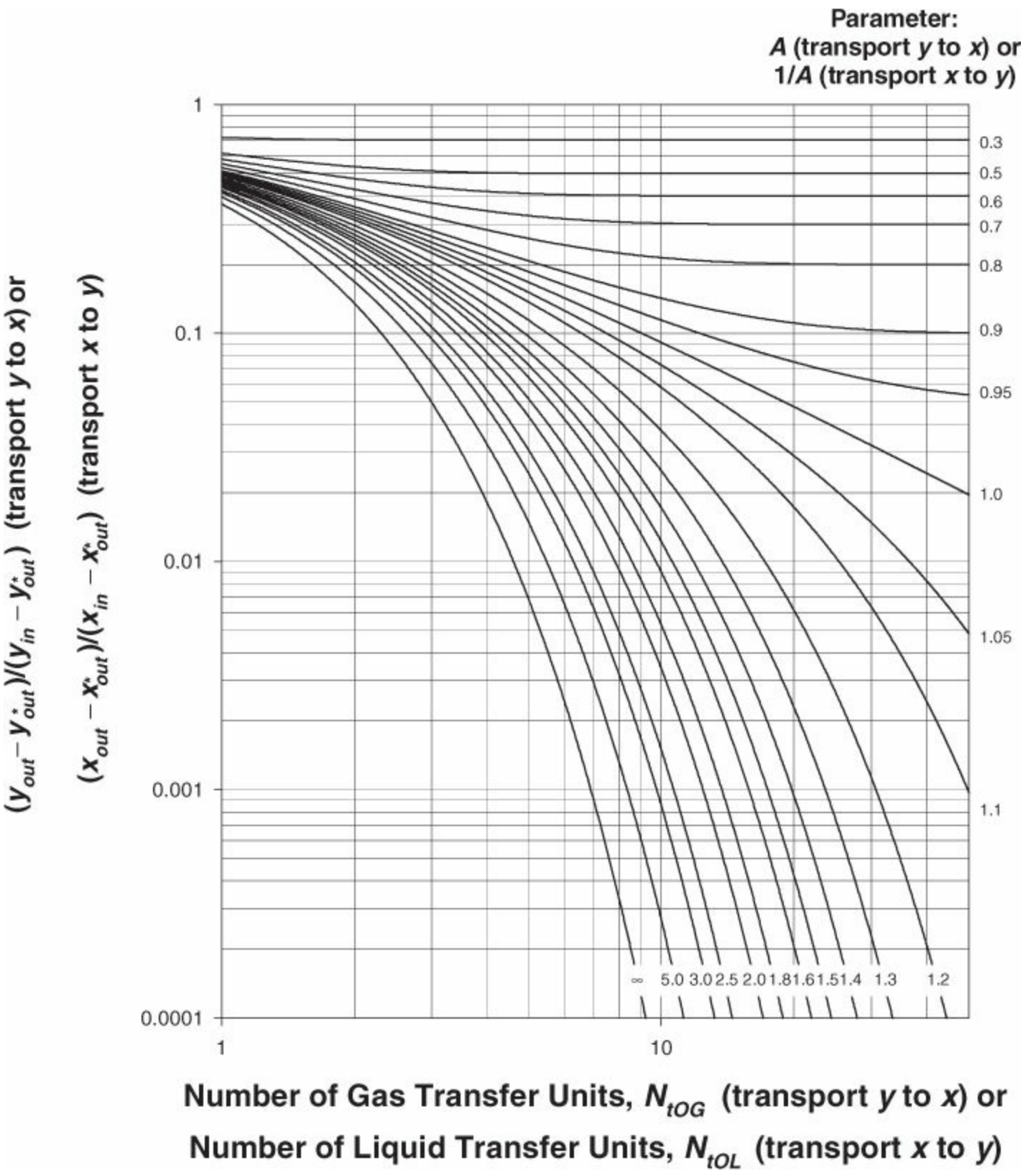


Figure 21.15. Plot of Colburn Equation, Number of Transfer Units for Countercurrent Operation, Henry's Law Equilibrium, and Constant A or $1/A$

As with the Kremser equation, the Colburn equation does not describe flooding behavior of a packed bed, which is specific to a particular column design. Flooding occurs when the vapor velocity upward through the column is so great that liquid is prevented from flowing downward. When a column is designed, the diameter is chosen so that the vapor velocity is below the flooding limit (typically 75%–80% of the limit). However, if the vapor velocity is increased, flooding can occur. Because flooding is specific to a particular column, it cannot be illustrated on the general performance curve. Care must be taken not to use the Kremser or Colburn graphs to obtain a result

that will cause flooding in a particular column or to recommend operation in the flooding zone.

Examples 21.9 and 21.10 illustrate the use of the Kremser and Colburn equations.

Example 21.9.

A tray scrubber with eight equilibrium stages is currently operating to reduce the acetone concentration in 40 kmol/h of air from a mole fraction of 0.02 to 0.001. The acetone is absorbed into a 20 kmol/h water stream, and it can be assumed that the water stream enters acetone free. Due to a process upset, it is necessary to increase the flow of air by 10%. Under the new operating conditions, what is the new outlet mole fraction of acetone in air?

The use of Figure 21.14 for this problem is illustrated in Figure E21.9. For the design case, $y_{A,in}$ = 0.02, $y_{A,out}$ = 0.001, and $x_{A,in}$ = 0, which means that $y^*_{A,out} = 0$. Therefore, the y-axis is 0.05. Because N = 8, the design case has a value of A = 1.2. This is shown as point "a" on Figure E21.9. If the flow of air (G) is increased by 10%, then the new value of A = 1.08. Following a vertical line (constant number of stages) from the original point to a value of A = 1.08 (point "b") yields a y-axis value of 0.08. Hence, the new value of $y_{A,out}$ = 0.0018.

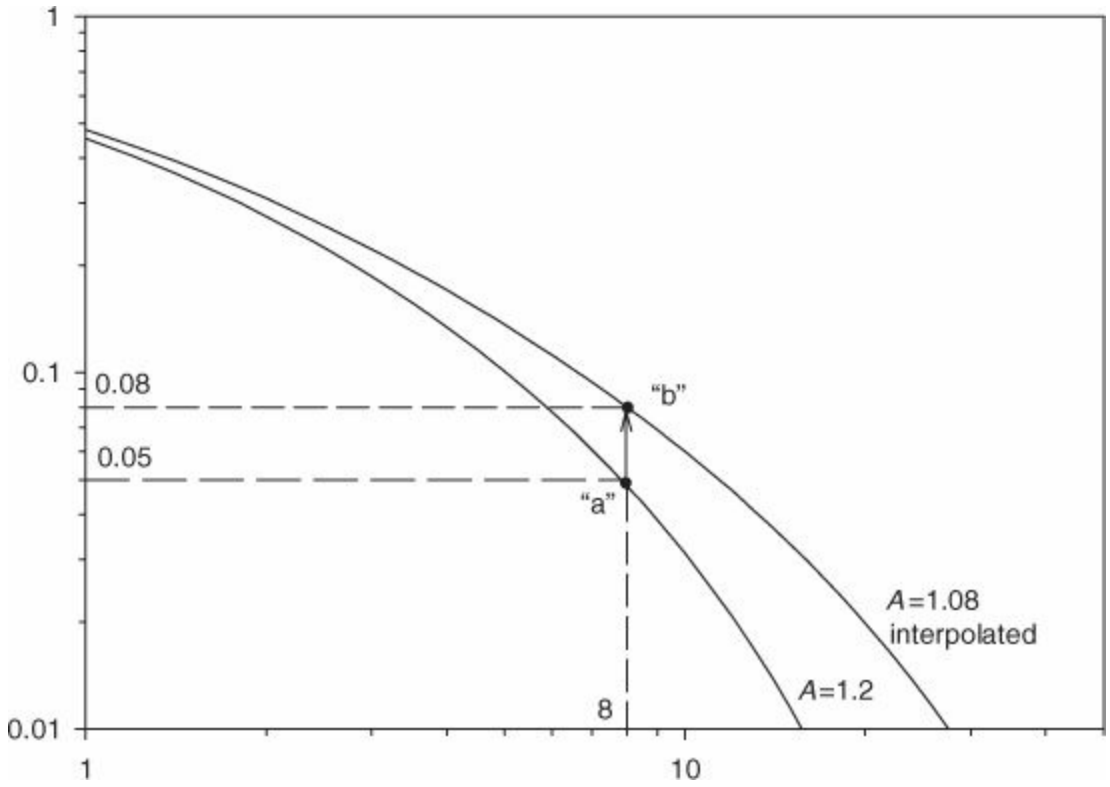


Figure E21.9. Use of Kremser Graph to Solve Example 21.9

Example 21.10.

For the situation described in Example 21.9, the inlet air flowrate and the inlet mole fraction of acetone in air may vary during process operation. Prepare a set of performance curves for the liquid rate necessary to maintain the outlet acetone mole fraction for a range of inlet acetone mole fractions. There should be curves for five different values of the inlet gas rate, including the original case and the following percentages of the original case: 80, 90, 110, and 120. The temperature and pressure in the scrubber are assumed to remain constant.

The result is shown on Figure E21.10. The curves are generated as follows. From the original

operating point, the value of m can be determined to be 0.417. By moving vertically on a line of constant number of equilibrium stages (eight in this case), values for the y-axis and A can be tabulated. The y-axis value is easily converted into $y_{A,in}$ because $y_{A,out}$ is known and constant. Then, for different values of G, values of L are obtained because m is known and constant.

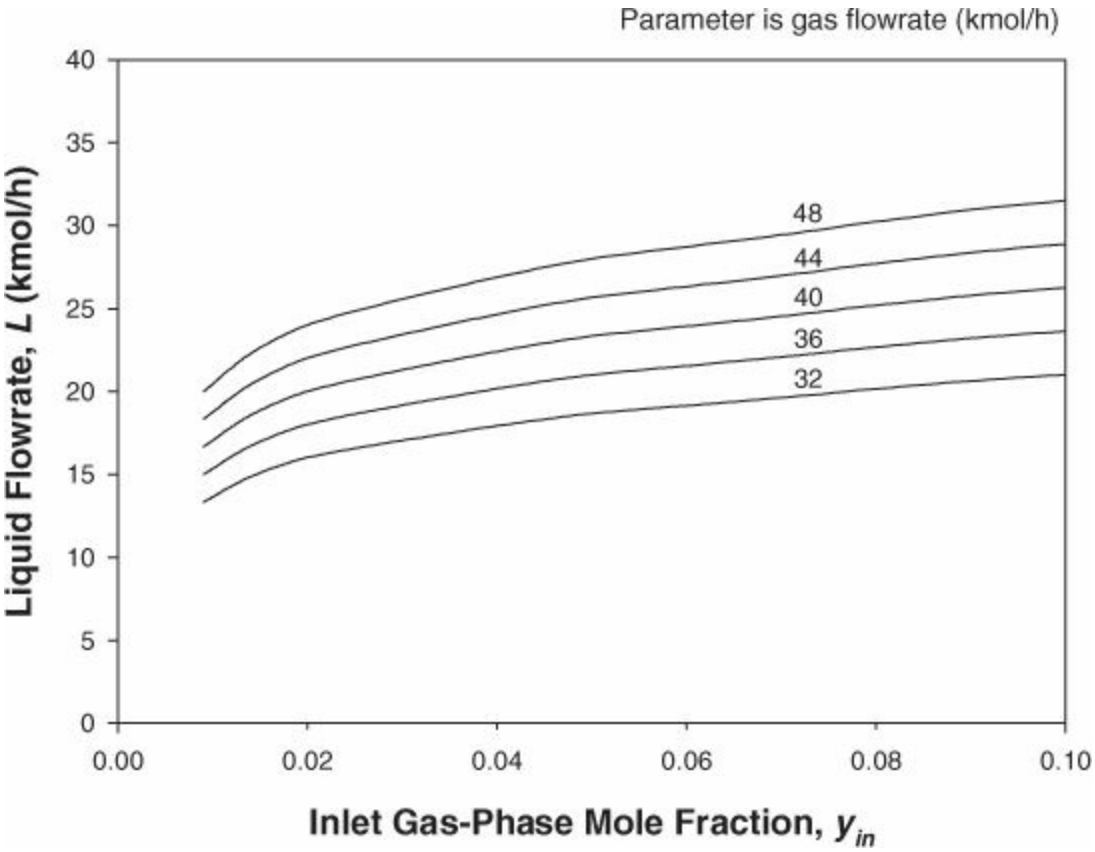


Figure E21.10. Performance Curves for Example 21.10

21.3.2. Distillation

For distillation, there is no universal set of performance curves as for multistage equilibrium separations involving mass separating agents. However, for a given situation, performance curves can be generated. This section demonstrates how this is done.

Figure 21.16 illustrates a multistage distillation system for separating benzene from a mixture of benzene and toluene. Figure 21.17 is a sketch of a typical distillation column. This problem is modified from Bailie and Shaeiwitz [1].

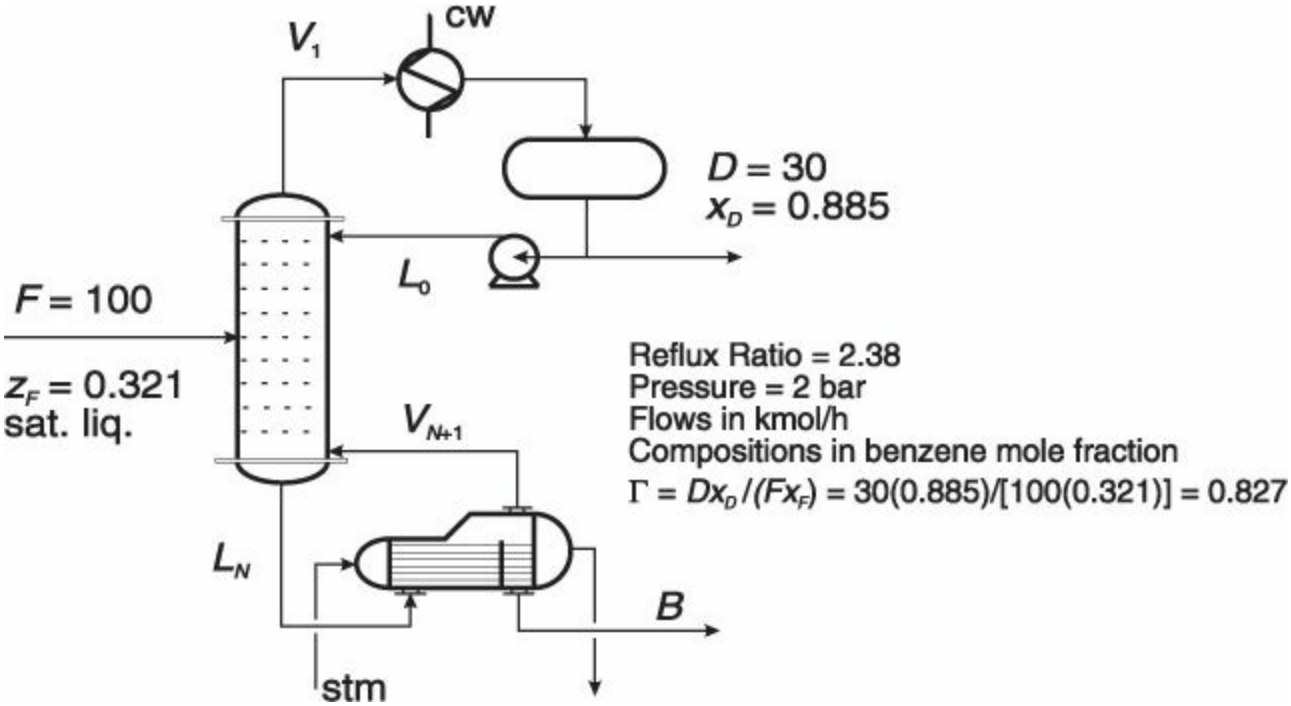


Figure 21.16. Plant Section for Distillation of Benzene from Toluene

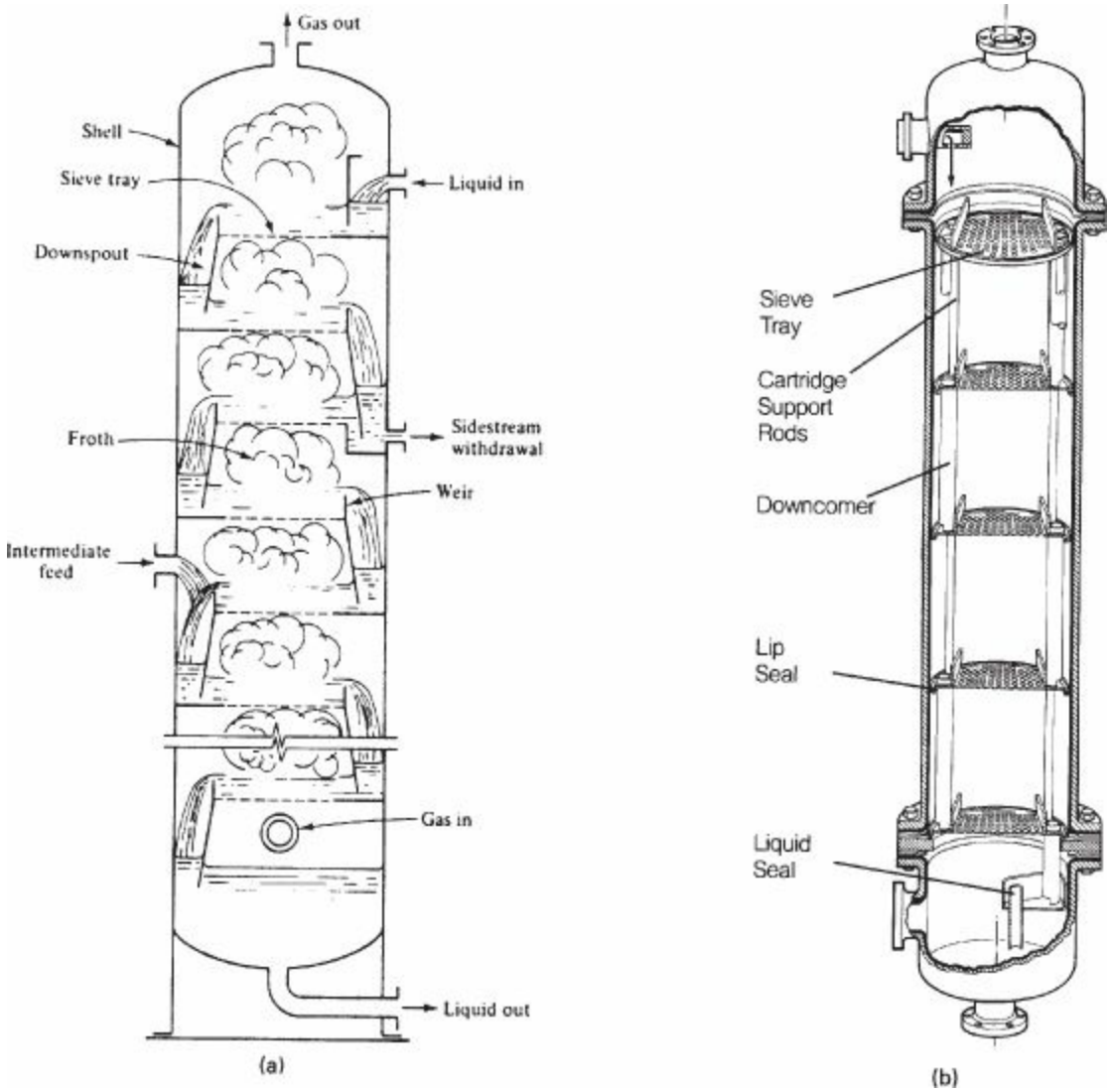


Figure 21.17. Details of Internal Construction of a Distillation Column (From S. Walas, *Chemical Process Equipment: Selection and Design.* Stoneham, MA: Butterworth, 1988. Reprinted with permission.)

Component separation takes place within the tower. Considering the tower alone, there are three input

and two output streams. Separation is achieved by the transfer of components between the two phases. For an operating plant, the size of the tower, the number and type of trays (or height of packing) in the tower, and other tower attributes are fixed. The output streams are established once the input flow streams to the tower are set.

In this section several performance diagrams will be developed for the distillation process shown in Figure 21.16. The tower is the separation unit, and the two phases needed for the separation are provided by the condenser and reboiler.

In a typical distillation system, two recycle streams are returned to the tower. A condenser is added at the top of the column, and a fraction of the overhead vapor, V_1, is condensed to form a liquid recycle, L_0. This provides the liquid phase needed in the tower. The remaining fraction is the overhead product, D. A vaporizer (reboiler) is added to the bottom of the column, and a portion of the bottom liquid, L_N, is vaporized and recycled to the tower as stream V_{N+1}. This provides the vapor phase needed in the tower.

Figure 21.16 provides some information on the distillation process taken from an operating plant.

> *Product benzene is separated from a benzene-toluene mixture. The feed stream,* F = *100 kmol/h, is a saturated liquid with composition* $z_F = 0.321$ *(mole fraction benzene) at a pressure P = 2 bar. The top product consists of a distillate stream, D = 30 kmol/h, with composition* $x_D = 0.885$ *and a corresponding benzene recovery,* $\Gamma = 0.827$. *The tower has a diameter of 0.83 m and contains 20 sieve plates with a 0.61 m plate spacing. Feed is introduced on Plate 13, and the tower operates at a reflux ratio of 2.38. No information is provided on the partial reboiler and total condenser. From a benzene balance,* B = *70 kmol/h and* $x_B = 0.079$.

Figure 21.18 provides a McCabe-Thiele diagram for the separation given in Figure 21.16. This was constructed from the equilibrium curve and by matching the concentrations, $x_D = 0.885$, $z_F = 0.321$, and $x_B = 0.079$, the reflux ratio, $R = 2.38$, and the condition of saturated liquid feed with plant operating conditions. This McCabe-Thiele construction yielded 13 theoretical stages (12 trays plus a reboiler). This means that the average plate efficiency was 60% (100[No. of theoretical plates/No. of actual plates] = 100(12/20). The 60% plate efficiency is within the range found for columns separating benzene from toluene. The feed is added on theoretical plate number 8 (13[0.60] ≈ 8). (*Note:* The number 13 appearing in the previous calculation refers to the actual feed location and not to the number of stages.)

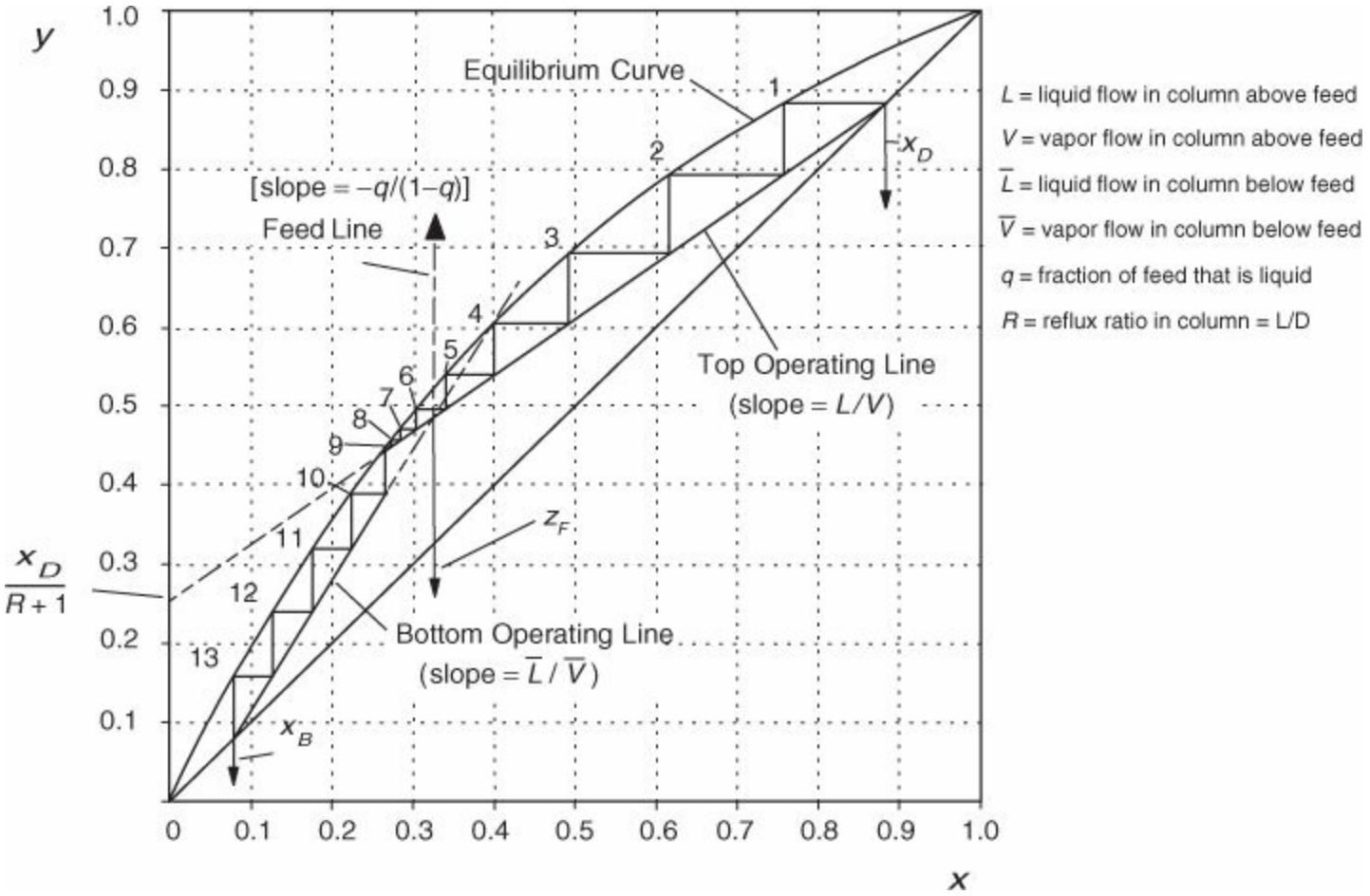


Figure 21.18. McCabe-Thiele Diagram for Benzene Separation: Base Case

The McCabe-Thiele method for evaluating theoretical stages is limited by the following assumptions and constraints:

1. It applies only to binary systems.
2. It assumes "constant molal overflow" and in most situations does not satisfy an overall energy balance.
3. It requires graphical trial-and-error solutions to solve performance problems.

Even though the speed of computation using the McCabe-Thiele method is far slower than for process simulators, it nevertheless remains an important analytical tool. Its graphical representation promotes a clarity of understanding that leads to valuable insights. This is illustrated by using the McCabe-Thiele diagram to glean some critical information required to construct a performance curve for the distillation process in Figure 21.18.

Upon studying Figure 21.18 the following factors are revealed:

1. Feed is not being introduced at the optimum location in the column. The optimal location is on Plate 10 (6/0.60 ≈ 10) and not Plate 13 as currently used.
2. Separation steps near the feed plate are small.

For the current conditions and feed plate location, there are more than the optimum number of stages in the rectifying (top) section. This suggests that the unit may have been designed to process a lower concentration of feed material or to produce a higher-concentration distillate stream than is required currently.

Increasing the slope of the top operating line, L/V, moves the operating lines away from the equilibrium line. This increases the separation of each stage (increases the **step size**). In the special

case when the distillate concentration remains the same, the concentration of the more volatile material (in this case, benzene) in the bottom stream will be lowered.

From an inspection of the McCabe-Thiele diagram, the tower appears to be oversized for the present separation. It could process a lower quality of feed (lower benzene concentration), produce a higher-quality product, and improve benzene recovery. These are points that may deserve further investigation and could be overlooked easily without the graphical representation provided by the McCabe-Thiele diagram.

The McCabe-Thiele analysis is difficult to utilize for developing all the information needed in a performance problem. It requires a graphical trial-and-error solution to match the number of stages to a set of values for z_F, x_D, and x_B. Fortunately, modern computer simulators can provide rigorous solutions for a large variety of separators, including distillation towers. The information needed to construct the performance diagrams for the distillation column in this chapter was obtained from a CHEMCAD simulation. As a base case, a column with 13 theoretical stages (fed on Tray 8) was selected. In the preliminary evaluation, it was assumed that the tray efficiency remained constant. This assumption will be revisited in the discussion of the limitations of these performance curves.

There are three input streams entering the tower shown in Figure 21.16. The flowrate and concentration of these streams, coupled with the performance of the equipment, establish the tower output. The remaining streams in the distillation system can be calculated once these streams are known.

The results of a computer simulation for the base-case conditions are shown in Table 20.1.

Table 20.1. Results of Computer Simulation for Base-Case Conditions

	Flowrate (kmol/h)	Mole Fractions	Concentration
Inputs			
F	100.0	z_F	0.321
Outputs from Simulation			
L_0	71.5	x_0	0.885
V_{N+1}	96.4	y_{N+1}	0.079
V_1	101.5	y_1	0.885
L_N	166.4	x_N	0.079

The value for the vapor flowrate changed from 101.5 kmol/h to 96.4 kmol/h moving from the top to the bottom of the column. Even for this “ideal” separation, the assumption of constant molal overflow is not satisfied.

The process simulator provides a rigorous solution by carrying out material balances, energy balances, and equilibrium calculations over each stage. The simulator provides tray-by-tray results that include the composition of liquid and vapor on each tray, temperature, pressure, and K-values for each component on each tray, along with transport properties of both phases. Using data from this simulation, performance diagrams may be obtained. The most important variables are the tower inputs. They cause the outputs to change. Selection of which performance diagrams to prepare depends on the problem being considered. This is illustrated in the following case study.

You are the engineer in charge of the toluene-benzene distillation section in a chemical plant.

You have just met with your supervisor and have been informed that, in the future, the feed concentration to this unit will no longer be constant but will vary between 25% and 40% benzene. You have also been told that it is important to maintain a constant distillate flow, D, and concentration, x_D, from this distillation unit to the downstream process.

At this meeting, possibilities for replacing parts of this process, replacing the whole system, and installing a storage system to blend feed and/or product distillate, or a combination of these alternatives, were discussed. The object is to maintain the distillate flow and concentration.

To make a responsible decision on this matter, it will be necessary to assess the effect that changes in feed concentration will have on the operation of the distillation process. Before making a decision, background material will be needed. You have been told to provide a performance diagram that shows the effects of changes in feed concentration on the reflux flowrate. For a preliminary assessment, you are to assume that the reboiler and condenser can meet any new demands. If they are found inadequate, they will be replaced or modified.

In addition, questions have been raised regarding the low benzene recovery in the current operation, and you have been told to consider the impact of using higher benzene recoveries.

For the situation described above, the important variables are the feed concentration, x_F, and the benzene recovery, Γ. The information needed to respond to the above request can be obtained by running simulations at different feed concentrations and reflux flowrates to determine the benzene recovery for each pair of conditions. Reflux is chosen as the dependent variable here because the flow of the reflux stream is the most common way to regulate the performance of a distillation column.

Figure 21.19 gives the performance curves for the reflux, L_0. The performance diagram shows the feed concentration, z_F, on the x-axis with the benzene recovery, Γ, as a parameter. The base case is identified as point “a” on the diagram.

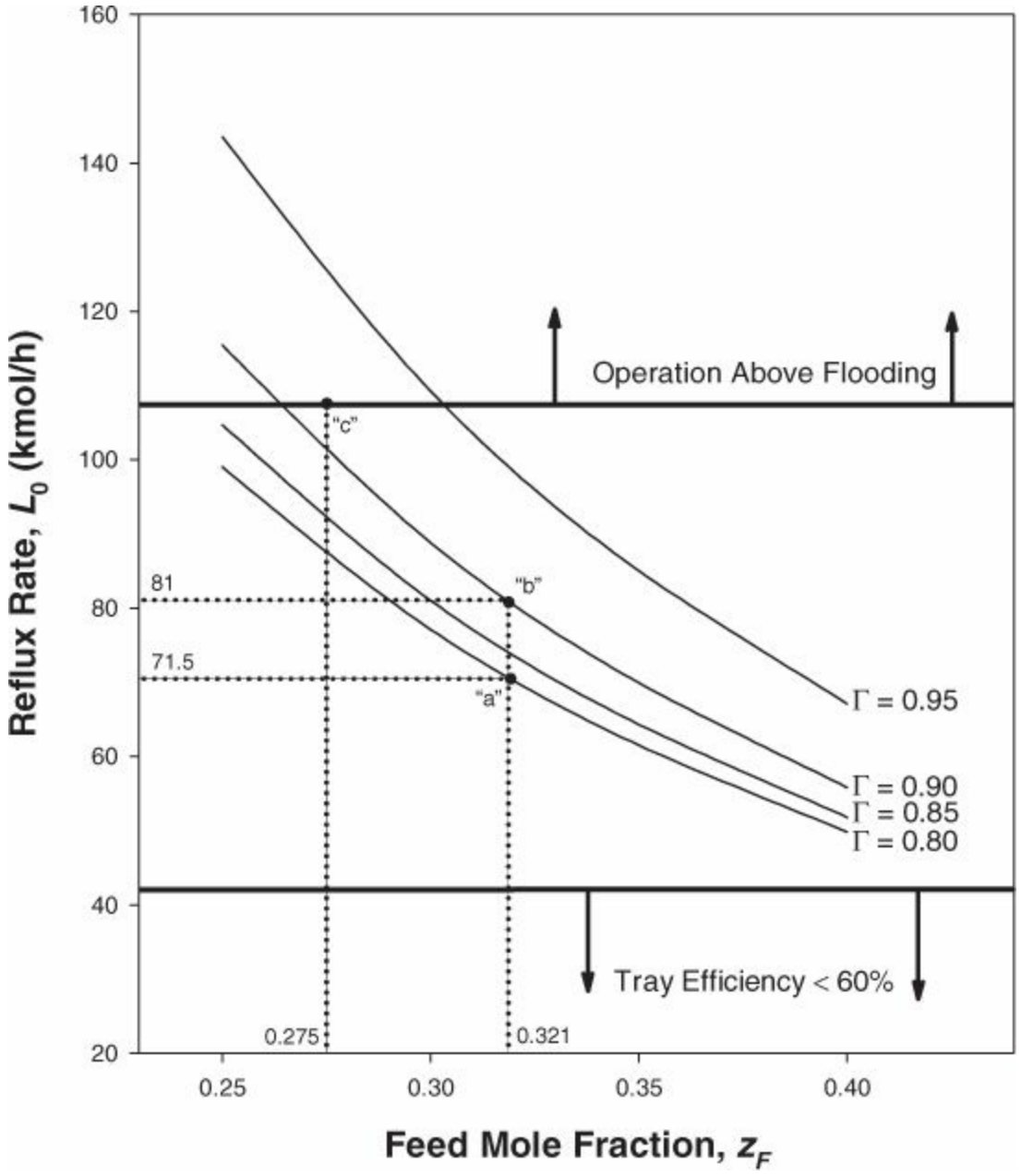


Figure 21.19. Performance Curve for Distillation Tower

The performance curves presented show the following trends:

1. **For constant recovery, Γ:** As z_F increases, the reflux decreases. The rate of decrease becomes less as z_F increases.
2. **For a constant feed concentration, z_F:** As Γ increases, the reflux increases. The rate of increase becomes greater as Γ increases.

The performance diagram given in Figure 21.19 is specific to the existing tower with fixed feed location, saturated liquid feed, and desired distillate conditions. The conditions or variables that are fixed in this problem are as follows:

D = 30 kmol/h

x_D = 0.885 mole fraction benzene

20 trays (12 theoretical equilibrium stages plus a reboiler)

Feed plate = 13 (theoretical equilibrium Stage 8)

Diameter of tower = 0.83 m

Tray spacing = 0.61 m

Overall tray efficiency = 60%

The independent input variables are the feed concentration, z_F, and the benzene recovery, Γ. One important point to note is that, as in all other performance problems, the parameters associated with the equipment are fixed. A second point to note is that with the information in Figure 21.19, it is possible to work backward and estimate the desired reflux flowrate, for example, that would be required to obtain the desired distillate conditions if the feed concentration changed from 0.321 to 0.295. The utility of the performance curves is best illustrated in Example 21.11. Additional problems involving construction and use of performance curves for distillation are given at the end of the chapter.

Example 21.11.

Using the performance diagram, Figure 21.19, find the changes to the tower input needed to achieve a recovery of 90% for the current feed concentration, $x_F = 0.321$.

New Feed Rate, F: $F = x_D D/(z_F \Gamma) = 0.885(30)/[(0.321)(0.9)] = 91.9$ kmol/h

New Reflux, L_0: From Figure 21.19 new feed rate (see point "b") $L_0 = 81$ kmol/h

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Example 21.11 showed that the distillation system could be operated at a recovery, Γ = 0.9. This reduces the feed that can be processed by 8.1%.

Installed equipment imposes operating limitations that restrict the range over which the performance diagrams can be used. Equipment manufacturers often provide technical information that gives the limitations of the equipment. This information may include, but is not limited to, operating temperature, pressure, installation instructions, and operating parameters such as plate efficiencies and flooding and weeping velocities. Thus this specific information adds additional constraints on the range of operations that may be considered.

From the technical information provided with the sieve trays used in the distillation tower in Figure 21.19, the following information was obtained:

1. Flooding gas velocity, $u_f = 1.07$ m/s
2. Weeping gas velocity, $u_w = 0.35$ m/s
3. Tray efficiency, $\epsilon = 0.60$ for $2.6 > u[\text{m/s}](\rho_v[\text{kg/m}^3])^{0.5} > 1.2$

Based on this information, two regions on Figure 21.19 are shown. These are "forbidden" or infeasible regions, in which the performance curves are not valid because of the limitations of the specific equipment or the assumptions made (e.g., $\epsilon = 0.60$). For any change to be made, the new condition must be checked to ensure that the new operating point lies within the feasible region for all the performance curves.

The flooding velocity limit is also shown on Figure 21.19. The limit related to weeping lies below that for tray efficiency; that is, the tray efficiency drops below 60% well before the weeping condition is reached. The constraint of operating below a tray efficiency of 60% is shown as the lower infeasible region in Figure 21.19.

Example 21.12 shows how the flooding limit of the equipment, illustrated on the performance graph,

identifies another equipment limitation.

Example 21.12.

Find the maximum recovery possible from the distillation equipment for a feed concentration, z_F = 0.275.

Point "c" on Figure 21.19 provides an estimate of the recovery, $\Gamma = 0.91$.

The constraints associated with the equipment must be included in any analysis of performance.

In the preliminary analysis, it was assumed that the tray efficiency was 60% and the reboiler and condenser were adequate. From the manufacturer's data, it was confirmed that the efficiencies were constant over the operating range given above. The limits on the reboiler and the condenser have not been considered in the above analysis and must be checked against the performance limits for these pieces of equipment. In addition, the curves obtained assume that the feed location would not change. However, by using the optimum location, as the feed concentration changes, the performance of the tower could be improved. The use of alternative feed locations requires that feed nozzles be present at different trays. Thus, once again, the constraints of the existing equipment dictate whether this option should be considered further.

21.4. Summary

In this chapter how to construct simple performance diagrams for some common individual pieces of equipment was presented. These performance diagrams show how a given piece of equipment responds to changes in input flows. They also can be used to predict what changes in input variables would be required in order to obtain a desired output condition. In some instances, as with valves, pumps, and compressors, performance curves are provided by equipment manufacturers. In other instances, as with the Kremser or Colburn equation, universal performance curves and equations exist subject to specific assumptions. In still other instances, as with heat exchangers or distillation columns, performance curves must be constructed by modeling equipment behavior.

In all real chemical processes, the final element that makes changes in flowrates possible is the regulating valve. Without such valves, it would be impossible for a process to adjust for unforeseen changes in operating conditions. In addition, it would be equally impossible to manipulate a process to give new desired outputs. Regulating valves are relatively simple and inexpensive pieces of equipment, and yet they are absolutely essential in the day-to-day operation of a chemical process. The use of regulating valves was illustrated for a simple flow system including a pump, piping system, process equipment, and a valve.

What You Should Have Learned

- How performance relates the output to the input when the equipment is fixed (already exists)
- The basic analytical method for doing performance calculations involving ratios
- That the constraints of chemical process equipment must be included in this analysis
- How to represent the performance of typical chemical process equipment graphically

Reference

1. Bailie, R. C., and J. A. Shaeiwitz, "Performance Problems," *Chem. Eng. Edu.* 28 (1994): 198–203.

Short Answer Questions

1. What is a pump curve? Sketch a typical pump curve, making sure that both axes are clearly labeled. On the same sketch, show a typical system curve. Indicate the typical region of good operating practice. Explain.
2. Comment on the following statement: *For a two-pump system, it is always best to run the two pumps in series rather than in parallel because greater scale-up will be possible.*
3. Explain the meaning of the intersection of the two curves on the diagrams in Figure P21.3.

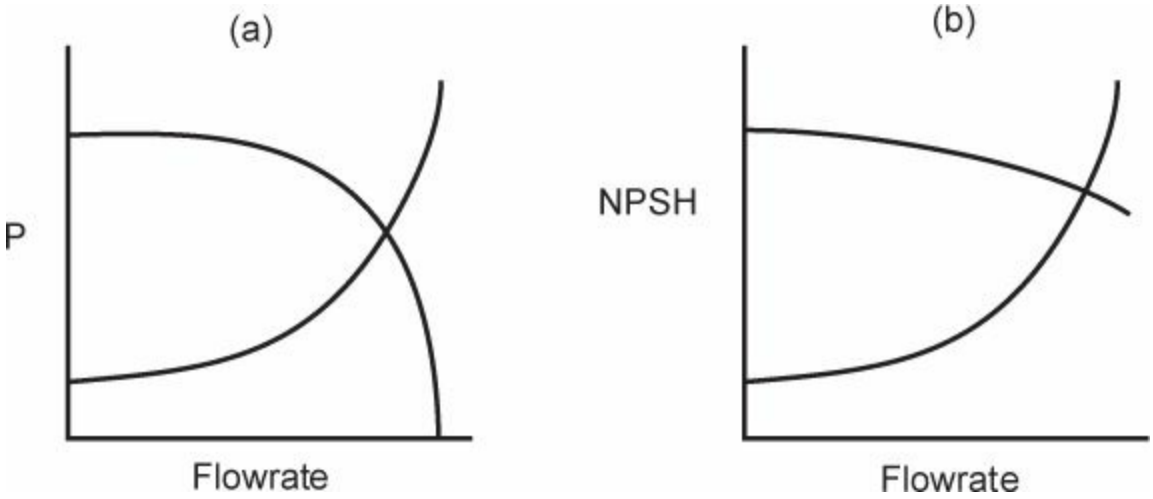


Figure P21.3. Diagrams for Problem 21.3

4. Comment on the following statement: *The film heat transfer coefficient always increases with flowrate to the 0.8 power.*
5. For a given flowrate, it is known that the pump through which the process flows cavitates. The pump has a spare, and a temporary fix to run both pumps simultaneously has been suggested. The pumps can be run either in series or parallel. Which arrangement *might* fix the cavitation problem?
6. A storage tank uses gravity flow to supply a liquid feed material to a holding tank. The pressures and levels in each tank can be considered to be constant. If the viscosity of the fluid is sensitive to temperature (increasing with decreasing temperature), what effect (large or small) will a decrease in temperature have on the flow of the material if the flow is (a) laminar or (b) turbulent? Explain your reasoning.
7. Two columns operate in a chemical plant. The first column operates at a pressure of 10 bar, and the second at a temperature of 1 bar. For process reasons, the pressures in the two columns are both reduced by 0.4 bar. If the internal flows in the columns (mass flows of liquid and vapor) are held constant during this pressure change, which column is more likely to flood?
8. For the separation of a binary mixture in a distillation column, what will be the effect of an increase in column pressure on the following variables?

   a. Tendency to flood at a fixed reflux ratio

b. Reflux ratio for a given top and bottom purity at a constant number of stages

c. Number of stages required for a given top and bottom purity at constant reflux ratio

d. Overhead condenser temperature

9. Explain, using equations where appropriate, why a pump located even with the bottom of a pressurized tank containing a vapor-liquid mixture of a pure component will likely not ever cavitate regardless of the ambient temperature.

10. A storage tank is connected to a pond (at atmospheric pressure!) by a length of 4-in pipe and a gate valve. From previous operating experience, it has been found that when the tank is at a pressure of 3 atm, the flow through the pipe is 35 m^3/h when the gate valve is fully open. If the pressure in the tank increases to 5 atm, what will be the maximum discharge rate from the tank?

11. Consider the pump and system curves in Figure P21.11 for identical pumps arranged in parallel and series.

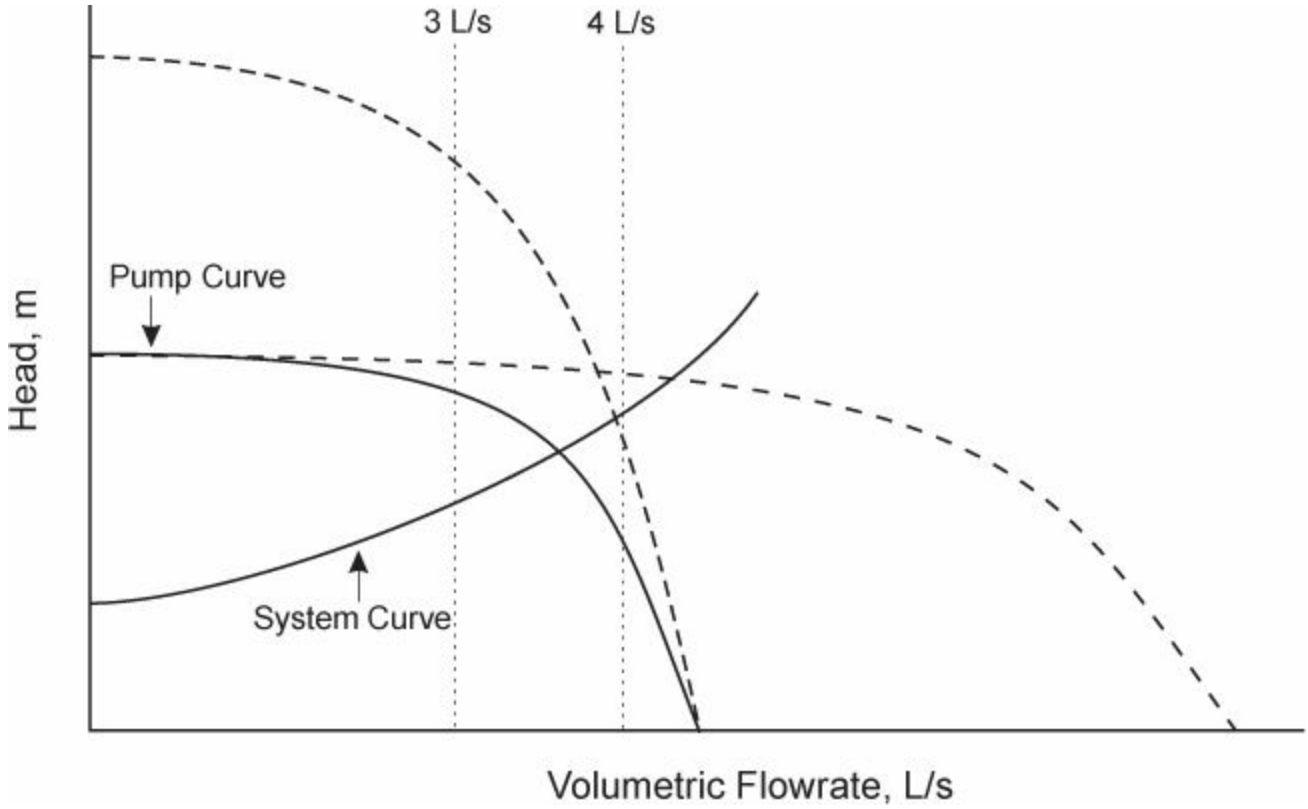


Figure P21.11. Pump and System Curves for Problem 21.11

a. If the flowrate is increased from 3 L/s to 4 L/s, which pump arrangement(s) (single pump, two in series, or two in parallel) will give you the desired flow increase?

b. For your answer(s) to Part (a), will the pump(s) cavitate?

Problems

Background Material for Problems 21.12–21.14

For the steam generator illustrated in Figure 21.1(a) and discussed in Section 21.1, the total resistance to heat transfer, $R_T = 1/(UA)$, is given by the following relationship:

$$R_T = R_i + R_o + R_p + R_{f,i} + R_{f,o}$$

In the above equation,

R_T = total resistance to heat transfer.

R_i = convective resistance of the light oil. This resistance is a function of the flowrate, as shown in Chapter 20. Subscript 1 refers to the base case, and subscript 2 refers to the new case.

$$R_{i2} = R_i(\dot{m}_2/\dot{m}_1)^{0.8}$$

R_o = convective resistance of the boiling water. This resistance is not a function of flowrate. It is a weak function of the temperature drop across the film of vapor on the outside of the tubes. For this analysis, it is assumed constant.

R_p = conductive resistance of the tube walls. This resistance is small and is ignored here.

$R_{f,i}$ and $R_{f,o}$ = fouling resistances on the inside and outside of the tubes, respectively. These two resistances are combined into a single fouling term.

$$R_f = R_{f,i} + R_{f,o}$$

For the conditions given above, the total resistance becomes

$$R_T = R_{i1}(\dot{m}_2/\dot{m}_1)^{0.8} + R_o + R_f$$

The only resistance affected by mass flowrate, $\dot{m}_i$, is R_i.

12. Operating data taken from the plant shortly following the cleaning of the reboiler tubes show that

$$T_{in} = 325°C,\ T_{out} = 293°C,\ \dot{m}_s = 1650 \text{ kg/h},\ T_s = 253°C$$

a. Find the overall heat transfer coefficient.

b. Estimate the overall resistance to heat transfer.

13. This is a continuation of Problem 21.12. Estimate the fouling resistance for the base case presented in Figure 21.1(a).

14. This is a continuation of Problem 21.12. Typical heat transfer coefficients given in Table 11.11 are used to predict the ratio of heat transfer resistances between boiling water and light oil. This ratio is estimated to be approximately 1:2. Estimate the individual resistance and heat transfer coefficient for both the oil and the boiling water.

Background Material for Problems 21.15–21.16

The performance curves presented in Figure 21.1 represent those obtained for the heat exchanger used in Problems 21.15–21.16.

15. a. Use the guideline from Tables 11.11 and 11.18 to establish "normal" limits on the amount of heat that could be exchanged.

b. How do these limits explain the fouling of the heat exchanger observed in the operating unit?

c. Under the constraints identified in Part (a), what is the highest temperature allowed (flowrates limited to range of M values shown)?

16. a. Estimate the relative increase in heat duty that would result from increasing the liquid level from the base case to cover the tubes completely. The input streams and vapor temperature remain the same as in the base case.

b. Explain why the duty increase is less than the increase in area.

Background Material for Problems 21.17–21.19 is given in Section 21.2

17. For the system presented in Example 21.3 you are asked to appraise the effects of adding a second pump and impeller set identical to the current pump in the system.

a. Prepare a performance diagram, for the two-pump system and for each impeller size, if the pumps are to be installed in series.

b. Prepare a performance diagram, for the two-pump system and for each impeller size, if the pumps are to be installed in parallel.

c. Estimate the pressure achieved for each pump/impeller system in Parts (a) and (b) at flowrates of 400 and 800 gallons/min.

18. Referring to Example 21.3, it has been decided that the storage tank should be kept at 1 bar and the reactor pressure at 1.2 bar. To provide the pressure head required, a pump is placed in line before the heat exchanger. For the 50% increase in flow desired in Example 21.3, answer the following:

a. What pressure head must be produced by the pump?

b. Which of the pump/impeller systems given in Figure 21.4 is capable of providing sufficient flow?

c. At what location in the system would you place the pump? Explain why.

19. A centrifugal pump produces head by accelerating fluid to a velocity approaching the tip velocity of the rotating impeller. The liquid leaving the pump is at a high velocity and is forced into the discharge pipe from the pump, where it comes into contact with relatively slow-moving fluid in the pipe. As the fluid decelerates, the velocity head is converted into pressure head. For a given pump the following relationships can predict performance:

$$h_2/h_1 = [(N_2/N_1)(D_2/D_1)]^2 \text{ and } \dot{v}_2/\dot{v}_1 = [(N_2/N_1)(D_2/D_1)]^3$$

where

N = speed of rotation of the impeller, rpm

h and $\dot{v}$ = head and volumetric flowrate, respectively

2 and 1 = new and base-case conditions, respectively

D = impeller diameter

The speed of rotation of the impeller can be adjusted, even when a constant speed motor is used, by the use of a pulley system as shown in Figure P21.19.

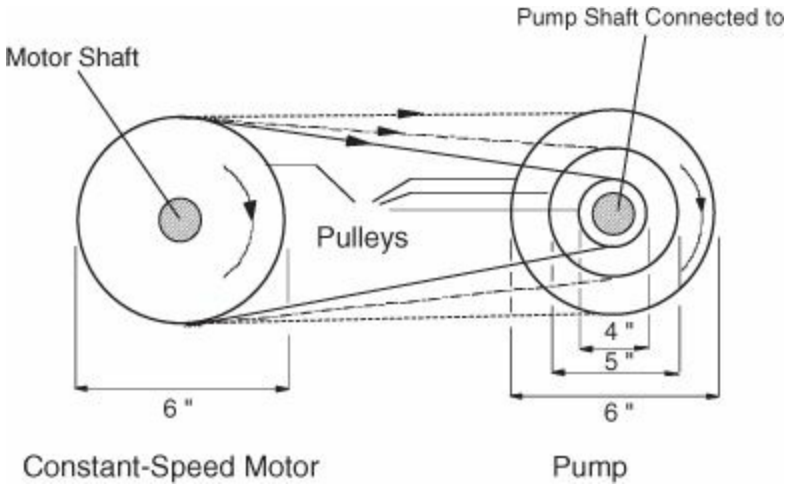


Figure P21.19. Pully System for Problem 21.19

The pump curve given in Figure 21.4 was obtained when the impeller was directly coupled to a constant-speed motor (3500 rpm). Develop performance curves for this pump, with a 7-in-diameter impeller, assuming that the pump is driven via a pulley system in which the constant-

speed motor (3500 rpm) has a 6-in-diameter pulley and the motor impeller is connected to a series of pulleys with diameters of 4 in, 5 in, and 6 in. Construct performance diagrams for each pulley combination.

20. Naphthalene is fed to a phthalic anhydride production process. The feed is available at 208°C and 79 kPa. The flowrate is 18,500 kg/h in 1.5-in schedule-40 pipe. A pump with NPSH characteristics as plotted in Figure 21.9 is used. Will this pump be suitable for the desired duty? If not, what modifications would be necessary in order to use the existing pump? Be quantitative.

21. Refer to Example 21.8. There are additional methods other than the two presented for increasing the NPSH in order to avoid pump cavitation. For the following situations, sketch the $NPSH_A$ curve on Figure 21.9, keeping head at 2 m and keeping the flowrate constant. Identify the operating point on the $NPSH_A$ curve in order to determine whether $NPSH_A > NPSH_R$.

    a. The diameter of the suction line can be increased. Examine the effect of increasing the diameter of the suction line to 1.25-in schedule 80.

    b. The temperature of the toluene can be decreased. Examine the effect of decreasing the temperature of the toluene to 40°C using the original pipe.

22. Refer to the compressor curves given in Figure 21.11.

    a. At a flowrate of 125 Mg/h, what is the exit pressure from the compressor operating at 3500 rpm if the inlet pressure is 2 bar?

    b. If the feed pressure is 4 bar and the compressor is operating at 2200 rpm, how can you obtain an outlet pressure of 9 bar at 125 Mg/h?

    c. It is necessary to raise the pressure from 2 bar to 24 bar at 125 Mg/h. How could this be accomplished at each rpm? Which method do you recommend?

23. A packed scrubber with 20 transfer units has been designed to reduce the solute concentration in 80 kmol/h of air from a mole fraction of 0.01 to 0.006. The solute is absorbed into a 20 kmol/h solvent stream, and it can be assumed that the solvent stream enters solute free. If the flow of solvent is decreased by 15%, what is the new outlet mole fraction of solute in air?

24. Prepare a set of performance curves similar to those in Example 21.10 for a packed scrubber with 10 transfer units that removes solute from air from a mole fraction of 0.02 to a mole fraction of 0.001. The flowrate of the inlet air stream is 80 kmol/h, and the solvent flowrate (assumed solute free) is 40 kmol/h.

25. Repeat Problem 21.24 and Example 21.10 with the following change: In each case, the gas flowrate remains constant at the original conditions. The parameter on the performance curve is now absorber temperature (assumed constant throughout the absorber). There should be five curves for each absorber: the original temperature, an increase of 5°C and 10°C from the original temperature, and a decrease of 5°C and 10°C from the original temperature.

26. The scrubber in Problem 21.23 has been running well for several years. It is now observed that the outlet solute mole fraction in air is 0.002. Suggest at least five reasons for this observation. Suggest at least five ways to compensate for this problem in the short term. Evaluate each compensation method as to its suitability.

27. It is necessary to increase the capacity of an existing distillation column by 25%. As a consequence, the amount of liquid condensed in the condenser must increase by 25%. In this condenser, cooling water is available at 30°C and, under present operating conditions, exits the

condenser at 45°C, the maximum allowable return temperature without a financial penalty assessed to your process. Condensation takes place at 75°C. You can assume that the limiting resistance is on the cooling water side. Can the existing condenser handle the scale-up without incurring a financial penalty? What is the new outlet temperature of cooling water? By what factor must the cooling water flow change?

28. In the previous problem, it may be necessary to scale up or scale down by as much as 50% from the original operating conditions. Prepare a performance curve similar to the one in Figure 21.1 for operation of the condenser over this range.

Background Material for Problems 21.29–21.33

In Section 21.3.2, it was shown that Figure 21.19 could be constructed from results of simulating the distillation column. Table P21.29 shows the results of such a simulation for the problem discussed in Section 21.3.2. The data used in Figure 21.19 are contained in this table. The data in Table P21.29 can be used to construct other performance curves, similar to Figure 21.19. In Problems 21.29–21.31, a performance curve should be constructed with the flooding and tray efficiency limits included (given on page 747), as in Figure 21.19.

Table P21.29. Performance Data from a Process Simulator for the Benzene-Toluene Tower

Feed Conc z_F	Benz Rcvry Γ	Feed F kmol/h	Bottm Prod B kmol/h	Reflux Ratio R	Ovhd Vapor V_1 kmol/h	Boil-Up V_{N+1} kmol/h	Liquid Reflux L_0 kmol/h	Cond Duty Q_c GJ/h	Rebl Duty Q_r GJ/h	Bottm Temp °C	Vapor Vel at Top u m/s
0.25	0.80	132.8	102.8	3.30	129.0	122.4	99.0	–3.93	3.87	133.4	1.01
0.30	0.80	110.6	80.6	2.57	107.1	101.7	77.1	–3.26	3.21	132.6	0.84
0.35	0.80	94.8	64.8	2.05	91.5	86.9	61.5	–2.79	2.75	131.8	0.73
0.40	0.80	83.05	53.0	1.66	79.8	75.7	49.8	–2.43	2.39	130.7	0.62
0.25	0.85	124.9	94.9	3.49	134.7	127.8	104.7	–4.10	4.04	134.1	1.05
0.30	0.85	104.1	74.1	2.70	111.0	105.4	81.0	–3.38	3.33	133.5	0.87
0.35	0.85	89.3	59.3	2.14	94.3	89.5	64.3	–2.87	2.83	132.8	0.74
0.40	0.85	78.1	48.1	1.73	81.8	77.6	51.8	–2.49	2.45	132.0	0.64
0.25	0.90	118.0	88.0	3.85	145.4	138.0	115.4	–4.42	4.36	134.9	1.14
0.30	0.90	98.3	68.3	2.96	118.8	112.7	88.8	–3.56	3.61	134.4	0.93
0.35	0.90	84.3	54.3	2.33	99.9	94.8	69.9	–3.04	3.00	133.9	0.78
0.40	0.90	73.8	43.8	1.86	85.5	81.4	55.8	–2.61	2.57	133.3	0.67
0.25	0.95	111.8	81.8	4.78	173.5	164.5	143.5	–5.26	5.20	135.6	1.36
0.30	0.95	93.2	63.2	3.64	139.2	132.1	109.2	–4.23	4.17	135.4	1.09
0.35	0.95	79.9	49.9	2.83	115.0	109.2	85.0	–3.50	3.45	135.1	0.90
0.40	0.95	69.9	39.9	2.24	97.1	92.0	67.1	–2.95	2.91	134.8	0.76

D = 30 kmol/h, x_D = 0.885, P_{bot} = 2 bar, overall tray efficiency = 60%.
Assume ideal system for evaluation of K values and other thermodynamic data.

29. Prepare a performance plot for vapor velocity as a function of feed composition with benzene recovery as a parameter.
30. Prepare a performance plot for boil-up rate as a function of feed composition with benzene recovery as a parameter.
31. Prepare a performance plot for reboiler duty as a function of feed composition with benzene recovery as a parameter.
32. For the distillation problem outlined in Section 21.3.2,
    a. Determine the values of F, B, and x_B required when the concentration of the feed becomes z_F = 0.25. Assume that the values of D and x_D are to remain the same (D = 30 kmol/h and x_D = 0.885) and that the recovery is to remain 90%.
    b. Report any risks associated with the solution.
    c. What are the values of L_0 and V_{N+1} for this case?
33. The information given in Figure 21.18 showed that the benzene recovery column was not operating at maximum benzene recovery.

a. Estimate the maximum value of benzene recovery for the base case ($z_F = 0.321$).

b. Give several reasons for operating the current column at less than maximum benzene recovery.

c. Plot a performance curve that shows estimated values for F, L_0, and V_1 at maximum benzene recovery as a function of feed composition.

Background Information for Problems 21.34 and 21.35

In preparing the performance diagrams for the benzene-toluene system in Section 21.3.2, it was noted that under current operation, the feed stream was not introduced at the optimum location. The performance curves, Figure 21.19, were constructed for this nonoptimal feed location.

34. For the same feed, distillate, and bottoms shown in Figure 21.16, determine the following:

a. The boil-up, V_{N+1}, and reflux, L_0, required if the feed is now introduced at the optimum location.

b. Using typical utility costs from Chapter 8, estimate the yearly savings ($/y) obtained by changing the feed location.

35. Assume that the distillation column in Figure 21.16 is to be operated at the same value of L_0, D, and B and the same feed as the base case.

a. Calculate x_D, x_B, and the benzene recovery, Γ, obtained by introducing the feed at the optimum location.

b. Assuming that the benzene lost in the bottom is valued at $0.20/lb, calculate the savings resulting from locating the feed at the optimum location.

36. A heat exchanger was put into service approximately one year ago. The design conditions are that process gas is cooled from 100°C to 50°C, with cooling water entering at 30°C and exiting at 40°C. Initially, the heat exchanger operated satisfactorily, meaning the temperatures for the cooling water and process streams were the same as the design conditions given above. However, over time, it has been observed that, due to impurities in the gas stream, a fouling layer of dirt has built up on the outside of the tubes. This dirt layer has caused the temperatures through the heat exchanger to change, and, in order to maintain the process gas outlet temperature at 50°C with the same design gas flowrate, the mass flow of water has had to be increased to 150% of the design flow, with a corresponding change in cooling water outlet temperature.

Assuming that, for the design case, all the resistance to heat transfer is on the process-gas side, estimate the fouling heat transfer coefficient for the current operation as a fraction or multiple of the gas-phase heat transfer coefficient.

37. In a process that produces a temperature-sensitive product, the final step is to cool the product from 70°C to 35°C prior to sending it to storage. This cooling is achieved using cooling water that is available at 30°C and exiting at 40°C. A shell-and-tube heat exchanger is used with cooling water in the tubes. The process-side resistance is dominant. It is desired to scale down this process. Answer the following questions:

a. If the flowrate of the process fluid decreases to 70% of its design value, by how much must the cooling water flowrate change to maintain the desired exit temperature of the process fluid of 35°C?

b. What is the exit temperature of the cooling water for this case?

38. A desuperheater permits the temperature of saturated steam entering a heat exchanger to be controlled. This is accomplished by having a valve that changes the pressure of the source steam to a known value. When the steam pressure is lowered, the steam becomes superheated. If the correct amount of bfw is sprayed into the stream, it can be resaturated, and at the lower pressure, the steam is at a lower temperature.

In a particular heat exchanger, condensing steam in the shell at 160°C is used to heat 2 kg/s of a process fluid from 50°C to 100°C. The condensing coefficient is 5000 W/m^{2}K, and the process-side coefficient is 200 W/m^{2}K. It is required that the process fluid flowrate be increased by 15%. What steam temperature and flowrate are needed to maintain the outlet process temperature at 100°C?

Chapter 22. Performance of Multiple Unit Operations

What You Will Learn

- How the analysis of the previous chapter can be applied to multiple unit operations

In Chapter 21, techniques for evaluating the performance of individual unit operations were introduced. The use of performance curves was illustrated. Performance curves describe the behavior of a unit over a wide range of inputs. The techniques developed in Chapter 20 were also used to obtain results for a single set of input conditions, which is one point on a performance curve.

In a chemical process, units do not operate in isolation. If the input to one unit is changed, its output changes. However, this output is usually the input to another unit. In certain cases, what is usually considered to be a single unit is actually multiple units operating together. A distillation column is an example of this situation, because the reboiler and condenser are part of the distillation unit. Any change in the column or in either of the heat exchangers will affect the performance of the other two. Therefore, it is necessary to understand the interrelationship between performance of multiple units and to gain experience in analyzing these types of problems.

Given the complexity of the performance of multiple units, performance curves will not be generated. The techniques developed in Chapters 19 through 21 will be used to solve for one point on a performance curve. As in Chapter 21, the case-study approach is used. Four examples of multiple units are illustrated in order to help you understand the approach to analyzing performance problems involving multiple units.

22.1. Analysis of a Reactor with Heat Transfer

Many industrially significant reactions are exothermic. Therefore, in a reactor, it is necessary to remove the heat generated by the heat of reaction. There are several ways to accomplish heat removal. For relatively low heats of reaction, staged adiabatic packed beds (packed with catalyst) with intercooling may be used. Here, no heat is removed in the reaction section of the equipment. Instead, the process fluid is allowed to heat up in the reactor and heat is removed in heat exchangers between short beds of catalyst (reactor sections). For larger exothermic heats of reaction, a shell-and-tube configuration, much like a heat exchanger, is often used. Here, the reaction usually occurs in the tubes, which are packed with catalyst. As the heat of reaction increases, tube diameter is decreased in order to increase the heat transfer area. For extremely large heats of reaction, fluidized beds with internal heat transfer surfaces are often used, due to the constant temperature of the fluid bed and the relative stability of such reactors because of the large thermal mass of well-mixed solid particles.

In all three of these cases, the performance of the reactor and the heat exchanger are coupled. It is not correct to analyze one without the other. In this section, an example of the performance of a shell-and-tube-type reactor (tube bundle containing catalyst immersed in a pool of boiling water) with heat removal is used to illustrate the interrelationship between reactor performance and heat transfer. In Chapter 23, other examples of reactor performance are presented.

A shell-and-tube reactor, as illustrated in Figure 22.1, is used for the following reaction to produce cumene from benzene and propylene.

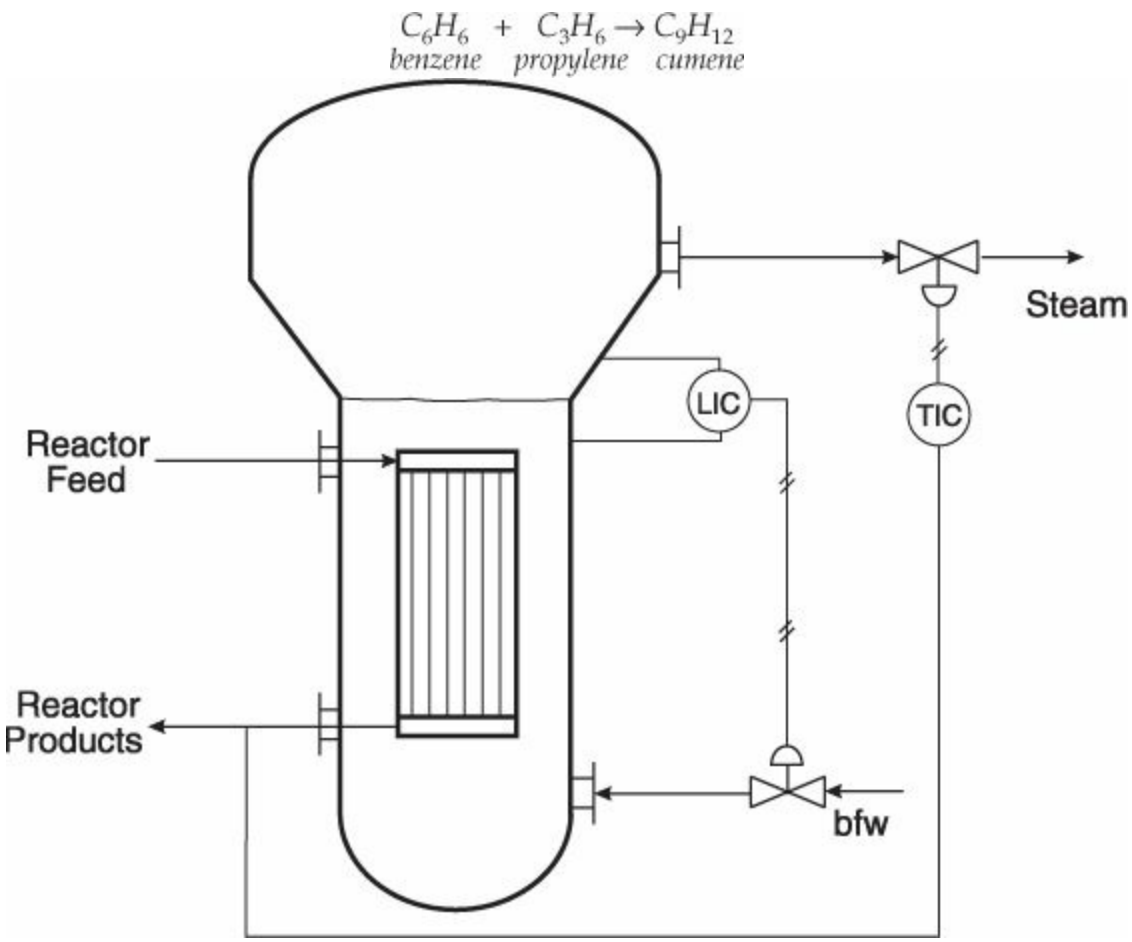


Figure 22.1. Shell-and-Tube-Type Packed-Bed Reactor

The reaction kinetics are as follows:

$$r = kc_b c_p \quad \text{mol/L s}$$

$$k = 3500 \exp(-13.28\ (\text{kcal/mol})/RT)$$

Normally, the reaction occurs at 350°C and 3000 kPa (the reaction is not really isothermal; see item 3 below). Heat evolved by the reaction is removed by producing high-pressure steam (4237 kPa, 254°C) from boiler feed water in the reactor shell. Propylene is the limiting reactant, with benzene present in excess. The feed propylene is a raw cut and contains 5 wt% propane impurity. Recently, the propane supplier has been having difficulty meeting specifications, and the propane impurity exceeds 5 wt%. The reduced feed concentration of propylene is causing a decrease in cumene production. In order to maintain the desired cumene production rate, it has been suggested that the reaction temperature be raised to compensate.

The following assumptions are made in order to simplify the problem:

1. There are no other impurities except for the propane.
2. The pressure drop in the reactor is negligible relative to the operating pressure.
3. The temperature profile in the reactor is flat; that is, the temperature is 350°C everywhere in the reactor. This is the most serious assumption, and it is clearly not correct. There will most likely be a hot spot near the reactor entrance. Figure 22.2 illustrates the temperature profiles for the reactor and for the steam. The dotted line is the anticipated temperature profile. By assuming a constant temperature, calculations are simplified, and the concept illustrated in this case study can still be understood.

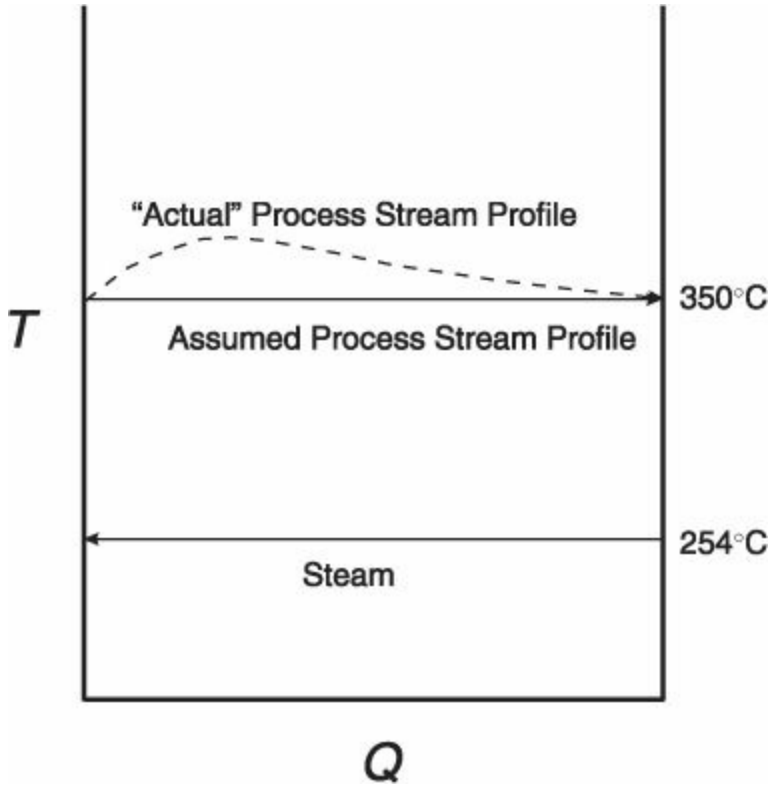


Figure 22.2. Temperature Profiles in Cumene Reactor

Before proceeding with a detailed analysis, it is instructive to understand why a temperature increase was suggested as compensation for decreased propylene feed concentration. If the total feed rate of impure propylene is consistently maintained, the feed rate of propylene decreases with increasing propane impurity. Because propylene is the limiting reactant, cumene production is related to propylene feed by the following relationship:

$$F_c = F_{po} X \qquad (22.1)$$

where

F_c = molar rate of cumene produced

F_{po} = molar rate of propylene feed

X = conversion of propylene

If the molar feed rate of propylene, F_{po}, is reduced, cumene production will decrease unless the conversion, X, is increased. In the reactor, the overall flow of material is constant, because propane replaces propylene; therefore, the space time remains constant. From the reaction expression, a reduced concentration of propylene results in a reduced reaction rate. Intuitively, a reduced reaction rate at constant space time results in reduced conversion. Therefore, from Equation (22.1), the cumene production rate is decreased because of both a decreased reactant feed rate and a decreased conversion.

One method to increase reaction rate is to increase the reactor temperature. The quantitative relationship between temperature increase and cumene production rate can be obtained by the methods learned in a typical reaction engineering class or by use of a process simulator. Example 22.1 illustrates this method.

Example 22.1.

Analyze the heat transfer consequences of increasing the reactor temperature by 10°C and 20°C,

increases that correspond to maintaining the desired cumene production rate at approximately 6% and 7% propane impurity, respectively.

The heat transfer performance equation must also be obeyed. Predicting trends shows that the temperature difference between the reaction side and steam side must remain constant:

$$\Delta T(¢) = \frac{Q(¢)}{U(¢)A(¢)} \qquad \text{(E22.1a)}$$

Because the cumene production rate is to remain constant, the heat load on the reactor remains constant. Because overall flows do not change, the heat transfer coefficient remains constant. Because the reactor is not modified, the heat transfer area remains constant. Therefore, ΔT must remain constant. Because the original ΔT was 96°C, the following table gives the temperatures that are required on the steam side. In order to produce higher-temperature steam, the boiler feed water pressure, and therefore steam pressure, must be increased on the shell side. This is because the temperature at which boiler feed water vaporizes to saturated steam increases with pressure.

Temperature Increase (°C)	Steam Temperature (°C)	Steam Pressure (kPa)
0	254	4237
10	264	5002
20	274	5853

For a 10°C increase in reactor temperature, the pressure on the shell side must increase by almost 20%, and for a 20°C increase in reactor temperature, the pressure on the shell side must increase by about 38%.

Without considering the heat transfer analysis, it would have been easy to suggest the temperature increases be implemented. However, they could not be accomplished without raising the shell-side temperature and pressure. Because the reactor is also a heat exchanger, the performance equation for a heat exchanger must be used in the analysis. Therefore, in order to increase the reactor temperature, the steam temperature, and consequently the steam pressure, must be increased. The unanswered question is whether the reactor can withstand the indicated pressure increases. It is unlikely that a vessel designed for a high pressure like 4237 kPa would be overdesigned to handle a 20% increase in pressure, and a design for 38% increase would be extremely uncommon.

It is instructive to continue this analysis and determine whether there are other ways to increase the conversion in the reactor to compensate for the reduced feed, and this is illustrated in Example 22.2.

Example 22.2.

Suggest another method for increasing the conversion in the reactor so that the cumene production rate remains constant with reduced propylene feed concentration.

The question to be answered is what can be adjusted, other than temperature, that will affect the reaction rate and/or the conversion. In the reaction rate expression, the primary temperature effect is in the Arrhenius expression. For gas-phase reactions, assuming ideal gas behavior, the concentrations $c_i = P_i/RT$. The increase in temperature discussed in Example 22.1 will actually reduce the concentrations; however, the exponential increase in the reaction rate constant is the primary effect. It is also observed that increasing the pressure increases the concentration, thereby increasing the

reaction rate. There is an additional effect. This can be seen from the equation of a plug flow reactor.

$$\frac{\tau}{c_{Ao}} = \int_0^X \frac{dX}{-r_A}$$

Because the mass flowrate $\dot{m} = \rho A v$, and increasing the pressure increases the density, at constant mass flowrate, the velocity drops. Therefore, the residence time, τ, in the reactor increases, which results in increased cumene conversion (upper limit of integral increases) and increased cumene production. Of course, pressure limitations of the equipment in the process or in the tube side of the reactor may limit the pressure increase possible.

In this case study, the most likely solution to the problem is some combination of temperature and pressure increase. If this is insufficient, it may be necessary to try to increase the feed rates of the reactants. However, consistent with the lesson of this case study, the performance of the pumping equipment may limit possible feed rate increases.

In summary, this case study introduces the concept that performance of any unit cannot be considered in isolation. For the reactor, it seems straightforward to do an analysis involving only reaction kinetics and conclude that a temperature increase is a solution to the problem of reduced feed. However, it is now clear that because the reactor is also a heat exchanger, both reactor and heat exchanger analyses must be done simultaneously in order to obtain a correct result. In order to get the correct numerical result, the correct temperature profile on the reaction side must be used. It is obtained by using a process simulator or by solving the differential equations for conversion and temperature simultaneously. The correct temperature profile, as illustrated in Figure 22.2, arises because of the reaction rate, $r \propto e^{-E/RT}$. Therefore, as the temperature increases, r increases by a large amount, generating even more heat, and the peak in the temperature profile may increase significantly, causing hot spots to develop. Hot spots can damage catalyst or promote undesired side reactions. Chapter 23 treats these issues in more detail.

22.2. Performance of a Distillation Column

A distillation column requires a reboiler to add the energy necessary to accomplish the separation. A condenser is also required to reject heat to the surroundings. The performance of a distillation column cannot be analyzed without consideration of the performance of both heat exchangers. This is illustrated in the following case study.

The distillation column illustrated in Figure 22.3 is used to separate benzene and toluene. It contains 35 sieve trays, with the feed on Tray 18. The relevant flows are given in Table 22.1. Your assignment is to recommend changes in the tower operation to handle a 50% reduction in feed. Overhead composition must be maintained at 0.996 mole fraction benzene. Cooling water is used in the condenser, entering at 30°C and exiting at 45°C. Medium-pressure steam (185°C, 1135 kPa) is used in the reboiler.

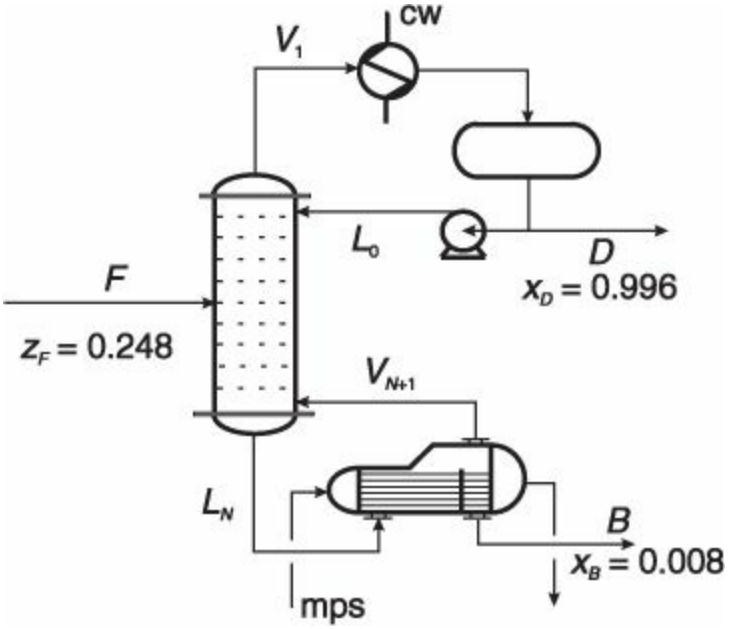


Figure 22.3. Distillation of Benzene from Toluene

Table 22.1. Operating Conditions for Process in Figure 22.3

Input/Output	Flow (kmol/h)	Mole Fraction Benzene	Temperature (°C)
Inputs			
Feed, F	141.3	0.248	90
Reflux, L_0	130.7	0.996	112.7
Boil-up, V_{N+1}	189.5	0.008	145.3
Outputs			
Distillate, D	34.3	0.996	112.7
Still bottoms, L_N	296.5	0.008	145.3
Bottoms product, B	107.0	0.008	145.3

The operating conditions of the tower before reduction in feed are in Table 22.1.

Among the several possible operating strategies for accomplishing the necessary scale-down are the following:

1. Scale down all flows by 50%. This is possible only if the original operation is not near the lower velocity limit that initiates weeping or reduced tray efficiency. If 50% reduction is possible without weeping, reduced tray efficiency, or poor heat-exchanger performance, this is an attractive option.
2. Operate at the same boil-up rate. This is necessary if weeping or reduced tray efficiency is a problem. The reflux ratio must be increased in order to maintain the reflux necessary to maintain the same liquid and vapor flows in the column. In this case, weeping, lower tray efficiency, or poor heat-exchanger performance caused by reduced internal flows is not a problem. The downside of this alternative is that a purer product will be produced and unnecessary utilities will be used.

In Example 22.3, the analysis will be done by assuming that it is possible to scale down all flows by 50% without weeping or reduced tray efficiency.

Example 22.3.

Estimate the pressure drop through the column. To what weir height does this correspond?

Interpolation of tabulated data [1] yields the following relationships for the vapor pressures in the temperature range of interest. Note that the temperatures predicted by these interpolated relationships differ slightly from those predicted by the simulator results in Table 22.1.

$$\ln P^* \text{ (kPa)} = 15.1492 - \frac{3706.84}{T(\text{K})} \quad \text{benzene}$$

$$\ln P^* \text{ (kPa)} = 15.3877 - \frac{4131.14}{T(\text{K})} \quad \text{toluene}$$

It is assumed that the bottom is pure toluene and the distillate is pure benzene. This is a good assumption for estimating top and bottom pressures given the mole fractions specified for the distillate and bottoms. Therefore, at the bottom temperature of 141.7°C, the vapor pressure of toluene, and hence the pressure at the bottom of the column, is 227.2 kPa. At the top temperature of 104.2°C, the vapor pressure of benzene, and hence the pressure at the top of the column, is 204.8 kPa.

Because there are 35 trays, the pressure drop per tray is

$$\Delta P = (227.2 - 204.8)/35 = 0.64 \text{ kPa/tray}$$

If it assumed that the weir height is the major contribution to the pressure drop on a tray, then

$$\Delta P = \rho g h$$

where h is the weir height. Assuming an average density of 800 kg/m^3, then

$$h = (640 \text{ Pa})/[(800 \text{ kg/m}^3)(9.8 \text{ m/s})] = 0.08 \text{ m} \approx 3 \text{ in}$$

This is a typical weir height and is consistent with the assumption that the weir height is dominant.

The pressure drop is assumed to remain constant after the scale-down because the weir height is not changed. In practice, there is an additional contribution to the pressure drop due to gas flow through the tray orifices. This would change if column flows changed, but the pressure drop through the orifices is small and should be a minor effect. Examples 22.4 and 22.5 illustrate how the performance of the reboiler and condenser affect the performance of the distillation column.

Example 22.4.

Analyze the reboiler to determine how its performance is altered at 50% scale-down.

Figure E22.4 shows the T-Q diagram for this situation. Because the amounts of heat transferred for the base and new cases are different, the Q values must be normalized by the total heat transferred in order for these profiles to be plotted on the same scale. The solid lines are the original case (subscript 1). For the new, scaled-down case (subscript 2), a ratio of the energy balance on the reboiled stream for the two cases yields

$$\frac{Q_2}{Q_1} = \frac{\dot{m}_2 \lambda}{\dot{m}_1 \lambda} \qquad \text{(E22.4a)}$$

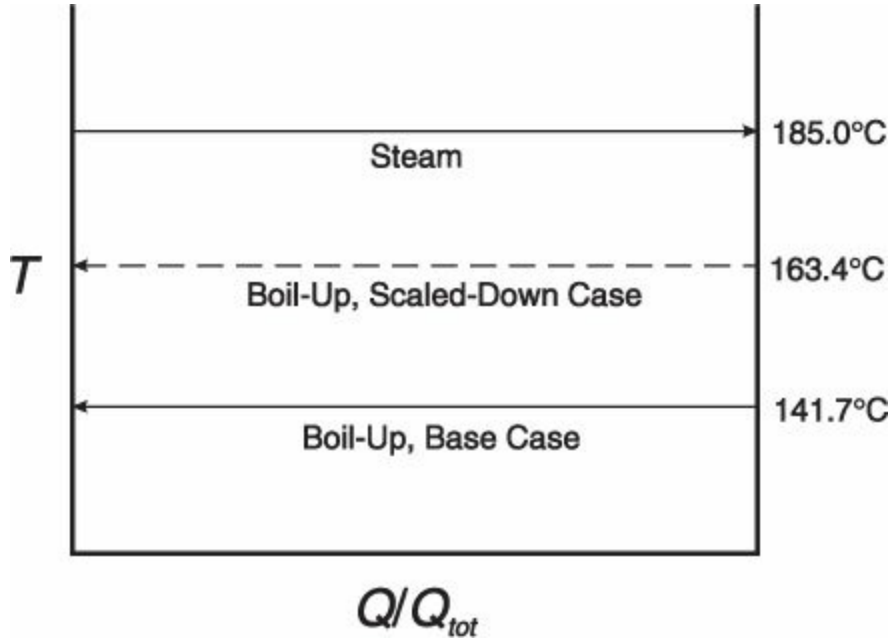


Figure E22.4. Temperature Profiles in Reboiler for Example 22.4

If it is assumed that the latent heat is unchanged for small temperature changes, then $Q_2/Q_1 = 0.5$, because at 50% scale-down, the ratio of the mass flowrates in the reboiler is 0.5. The ratio of the heat transfer equations yields

$$\frac{Q_2}{Q_1} = 0.5 = \frac{U_2 A \Delta T_2}{U_1 A \Delta T_1} \approx \frac{\Delta T_2}{43.3} \qquad \text{(E22.4b)}$$

In Equation (E22.4b), it is assumed that the overall heat transfer coefficient is constant. It is assumed here that $U \neq f(T)$. This assumption should be checked, because for boiling heat transfer coefficients with large temperature differences, the boiling heat transfer coefficient may be a strong function of temperature difference.

From Equation (E22.4b), it is seen that $\Delta T_2 = 21.7°C$. Therefore, for the reboiler to operate at 50% scale-down, with the steam side maintained constant, the boil-up temperature must be 163.4°C. This is shown as the dotted line in Figure E22.4.

From the vapor pressure expression for toluene, the pressure at the bottom of the column is now 372.5 kPa. It would have to be determined whether the existing column could withstand this greatly increased pressure.

Example 22.4 shows that the reboiler operation requires that the pressure of the boil-up stream be increased. This is not the only possible alternative. All that is necessary is that the temperature difference be 21.7°C. This could be accomplished by reducing the temperature of the steam to 163.4°C. In most chemical plants, steam is available at discrete pressures, and the steam used here is typical of medium-pressure steam. Low-pressure steam would be at too low a temperature to work in the scaled-down column. However, the pressure and temperature of medium-pressure steam could be reduced if there were a throttling valve in the steam feed line to reduce the steam pressure. The resulting steam would be superheated, so desuperheating would also be necessary. This could be accomplished by spraying water into the superheated steam. A change in a utility stream is almost always preferred to a change in a process stream. The condenser is now analyzed in Example 22.5.

Example 22.5.

Using the results of Example 22.4, analyze the condenser for the scaled-down case.

Under the assumption that the pressure drop for the column remains at 22.4 kPa, the pressure in the condenser is now 350.0 kPa. From the vapor pressure expression for benzene, the new temperature in the condenser is 126.0°C. The remainder of the analysis is similar to Example 21.1. The *T*-*Q* diagram is illustrated in Figure E22.5. Because an organic is condensing, it is assumed that the resistance on the cooling water side is approximately equal to the resistance on the condensing side. Therefore,

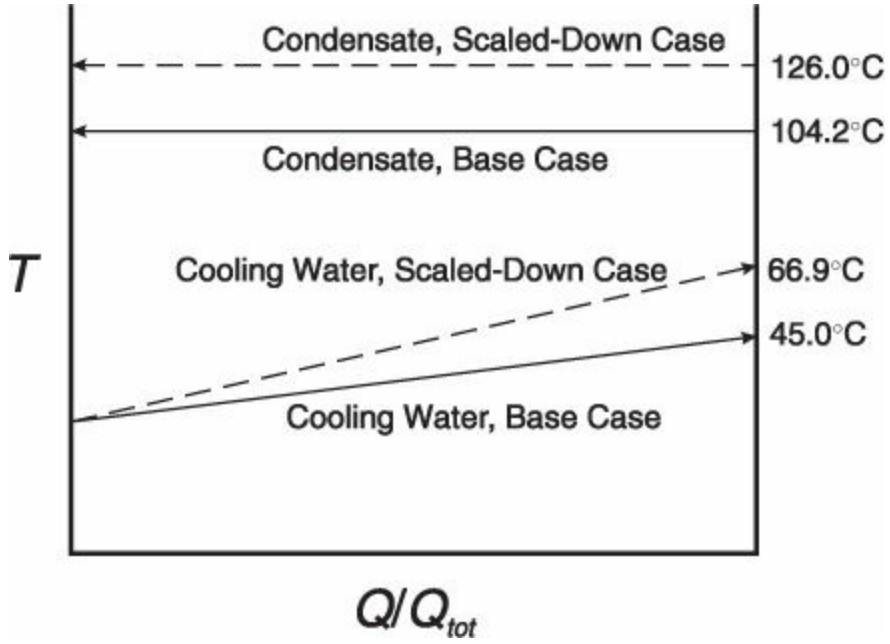


Figure E22.5. Temperature Profiles in Condenser for Example 22.5

$$\frac{U_2}{U_1} = \frac{\dfrac{1}{h_{o1}} + \dfrac{1}{h_{i1}}}{\dfrac{1}{h_{o2}} + \dfrac{1}{h_{i2}}} = \frac{\dfrac{2}{h_{o1}}}{\dfrac{1}{h_{o1}} + \dfrac{1}{h_{o1}M^{0.8}}} = \frac{2}{1 + \dfrac{1}{M^{0.8}}} \qquad \text{(E22.5a)}$$

where $M = \dot{m}_2/\dot{m}_1$.

The ratio of the base cases for the energy balance on the condensing stream is

$$\frac{Q_2}{Q_1} = \frac{\dot{m}_2\lambda}{\dot{m}_1\lambda} \qquad \text{(E22.5b)}$$

Because the ratio of the mass flowrates is 0.5, and assuming that the latent heat is unchanged with temperature in the range of interest, $Q_2/Q_1 = 0.5$.

The ratio of the base cases for the energy balance and the heat-exchanger performance equation are, respectively,

$$0.5 = M\frac{T - 30}{15} \qquad \text{(E22.5c)}$$

$$0.5 = \frac{2(T - 30)}{(66.42)\left(1 + \dfrac{1}{M^{0.8}}\right)\ln\left(\dfrac{96}{126 - T}\right)} \qquad \text{(E22.5d)}$$

Solution of Equations (E22.5c) and (E22.5d) yields

$$M = 0.203$$

$$T = 66.9°C$$

Therefore, the cooling water rate must be reduced to 20% of the original rate, and the outlet water

temperature is increased by about 22°C. This would cause increased fouling problems on the cooling water side. Therefore, it may be better to use a higher reflux ratio rather than reduce the flows in the column.

Observation indicates that in order to operate the distillation column at 50% scale-down with process flows reduced by 50%, a higher pressure is required and the cooling water will be returned at a significantly higher temperature than before scale-down. The operating pressure of the column is determined by the performance of the reboiler and condenser.

Examples 22.4 and 22.5 reveal a process bottleneck at the reboiler that must be resolved in order to accomplish the scale-down. In the process of changing operating conditions (capacity) in a plant, a point will be reached where the changes cannot be increased or reduced any further. This is called a **bottleneck**. A bottleneck usually results when a piece of equipment (usually a single piece of equipment) cannot handle additional change. In this problem, one bottleneck is the high cooling water return temperature, which would almost certainly cause excessive fouling in a short period of time. Another potential bottleneck is tray weeping due to the greatly reduced vapor velocity. In addition to the solution presented here, there are a variety of other possible adjustments, or debottlenecking strategies, which follow with a short explanation for each. Another debottlenecking problem is presented in Chapter 24.

1. **Replace the Heat Exchangers:** Equation (E22.4b) shows that a new heat exchanger with half of the original area allows operation at the original temperature and pressure. The heat transfer area of the existing exchanger could be reduced by plugging some of the tubes, but this modification would require a process shutdown. This involves both equipment downtime and capital expense for a new exchanger. Your intuitive sense should question the need to get a new heat exchanger to process less material. You can be assured that your supervisor would question such a recommendation.
2. **Keep the Boil-Up Rate Constant:** This would maintain the same vapor velocity in the tower. If the operation occurs near the lower velocity limit that initiates weeping or lower tray efficiency, this is an attractive option. The constant boil-up increases the tower separation. This is an attractive option that results in much smaller temperature and pressure changes.
3. **Introduce Feed on a Different Plate:** This must be combined with Option 4. The plate should be selected to decrease the separation and increase the bottoms concentration of the lower boiling fraction. This lowers the process temperature, increases the ΔT for heat transfer and the reboiler duty. This may or may not be simple to accomplish depending on whether the tower is piped to have alternate feed plates. As in Option 2, the reflux and coolant inputs will change.
4. **Recycle Bottoms Stream and Mix with Feed:** This must be combined with Option 3. By lowering the concentration of the feed, the concentration of the low boiler in the bottoms can be increased, the temperature lowered, and the reboiler duty increased. This represents a modification of process configuration and introduces a new (recycle) input stream into the process.

The adjustments outlined were based on the following:

1. Replace the exchanger (Option 1).
2. Modify utility stream (discussed after Example 22.4).
3. Modify process stream (Option 2).

4. Modify equipment (Option 3 or Option 1, if plugging of tubes to reduce area is chosen).
5. Modify process configuration (Option 4).
6. Modify operating conditions T and P (as in Examples 22.4 and 22.5).

It has been shown that there are a number of paths that remove the bottleneck that exists at the reboiler. Adjustments 1 and 2 required no changes in process inputs. All others required modifications of several input streams to maintain the output quality.

It should be noted that, at 50% scale-down, it is possible that weeping or low tray efficiency may be observed (see Section 21.3.2 and Figure 21.19). This must be considered before recommending such a scale-down. Furthermore, reduction of the cooling water flowrate in the condenser, combined with increased cooling water temperatures, could cause fouling problems, as pointed out in Example 22.5. Care must taken to understand the consequences of process modifications.

During plant operations, when seeking the best operating conditions, incremental changes can be made and the effects observed. This is termed “evolutionary operation” [2]. Amoco has reported a significant increase in its annual income from evolutionary operation [3]. In the design case, changes recommended are necessarily conservative to ensure that equipment purchased and installed is adequate to meet the conditions when the plant is operated.

22.3. Performance of a Heating Loop

In Section 22.2, it was noted how the performance of a distillation column was affected by the performance of the reboiler and condenser. It was possible to analyze the reboiler, column, and condenser sequentially in order to solve the scale-down problem. In this section, the performance of a reactor in which the large, exothermic heat of reaction is removed by a heat transfer fluid is examined. It will be seen that the bottleneck for scale-up of this process is the performance of the heat removal loop. The analysis of this problem is more complex than for the distillation column, because all units involved must be analyzed simultaneously in order to solve the problem.

The problem to be analyzed is illustrated in Figure 22.4. It is a part of the allyl chloride problem discussed in more detail in Appendix C, on the accompanying CD.

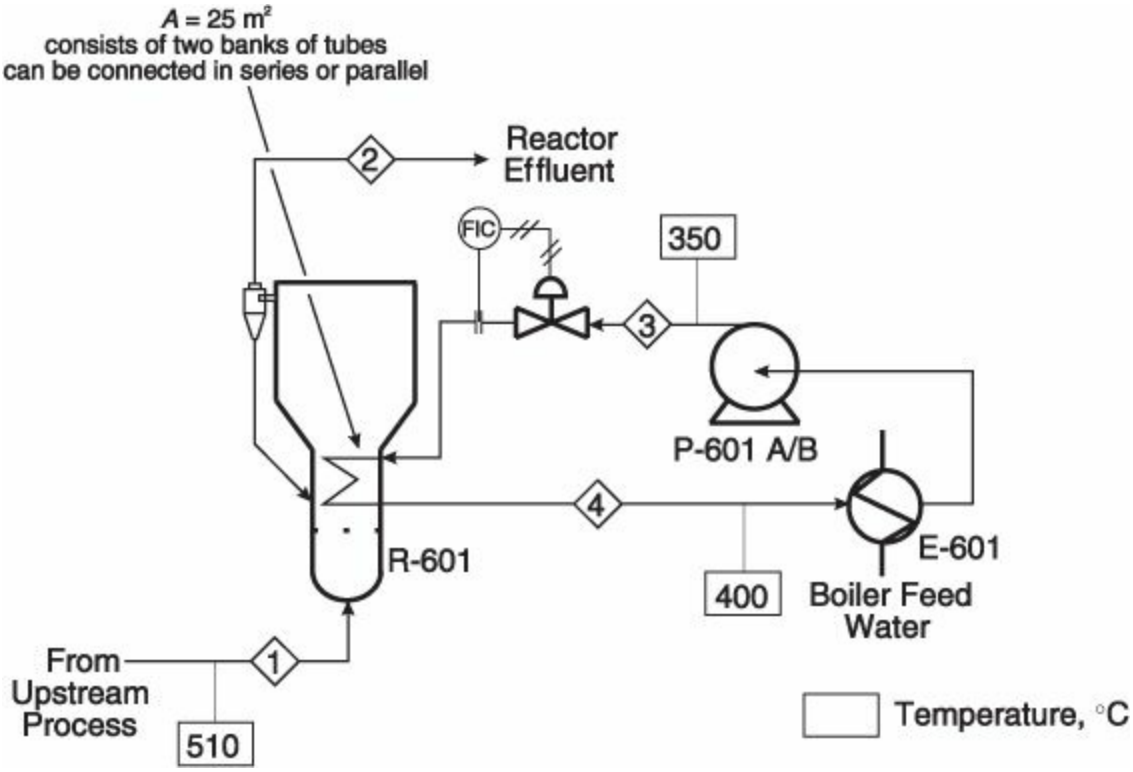


Figure 22.4. Dowtherm A Loop for Allyl Chloride Reactor

Due to an emergency, an unscheduled shutown at an another allyl chloride production plant operated by your company, it is necessary to increase production temporarily at your plant. Your job is to determine the maximum scale-up possible for the allyl chloride production reactor. The reactor is a fluidized bed, with a cyclone for solids recovery, operating isothermally at 510°C. The reactor is operating at two times the minimum fluidization velocity. Based on the cyclone design and the solids handling system, it is known that an increase of at least 100% of process gas flow can be accommodated. The reaction proceeds to completion as long as the reactor temperature remains at 510°C. A temperature increase destroys the catalyst, and a temperature decrease results in incomplete reaction and undesired side products. The reaction is exothermic and heat is removed by Dowtherm A circulating in the loop. The maximum operating temperature for Dowtherm A is 400°C, and its minimum operating pressure at this temperature is 138 psig. There are two heat-exchanger units in the reactor, and they are currently operating in series. The heat transfer resistance on the reactor side is four times that on the Dowtherm A side. The inside of the reactor is always at 510°C due to the well-mixed nature of the fluidized solids. There is a spare pump. High-pressure steam is made from boiler feed water in the heat exchanger. The boiler feed water is available at 90°C and has been pumped to 600 psig by a pump that is not shown. The pool of liquid being vaporized can be assumed to be at the vaporization temperature, 254°C. All resistance in the heat exchanger is assumed to be on the Dowtherm A side. At normal operating conditions, Dowtherm A circulates at 85 gal/min in the loop. The temperatures of each stream are shown on Figure 22.4. The pump curve for the pump in the loop is shown on Figure 22.5.

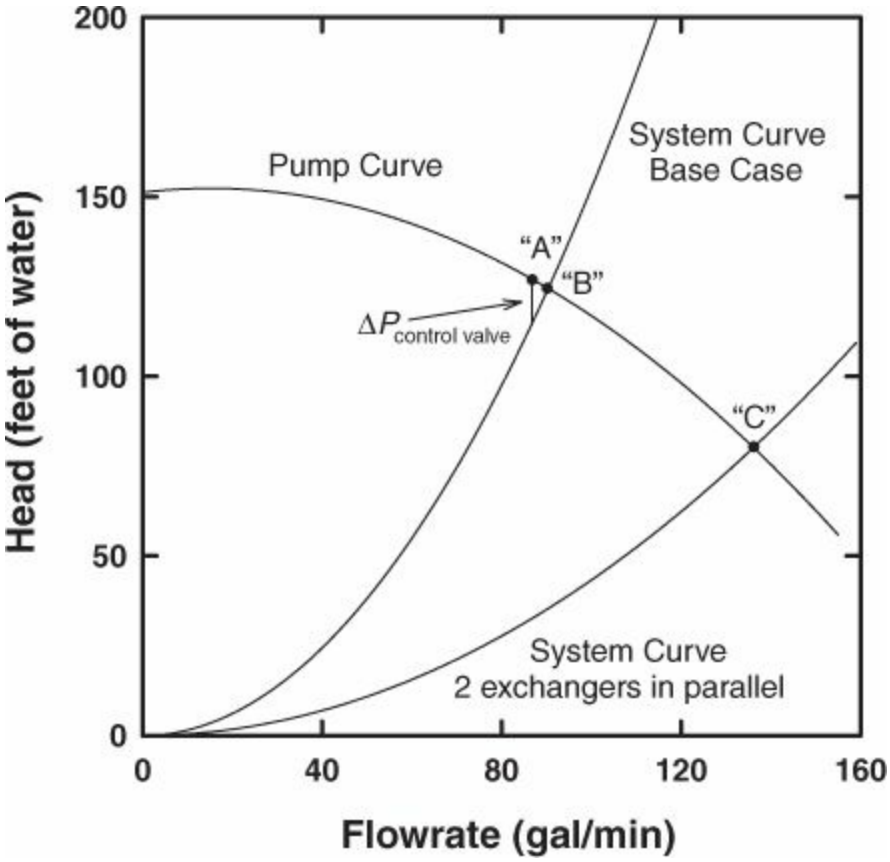


Figure 22.5. Performance of Dowtherm A Loop

An energy balance on the process fluid in the reactor yields

$$Q_R = \dot{n}_{Cl}\Delta H_{rxn} \qquad (22.2)$$

where $\dot{n}_{Cl}$ is the molar flowrate of chlorine (the limiting reactant), and the subscript *R* refers to the reactor. The heat of reaction term in Equation (22.2) is on a unit mole basis. Because the heat of reaction is constant during scale-up, Equation (22.2) shows that the amount of heat removed increases proportionally with the amount of scale-up. From this energy balance, there is nothing to suggest that the reactor cannot be scaled up by a factor of 2, the maximum allowed by the reactor. However, the question that must be answered is whether twice the heat can be removed from the reactor by the heat-exchange loop. An energy balance on the Dowtherm A in the reactor yields

$$Q_R = \dot{m}_D C_{pD}(T_4 - T_3) \qquad (22.3)$$

where the subscript *D* refers to the Dowtherm A. From Equation (22.3), it is observed that the heat removal rate is proportional to both the mass flowrate and the temperature increase of the Dowtherm A. Therefore, the most obvious method is to increase the flowrate of Dowtherm A, so it is necessary to determine the maximum flowrate possible for Dowtherm A. Example 22.6 illustrates this calculation.

Example 22.6.

For the pump curve provided in Figure 22.5, determine the maximum possible flowrate for Dowtherm A in the loop. The pump operates at only one speed, described by the curve given in the figure. The pressure drops between streams are shown in Figure E22.6.

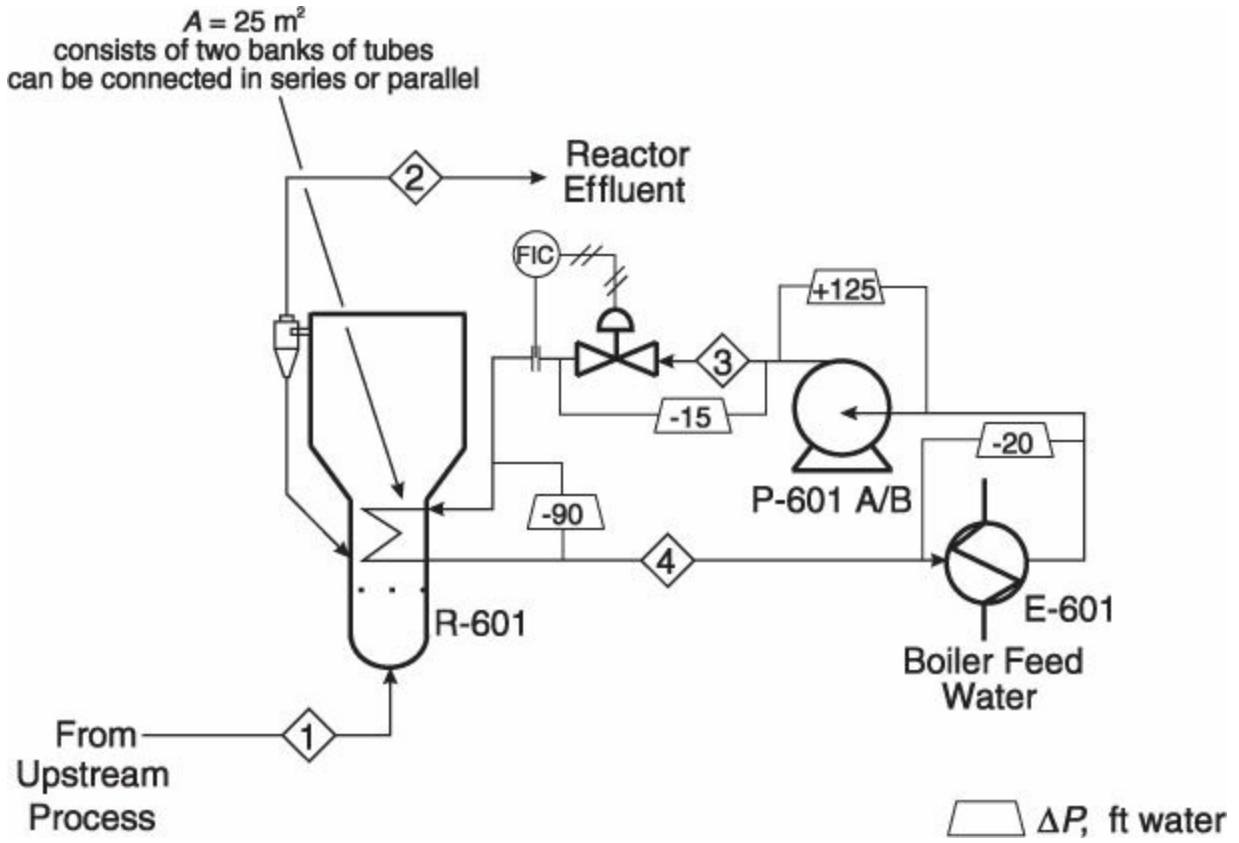


Figure E22.6. Pressure Drops in Dowtherm A Loop for Allyl Chloride Reactor

The pump operates only at conditions shown on the pump curve. The pressure drop in the system and regulating valves must equal the pressure delivered by the pump. The base-case solution gives one point on this line (point "a"). Of this total pressure drop, 15 feet of water is from the control valve, which can be adjusted independently. The remaining pressure drop, 110 feet of water (125 – 15 feet of water), is the **system pressure drop** and is dependent on the flowrate through the system. The system pressure drop can be obtained from the equation for frictional pressure losses.

$$\Delta P = \frac{2\rho f L_{eq} v^2}{D} \qquad \text{(E22.6a)}$$

Taking the ratio of Equation (22.6a) for the scaled-up case (subscript 2) to the base case (subscript 1) for constant L, D, and the assumed constant friction factor (high Reynolds number, fully developed turbulent flow) yields

$$\frac{\Delta P_2}{110} = \frac{v_2^2}{v_1^2} = \frac{\dot{m}_2^2}{\dot{m}_1^2} \qquad \text{(E22.6b)}$$

where M is the scale-up factor, the ratio of the scaled-up Dowtherm A flowrate to that for the base case. Equation (22.6b) is plotted with the pump curve on Figure 22.5. The maximum flowrate occurs when the valve is wide open. When the valve is wide open, there is no (or very little) pressure drop across the valve. This is shown as point "b" and occurs at 89 gal/min.

Example 22.6 shows that the maximum scale-up is limited to about 5% by the Dowtherm A flowrate in the loop. A bottleneck has been identified. In order for additional scale-up to be possible, a method for increasing the maximum Dowtherm A flowrate must be found. Several options are possible:

1. Run only one pump, but operate the reactor heat exchangers in parallel.
2. Run both pumps (the operating pump and the spare) in parallel, with the reactor heat exchangers in series.

3. Run both pumps in series, with the reactor heat exchangers in series.
4. Run both pumps (series or parallel), and operate the reactor heat exchangers in parallel.

Option 1 is illustrated in Example 22.7. The remaining options are the subject of a problem at the end of the chapter.

Example 22.7.

Determine the maximum possible Dowtherm A flowrate for one pump operating with the two reactor heat exchangers operating in parallel.

From Equation (E22.6a), it is seen that

$$\Delta P \propto L_{eq} v^2 \qquad \text{(E22.7a)}$$

The equivalent length in the heat exchanger is reduced by half for operation in parallel. Half the flowrate goes through each heat exchanger, which means that the Dowtherm A has half the original velocity. Therefore, the pressure drop through the reactor heat exchangers drops by a factor of 8 and becomes 11.25 feet of water. The base-case pressure drop is now 31.25 feet of water. Therefore, a new system curve is obtained. Its equation is

$$\Delta P = 31.25\, M^2 \qquad \text{(E22.7b)}$$

The new system curve along with the pump curve is plotted on Figure 22.5. Point "c" represents the maximum possible flowrate of Dowtherm A, 135 gal/min. This represents a 58.8% scale-up.

Therefore, if only the original pump is used with the reactor heat exchangers in parallel, the Dowtherm A circulation rate can be increased by almost 50%. For Options 2 through 4, additional increases are possible. It should be noted that liquid velocities exceeding 10 ft/sec are not recommended due to potential erosion problems. Therefore, if the original case was designed for the maximum recommended velocity, operation at a 50% higher velocity for an extended period of time is not a good idea. Proceeding with this problem, the assumption is that the original design permits 50% scale-up without exceeding the maximum recommended velocity.

Because the flowrate of the Dowtherm A can be scaled up by 50% does not mean that the heat removal rate can be scaled up by the same factor. Analysis of the heat transfer in both heat exchangers is required. For the reactor, the energy balances were given by Equations (22.2) and (22.3), for the process side and the Dowtherm A side, respectively. The performance equation for the reactor heat exchanger is

$$Q_R = U_R A_R \Delta T_{lm} \qquad (22.4)$$

For the heat exchanger producing steam, there are two additional equations. One is the energy balance on the boiler feed water to steam side.

$$Q_h = \dot{m}_s (C_{p,bfw} \Delta T + \lambda) \qquad (22.5)$$

where $\dot{m}_S$ is the mass flowrate of steam, ΔT is the temperature difference between the boiler feed water inlet and the vaporization temperature, and λ is the latent heat of vaporization of the steam. The second equation is the performance equation for the heat exchanger.

$$Q_h = U_h A_h \Delta T_{lm} \qquad (22.6)$$

The energy balance on the Dowtherm A side is identical (with the temperature difference reversed) to Equation (22.3). It is assumed that all heat removed from the reactor is transferred to make steam (Q_R

$= Q_h$).

Therefore, there are five independent equations that describe the performance of the loop. The unknowns are T_3, T_4, $Q_R = Q_h$, $\dot{m}_p$, $\dot{m}_D$, and $\dot{m}_s$. For a given value of $\dot{m}_D$, the mass flowrate of Dowtherm A, a unique solution exists. The method for obtaining this solution is illustrated in Example 22.8.

Example 22.8.

From a heat transfer analysis, determine the maximum scale-up possible for the allyl chloride reactor for the original case and for the case of one pump with the reactor heat exchangers operating in parallel.

Ratios of the scaled-up case (subscript 2) to the base case (subscript 1) will be used. Q_2/Q_1 is the ratio of the heat transfer rates, M is the ratio of the mass flowrates of Dowtherm A, and M_s is the ratio of the mass flowrates of steam. Only three of the five equations are coupled. Base-case ratios of Equations (22.3), (22.4), and (22.6) must be solved for T_3, T_4, and Q_2/Q_1. Then M_s and M are determined from Equations (22.5) and (22.2), respectively. The value of Q_2/Q_1 defines the level of scale-up possible.

The base-case ratios for Equations (22.3), (22.4), and (22.6) are

$$\frac{Q_2}{Q_1} = \frac{M(T_4 - T_3)}{50} \qquad \text{(E22.8a)}$$

$$\frac{Q_2}{Q_1} = \frac{5(T_4 - T_3)}{133.44\left(4 + \frac{1}{M^{0.8}}\right) \ln\left(\frac{510 - T_3}{510 - T_4}\right)} \qquad \text{(E22.8b)}$$

$$\frac{Q_2}{Q_1} = \frac{M^{0.8}(T_4 - T_3)}{119.26 \ln\left(\frac{T_4 - 254}{T_3 - 254}\right)} \qquad \text{(E22.8c)}$$

For the case of maximum scale-up with the original heat-exchanger configuration, $M = 89/85 = 1.05$. The solutions are

$$T_3 = 348.7°\text{C}$$

$$T_4 = 397.4°\text{C}$$

$$Q_2/Q_1 = 1.02$$

From Equation (22.2), because $Q_2/Q_1 = 1.02$, and because the heat of reaction is constant, the process flowrate increases by 2%. So only 2% scale-up is possible.

For one pump with the reactor heat exchangers in parallel, the mass flowrate in each reactor heat exchanger is half of the total flow. Therefore, Equation (E22.8b) becomes

$$\frac{Q_2}{Q_1} = \frac{5(T_4 - T_3)}{133.44\left(4 + \left(\frac{2}{M}\right)^{0.8}\right) \ln\left(\frac{510 - T_3}{510 - T_4}\right)} \qquad \text{(E22.8d)}$$

For $M = 1.588$, solution of Equations (E22.8a), (E22.8c), and (E22.8d) yields

$$T_3 = 331.7°\text{C}$$

$$T_4 = 367.8°\text{C}$$

$$Q_2/Q_1 = 1.15$$

Therefore, 15% scale-up is possible.

Performance of the heat-exchange loop is illustrated on the *T*-*Q* diagram shown in Figure 22.6. The lines for the reactor and the steam-generating heat exchanger are unchanged. The line for the Dowtherm A changes slope as the mass flowrate, the reactor heat-exchanger configuration, or the number and configuration of pumps change.

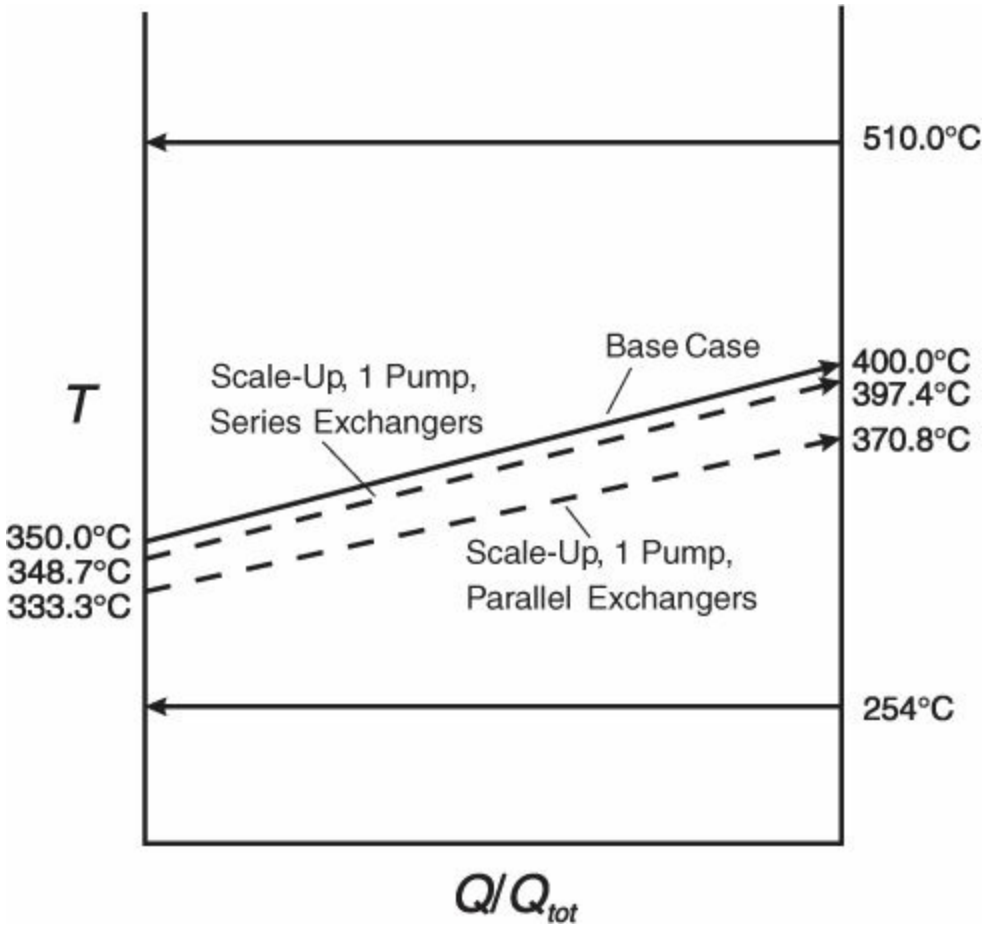


Figure 22.6. Temperature Profiles for Exchangers in Dowtherm A Loop

This complex problem illustrates an important feature of chemical processes. Often the bottleneck to solving a problem is elsewhere in the process. In this problem, the bottleneck to reactor scale-up is not in the reactor itself, but in the heat removal loop. Nevertheless, several alternatives are available to increase the Dowtherm A flowrate and scale up the process.

22.4. Performance of the Feed Section to a Process

A very common feature of chemical processes is the mixing of reactant feeds prior to entering a reactor. When two streams mix, they are at the same pressure. The consequences of this are illustrated by the following scenario.

Phthalic anhydride can be produced by reacting naphthalene and oxygen. The feed section to a phthalic anhydride process is shown in Figure 22.7. The mixed feed enters a fluidized bed reactor operating at five times the minimum fluidization velocity. A stream table is given in Table 22.2. It is assumed that all frictional pressure losses are associated with equipment and that frictional losses in the piping are negligible. It is temporarily necessary to scale down production by 50%. Your job is to determine how to scale down the process and to determine the new flows and pressures.

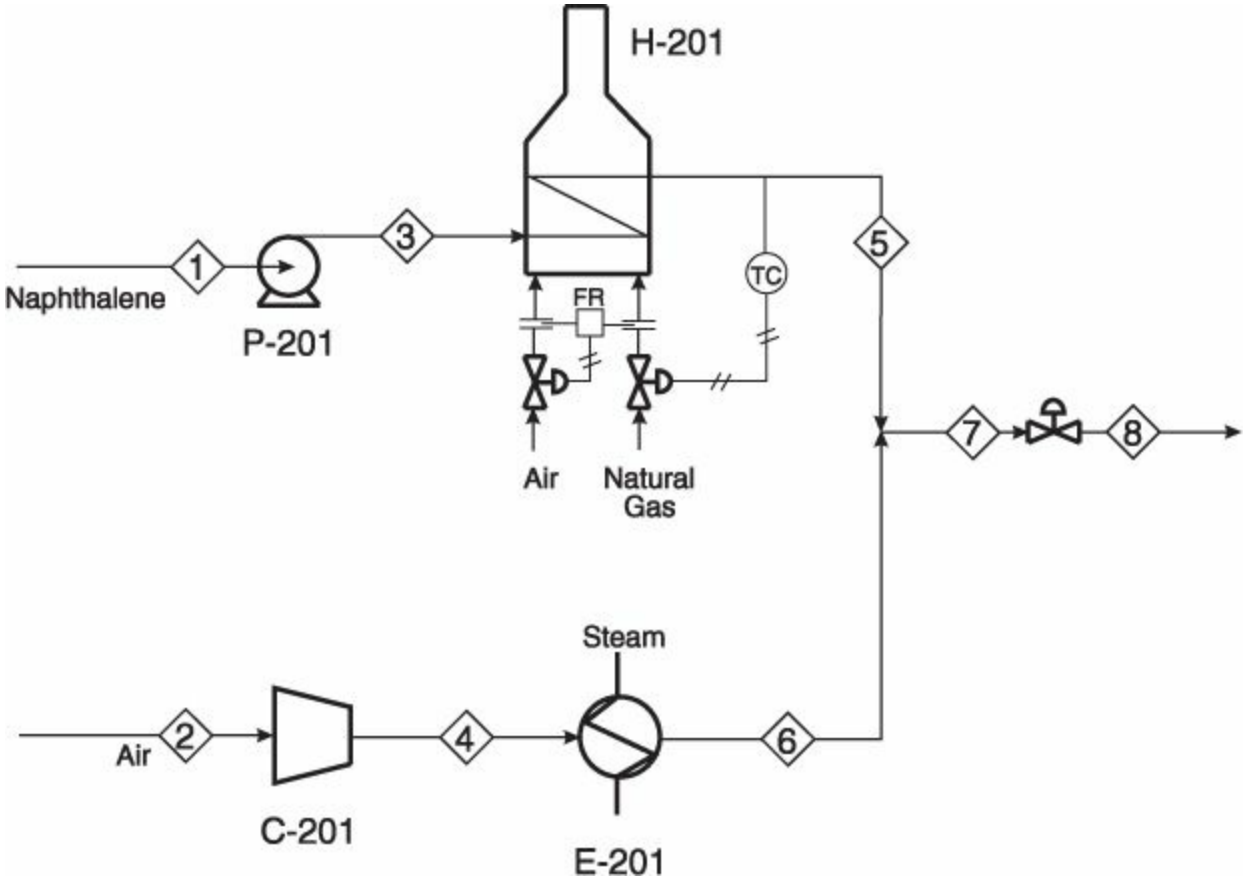


Figure 22.7. Feed Section to Phthalic Anhydride Process

Table 22.2. Partial Stream Table for Feed Section in Figure 22.7

	Stream							
	1	2	3	4	5	6	7	8
P (kPa)	80.00	101.33	343.00	268.00	243.00	243.00	243.00	200.00
Phase	L	V	L	V	V	V	V	V
Naphthalene (Mg/h)	12.82	—	12.82	—	12.82	—	12.82	12.82
Air (Mg/h)	—	151.47	—	151.47	—	151.47	151.47	151.47

It is necessary to have pump and compressor curves in order to do the required calculations. In this example, equations for the pump curves are used. These equations can be obtained by fitting a polynomial to the curves provided by pump manufacturers. As discussed in Chapter 21, pump curves are usually expressed as pressure head versus volumetric flowrate. This is so that they can be used for a liquid of any density. In this section, pressure head and volumetric flowrate have been converted to absolute pressure and mass flowrate using the density of the fluids involved. Pump P-201 operates at only one speed, and an equation for the pump curve is

$$\Delta P(\text{kPa}) = 500 + 4.663\dot{m} - 1.805\dot{m}^2 \quad \dot{m} \leq 16.00 \text{ Mg/h} \tag{22.7}$$

Compressor C-201 operates at only one speed, and the equation for the compressor curve is

$$\frac{P_{out}}{P_{in}} = 5.201 + 2.662 \times 10^{-3}\,\dot{m} - 1.358 \times 10^{-4}\,\dot{m}^2 + 4.506 \times 10^{-8}\dot{m}^3 \quad \dot{m} \leq 200 \text{ Mg/h} \tag{22.8}$$

From Figure 22.7, it is seen that there is only one valve in the feed section, after the mixing point. Therefore, the only way to reduce the production of phthalic anhydride is to close the valve to the point at which the naphthalene feed is reduced by 50%. Example 22.9 illustrates the consequences of reducing the naphthalene feed rate by 50%.

Example 22.9.

For a reduction in naphthalene feed by 50%, determine the pressures and flows of all streams after the scale-down.

Because it is known that the flowrate of naphthalene has been reduced by 50%, the new outlet pressure from P-201 can be calculated from Equation (22.7). The feed pressure remains at 80 kPa. At a naphthalene flow of 6.41 Mg/h, Equation (22.7) gives a pressure increase of 455.73 kPa, so P_3 = 535.73 kPa. Because the flowrate has decreased by a factor of 2, the pressure drop in the fired heater decreases by a factor of 4 (see Equation [E22.7a]). Therefore, P_5 = 510.73 kPa. Therefore, the pressure of Stream 6 must be 510.73 kPa. The flowrate of air can now be calculated from the compressor curve equation.

There are two unknowns in the compressor curve equation: the compressor outlet pressure and the mass flowrate. Therefore, a second equation is needed. The second equation is obtained from a base-case ratio for the pressure drop across the heat exchanger. The two equations are

$$\frac{P_4}{101.33} = 5.201 + 2.662 \times 10^{-3}\dot{m}_{2,new}^2 - 1.358 \times 10^{-4}\dot{m}_{2,new}^2 + 4.506 \times 10^{-8}\dot{m}_{2,new}^3 \qquad \text{(E22.8a)}$$

$$P_4 - 510.73 = 25\left(\frac{\dot{m}_{2,new}}{151.47}\right)^2 \qquad \text{(E22.8b)}$$

The solution is

$$P_4 = 512.84 \text{ kPa}$$

$$\dot{m}_2 = 43.80 \text{ Mg/h}$$

The stream table for the scaled-down case is given in Table 22.3. Although it is not precisely true, for lack of additional information, it has been assumed that the pressure of Stream 8 remains constant.

Table 22.3. Partial Stream Table for Scaled-Down Feed Section in Figure 22.7

	Stream							
	1	2	3	4	5	6	7	8
P (kPa)	80.00	101.33	535.73	512.84	510.73	510.73	510.73	200.00
Phase	L	V	L	V	V	V	V	V
Naphthalene (Mg/h)	6.41	—	6.41	—	6.41	—	6.41	6.41
Air (Mg/h)	—	43.80	—	43.80	—	43.80	43.80	43.80

It is observed that the flowrate of air is reduced by far more than 50% in the scaled-down case. This is because of the combination of the compressor curve and the new pressure of Streams 5 and 6 after the naphthalene flowrate is scaled down by 50%. The total flowrate of Stream 8 is now 50.21 Mg/h, which is 30.6% of the original flowrate to the reactor. Given that the reactor was operating at five

times minimum fluidization, the reactor is now in danger of not being fluidized adequately. Because the phthalic anhydride reaction is very exothermic, a loss of fluidization could result in poor heat transfer, which might result in a runaway reaction. The conclusion is that it is not recommended to operate at these scaled-down conditions.

The question is how the air flowrate can be scaled down by 50% to maintain the same ratio of naphthalene to air as in the original case. The answer is in valve placement. Because of the requirement that the pressures at the mixing point be equal, with only one valve after the mixing point, there is only one possible flowrate of air corresponding to a 50% reduction in naphthalene flowrate. Effectively, there is no control of the air flowrate. A chemical process would not be designed as in Figure 22.7. The most common design is illustrated in Figure 22.8. With valves in both feed streams, the flowrates of each stream can be controlled independently. Design of control systems was discussed in more detail in Chapter 18.

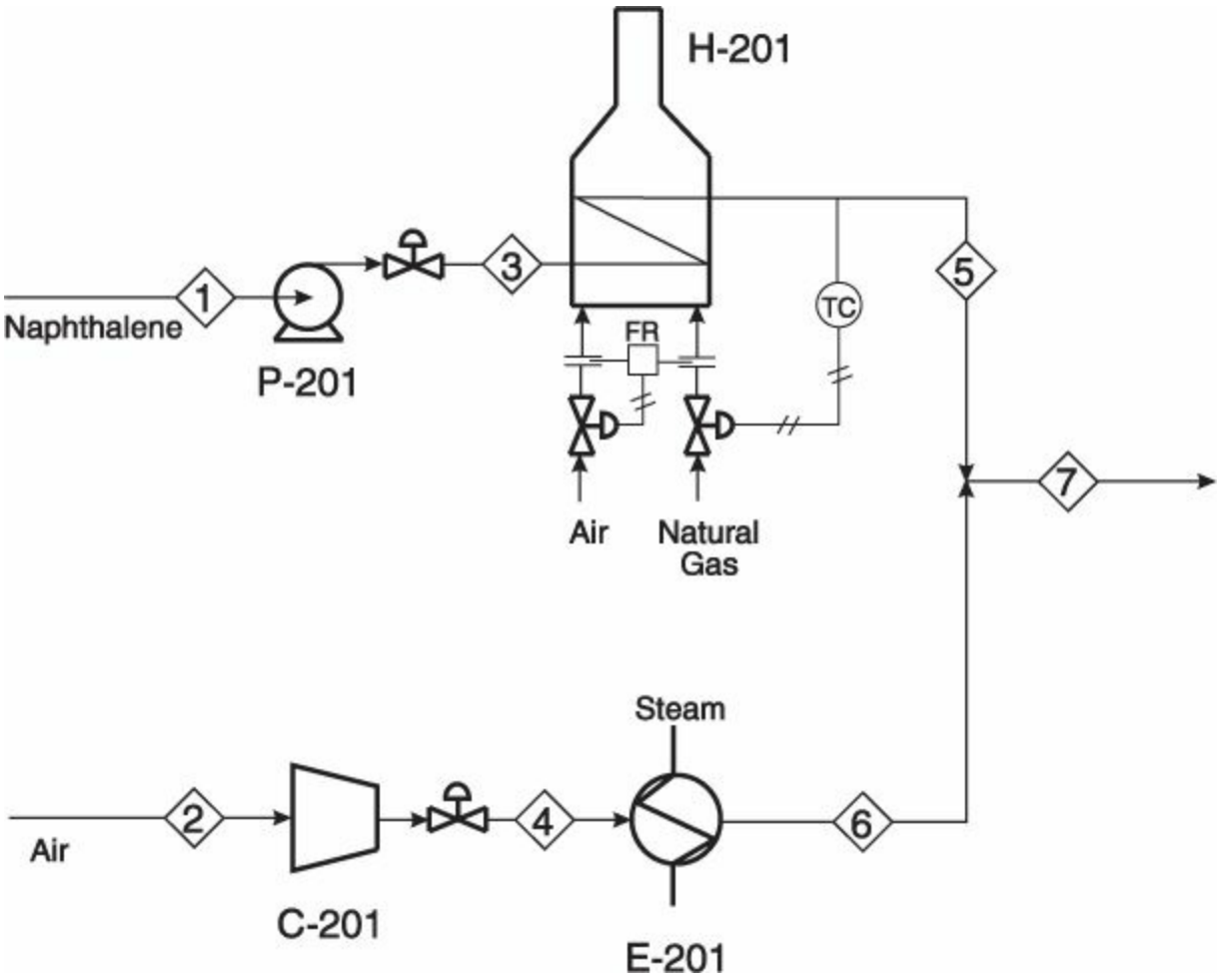


Figure 22.8. Feed Section to Phthalic Anhydride Process with Better Valve Placement than Shown in Figure 22.7

22.5. Summary

In this chapter, it has been demonstrated that performance of existing equipment is affected by other equipment. The input/output models discussed in Chapter 19 suggested this outcome. If the input to a unit is altered, its output is altered. Because the output from one unit is the input to the next, the interaction observed in the case studies in this chapter are expected. It is always important to remember the interaction between equipment performance in a chemical process.

In terms of obtaining numerical solutions for performance problems involving multiple units, examples such as the reactor heat exchanger and the distillation column have been used, in which the

adjacent units were analyzed sequentially. Other examples have been used, such as the heat-exchange loop and the feed section in which simultaneous solution of the relationships for multiple units was required. The exact set of calculations necessary and the difficulty of these calculations are specific to each problem encountered. However, the tools developed in Chapter 20, such as determining trends, base-case ratios, and *T*-*Q* diagrams, are essential to obtaining desired solutions.

What You Should Have Learned

- The analysis of the previous chapter can be applied to multiple unit operations.
- The general procedure is the same as for single unit operations.
- The input to any unit operation that is the output of another unit operation cannot be assumed; it must be calculated.

References

1. Perry, R. H., and D. W. Green, eds., *Perry's Chemical Engineers' Handbook*, 7th ed. (New York: McGraw-Hill, 1997), 2-61–2-75.
2. Box, G. E. P., *Evolutionary Operation: A Statistical Method for Process Improvement* (New York: John Wiley and Sons, 1969).
3. Kelley, P. E., "EVOP Technique Improves Operation of Amoco's Gas Producing Plants," *Oil and Gas Journal* 71, no. 44 (1973): 94.

Short Answer Questions

1. In the process to produce acetone from isopropyl alcohol (see process description on the CD), heat is supplied to the endothermic reaction using a Dowtherm A (or molten salt) loop and a fired heater. During the start-up of a new plant, it is found that the activity of the catalyst (k_o in the kinetics expression) is less than designed. How would you adjust the flow of heat transfer fluid (up or down) to compensate for this error? Explain your reasoning.
2. In a distillation column, if the bottom pressure decreases, what is the effect on the bottom temperature, the top pressure, the top temperature, and the flooding situation? Assume that all flows, temperatures, and pressures for the utility streams remain constant.

Problems

3. It is possible to generate performance curves for the reactor in Section 22.1. One type of performance curve would have the rate of cumene production (kmol/h) on the *y*-axis, and the percent propane impurity in the propylene on the *x*-axis. There would be lines for different operating temperatures all at constant pressure.

   Assume that the feed to the reactor is 108 kmol/h propylene, 8 kmol/h propane, and 203 kmol/h benzene. The pressure is kept constant at 3000 kPa. Prepare performance curves on the same graph for temperatures from 350°C to 400°C in 10°C intervals. Superimpose on this graph the maximum allowable conditions, which correspond to a steam-side pressure of 4800 kPa. A process simulator should be used to generate points on the performance curves. Other data: reactor volume = 7.89 m^3, heat transfer area A = 436 m^2, overall heat transfer coefficient = 65 $W/m^2°C$.

4. Repeat Problem 22.3 for varying reaction pressure at a constant temperature of 350°C. The pressure range is 3000 kPa to 3300 kPa, in intervals of 50 kPa.
5. For the distillation performance problem in Section 22.2, assume that scale-down occurs while maintaining constant boil-up rate. Determine the conditions in the reboiler, column, and condenser for these operating conditions. A process simulator should be used for the distillation column.
6. The benzene-toluene distillation column in Section 22.2 must temporarily handle a 25% increase in throughput while maintaining the same outlet concentrations. Determine the operating conditions required if the reflux ratio remains constant. What other factors must be considered in order to determine whether the column can handle this amount of increased throughput?
7. Suggest alternative changes in process conditions or addition of new equipment in the distillation column in Section 22.2 that would allow 50% scale-down. Suggest as many alternatives as you can think of, and discuss the advantages and disadvantages of each.
8. Consider the Dowtherm A loop described in Section 22.3. For the options involving multiple pumps either in series or parallel, determine the configuration that provides the maximum scale-up capacity. What are the temperatures of Dowtherm A, T_3, and T_4, and the maximum percent scale-up?
9. Repeat the analysis in Section 22.3 for the case when cooling water is used in the heat exchanger in place of boiler feed water. The cooling water enters at 30°C and must exit at 45°C.
10. Repeat the analysis in Problem 22.8 using cooling water as described in Problem 22.9.
11. Suggest alternative solutions, not involving increasing the Dowtherm A flowrate, to obtain the maximum scale-up possible in the Dowtherm A loop in Section 22.3. Suggest as many alternatives as you can think of, and discuss the advantages and disadvantages of each.
12. Consider the molten salt loop for removal of the heat of reaction in the production of phthalic anhydride described in Appendix C (on the CD) and illustrated in Figure C.5. It is necessary to scale down phthalic anhydride production by 50%. Estimate the flow of molten salt for the scaled-down case and the temperatures of molten salt entering and exiting the reactor. You may assume that sensible heat effects (energy necessary to heat reactants to reaction temperature) are negligible.
13. Consider the situation illustrated in Figure P22.13. Due to downstream considerations, P_8 is always maintained at 200 kPa. It is known that P_1 = 100 kPa and P_4 = 100 kPa, and because the feeds come from storage tanks maintained at constant pressure, they are always constant. It is also known that P_3 = 225 kPa, P_5 = 375 kPa, P_6 = 250 kPa, P_7 = 225 kPa, and $\dot{m}_1$ = 15,500 kg/h. The pump curves are given by the following equations, with ΔP in kPa and $\dot{m}$ in Mg/h:

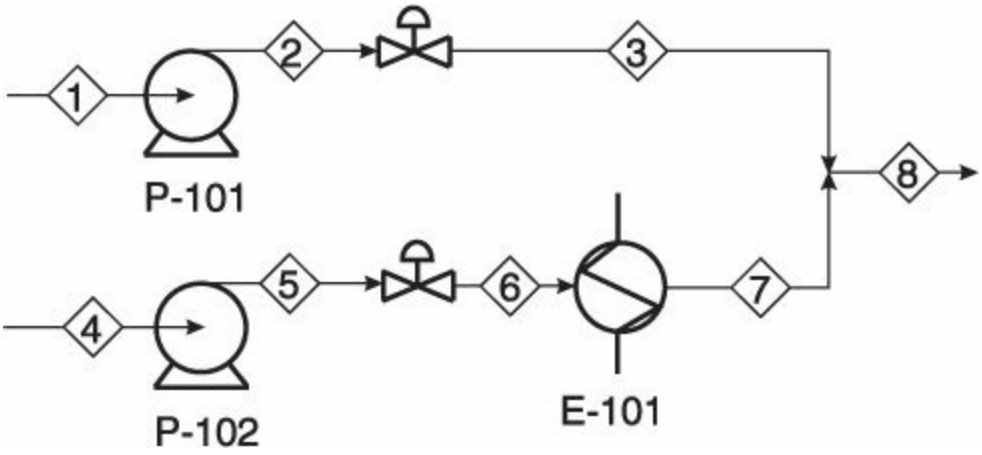


Figure P22.13. Process for Problem 22.13

Pump 1: $\Delta P = 340 - 0.913\ \dot{m} + 0.0535\dot{m}^2 - 0.0101\dot{m}^3$

Pump 2: $\Delta P = 312 - 1.924\ \dot{m} + 0.0302\ \dot{m}^2 - 0.01124\ \dot{m}^3$

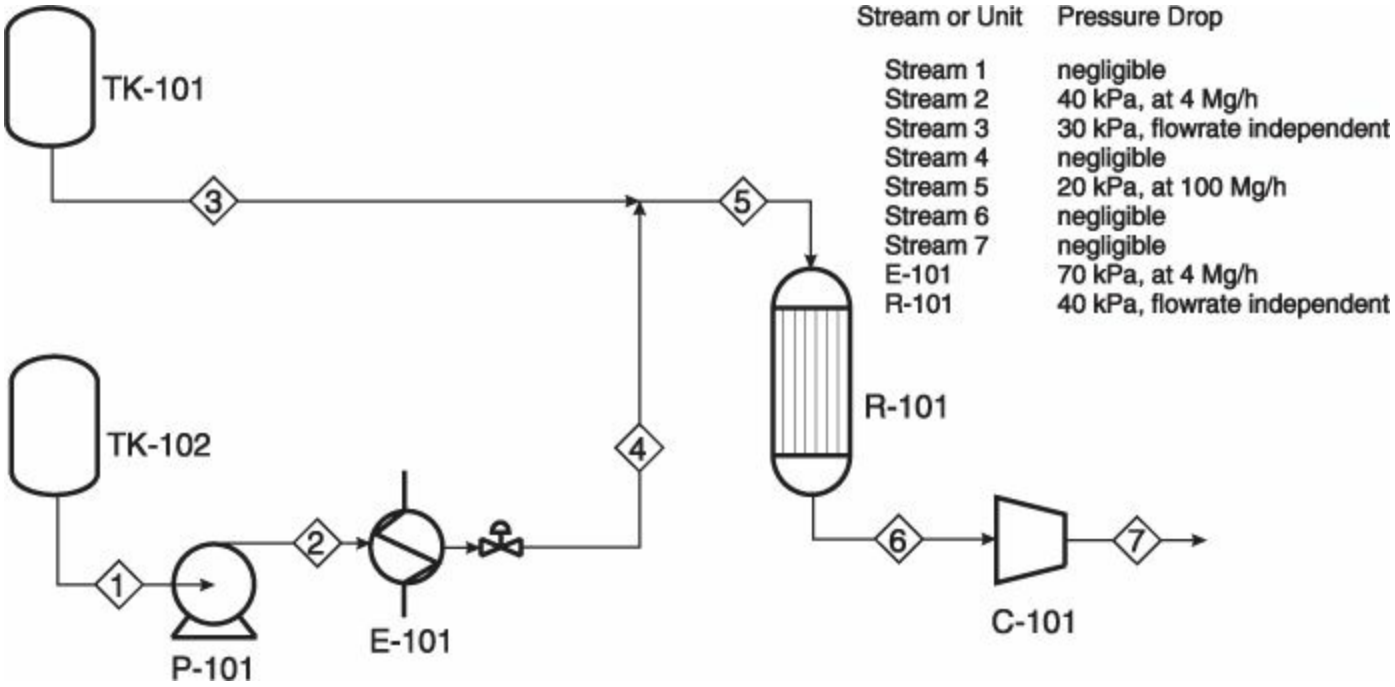
a. Calculate $\dot{m}_4$ and ΔP_{23} for this situation.

b. Sketch the pump and system curves for this situation as illustrated in Section 21.2.1. Identify the pressure drop across the valves on the sketch.

14. Refer to Figure P22.14 and the data provided with the figure. The compressor (C-101) exhausts to 101 kPa. Tank TK-102 is controlled to be always 101 kPa. Assume all flows are turbulent.

a. If the valve is closed, the flowrate from the compressor exhaust (Stream 7) is 100 Mg/h. What is the pressure in the storage tank (TK-101)?

b. If the pressure of TK-101 is kept constant at the pressure calculated in Part (a), what is the maximum flowrate of liquid (Stream 2) when the valve is wide open (i.e., no pressure drop across the valve)?



Stream or Unit	Pressure Drop
Stream 1	negligible
Stream 2	40 kPa, at 4 Mg/h
Stream 3	30 kPa, flowrate independent
Stream 4	negligible
Stream 5	20 kPa, at 100 Mg/h
Stream 6	negligible
Stream 7	negligible
E-101	70 kPa, at 4 Mg/h
R-101	40 kPa, flowrate independent

Figure P22.14. Process for Problem 22.14

c. What is the flowrate of the compressor exhaust (Stream 7) when the valve is wide open?

C-101 compressor curve:

$$\frac{P_{out}}{P_{in}} = 4.015 + 5.264 \times 10^{-3}\dot{m} - 1.838 \times 10^{-4}\dot{m}^2$$

P-101 pump curve:

$$\Delta P = 500 + 4.662\dot{m} - 1.805\dot{m}^2$$

where P is in kPa and $\dot{m}$ is in Mg/h.

15. Consider a process in which a fluid is pumped from a storage tank through a heat exchanger, where it is heated and then pumped into another storage tank. The process flow diagram for this process is shown in Figure P22.15(a), and the pump and system curves are shown in Figure P22.15(b).

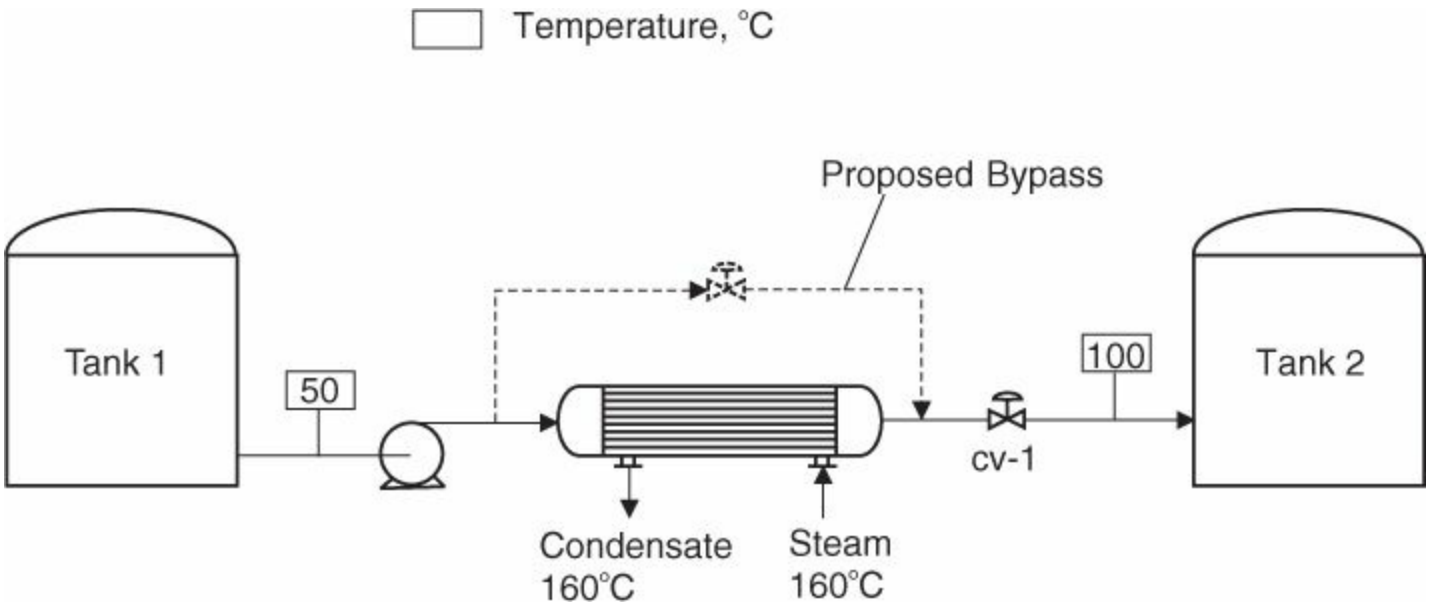


Figure P22.15(a). Process Flow Diagram for Problem 22.15

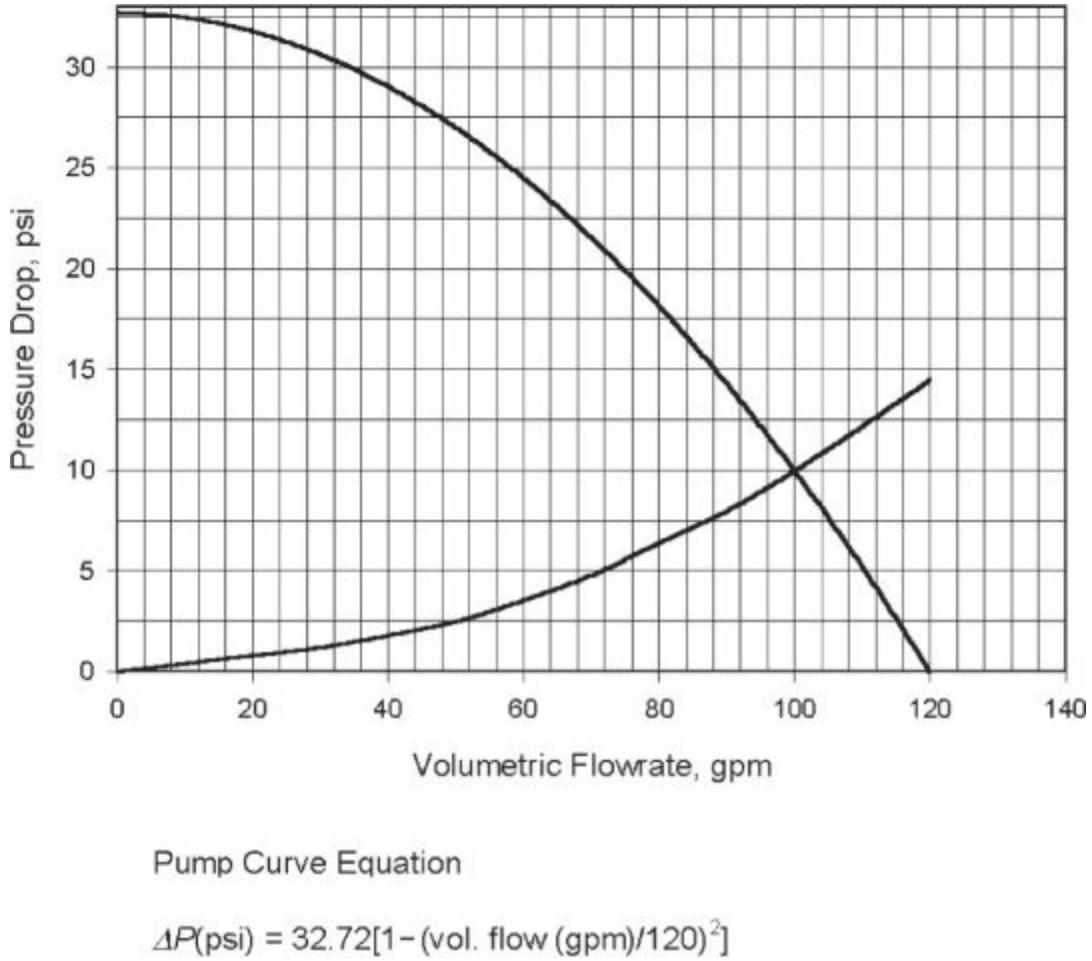


Figure P22.15(b). Pump Curve and System Curve for Problem 22.15

Currently, the system is operating with the control valve (cv-1) wide open, and the flow through the pump is measured at 100 gallons per minute (gpm). The elevations and pressures of both tanks are equal, and the pressure drop across the heat exchanger is 5 psi, with the remaining 5 psi pressure drop occurring in the piping. It has been noted that the current velocity through the heat exchanger is very high and must be reduced by half. It is proposed to add a bypass line with a valve around the heat exchanger. The valve will be adjusted so that the flow through the heat exchanger is 50% of the current flow. The control valve, cv-1, will remain wide open. For the proposed change, find the following:

a. The pressure drop across the heat exchanger.

b. The total flowrate of fluid passing through the pump.

c. Assume that all the resistance to heat transfer is on the process fluid side and that the temperature of the condensing steam remains constant. Determine the temprature of the fluid entering Tank 2.

16. During the retrofit of a chemical plant, it was decided to place valves and bypass lines around two exchangers placed in series. The flows through each of the bypass lines are controlled by the valves so that 40% of the flow bypasses each exchanger. Because of safety concerns, the bypass lines must be removed. These situations are illustrated in Figure P22.16(a), and the pump curve is in Figure P22.16(b). From the information given in the following table, find the following:

a. For the base case, what is the flowrate through the pump?

b. For the new case, what the maximum flow that can be sent through the two exchangers?

Pressure Profile for Base Case

Location	Pressure (kPa)
1	300
2	290
3	250
4	240
5	200
6	170

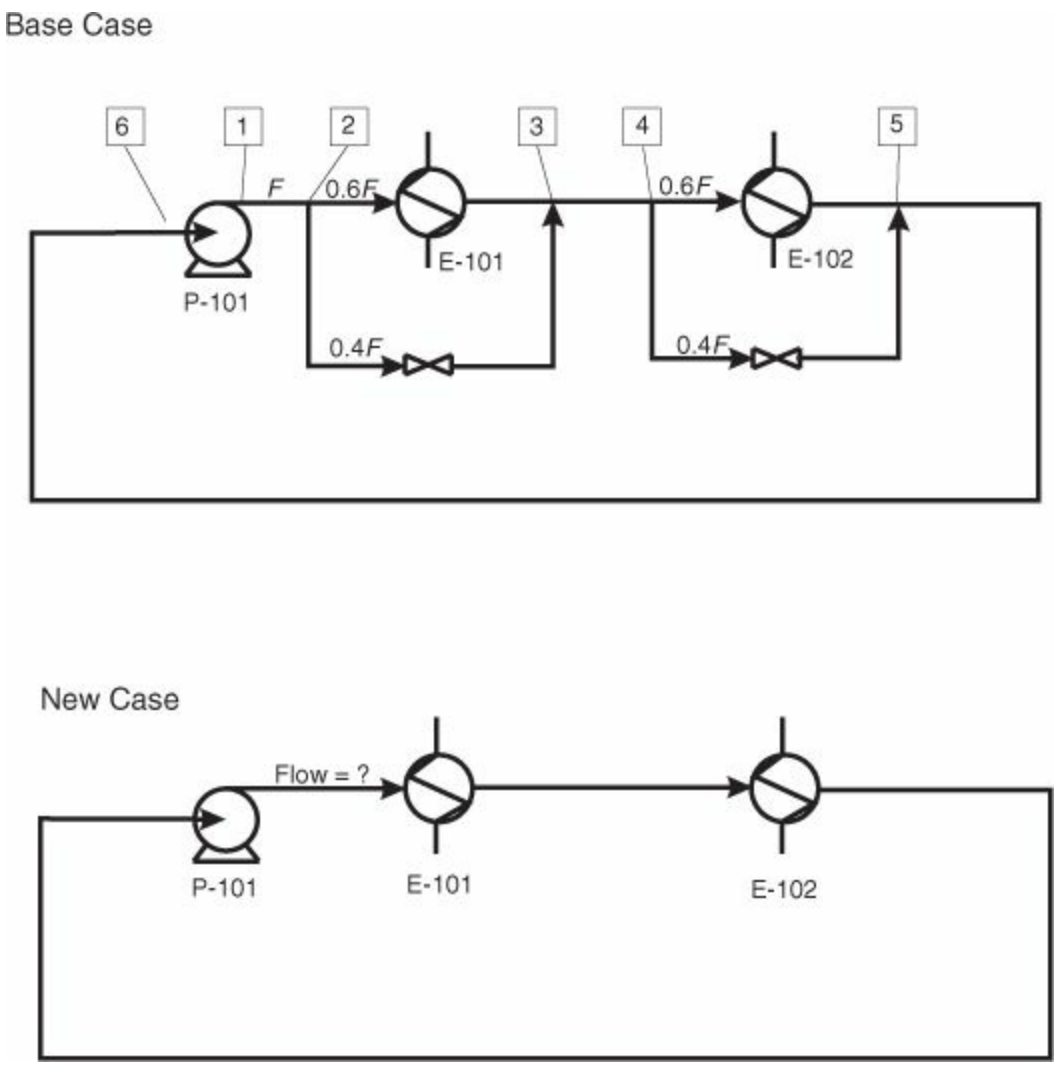


Figure P22.16(a). Process Flow Diagram for Problem 22.16

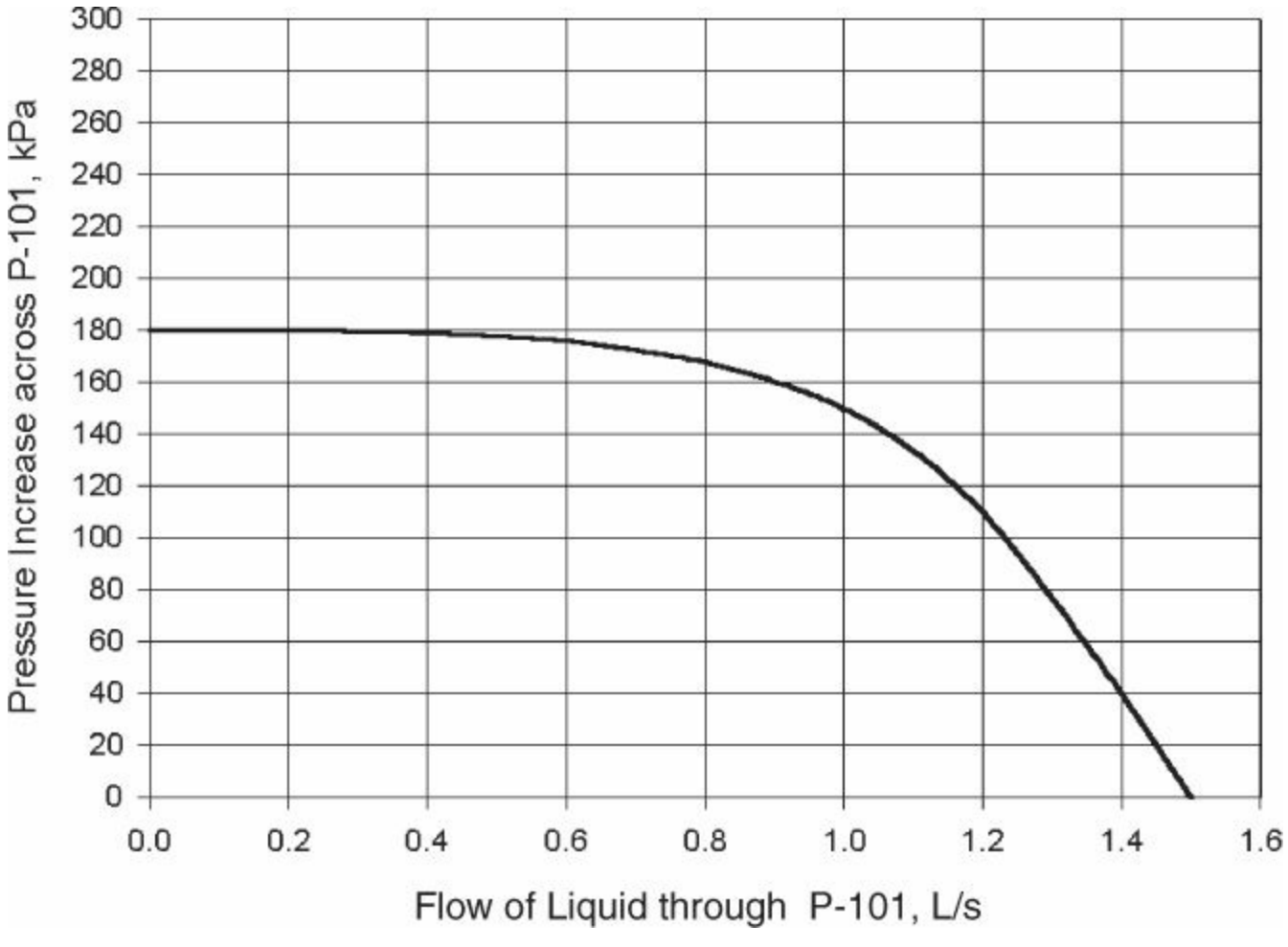


Figure P22.16(b). Pump Curve for P-101

17. The feed system for a distillation process is shown in Figure P22.17(a). The feed to be distilled is an organic liquid stored in V-301 under a nitrogen blanket at a constant pressure of 21 psi. The liquid is pumped through a pump, heat exchanger, and control valve to the distillation column. The pressure profile for the design flow of 50 gpm is shown in the diagram. Also shown are the elevations of the liquid level in the tank and the feed tray in the column. Using the pump characteristics shown in Figure P22.17(b), answer the following questions:
    a. What is the maximum flowrate that can be pumped through this system assuming that the feed and destination pressures remain constant?
    b. What would the vapor pressure of the liquid have to be at the entrance to the pump so that the pump would just cavitate at the design flow?
    c. In order to design the heat exchanger, a maximum design pressure needs to be specified. It has been determined that the maximum pressure to which E-301 can be exposed occurs when the control valve fails closed while the pump continues to operate. What is this maximum pressure?

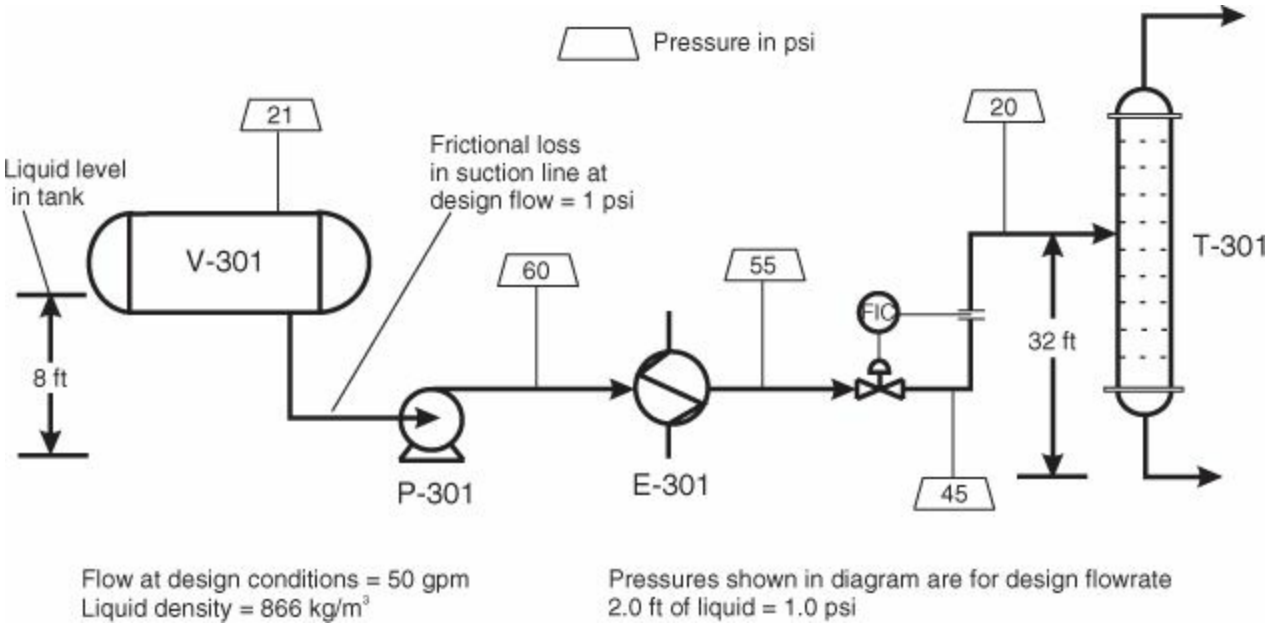


Figure P22.17(a). Process Flow Diagram for Problem 22.17

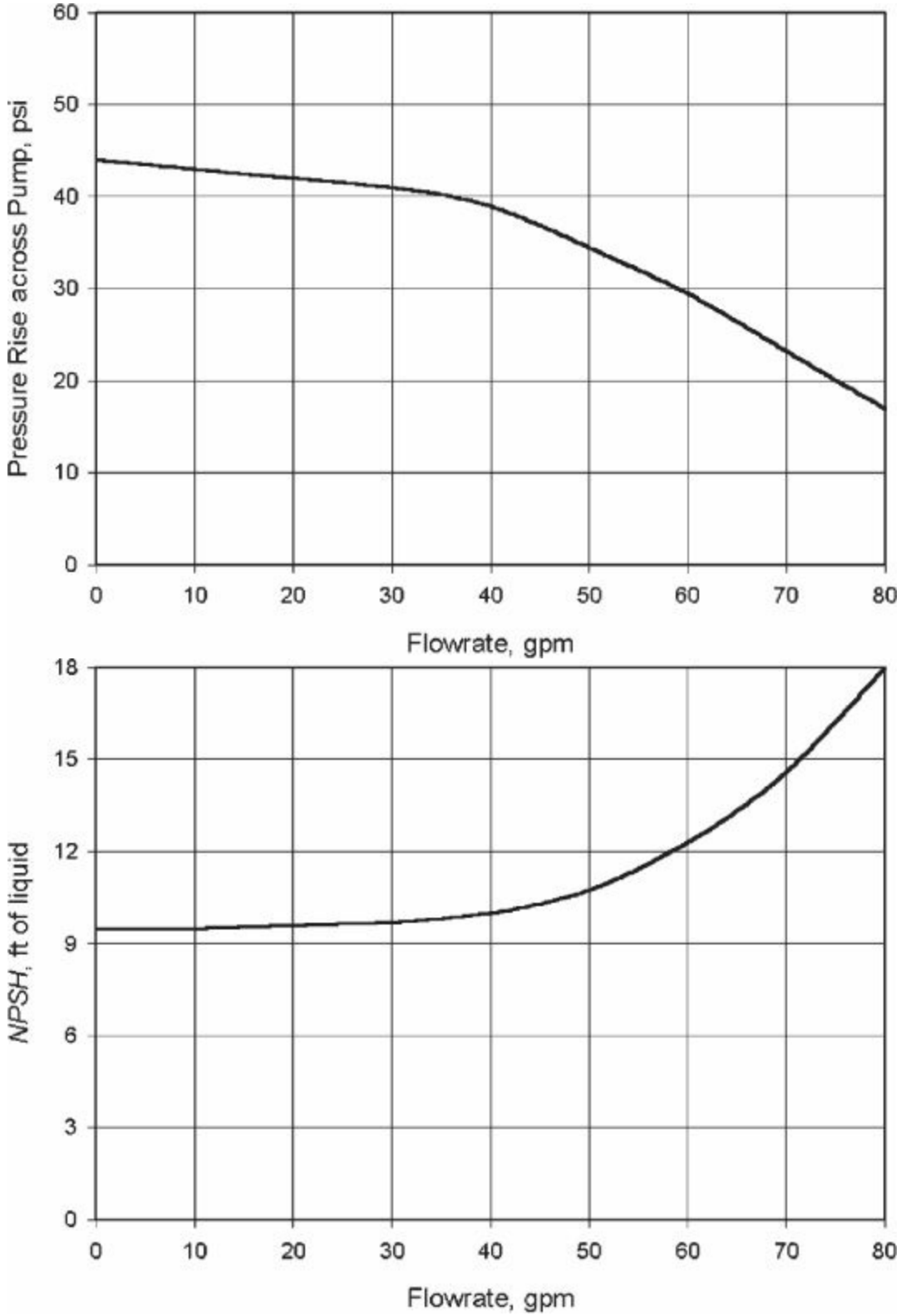


Figure P22.17(b). Pump Characteristics for P-301

18. In the production of acrylic acid, the final step is distillation of an acrylic acid/acetic acid mixture. The acrylic acid, which is the bottoms product, may not exceed 90°C due to spontaneous polymerization above that temperature. Both the acrylic acid and the acetic acid may be considered pure at the bottom and the top of the column, respectively.

In the current design, a vacuum column with low-pressure-drop, structured packing is used. The pressure drop in the column is 9.5 kPa. The reboiler uses low-pressure steam, but the reboiler feed is equipped with a desuperheater, so the steam temperature is 120°C. There is a control system designed to maintain the temperature difference between the boiling acrylic acid and the steam constant by varying the desuperheater settings. The acrylic acid is reboiled at 89°C. In the

condenser, the current design is for cooling water entering at 30°C and leaving at 40°C.

a. What is the pressure at the bottom of the column?

b. What is the temperature of the condensing acetic acid at the top of the column?

c. Based on customer complaints, it is believed that the product is off spec. Investigation shows that the cooling water is flowing at the design rate and that the heat load on the condenser is at design specifications. However, due to a heat wave, the cooling water appears to be entering at 35°C. Could this explain the off-spec product? Support your argument with calculations. What else in the column (temperatures, pressures, etc.) must have changed? What are these new values? Comment on the reboiler control strategy.

Vapor pressure data:

$$\text{For acrylic acid:} \quad \ln P^*\,(kPa) = 17.31 - \frac{5264.4}{T(K)}$$

$$\text{For acetic acid:} \quad \ln P^*\,(kPa) = 17.54 - \frac{4981.5}{T(K)}$$

19. The distillate stream from a distillation column (flowrate 35 m^3/h, density of water) is recycled. The destination of the recycle stream is at a location 3 m below the fluid level in the reflux drum. First, the recycle passes through a pump to supply sufficient head to overcome frictional losses (20 kPa) and reach the pressure of the stream with which it is mixed (250 kPa above distillate stream). Then it is heated from 90°C to 120°C using low-pressure steam at 140°C. Assume that all resistance is on the process-stream side of the exchanger (tube side).

It is desired to scale up the entire plant capacity by 15%. It has been determined that the distillation column can be modified to maintain the recycle stream temperature at 90°C. It has also been determined that, with the required changes in the feed section of the process, the minimum temperature of the recycle stream must be between 119°C and 121°C to satisfy liquid-phase reactor inlet conditions after mixing with fresh feed.

a. Can the temperature criterion be satisfied?

b. Can the flows in this portion of the process be scaled up by 15%? The pump curve is in Figure P22.19.

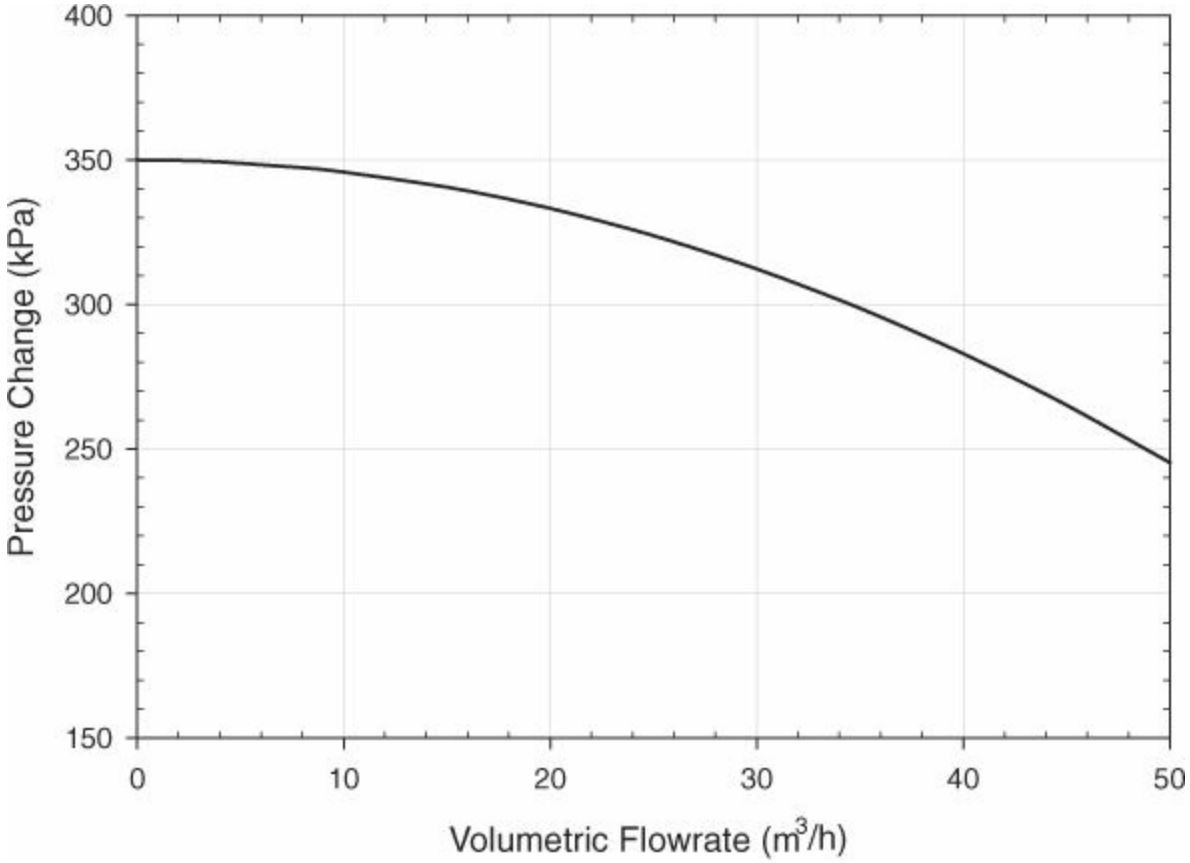


Figure P22.19. Pump Curve for Problem 22.19

c. With a scale-up of 15% desired, what feature must be included in this distillation column so that column operation can be modified to maintain the recycle stream at 90°C?

d. It is suggested that because a lower temperature of the recycle stream would reduce the reaction rate, if needed, the pumps in the feed section could be used to increase the reactor pressure and hence the reaction rate. What is your opinion of this suggestion?

20. A process heat exchanger has a bypass around it that is normally closed, thus forcing all the process flow through the exchanger. The process fluid (vapor) flows through the shell side of an exchanger, and cooling water flows through the tubes. You may assume that all the heat transfer resistance is on the shell side. During a planned change in operations, it has been determined that additional gas flow will be generated, resulting in an increase of 70% above the current flow. However, the pressure drop across the exchanger would be excessive if all of this flow passed through the exchanger. Therefore, the bypass will be opened so that the pressure drop across the process exchanger increases by only 69%. For this situation answer the following questions:

a. By how much does the flow through the heat exchanger increase?

b. What fraction of the new flow will flow through the bypass?

c. What will be the new overall heat transfer coefficient?

21. You are trying to evaluate whether an existing, idle distillation column can be used for a separation for which it was not originally designed. Answer the following questions about this column:

a. The reflux pump (there are two in parallel) must pump fluid from the reflux drum to the top of the column. The fluid density is 775 kg/m^3. The reflux drum is 6 m above the pump inlet. The top of the tower is 42 m above the pump discharge. Frictional pressure drop for the entire length of pipe is calculated to be 130 kPa. The desired flowrate is 7 L/s. The pump curve and

$NPSH_R$ curves are in Figure P22.21. Determine whether this pump can be used for this job and, if so, what configuration is necessary. The frictional pressure drop seems high. Suggest a possible explanation.

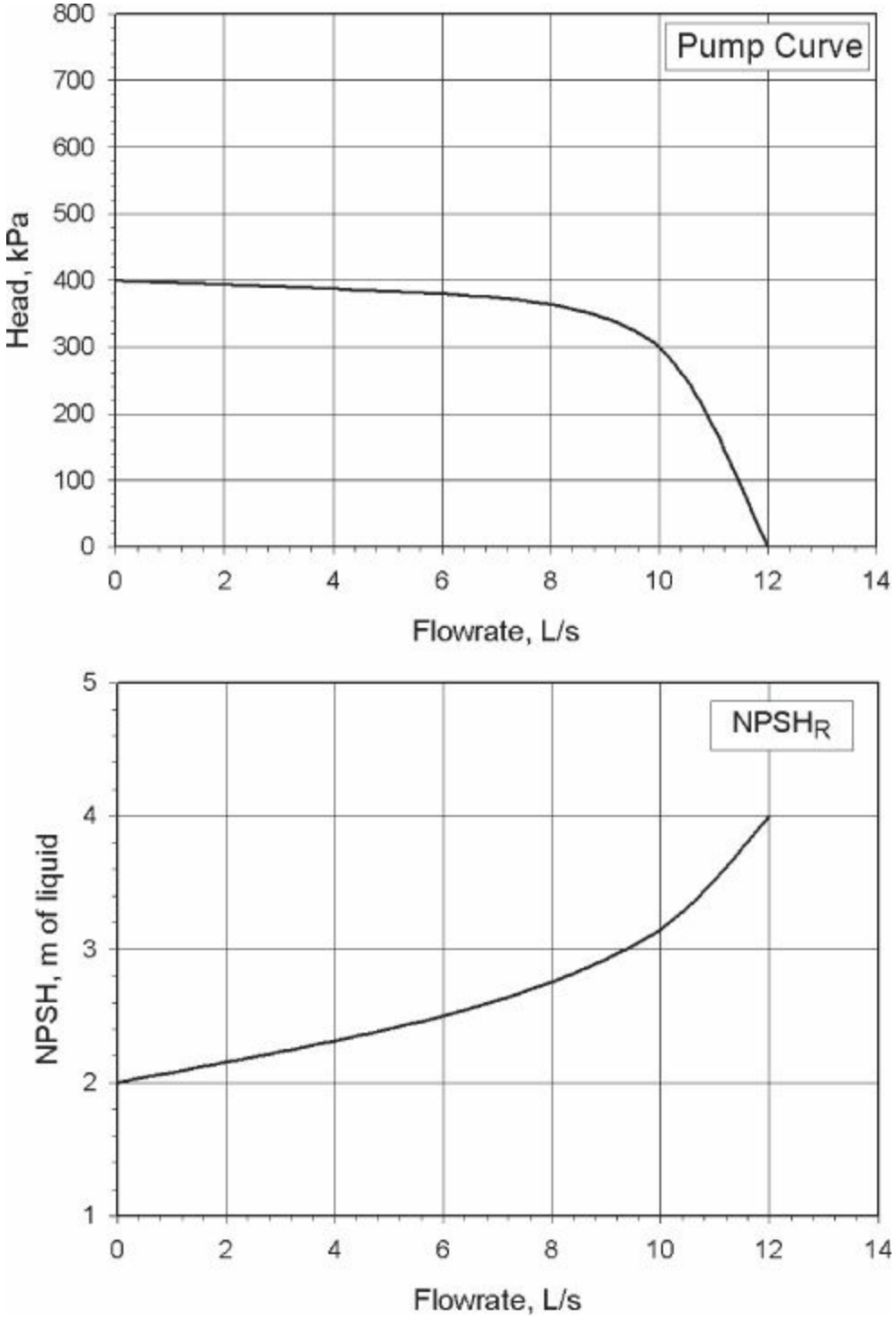


Figure P22.21. Pump and NPSH Curves for Problem 22.21

b. The reboiler is connected to the low-pressure steam line (160°C). However, there is also a desuperheater. The area of the exchanger is 300 m^2, and the heat transfer coefficients have been estimated to be 5000 W/m^2K and 3000 W/m^2K for the boiling side and the condensing side, respectively. The boiling point of the process fluid is 87°C, and the required heat load is 6000 kW. What is the saturated steam temperature required at the desuperheater exit?

c. List at least three items you would investigate regarding the ability of this column to do the desired separation. For each item, discuss what you would look for or calculate to determine the suitability of the column for this duty.

22. During the design of a new separation system, a reboiler using throttled and desuperheated low-pressure steam (5 barg, T_{sat} = 160°C) was specified. The details of this design are given below:

Duty = 5000 kW

Overall heat transfer coefficient = 1500 W/m^2°C

Steam-side coefficient = process-side coefficient

$T_{process}$ = 70°C

T_{steam} (after throttling and desuperheating) = 110°C

The heat transfer coefficient for the boiling process fluid as a function of the temperature difference between the wall and the process fluid for this design is given in Figure P22.22.

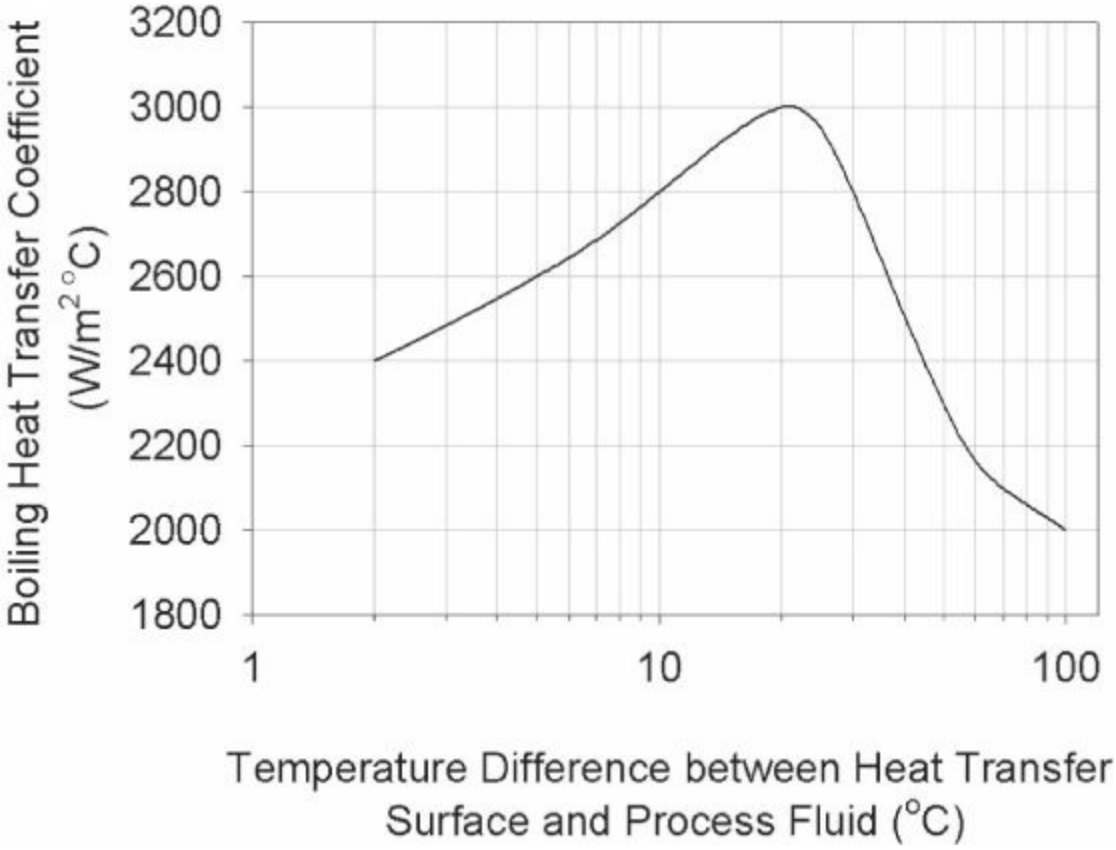


Figure P22.22. Boiling Heat Transfer Coefficient as a Function of Temperature Difference

a. During the construction of this new separation system, the throttling valve and desuperheating unit have been omitted. By how much will the new reboil rate change (magnitude as a percent of the base case), assuming that the column pressure and temperature do not change?

Hint: You may assume that the steam-side heat transfer coefficient does not change but the process-side heat transfer coefficient will change. *This means that the wall temperature will also change, and the solution to the problem will require trial and error.*

b. If the column were allowed to operate without the desuperheater and throttling units and no adjustments or changes were made to the column operation, how would the pressure in the column change? This answer should be consistent with your answer to Part (a).

23. The bottoms product from a distillation column is pumped through two heat exchangers to recover energy and is then sent to a storage tank, which is at atmospheric pressure. The system is shown in Figure P22.23(a).

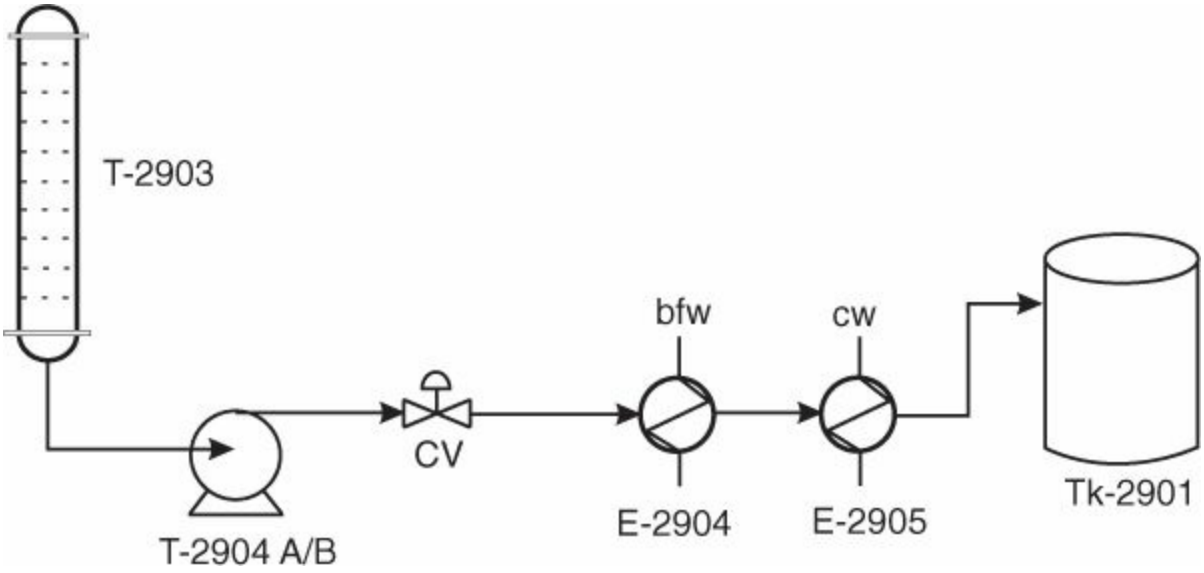


Figure P22.23(a). Process Flow Diagram for Problem 22.23

The pump curve for P-2904A/B is shown in Figure P22.23(b). At design conditions, the flow through the pump is 5 L/s, the pressure in T-2903 is 200 kPa, and the frictional loss (for the process fluid) through the piping and heat exchangers, but excluding the control valve, is 250 kPa. You may assume that the difference in height between the liquid level in T-2903 and Tk-2901 is negligible. For this system, answer the following questions:

a. What is the pressure drop across the control valve at design conditions?

b. Under design conditions, the 250 kPa frictional pressure drop is distributed as shown in Table P22.23.

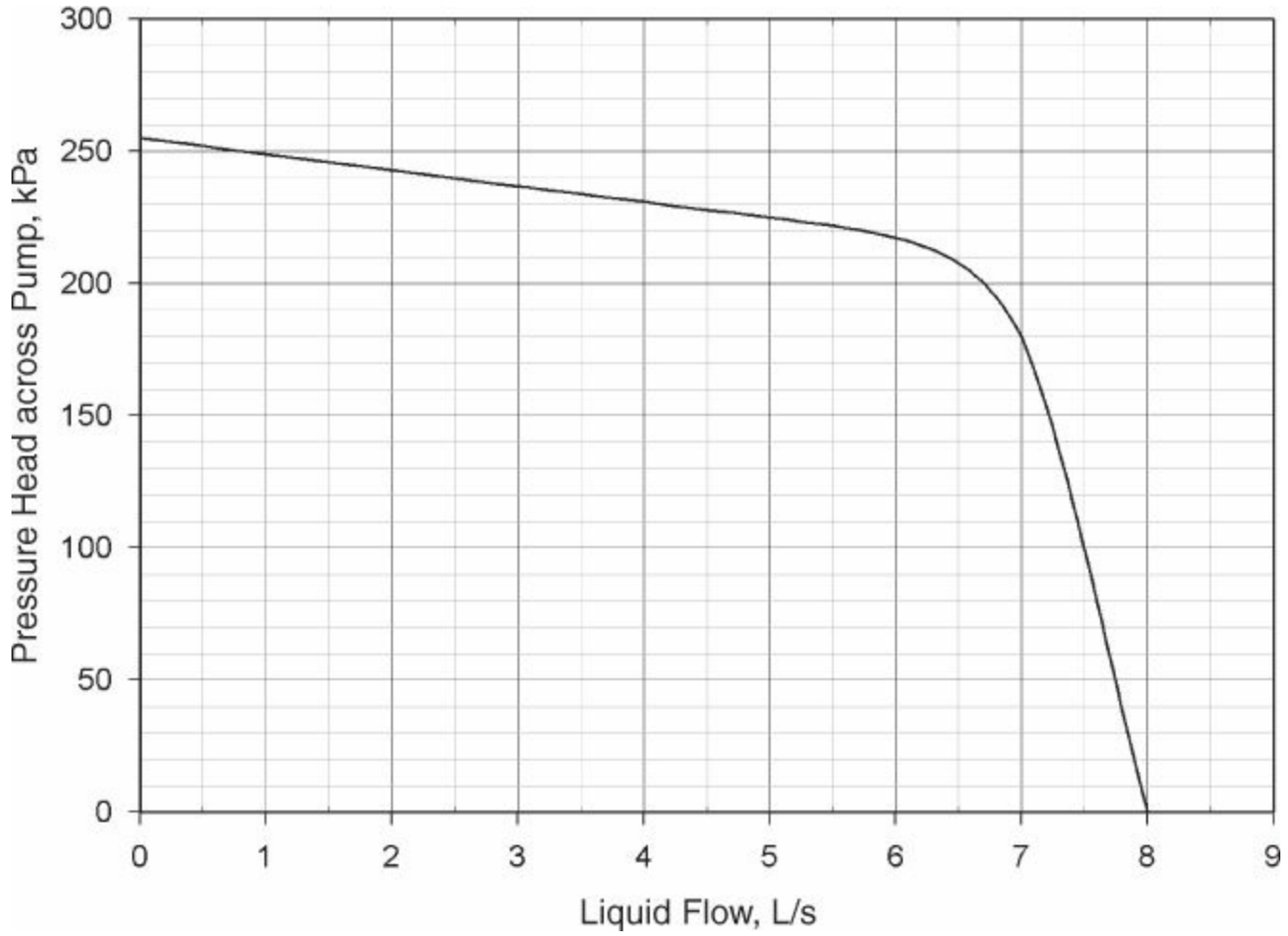


Figure P22.23(b). Pump Curve for Problem 22.23

Table P22.23. Pressure Drops in Pipe Sections

Equipment or Pipe	Pressure Drop at Design Flowrate (kPa)
Suction piping	5
Piping from P-2904 to CV	10
Piping from P-2904 to CV	10
E-2904	50
Piping from E-2904 to E-2905	25
E-2905	50
Piping from E-2905 to Tk-2901	100

c. What is the pressure of the liquid entering E-2904 and E-2905 at a scaled-up condition, which is 150% of the base-case flowrate?

24. Two heat exchangers of equal area have been designed to heat a certain process fluid from 50°C to 100°C using condensing saturated steam at 150°C. The designs of the two exchangers are different and result in different pressure drops and different overall heat transfer coefficients. Pilot-test results for the two heat exchangers operating individually are given in Table P22.24 for a single set of operating conditions.

Table P22.24. Heat-Exchanger Pilot-Test Results

Process Variable	Exchanger 1	Exchanger 2
Mass flow of process liquid (tube side)	2.0 kg/s	1.5 kg/s
Inlet temperature of liquid	50°C	50°C
Outlet temperature of liquid	100°C	100°C
Process liquid C_p	1000 J/kgK	1000 J/kgK
Steam temperature (shell side)	150°C	150°C
ΔT_{lm}	72.13°C	72.13°C
Area	6.93 m^2	6.93 m^2
Condensing steam heat transfer coefficient	1000 W/m^2K	1000 W/m^2K
U	200 W/m^2K	150 W/m^2K
Tube-side pressure drop	40 kPa	25 kPa

In the plant, these two exchangers are now to be piped in parallel, and at the current operating conditions, the pressure drop across both heat exchangers is measured at 52 kPa.

Assuming that the physical properties and inlet temperature of the process stream (in the tube side) are the same as given in Table P22.24 and that condensing steam is used in the shell side, answer the following questions:

a. What is the mass flowrate of process fluid through Exchanger 1?

b. What is the mass flowrate of process fluid through Exchanger 2?

c. What is the new overall heat transfer coefficient for Exchanger 1?

d. What is the new overall heat transfer coefficient for Exchanger 2?

e. If the process exit stream from Exchanger 1 is to be maintained at 100°C, what must be the

temperature of the condensing steam that is fed to this exchanger?

f. If the process exit stream from Exchanger 2 is to be maintained at 100°C, what must be the temperature of the condensing steam that is fed to this exchanger?

g. Under another set of conditions, if the two exchangers were piped in parallel and the flow measured through Exchanger 1 was 3.1 kg/s, what would the flow be through Exchanger 2?

25. Consider the system illustrated in Figure P22.25(a). The process is to be scaled up from a design flowrate of 120 m^3/h. The fluid is a liquid, and it is to be fed to a reactor. The heating medium is condensing, medium-pressure steam throttled and desuperheated to saturated steam at 180°C. In the heat exchanger, the resistances are such that the process-side resistance (tubes) is three times that of the condensing steam (shell). The pump and system curves are shown in Figure P22.25(b).

a. What is the maximum percent scale-up possible in this system and the corresponding outlet temperature of E-101?

b. If it is necessary for the minimum reactor feed temperature to be 153°C, what is the maximum possible scale-up?

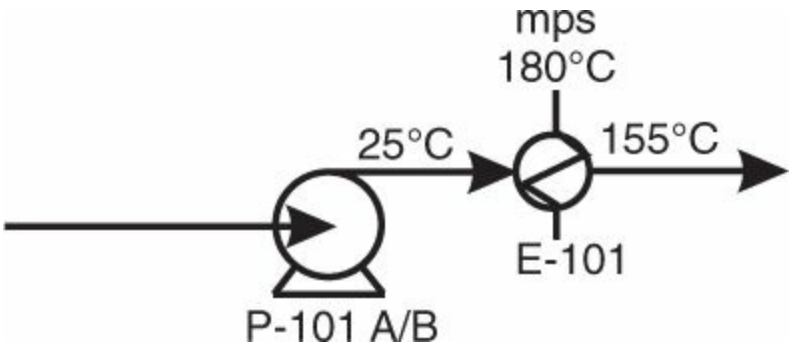


Figure P22.25(a). PFD for Problem 22.25

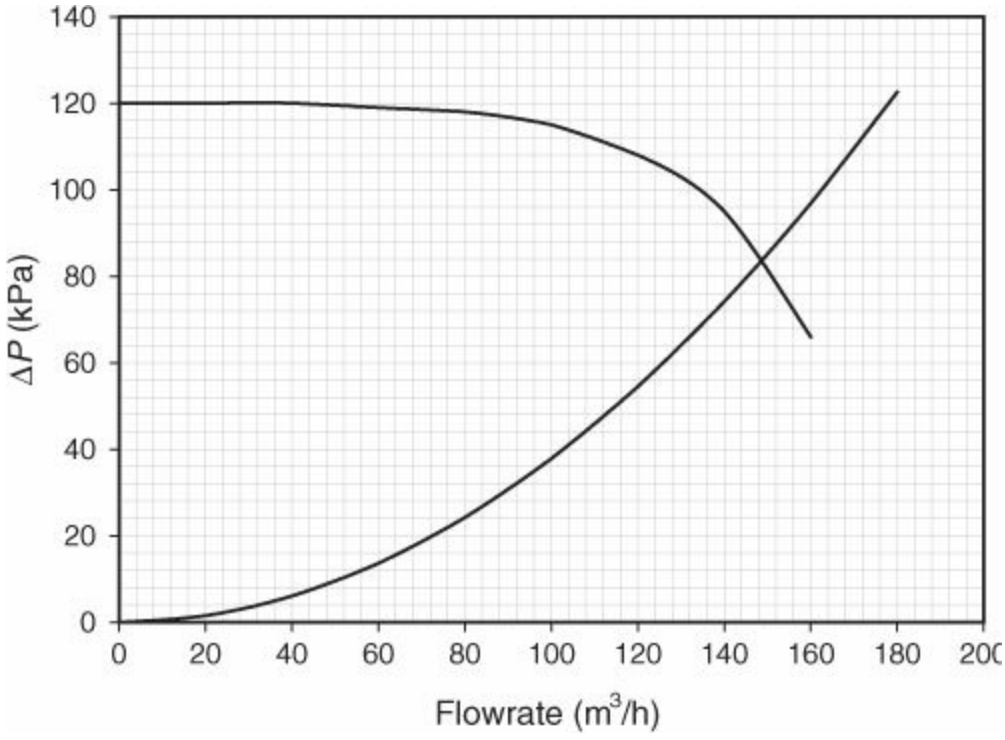


Figure P22.25(b). Pump and System Curves for P-101 A/B in Problem 22.25

Chapter 23. Reactor Performance

What You Will Learn

- Reactor performance is affected by multiple parameters.
- All of these parameters must be considered appropriately.

Chemical reactors are used to produce high-value chemicals from lower-value chemicals. Reactor performance depends on the complex interaction between four effects, as is illustrated in Figure 23.1. In order to understand fully the performance of a chemical reactor in the context of a chemical process, all four effects must be considered.

1. **Reaction Kinetics and Thermodynamics:** The influence of extensive variables (pressure, temperature, concentration) on reactor performance is defined by reaction kinetics and reaction equilibrium. These extensive variables affect the reaction rate and determine the extent to which reactants can be converted into products in a given reactor or the size of reactor needed to achieve a given conversion. Additionally, catalysts are used to increase the rate of reaction. Thermodynamics sets a theoretical limit on the extent to which reactants can be converted into products and cannot be changed by catalysts.
2. **Reactor Parameters:** These include the reactor volume, space time (reactor volume/inlet volumetric flowrate), and reactor configuration. For given kinetics, thermodynamics, reactor and heat transfer configuration, and space time, the reactor volume needed to achieve a given conversion of reactants is determined. This is the design problem. For a fixed reactor volume, the conversion is affected by the temperature, pressure, space time, catalyst, and reactor and heat transfer configuration. This is the performance problem.

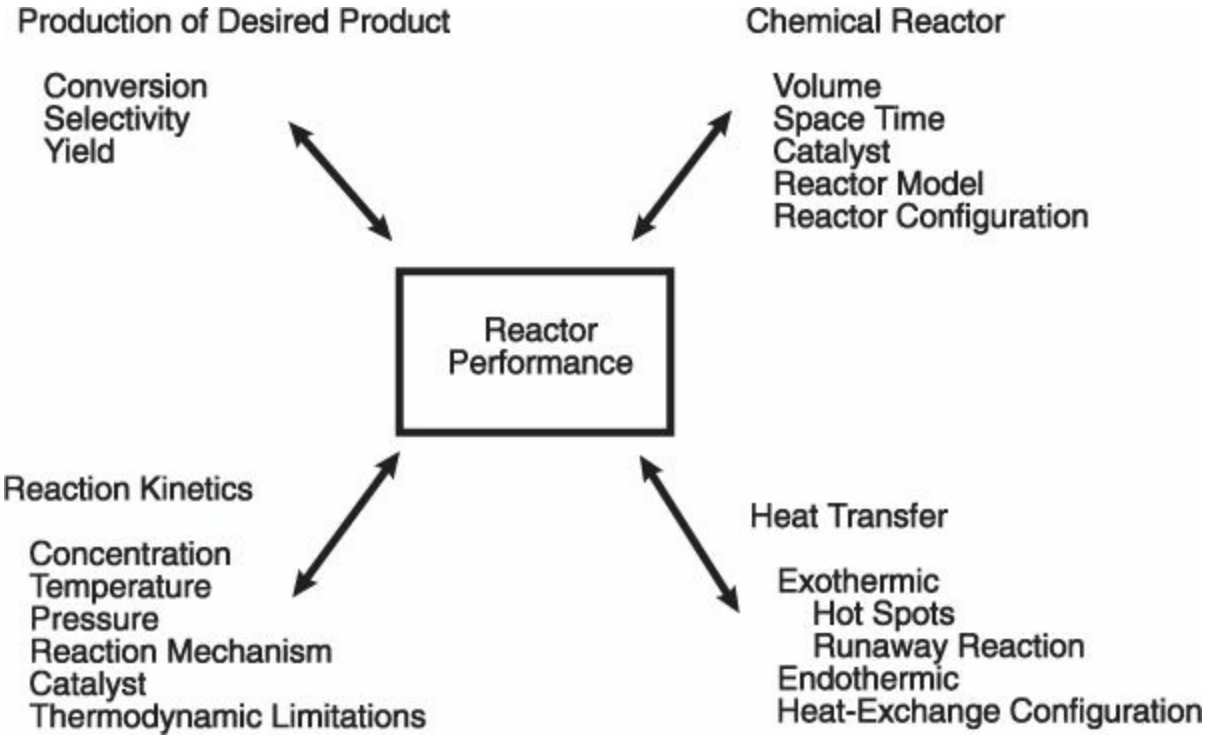


Figure 23.1. Phenomena Affecting Reactor Performance

3. **Production of Desired Product:** *Conversion*, *selectivity*, and *yield* are terms that quantify the amount of reactants reacted to form desired products. Reactor performance is expressed in

terms of these parameters. For a fixed reactor volume, these parameters are functions of the temperature, pressure, reactor and heat transfer configuration, and space time.

4. **Heat Transfer in Reactor:** This important effect is often overlooked. Energy is released or consumed in chemical reactions. The rate of chemical reaction is highly temperature dependent. The key point to consider is the interaction between chemical kinetics and heat transfer (see Example 22.1). For exothermic reactions, the heat of reaction must be removed efficiently to avoid large temperature increases that can damage catalyst and to prevent runaway reaction. For endothermic reactions, heat must be supplied efficiently so that the reaction can proceed. The rate of heat transfer depends on reactor configuration (including the heat transfer configuration), the properties of the reacting stream, the properties of the heat transfer medium, and the temperature driving force.

In this chapter, the basic concepts needed for prediction of reactor performance are reviewed. Multiple reaction systems, reactor models, and heat transfer considerations are emphasized. Case studies are presented based on reactors found in the processes used as examples throughout the text and in the appendixes.

23.1. Production of Desired Product

Consider the following reaction scheme:

$$aA + bB \xrightarrow[rxn\ 1]{k_1} pP \xrightarrow[rxn\ 2]{k_2} uU \qquad \beta B \xrightarrow[rxn\ 3]{k_3} vV \tag{23.1}$$

Equation (23.1) shows three reactions involving five species *A, B, P, U*, and *V*, with stoichiometric coefficients *a*, *b*, *p*, *u*, and *v*, respectively. It is assumed that *P* is the desired product and that *U* and *V* are unwanted by-products. The reaction scheme in Equation (23.1) can be used to illustrate the effects commonly observed in actual reaction kinetics.

1. A **single reaction** produces desired product. Here $k_2 = k_3 = 0$, and only the first reaction proceeds. Acetone production (Appendix B, Figure B.10.1) is an example of this situation. Hydrodealkylation of toluene to benzene behaves like this because the catalyst suppresses the undesired reactions sufficiently so that single-reaction behavior is approached.
2. **Parallel** (competing) reactions produce desired products and unwanted by-products. Here $k_2 = 0$, and no *U* is formed. Species *B* reacts to form either *P* or *V*. In the phthalic anhydride reaction sequence (Appendix C, Figure C.5), the reaction of o-xylene to form either phthalic anhydride, maleic anhydride, or combustion products (Appendix C, Table C.10, Reactions 1, 3, and 4) is an example of a parallel reaction.
3. **Series** (sequential) reactions produce desired products and unwanted by-products. Here $k_3 = 0$, and no *V* is formed. Species A reacts to form desired product *P*, which further reacts to form unwanted by-product *U*. In the phthalic anhydride reaction sequence (Appendix C, Table C.10), the reaction of o-xylene to phthalic anhydride to combustion products (Reactions 1 and 2) is an example of a series reaction.
4. **Series** and **parallel** reactions produce desired products and unwanted by products. Here, all

three reactions in Equation (23.1) occur to form desired product P and unwanted by-products U and V. The entire phthalic anhydride sequence (Appendix C, Table C.10) as well as the cumene production reaction (Appendix C, Table C.17) are examples of series or parallel reactions.

For reaction schemes like the one shown in Equation (23.1), there are three key definitions used to quantify production of desired product.

The term **conversion** quantifies the amount of reactant reacted. The single-pass conversion (or reactor conversion) is

$$\text{Single-pass conversion} = \frac{\text{Reactant consumed in reactor}}{\text{Reactant fed to reactor}} \tag{23.2}$$

and is generally reported in terms of the limiting reactant. This is different from the overall process conversion, which is defined as

$$\text{Overall conversion} = X = \frac{\text{Reactant consumed in process}}{\text{Reactant fed to process}} \tag{23.3}$$

Most processes recover and recycle unreacted material to provide a high overall conversion.

High reactor conversions are neither necessary nor desirable for optimum reactor performance. At low reactor conversions, high overall conversions can be achieved with increased recycle.

The term **selectivity** quantifies the conversion to desired product.

$$\text{Selectivity} = \eta = \frac{\text{Rate of production of desired product}}{\text{Rate of production of undesired by-products}} \tag{23.4}$$

A high selectivity is always desirable.

Competition from undesired reactions limits conversion to the desired product.

Another term used to quantify production of the desired product is **yield**, defined as

$$\text{Yield} = \frac{\text{Moles of reactant reacted to produce desired product}}{\text{Moles of limiting reactant reacted}} \tag{23.5}$$

The terms defined in this section will be used in examples and the case studies presented later in this chapter.

23.2. Reaction Kinetics and Thermodynamics

The kinetics of a reaction quantify the rate at which the reaction proceeds. When designing a new reactor for a given conversion, a faster reaction requires a smaller volume reactor. When analyzing an existing reactor of fixed volume, a faster reaction means increased conversion. As stated previously, thermodynamics provides limits to the conversions obtainable from a chemical reaction.

23.2.1. Reaction Kinetics

The reaction rate, r_i, is defined as

$$r_i = \frac{1}{V}\frac{dN_i}{dt} = \frac{\text{moles of } i \text{ formed}}{(\text{volume of reactor})\,(\text{time})} \tag{23.6}$$

The reaction rate is an intensive property. This means that the reaction rate depends only on state variables such as temperature, concentration, and pressure, and not on the total mass of material present.

For solid catalyzed reactions, the reaction rate is often defined based on the mass of catalyst present, W:

$$r_i = \frac{1}{W}\frac{dN_i}{dt}\rho_b = \frac{1}{V}\frac{dN_i}{dt} \qquad (23.7)$$

where ρ_b is the bulk catalyst density (mass catalyst/volume reactor). The density of solid catalyst is defined as ρ_{cat} (mass catalyst particle/volume catalyst particle). So the bulk density of the catalyst, ρ_b, is defined as

$$\rho_b = (1-\varepsilon)\rho_{cat} \qquad (23.8)$$

Here, ε is the void fraction in the reactor; so $(1-\varepsilon)$ is volume of catalyst/volume of reactor.

If a reaction is an elementary step, the kinetic expression can be obtained directly from the reaction stoichiometry. For example, in Equation (23.1), if the first reaction is an elementary step, the rate expression is

$$-r_A = k_1 c_A^{\alpha} c_B^{\beta} \qquad (23.9)$$

For catalytic reactions, the rate expressions are often more complicated because the balanced equation is not an elementary step. Instead, the rate expression can be obtained by an understanding of the details of the reaction mechanism. The resulting rate expressions are often of the form

$$r_i = \frac{k_1 \prod_{i=1}^{n} c_i^{\alpha_i}}{\left[1 + \sum_{j=1}^{m} K_j c_j\right]^{\gamma}} \qquad (23.10)$$

Equation (23.10) describes a form of Langmuir-Hinshelwood kinetics. The constants (k_1 and K_j) in Equation (23.10) are catalyst specific. The constants in Equation (23.10) must be obtained by fitting reaction data.

In heterogeneous catalytic reacting systems, reactions take place on the surface of the catalyst. Most of this surface area is internal to the catalyst pellet or particle. The series of resistances that can govern the rate of catalytic chemical reaction are as follows:

1. Mass film diffusion of reactant from bulk fluid to external surface of catalyst
2. Mass diffusion of reactant from pore mouth to internal surface of catalyst
3. Adsorption of reactant on catalyst surface
4. Chemical reaction on catalyst surface
5. Desorption of product from catalyst surface
6. Mass diffusion of product from internal surface of catalyst to pore mouth
7. Mass diffusion from pore mouth to bulk fluid

Each step offers a resistance to chemical reaction. Reactors often operate in a region where only one or two resistances control the rate. For a good catalyst, the intrinsic rates are so high that internal

diffusion resistances are usually controlling.

For solid catalyst systems, reactor performance is usually controlled by resistances to mass transfer.

The temperature dependence of the rate constants in Equations (23.9) and (23.10) is given by the Arrhenius equation

$$k_i = k_o e^{-\frac{E}{RT}} \qquad (23.11)$$

where k_o is called the **pre-exponential factor**, and E is the **activation energy** (units of energy/mol, always positive). Equation (23.11) reflects the significant temperature dependence of the reaction rate. For gas-phase reactions, the concentrations can be expressed or estimated from the ideal gas law, so $c_i = P_i/RT$. This is the origin of the pressure dependence of gas-phase reactions. As pressure increases, so does concentration, and so does the reaction rate. The temperature dependence of the Arrhenius equation usually dominates the opposite temperature effect on the concentration.

As temperature increases, the reaction rate always increases, and usually significantly.

23.2.2. Thermodynamic Limitations

Thermodynamics provides limits on the conversion obtainable from a chemical reaction. For an equilibrium reaction, the equilibrium conversion may not be exceeded.

Thermodynamics sets limits on possible conversions in a reacting system.

The limitations placed on conversion by thermodynamic equilibrium are best illustrated by Example 23.1.

Example 23.1.

Methanol can be produced from syngas by the following reaction:

$$CO + 2H_2 = CH_3OH$$

For the case when no inerts are present and for stoichiometric feed, the equilibrium expression has been determined to be

$$K = \frac{X(3-2X)^2}{4(1-X)^3 P^2} = 4.8 \times 10^{-13} \exp(11{,}458/T) \qquad (E23.1)$$

where X is the equilibrium conversion, P is the pressure in atmospheres, and T is the temperature in Kelvin. Construct a plot of equilibrium conversion versus temperature for four different pressures: 15 atm, 30 atm, 50 atm, and 100 atm. Interpret the significance of the results.

The plot is shown on Figure E23.1. By following any of the four curves from low to high temperature, it is observed that the equilibrium conversion decreases with increasing temperature at constant pressure. This is a consequence of Le Chatelier's principle, because the methanol formation reaction is exothermic. By following a vertical line from low to high pressure, it is observed that the

equilibrium conversion increases with increasing pressure at constant temperature. This is also a consequence of Le Chatelier's principle. Because there are fewer moles on the right-hand side of the reaction, increased conversion is favored at high pressures.

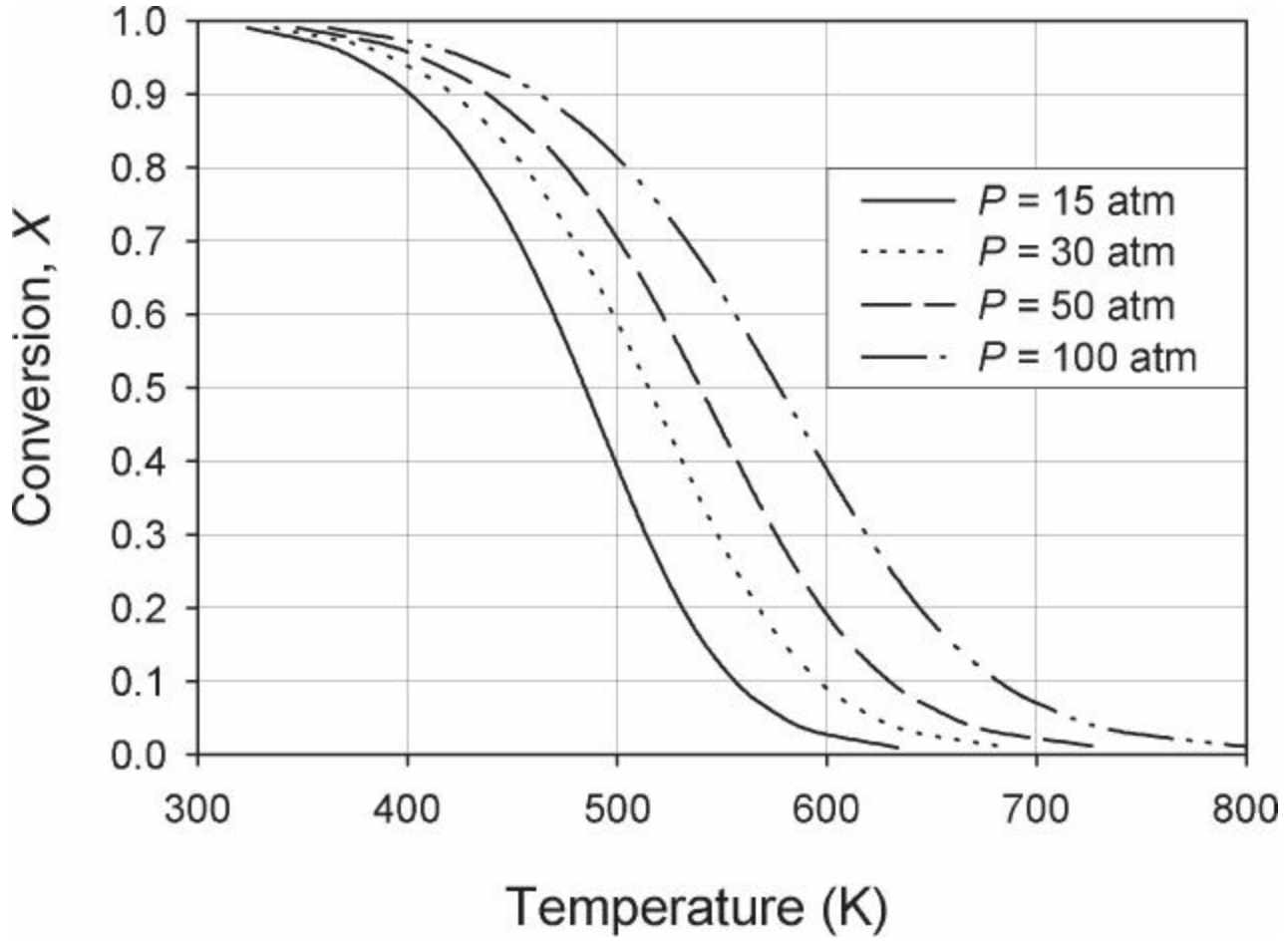


Figure E23.1. Temperature and Pressure Dependence of Conversion for Methanol from Syngas

From thermodynamic considerations alone, it appears that this reaction should be run at low temperatures in order to achieve maximum conversion. However, as discussed in Section 23.2.1, because the rate of reaction is a strong function of temperature, this reaction is usually run at higher temperatures, with low single-pass conversion, in order to take advantage of the faster kinetics. As discussed in Section 23.1, despite a low single-pass conversion in the reactor, a large overall conversion is still achievable by recycling unreacted reactants.

23.3. The Chemical Reactor

For continuous flow reactors, the two ideal models are the plug flow reactor and the continuous stirred tank reactor. In the plug flow reactor (PFR), which is basically a pipe within which the reaction occurs, the concentration, pressure, and temperature change from point to point. The performance equation is

$$\frac{V}{F_{Ao}} = \frac{\tau}{c_{Ao}} = \int_0^{X_A} \frac{dX_A}{-r_A} \qquad (23.12)$$

In the continuous stirred tank reactor (CSTR), the reactor is assumed to be well mixed, and all properties are assumed to be uniform within the reactor. The performance equation is

$$\frac{V}{F_{Ao}} = \frac{\tau}{c_{Ao}} = \frac{X_A}{-r_A} \qquad (23.13)$$

where

V = volume of the reactor

F_{Ao} = molar flow of limiting reactant A

τ = space time (reactor volume/inlet volumetric flowrate)

c_{Ao} = inlet concentration of A

X_A = conversion of A

r_A = rate of reaction of A

Equations (23.12) and (23.13) must be solved for a given rate expression to get the actual relationship between the indicated parameters. However, several generalizations are possible. The reactor volume and conversion change in the same direction. As one increases, so does the other; as one decreases, so does the other. As the reaction rate increases, the volume required decreases, and vice versa. As the reaction rate increases, the conversion increases, and vice versa. It has already been discussed how temperature, pressure, and concentration affect the reaction rate. Their effect on conversion and reactor volume is derived from their effect on reaction rate. Example 23.2 illustrates these qualitative generalizations.

Example 23.2.

Discuss qualitatively the effect of temperature and pressure on the space time and conversion in a chemical reactor.

Gas-Phase Reaction: From the Arrhenius equation in Equation (23.11), the reaction rate constant increases exponentially with temperature. From the ideal gas law, the concentration decreases less drastically. From Equations (23.12) and (23.13), at constant pressure, if the reaction rate increases, at constant conversion, a smaller reactor volume (and space time) is required. At constant reactor volume and space time, the conversion increases.

From a typical reaction rate expression such as Equation (23.9), as the pressure increases, so do the concentration and the reaction rate. Therefore, the same trends are observed as with temperature. However, the quantitative effect is not as great, because the concentration dependence on pressure is not exponential.

Liquid-Phase Reaction: For a liquid-phase reaction, temperature and pressure do not affect concentration. Therefore, there is no effect of pressure on reactor performance for a liquid-phase reaction. Because the temperature effect is determined by the Arrhenius equation only, the reaction rate increases exponentially with temperature.

The PFR is a hypothetical system. PFRs are elementary models for packed-bed reactors. The PFR model excludes the effects of axial mixing resulting from molecular movement and fluid turbulence while assuming radial mixing is complete. This mixing takes place between adjacent fluid elements of approximately the same conversion. Reactors approximating PFRs are often built using many small-diameter tubes (less than 3 in) of significant length (20 to 30 ft) operated at high fluid velocity with small space times. This minimizes axial fluid mixing, limits radial temperature profiles, and provides needed heat transfer area. Tubes are arranged in a bundle characteristic of those found in many heat exchangers. If heat exchange is not desired in the reaction zone, a single or series of larger-diameter

packed beds can be used.

The CSTR is also a hypothetical system in which there is perfect mixing so that temperature, pressure, concentration, and reaction rate are constant over the reactor volume. Reactors approximating CSTRs are used for liquid-phase reactions. This represents a theoretical limit because perfect mixing can only be approached. Transit time for fluid elements varies. The exit stream is at the same temperature, pressure, and conversion as the reactor contents. Feed is mixed with the reactor contents that have a high conversion. As a result, the CSTR requires a higher volume than a PFR when operated isothermally at the same temperature and conversion for simple, elementary reactions.

Reactors are modeled using different combinations and arrangements of CSTRs and PFRs. Intermediate degrees of mixing are obtained that can be used to model various real reactor systems. Some of these models are shown in Figure 23.2 and described below.

System (a) is a PFR for an exothermic reaction. The concentration and temperature vary from point to point in the reactor. This model is used to simulate the cumene reactor in Appendix C.

System (b) is a CSTR. The temperature and concentration are constant within the reactor.

System (c) consists of a PFR and CSTR in parallel. By increasing the ratio of CSTR feed rate to PFR feed rate, the degree of mixing is increased. By increasing the ratio of PFR feed rate to CSTR feed rate, dead space (regions that are not well mixed) in a CSTR can be simulated.

System (d) consists of a series of CSTRs in series. The degree of mixing is less than that in a single CSTR. Although each reactor is completely mixed, there is no mixing between each section. In the limit of an infinite number of CSTRs in series, PFR behavior is approached.

System (e) consists of an isothermal PFR with a bypass stream. In a fluidized bed, solid catalyst is circulated within the bed; however, the fluid moves through the bed essentially in plug flow. Maldistribution of fluid, due to the formation of bubbles and voids, and channeling may cause some fluid to bypass the catalyst. This model is used in catalytic fluidized bed applications or in any other application where the solid does not react. A portion of the reactants forms an emulsion phase with little mixing (plug flow). The remaining fluid forms bubbles that move upward at a higher velocity, contact only a small portion of the solid catalyst, and do not react as much as in the emulsion phase. An important feature of the fluidized bed is that it operates isothermally as a result of the mixing of the solids. The model shown in System E is a crude approximation of what happens in a real fluidized bed, but it predicts the trends found in fluidized beds. This model is used to simulate the acrylic acid reactor in Appendix B.

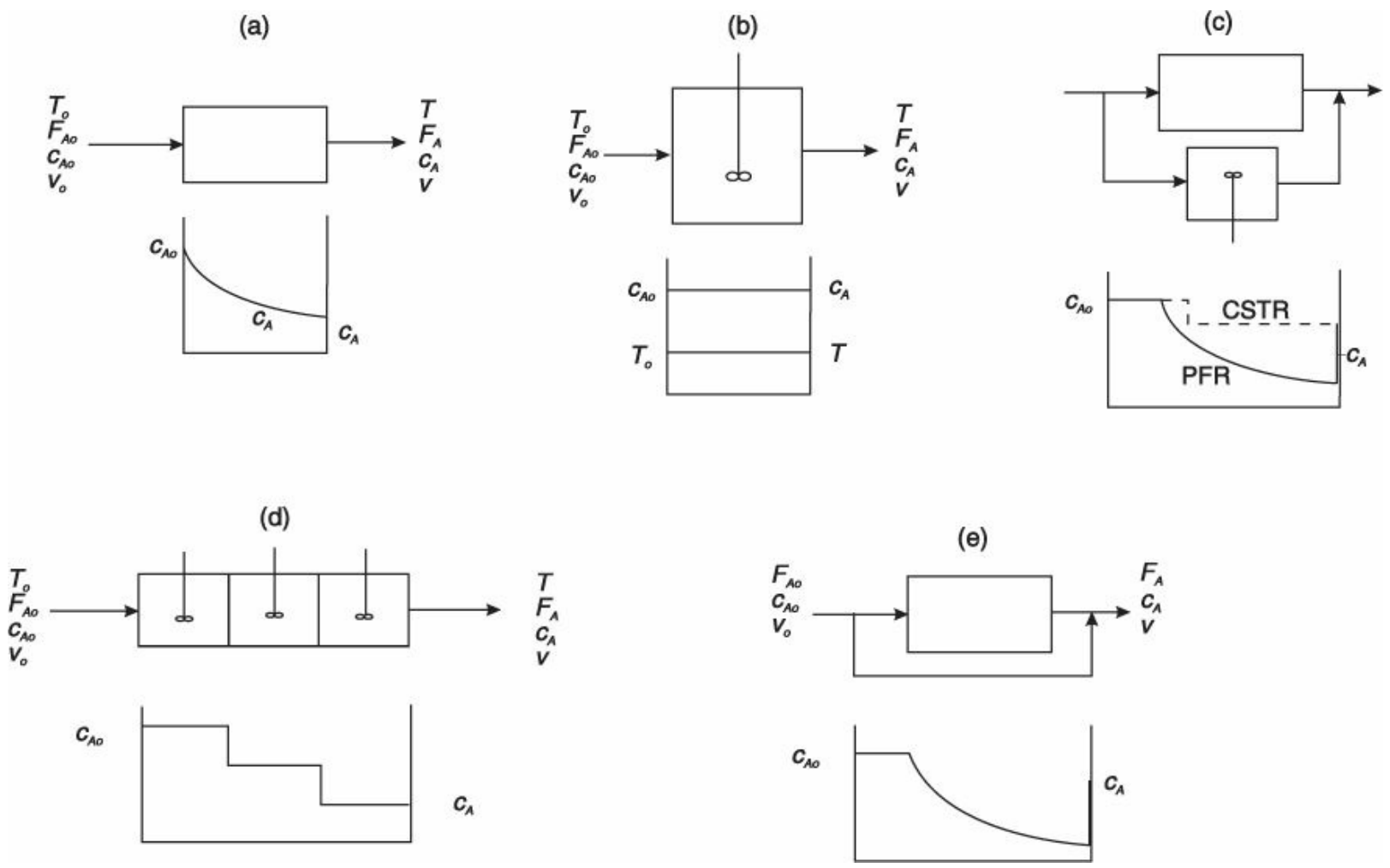


Figure 23.2. Mixing Patterns with Characteristic Concentration Profiles

As the reactor model becomes more complex, it becomes more difficult to solve Equations (23.12) and (23.13) to predict reactor performance. Because process simulators are already programmed to do this, they are a logical choice for analyzing reactor performance, especially because real reactors must be simulated in the context of an entire process. For the chemical reactor, the required input data include identification of the dominant reactions that take place, the form of the reaction rate, and values of the kinetic constants. All these may change with operating conditions, and a given set of values applies only to a limited range of operations. They must be obtained experimentally. If the experimental data are flawed or the simulation operating conditions are outside the range of the experimental studies, the answer obtained can lead to poor prediction of reactor performance. The computer can do the calculations but is unable to recognize the reliability of the input.

Example 23.3. summarizes the concepts presented thus far in this chapter.

Example 23.3.

Consider the reaction scheme given in Equation (23.1) where P is the desired product, with both U and V as undesired by-products. Assume that Equation (23.1) represents elementary steps, that $a = b = p = u = \upsilon = 1$, that $\beta = 2$, and that the activation energies for the reactions are as follows: $E_1 > E_2 > E_3$.

a. For the case where $k_2 = 0$, what conditions maximize the selectivity for P?

b. For the case where $k_3 = 0$, what conditions maximize the selectivity for P?

Solution

a. For this case, from Equation (23.4), the selectivity is written as

$$\eta = \frac{r_P}{r_V} = \frac{k_1 c_A c_B}{k_3 c_B^2} = \frac{k_1 c_A}{k_3 c_B} \qquad \text{(E23.3a)}$$

There are several ways to maximize the selectivity. Increasing c_A/c_B increases the selectivity. This means that excess A is needed and that B is the limiting reactant. Many reactions are operated with one reactant in excess. The reason is usually to improve selectivity as shown here. Because pressure affects all concentrations equally, it is seen that pressure does not affect the selectivity here. Temperature has its most significant effect on the rate constant. Because the activation energy for rxn 1 is larger than that for rxn 3, k_1 is more strongly affected by temperature changes than is k_3. Therefore, increasing the temperature increases the selectivity. In summary, higher temperatures and excess A maximize the selectivity for P.

b. For this case, the selectivity is written as

$$\eta = \frac{r_P}{r_U} = \frac{k_1 c_A c_B - k_2 c_P}{k_2 c_P} = \frac{k_1 c_A c_B}{k_2 c_P} - 1 \qquad \text{(E23.3b)}$$

Because pressure appears to the second power in the numerator and to the first power in the denominator (it is in each concentration term), increasing the pressure increases the selectivity. Because the activation energy for rxn 1 is larger, increasing the temperature increases the selectivity. Increasing both reactant concentrations increases the selectivity, but increasing the concentration of Component P decreases the selectivity. The question is how the concentration of Component P can be kept to a minimum. The answer is to run the reaction at low conversions (small space time, small reactor volumes). Quantitatively, the selectivity in Equation (23.3b) is maximized. Intuitively, because this is a series reaction with the desired product intermediate in the series, a low conversion maximizes the intermediate product and minimizes the undesired product. This can be illustrated by the concentration profiles obtained by assuming that these reactions take place in a PFR, as shown in Figure E23.3. It is seen that the ratio of P/U is at a maximum at low reactor volumes, which corresponds to low conversion. Therefore, increasing the temperature and pressure both increases the selectivity for Component P. Running at low conversion probably does more to increases the selectivity than can be accomplished by manipulating temperature and pressure alone. However, there is a trade-off between selectivity and overall profitability, because low conversion per pass means very large recycles and larger equipment.

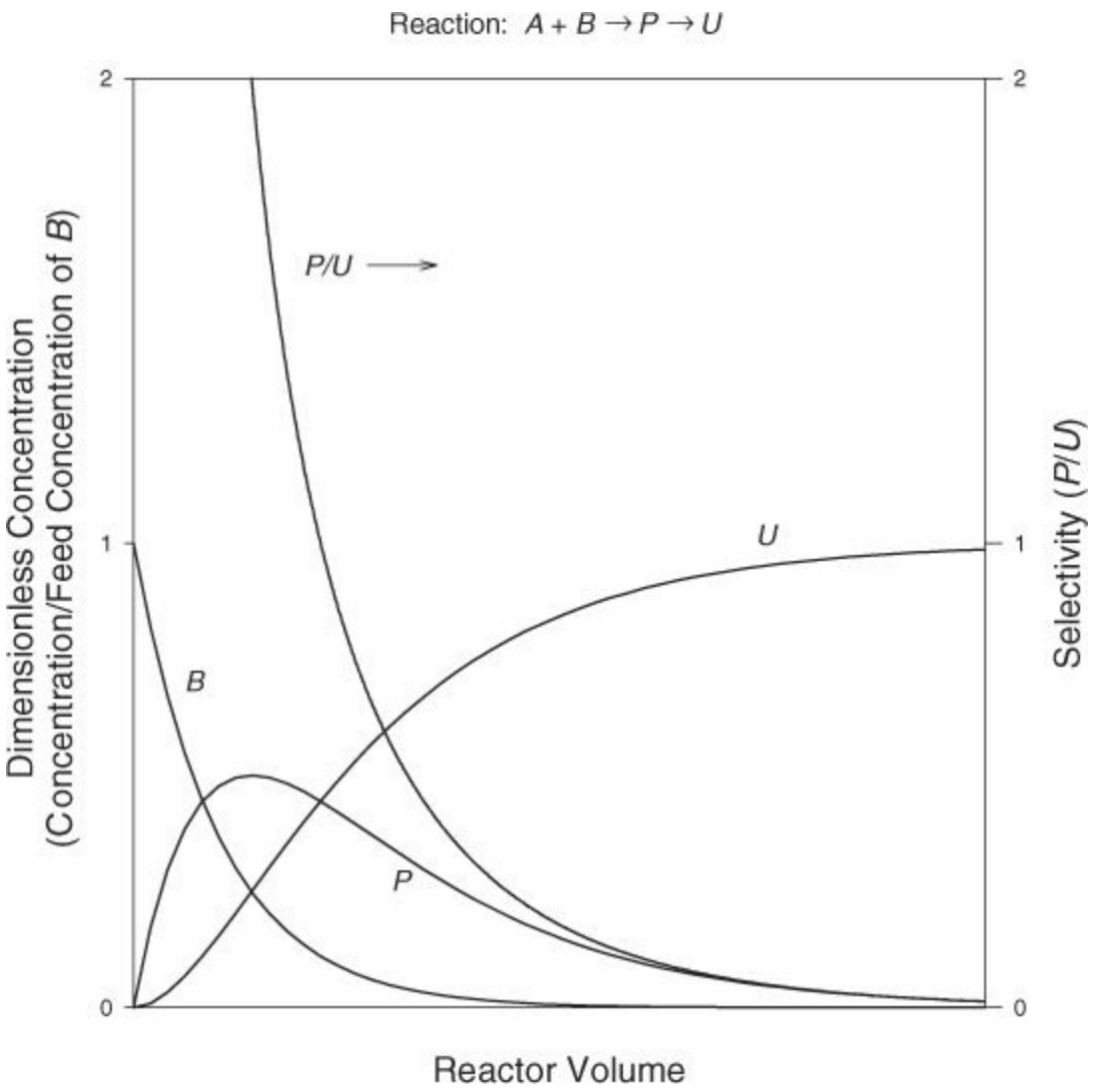


Figure E23.3. Concentration Profiles in a PFR for Series Reaction

23.4. Heat Transfer in the Chemical Reactor

Chemical reactions are either exothermic (release heat) or endothermic (absorb heat). Therefore, heat transfer in reactor systems is extremely important. For exothermic reactions, heat may have to be removed so that the temperature in the reactor does not increase above safe limits. For endothermic reactions, heat may have to be added so that the reaction will occur at an acceptable rate.

Reactor performance is often limited by the ability to add or remove heat.

Most industrially significant chemical reactions are exothermic. Highly exothermic reactions, especially in a reactor behaving like a PFR, can be dangerous if the rate of heat removal is not sufficient. For a rate expression such as Equation (23.9), the concentration of reactants is largest at the entrance to the reactor. The reaction at the entrance generates heat if the reaction is exothermic. The concomitant increase in temperature increases the reaction rate even further, which increases the temperature further, and so forth. Therefore, it is possible to have large temperature increases, called **hot spots.** The large temperature increase can be offset by removing heat from the reactor. This can cause radial temperature gradients, with severe hot spots near the center of the tube. Hot spots can damage and deactivate catalyst particles. In the extreme case, if the rate of heat removal is not sufficient to offset the rate of heat production by reaction, the temperature may increase rapidly,

causing damage to the reactor and its contents or an explosion. This is called **runaway reaction**. Reactor temperature profiles illustrating the situation leading to runaway reaction are illustrated in Figure 23.3(b).

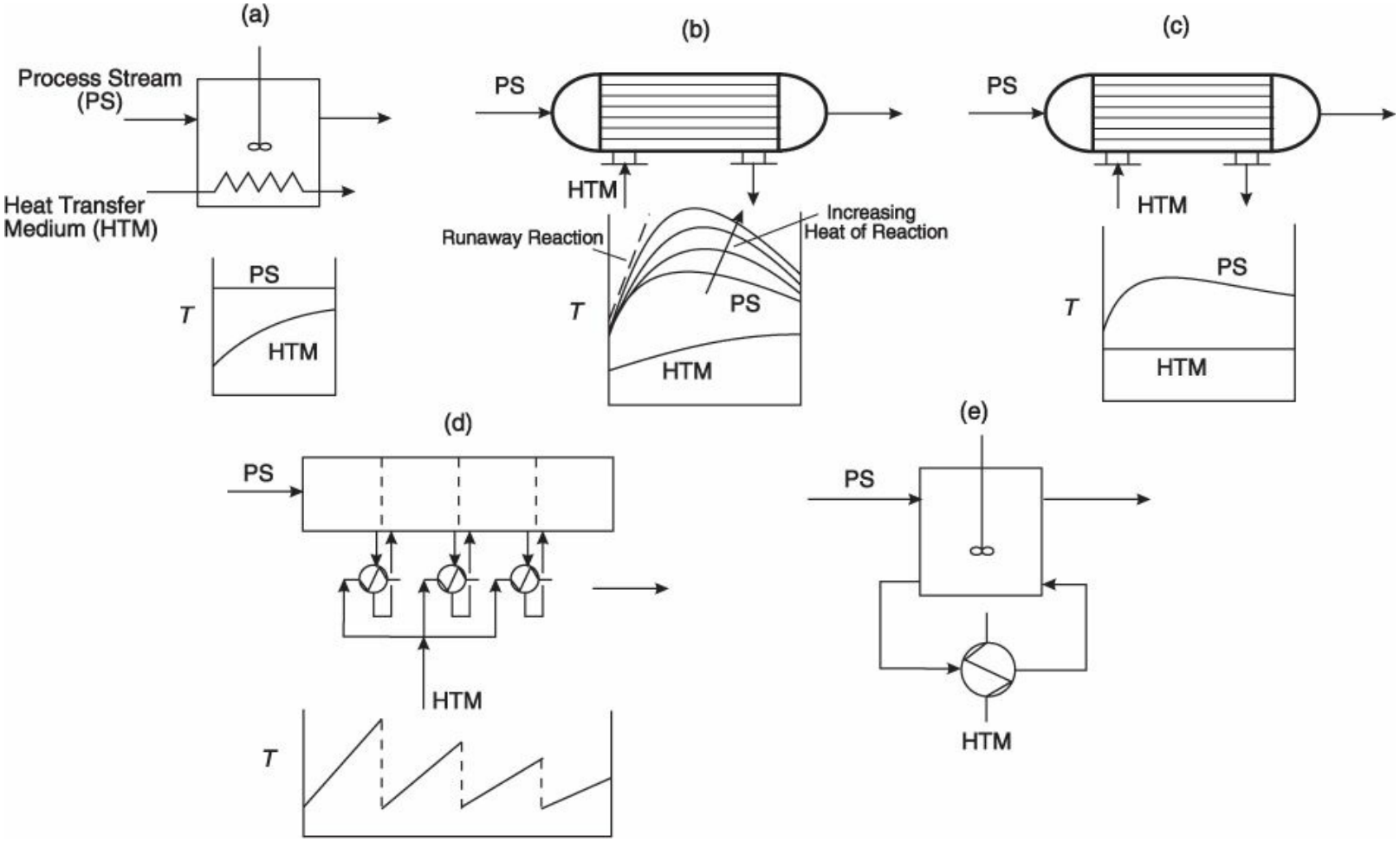


Figure 23.3. Alternative Heat-Exchange Systems for Reactors Shown for Exothermic Reaction: a–c, Internal Heat Exchanger; d–e, External Heat Exchanger

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Beware of exothermic reactions! Runaway reaction is possible if there is insufficient heat removal.

For endothermic reactions, heat must be added to the reactor. **Cold zones** are possible based upon the same logic as for the hot spots for exothermic reactions. However, if there is insufficient heat addition to an endothermic reaction, the reaction will be quenched. Therefore, endothermic reactions are inherently safe.

There are many methods used to avoid hot spots in a reactor with an exothermic reaction. Some of these methods are as follows:

1. **Run Heat Transfer Medium Cocurrently:** The heat transfer medium enters at its lowest temperature. By matching this low temperature with the highest temperature zone in the reactor, the temperature gradient is largest at the reactor entrance, providing more heat removal.
2. **Use Inert Solid:** By randomly packing the bed with inert solid (no catalytic activity), the heat released per unit volume of reactor is reduced, thereby minimizing hot spots. This results in a larger reactor.
3. **Use Catalyst Gradients in Reactor:** This is similar to item 2. Here, a larger fraction of inert

solid is used where hot spots are anticipated. This minimizes hot spots but also results in a larger reactor.

4. **Use a Fluidized Bed:** Due to the mixing behavior in a fluidized bed, isothermal operation is approached.

Both internal and external heat exchangers can be used to exchange heat with a reactor. In the internal systems (Figure 23.3[a–c]), the heat transfer area is in contact with the reacting fluid. Quite often, this is like a shell-and-tube heat exchanger, with the catalyst most often placed in the tubes. In the external systems (Figure 23.3[d–e]), reaction fluid is withdrawn from the reactor, sent to a heat exchanger, and then returned to the reactor.

a. **CSTR with Single-Phase Heat Transfer Medium:** The temperature profile is similar to that for the condensation of a single component vapor. The volume taken up by the heat exchanger increases the reactor volume. The mixing intensity of the reacting fluid may be reduced, and the potential for local nonisothermal behavior close to the heat-exchanger surfaces exists.

b. **PFR with Single-Phase Heat Transfer Medium:** Temperature on the process side goes through a maximum.

c. **PFR Heat Transfer Medium Boils:** Temperature on the utility side remains constant and goes through a maximum on the process side.

d. **Adiabatic PFR with Heat Removal between Stages:** This configuration is usually used for exothermic reactions that do not have extremely large heats of reaction. The reaction proceeds adiabatically with a temperature rise, and fluid is removed periodically to be cooled.

e. **External Heat Exchanger in CSTR:** Fluid in the reactor is circulated through an external heat exchanger.

In order to solve a problem involving a chemical reactor with heat transfer, the following equations must be solved:

1. Reactor performance equation, such as Equations (23.12) and (23.13)
2. Energy balance on reaction side
3. Energy balance on heat transfer medium side
4. Heat transfer performance equation ($Q = UA\Delta T_{lm}$)
5. Pressure drop in packed bed (Ergun equation)

Therefore, as the heat transfer configuration becomes more complex, it becomes very difficult to solve the necessary equations to predict reactor performance. Because process simulators are already programmed to do this, they are a logical choice for analyzing reactor performance with heat transfer.

For a chemical reactor with heat transfer, in addition to the input discussed earlier, the required input data must include the heat transfer coefficient, the heat transfer area, the length and diameter of tubes, and the number of tubes. The output obtained is the temperature, pressure, and concentration of each component at each point in the reactor.

Heterogeneous catalytic reactions are even more difficult to simulate. The major resistance to reaction can change from chemical reaction to external diffusion or to pore diffusion within a single reactor. Stream temperatures are not necessarily the temperatures of the catalyst surface where the reaction takes place. Large temperature gradients may exist in the radial direction and within the catalyst particles. Although they do not consider these important factors, process simulators can often

be used to obtain approximate solutions.

23.5. Reactor System Case Studies

This section contains case studies involving reactors from process flow diagrams presented throughout this text. The process changes presented illustrate typical problems a chemical engineer working in production may face on a routine basis.

All studies presented contain three parts:

Part A: A statement of the problem.

Part B: A solution to the specific problem, which includes discussion of the strategy used in the solution.

Part C: A discussion of the significance of the solution to a wider range of applications. Figures showing process response to important process variables are developed and used to reveal trends that yield insight into the problem. These performance curves provide better understanding of reactor behavior. They are also used as a guide to develop alternative problem solutions.

The availability of computers and computer software permits process simulation. Once the process is simulated, variables are easily varied to discover important performance characteristics that can be plotted over a wide range of operating conditions.

23.5.1. Replacement of Catalytic Reactor in Benzene Process

Problem. The catalyst in our benzene reactor has lost activity and must be replaced. The benzene process presented in Chapter 1 (Figure 1.5) is used to produce benzene. The reaction is carried out in an adiabatic PFR. Because of the cost of periodic catalyst replacement, it has been suggested that the catalytic reactor system could be replaced with a noncatalytic adiabatic PFR system that might be less costly. The new system is to match the input/output conditions of the current system so that the remainder of the plant will operate with little, if any, modification. You are asked to investigate the merits of this suggestion by identifying major cost items. Table 23.1 provides reactor information based on experimental studies on the toluene/benzene reaction.

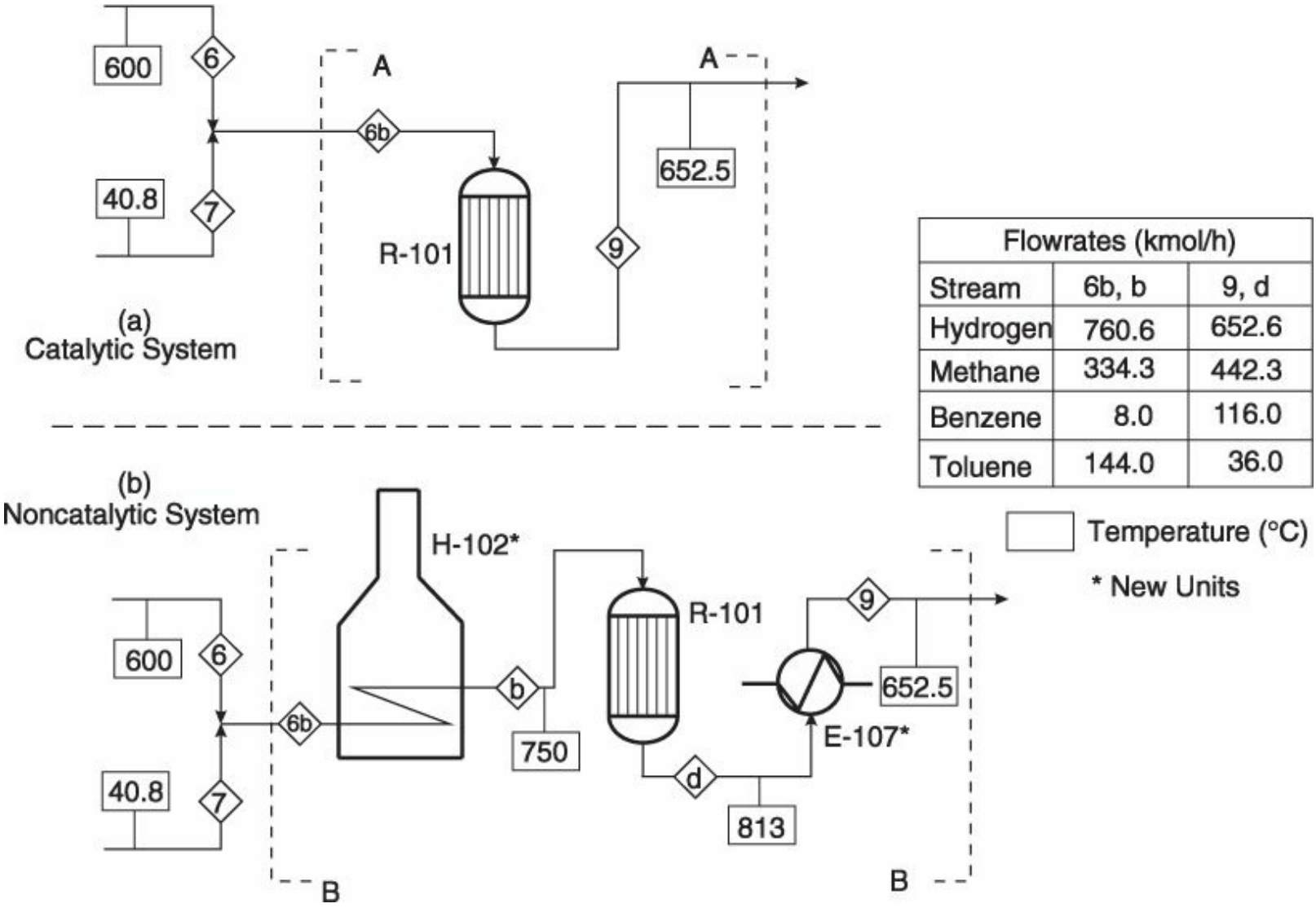
Table 23.1. Findings from Experimental Studies on Dealkylation of Toluene [1]

1. Reaction rate (mol/liter reactor s)	$-r_{tol} = 3.0 \times 10^{10} \exp(-25{,}164/T)\, c_{tol} c_H^{0.5}$
2. Temperature range	700–950°C
3. Carbon formation	None observed < 850°C with ratio of H_2/Tol > 1.5
4. Selectivity	Benzene/Unwanted > 19/1 with toluene conversion < 0.75
5. H_2/toluene	>2
6. By-product yield W = mass of all by-products/mass feed	W(Mass % of feed) = $1.0 \times 10^8\, (\theta/b) \exp(-25{,}667/T)$ where θ is the residence time (in seconds) and b is the H_2/toluene ratio
7. Observed components in output	Hydrogen, methane, toluene, various diphenyls

T in K, c in mol/liter.

Figure 23.4(a) provides a flow diagram of the current reactor taken from Figure 1.5. A-A identifies

the boundaries of the reactor system to be replaced. Flowrates and stream temperature and pressure at these boundaries are given.



Flowrates (kmol/h)		
Stream	6b, b	9, d
Hydrogen	760.6	652.6
Methane	334.3	442.3
Benzene	8.0	116.0
Toluene	144.0	36.0

Figure 23.4. Reactor Systems for Production of Benzene from Toluene

The dominant chemical reaction at plant operating conditions is

$$\underset{\text{toluene}}{C_7H_8} + \underset{\text{hydrogen}}{H_2} = \underset{\text{benzene}}{C_6H_6} + \underset{\text{methane}}{CH_4}$$

Reactor conversion, $X_{toluene} = 1 - (36.1/144.0) = 0.749$. The amount of by-product formed by side reaction is negligible; however, the small amounts of carbon formed can deposit on the catalyst surface.

Solution. The reactor volume calculated for a noncatalytic adiabatic PFR using the kinetics expression given in Table 23.1 that met the conditions shown in Figure 23.4(a) is 257 m^3 (7800 ft^3). This is six times as great as the current catalytic reactor (41.5 m^3; see Table 1.7).

Intuitively, the reactor volume can be reduced by increasing the pressure and/or temperature in the new reactor system. Increasing the pressure increases the concentrations in the rate expression, and increasing the temperature increases the rate constant. This requires that a gas compressor and/or a heat exchanger (additional fired heater) be added to the new reactor system.

Installing an additional fired heater that increases the feed temperature to 750°C was also analyzed. The calculated reactor size is about 5 m^3 and the outlet temperature is 814°C.

An evaluation of the preliminary findings for the noncatalytic reactor configuration shows the following:

1. Using the same inlet conditions as for the catalytic reactor (inlet temperature 588°C),
   a. Extrapolation of the data in Table 23.1 is uncertain. This is because the reaction rate expression is extrapolated outside the region of experimental data (see item 1 of Table 23.1).
   b. The predicted reactor size is much larger than that of the current reactor.
2. At increased temperature (inlet temperature 750°C),
   a. The reaction rate is known from experimental data.
   b. The reaction volume is much smaller than in the current reactor.
   c. The temperature, H_2/toluene ratio, and conversion are all in a range that gives high benzene selectivity.
3. Increasing reactor feed pressure: This is considered an expensive option due to gas compression costs and was not evaluated.

The noncatalytic replacement system is shown in Figure 23.4(b) as region B-B. It is a more complicated system. Higher feed temperature requires the addition of another fired heater before the reactor and a gas cooler following the reactor. (Heat integration might be another alternative.) Major capital costs are required for the reactor, fired heater, and cooler. Materials of construction for the reactor are more expensive at the higher temperature (at the exit temperature of 814°C, a reactor vessel would glow red). Fuel for the fired heater increases operating cost. The economically optimum reactor temperature that considered these items could be determined if needed.

Unless the cost of catalyst is extremely high, replacement of the catalytic reactor with a noncatalytic system does not appear to be an attractive option.

Discussion. It is observed that the low-temperature reactor (at the temperature of the catalytic reaction) was very large, a result obtained by assuming that it is valid to extrapolate the data in Table 23.1 outside the stated temperature range. Assuming the data to be accurate in the low temperature range, reasons a large reactor was obtained can be investigated.

Several important factors considered in selecting a chemical reactor are revealed in this case study. Normally the advantages of a catalytic over a noncatalytic reactor are reduction in operating temperature and pressure and improvement in product selectivity.

In this case study, the catalyst reduced the temperature and pressure requirements, as expected. However, high selectivity for the desired product could be obtained from both the catalytic and noncatalytic reactors.

Carbon is a common by-product formed during organic reactions carried out in high-temperature reactors. It is most significant in catalytic reactors where carbon forms on the catalyst surface and reduces activity. High hydrogen concentrations discourage carbon formation. This helps explain the high H_2-to-toluene ratio of 5:1 used in the catalytic system compared to the lower value of 2.0 required for the noncatalytic reactor.

Equilibrium constants for the reactions involving the components found in the laboratory studies on the benzene reaction are published [2]. The primary by-product at high temperatures is diphenyl, formed by the following reaction:

$$\underset{\text{benzene}}{2C_6H_6} = \underset{\text{diphenyl}}{C_{12}H_{10}} + \underset{\text{hydrogen}}{H_2}$$

At equilibrium, excess H_2 increases the toluene conversion, decreases diphenyl conversion, and improves benzene selectivity. This trend is assumed to hold for nonequilibrium conditions, which suggests that high excess H_2 be used.

Increasing the reaction temperature decreases the equilibrium constant of the benzene reaction, because the main reaction is exothermic and increases the equilibrium constant of the diphenyl reaction because the side reaction is endothermic. As a result, the selectivity decreases and the raw material costs increase.

In our system, any diphenyl present in the reactor effluent, Stream 9, would be largely removed in the separation section and recycled with the toluene to the reactor. The concentration of diphenyl in the reactor feed, Stream b, would be increased. When sufficient diphenyl is introduced in Stream b to provide the equilibrium concentration, little diphenyl is formed in the reactor. This retains a high benzene selectivity at higher reactor temperatures.

For a new design, it may be desired to consider scenarios to increase the reaction rate for the noncatalytic reaction. Figure 23.5 shows the reaction rate, temperature, and toluene mole fraction plotted against the reactor volume for the original feed temperature. This figure shows that low reaction rates exist at the feed end of the reactor, with rapidly falling reaction rates at the reactor exit. The reactor temperature increases over the volume of the reactor. Figure 23.5 identifies steps to take that would improve reactor performance. Increased performance can be obtained by

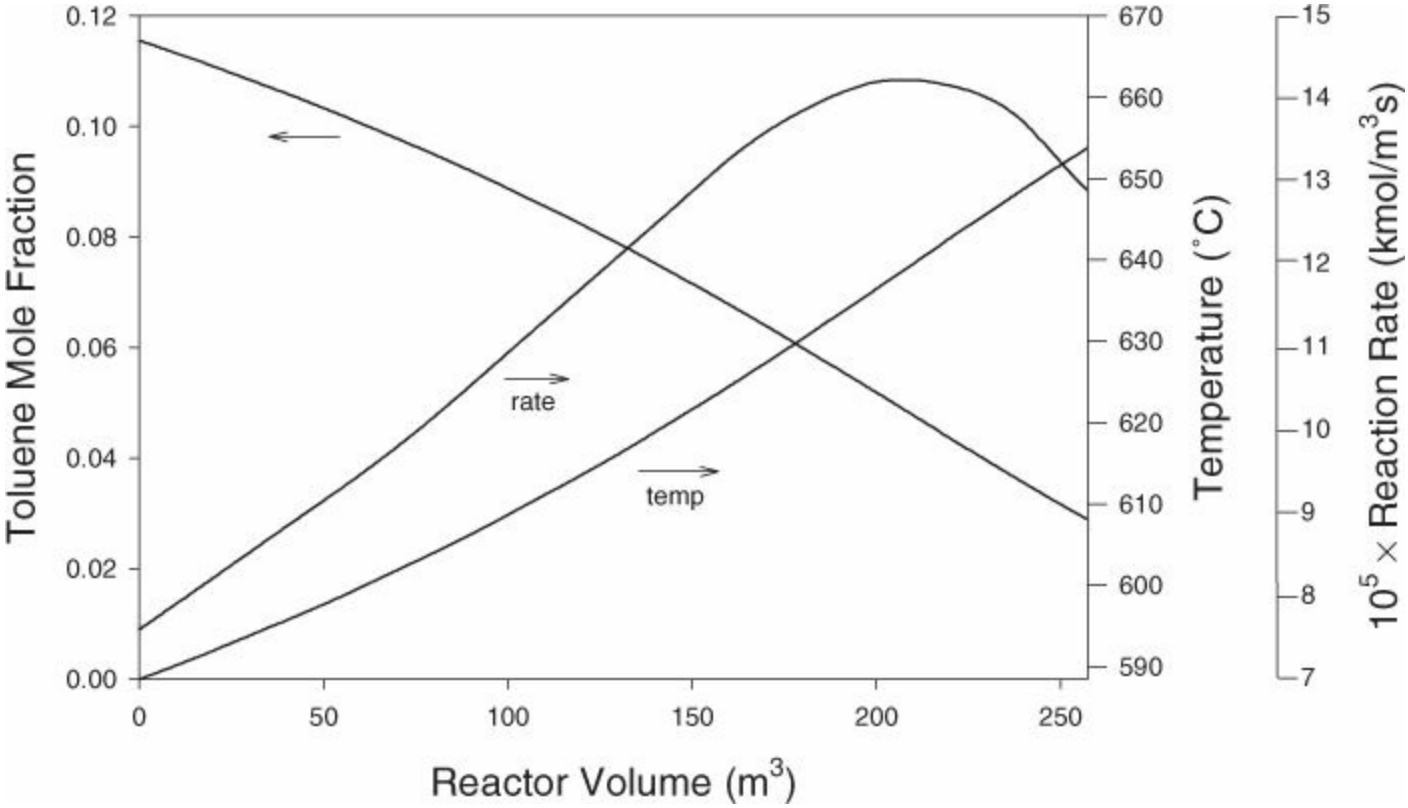


Figure 23.5. Behavior of Benzene PFR at Original Feed Temperature (585°C)

a. Elimination of the low reaction rate region at the beginning of the reactor. The low reaction rates are due to the low reaction rate constant, *k*, at low temperature. Increasing the feed temperature would increase reaction rate in this section.

b. Avoidance of operating in the region at the end of the reactor where the reaction rate falls rapidly. The falling reaction rate results from the lowering of toluene concentrations at high

conversions. This region can be avoided by operating at lower reactor conversion (and higher recycle rates of unreacted feed).

This case study demonstrates that a dramatic decrease in the reactor volume required for a given conversion results from an increase in feed temperature.

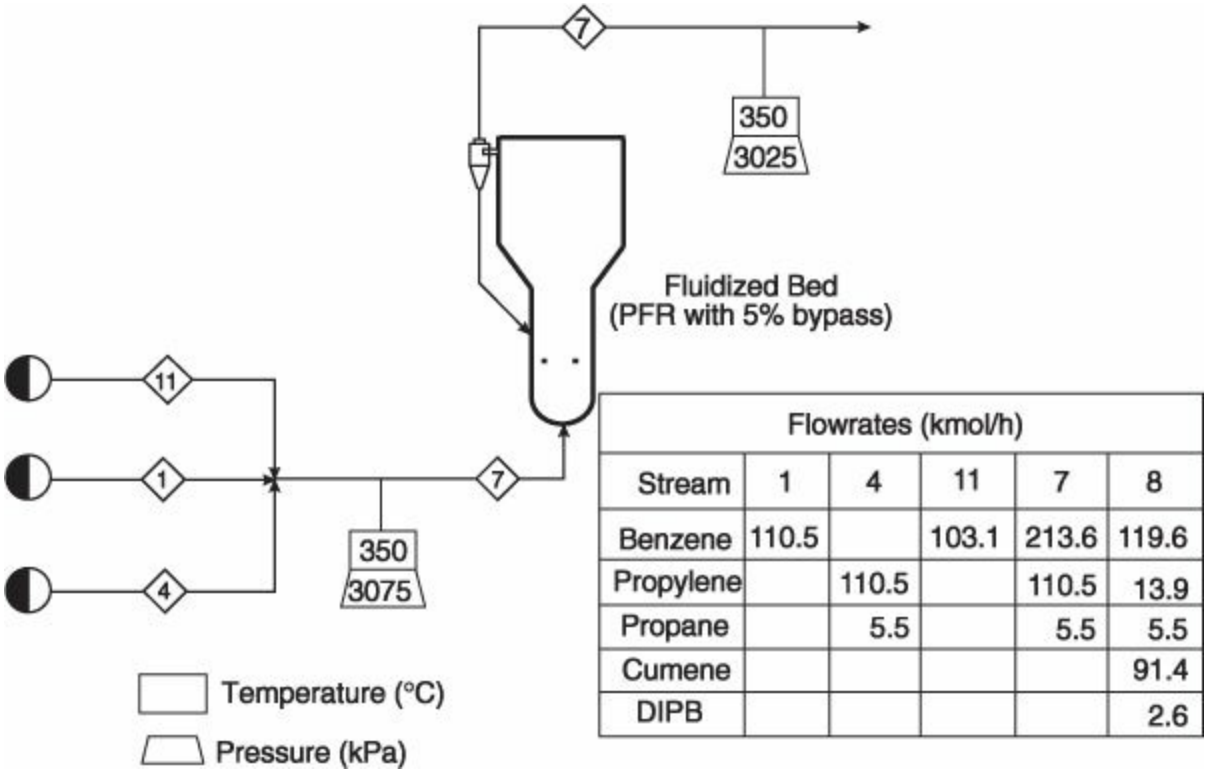
One could consider replacing the current reactor with an adiabatic CSTR. The reaction rate throughout the reactor would be constant at reactor exit conditions. This reaction rate is shown in Figure 23.5. The average reaction rate for the PFR is less than that of the CSTR, and the volume for a CSTR is less than that of the PFR. The elimination of the low-temperature region in the PFR overcomes the effect of lower toluene concentration in the CSTR.

The conclusion of this case study is that replacing the reactor with a non-catalytic PFR is not an attractive option. This may not be the conclusion if a new plant were to be built. In a new plant, the excess hydrogen could be substantially reduced. This would increase the toluene concentration and reduce the amount of recycle. Lower reactor conversions could be considered. Higher temperatures, higher toluene concentrations, and lower conversions would all contribute to a smaller reactor.

23.5.2. Replacement of Cumene Catalyst

Problem. Your company produces cumene. At your plant, the shell-and-tube, packed-bed reactor shown in Appendix C, Figure C.8, is used. At other plants owned by your company, proprietary fluidized bed reactors providing low gas bypass are used. The remainder of the process is identical at all locations. Your supplier has informed you that it has developed a new cumene catalyst that will improve fluidized bed reactor performance. The new catalyst is supported on the same inert material as the old catalyst. Therefore, the fluidizing properties are identical to those of the old catalyst. You are assigned the task of verifying claims of improved performance and identifying changes in operating conditions that would maximize the improvement this new catalyst could provide.

Figure 23.6 provides the operating conditions for this base case. In addition to the general process information provided with the process flow diagram (see the cumene flow diagram, Figure C.8, in Appendix C), the following specific background information is provided for your plant.



Flowrates (kmol/h)					
Stream	1	4	11	7	8
Benzene	110.5		103.1	213.6	119.6
Propylene		110.5		110.5	13.9
Propane		5.5		5.5	5.5
Cumene					91.4
DIPB					2.6

Figure 23.6. Base-Case Flow Diagram of Cumene Reactor System

In the first stage of a plant start-up, the plant is operated without the recycle stream, Stream 11. Benzene normally provided by this recycle stream is added with the feed stream. In the initial plant start-up, the plant operated for a substantial period without the recycle. During this time, the plant was operated at a range of temperatures, pressures, and excess benzene rates. These data were used to determine effective kinetics that are presented in Table 23.2. The active reactor volume is 7.88 m^3. It was found that the fluidized bed could be modeled accurately over a narrow range of superficial velocities as a PFR with 5% bypass.

Table 23.2. Kinetic Constants Obtained for Hypothetical Cumene Catalysts

Catalyst	Current	New
Reaction Rate (mol/liter s)		
Reaction 1 (cumene formation)	$r_1 = k_1 c_p c_b$	$r_1 = k_1 c_p c_b$
Reaction 2 (DIPB formation)	$r_2 = k_2 c_p c_c$	$r_2 = k_2 c_p c_c$
Rate Constant (liter/mol s)		
Reaction 1	$k_1 = 3500\exp(-6680/T)$	$k_1 = 2.8 \times 10^7 \exp(-12{,}530/T)$
Reaction 2	$k_2 = 290\exp(-6680/T)$	$k_2 = 2.32 \times 10^9 \exp(-17{,}650/T)$

T has the units of K, liters refers to liters of reactor.

The information from the open system (no recycle) was used to establish a base case. At each plant start-up following a catalyst change, the plant is run at base-case conditions. If the same reactor performance is not obtained, the catalyst and flow pattern in the reactor are examined. Problems of reactor performance are resolved before continuing plant start-up.

Solution. The dominant reactions involved within the cumene plant are

$$\underset{\text{propylene}}{C_3H_6} + \underset{\text{benzene}}{C_6H_6} \xrightarrow{k_1} \underset{\text{cumene}}{C_9H_{12}} \qquad \text{Reaction 1}$$

$$\underset{\text{propylene}}{C_3H_6} + \underset{\text{cumene}}{C_9H_{12}} \xrightarrow{k_2} \underset{\text{p-diisopropyl benzene}}{C_{12}H_{18}} \qquad \text{Reaction 2}$$

The kinetics for the catalyst are provided in Table 23.2.

In this analysis, to ensure a low bypass ratio (5%), the superficial gas velocity was held constant at the base-case conditions. For higher reactor temperatures, the molar flowrate to the reactor was decreased slightly so as to maintain the same superficial velocity. This was done by retaining the base-case flows of Stream 11 and Stream 4, and lowering the excess benzene Stream 1. The fluidized bed was assumed to behave as an isothermal PFR with a 5% bypass stream. This is shown in Figure 23.7. Some of the simulation results are shown in Figures 23.8 and 23.9. Figure 23.8 presents the production of cumene obtained for the current and new catalyst for temperatures ranging from 350°C to 410°C. The new catalyst is more sensitive to a change in temperature than is the current catalyst. At the base-case temperature, the new catalyst produces only 81 kmol/h, point "a," compared with 91 kmol/h, point "b," for the current catalyst. At a reactor temperature of 361°C, the new catalyst produces the same amount of cumene, point "c," as the old catalyst operating at the base-case temperature. At 367°C, both systems produce the same amount of cumene, point "d." The maximum

production rate of 101 kmol/h is obtained for the new catalyst at about 390°C, point "e." The current catalyst provides a maximum cumene production of 96 kmol/h, point "f."

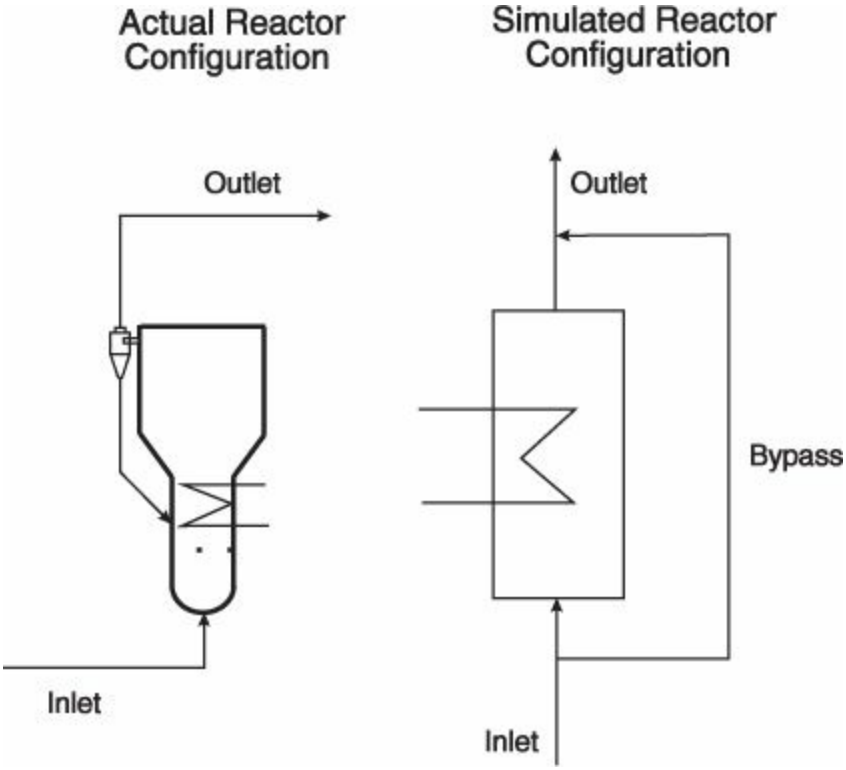


Figure 23.7. Fluidized Bed Reactor Showing Configuration (5% Bypass) Used for Simulation

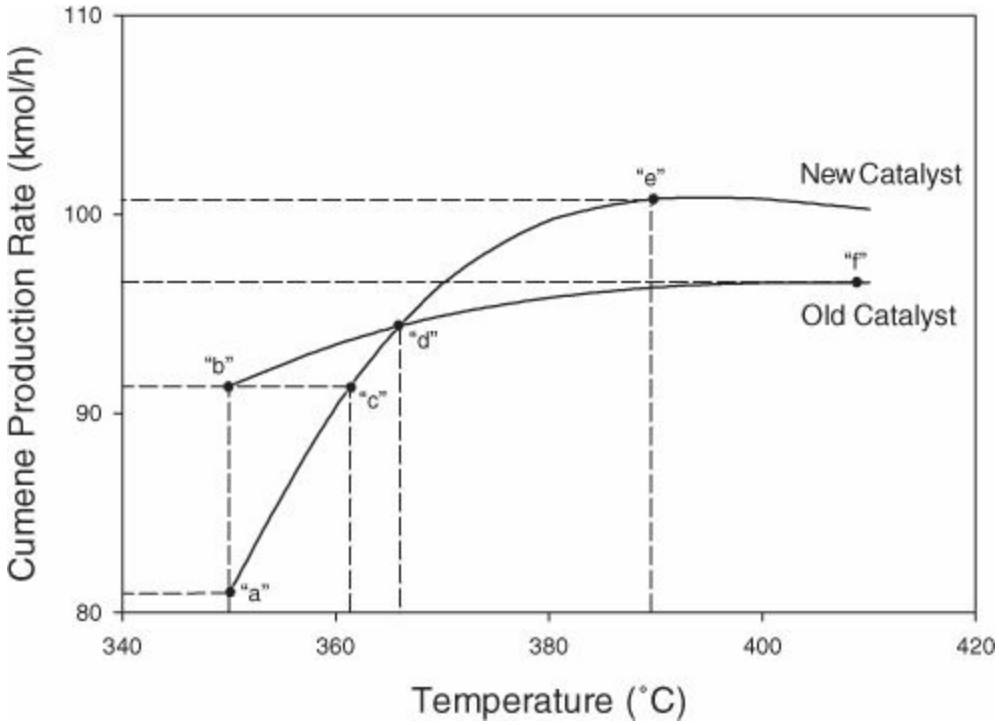


Figure 23.8. Cumene Production Rates at Constant Reactor Volume and Superficial Velocity

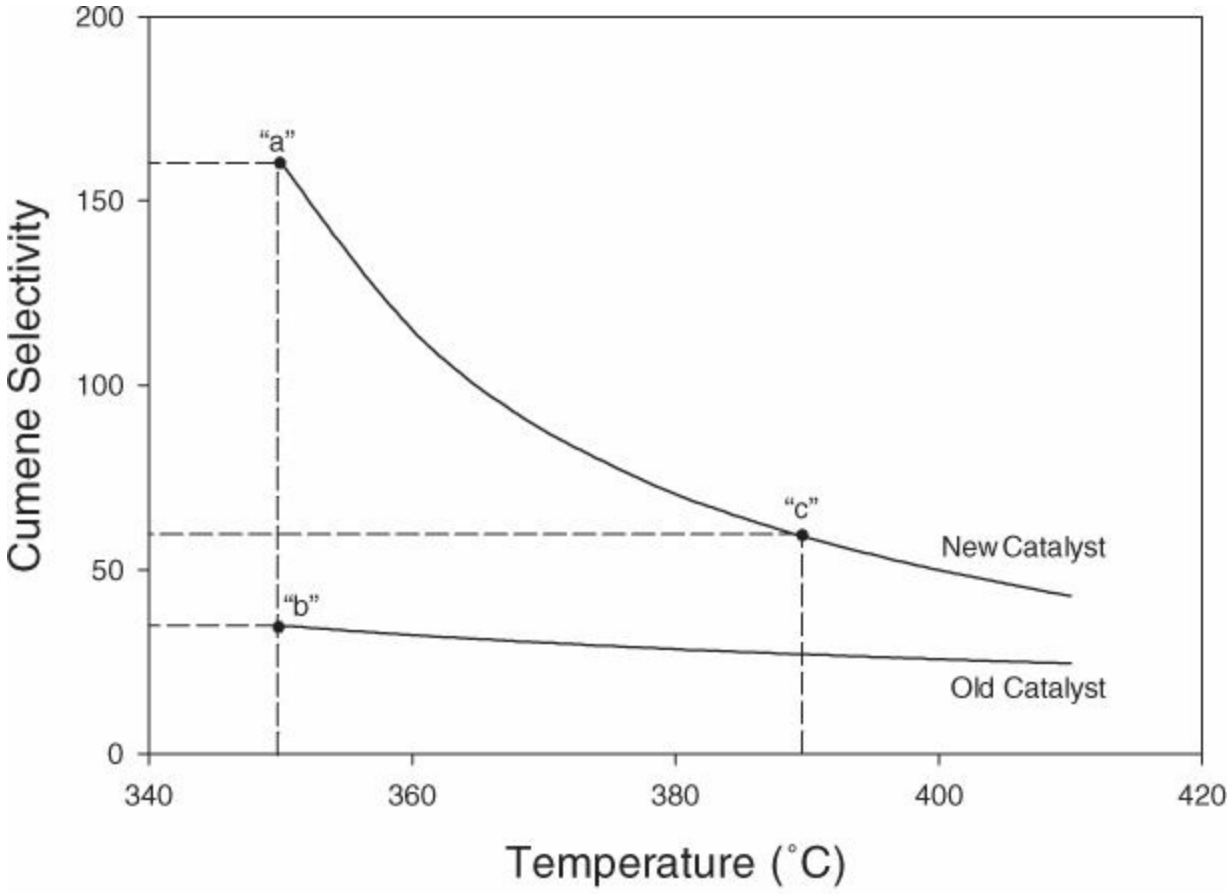


Figure 23.9. Selectivity for Cumene

Figure 23.9 shows the trends in product selectivity (moles of cumene produced per mole of DIPB produced) for both catalysts. At 350°C, the selectivity of the new catalyst is 160, point "a," compared with 35 for the current catalyst, point "b." At a temperature of 390°C, where the cumene reaches maximum production for the new catalyst, the selectivity is 59, point "c," well above that for the current catalyst.

In conclusion, the new catalyst is expected to provide higher product selectivity and higher cumene production at increased reactor temperature.

Discussion. It was found in the simulation of the dominant reactions in the production of cumene using the new catalyst that high temperatures increase the formation of the undesirable product, DIPB. This is expected based on the relative activation energies of the two reactions. The higher activation energy for the DIPB reaction leads to a more rapid increase in the rate of reaction of DIPB with temperature compared with cumene. Therefore, it is important to avoid hot spots in the reactor to avoid DIPB production. From a reaction point of view, isothermal reactors represent a desirable goal. This goal is obtained with a CSTR but is not easy to obtain in a PFR with a high heat of reaction. The fluidized bed system can approach isothermal behavior because of rapid mixing of the solid particles making up the bed. For highly exothermic reactions, the fluidized bed is inherently safe, hot spots do not develop, and heat can be removed from the bed.

However, fluid bypassing takes place in a fluidized bed. This adversely affects performance. This is because the bypassed fluid fraction does not come into contact with the catalyst and so a portion of the feed does not react. In the case study given above, the bypass fraction had a low value for a fluidized bed, 5%. As a result, the highest conversion that can be achieved is 95%.

If the products from the reactor are easily separated, the unreacted reactants can be recovered and

recycled to achieve high overall conversion. From a kinetic point of view, the formation of DIPB in the product could be effectively eliminated by operating at low reactor conversions. This can be seen from the reaction rate expression, which shows that the formation of DIPB is directly proportional to the concentration of cumene. If cumene concentration is kept low, the amount of DIPB formed is small.

Separation of the reactor products containing propane or propylene presents a problem. Propylene and propane have similar volatilities and are difficult to separate. If propylene and propane are not separated, there are three options to be evaluated:

1. Propylene-propane mix is discarded as waste. Fuel value may be recovered.
2. Total recycle of propylene-propane mix. This is not possible. Because the propane does not react, it must be purged from the system.
3. Partial recycle of propylene-propane mix. The propane in the feed would increase. This decreases the concentrations of the reactants and reduces the production of cumene. The superficial velocity in the reactor would increase. This reduces residence time and the fraction bypassed in the fluidized bed.

In the case study, the constant superficial velocity was maintained at higher temperatures by decreasing the excess benzene. The total concentration of gas in the reactor was reduced. This tends to decrease the reaction rate. In addition, the reaction equations show that the lower benzene concentration reduces the cumene reaction rate and has no impact on the DIPB reaction. As a result of maintaining a constant required superficial velocity by lowering the excess benzene, the selectivity is reduced.

An alternative approach to maintain the superficial velocity at increased temperature and retain the excess benzene flow is to increase the system pressure. This should provide higher reaction rates at a given temperature, resulting in higher conversions, and would not effect the selectivity.

The conclusions given regarding the catalyst replacement assumed that the reaction took place in a region where chemical reaction controlled. When chemical reaction controls, the effect of temperature is large. Figure 23.8 indicates there was little effect of temperature on cumene production using the current catalyst, but temperature had major impact on cumene production for the new catalyst. The low sensitivity in the base case suggests that the reaction is not chemical reaction controlled. Often when dealing with catalytic reactions, one finds that due to high catalyst activity, the reaction may be diffusion controlled. The activation energy for diffusion is significantly lower than that for chemical reactions. Therefore, the effective activation energy for a diffusion-controlled reaction is also significantly lower. This means that intrinsic reaction kinetics supplied by manufacturers may not be directly applicable in process simulation. The reader is referred to standard reaction engineering texts.

For catalytic reactions, always consider mass transfer effects. If present, they reduce the temperature sensitivity of the reaction.

23.5.3. Increasing Acetone Production

Problem. You are responsible for the operation of the acetone production unit in your plant. The acetone produced is used internally elsewhere in your plant. A need to increase internal production

by as much as 50% is anticipated. If this full increase cannot be met from your acetone unit, you will have to purchase additional acetone. You have been requested to evaluate how much increase in capacity can be obtained using the current chemical reactor.

Acetone is produced by the endothermic reaction

$$\underset{\text{isopropyl alcohol}}{(CH_3)_2CHOH} \rightarrow \underset{\text{acetone}}{(CH_3)_2CO} + \underset{\text{hydrogen}}{H_2}$$

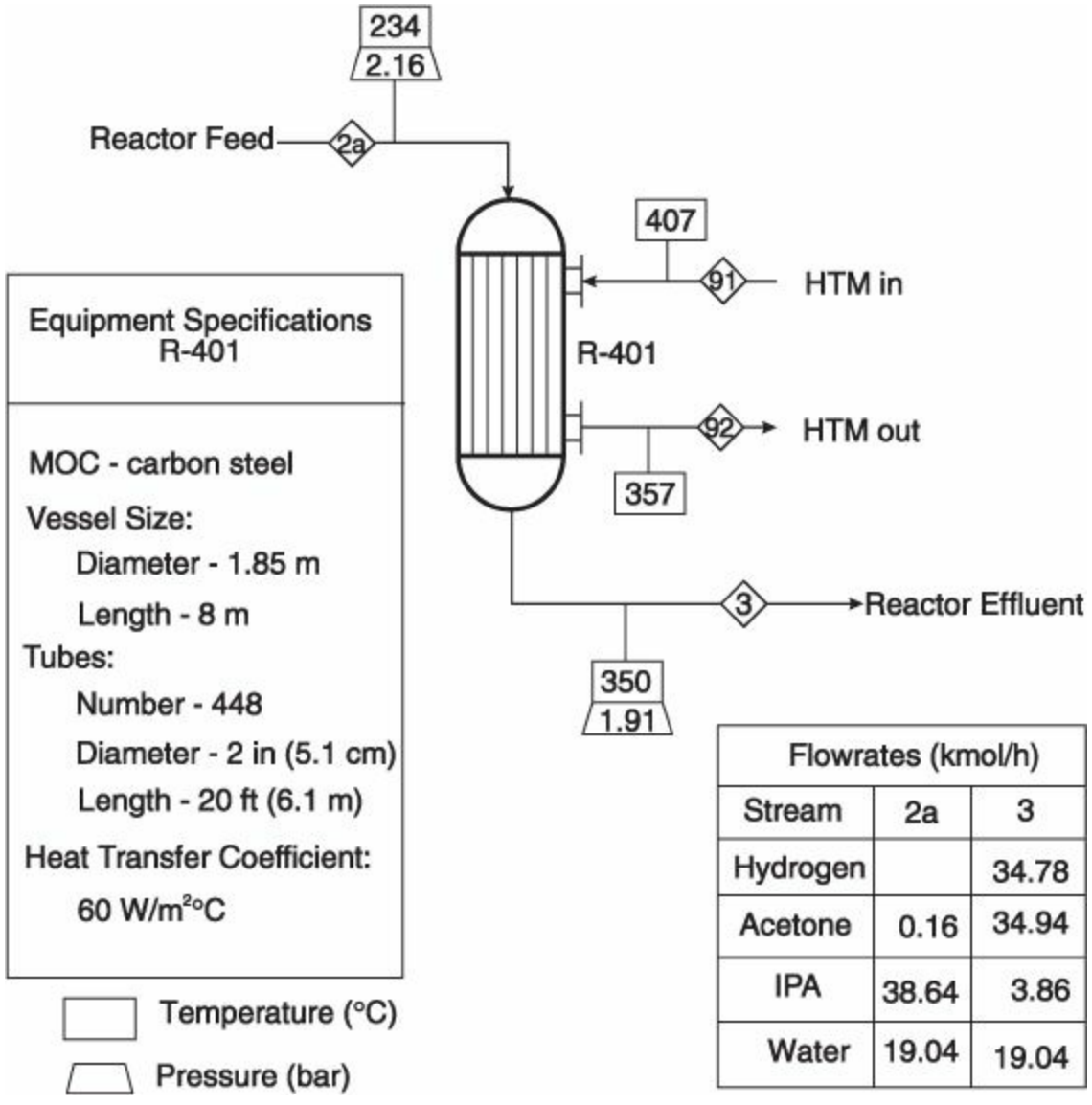
There are no significant side reactions. The reaction is endothermic and takes place in the gas phase on a solid catalyst. The reaction kinetics are given by

$$-r_{IPA} = kc_{IPA} \text{ kmol/m}^3 \text{ reactor s}$$

where

$$k = [3.156 \times 10^5 \text{ m}^3 \text{ gas/(m}^3 \text{ reactor s)}]\exp[-8702/T]$$

where T is in Kelvin. The process flowsheet for the plant is given in Appendix B, Figure B.3.1. Figure 23.10 shows the reactor portion of this process along with reactor specifications obtained from Table B.10.1. The process uses a PFR with the heat transfer medium, HTM, on the shell side. Because there is concern about operation of the downstream separation section, the IPA reaction conversion is held constant at 90% to ensure a constant feed composition to the separation section even though the flowrate of this stream may change.



Flowrates (kmol/h)		
Stream	2a	3
Hydrogen		34.78
Acetone	0.16	34.94
IPA	38.64	3.86
Water	19.04	19.04

Figure 23.10. Reaction Section of Acetone Process (from Figure B.10.1 and Table B.10.1)

Solution. The conversion of an endothermic reaction is most often limited by the amount of heat that can be provided to the reaction. Current operating conditions define the base case. Figure 23.11(a) shows the temperature profile in the reactor for the reacting stream and HTM for the base case. There is a small temperature driving force for heat transfer over most of the reactor. Only in a small region near the reactor entrance is there a large temperature difference needed to provide a high heat flux. To increase production, it is necessary to increase the overall heat flux into the reactor.

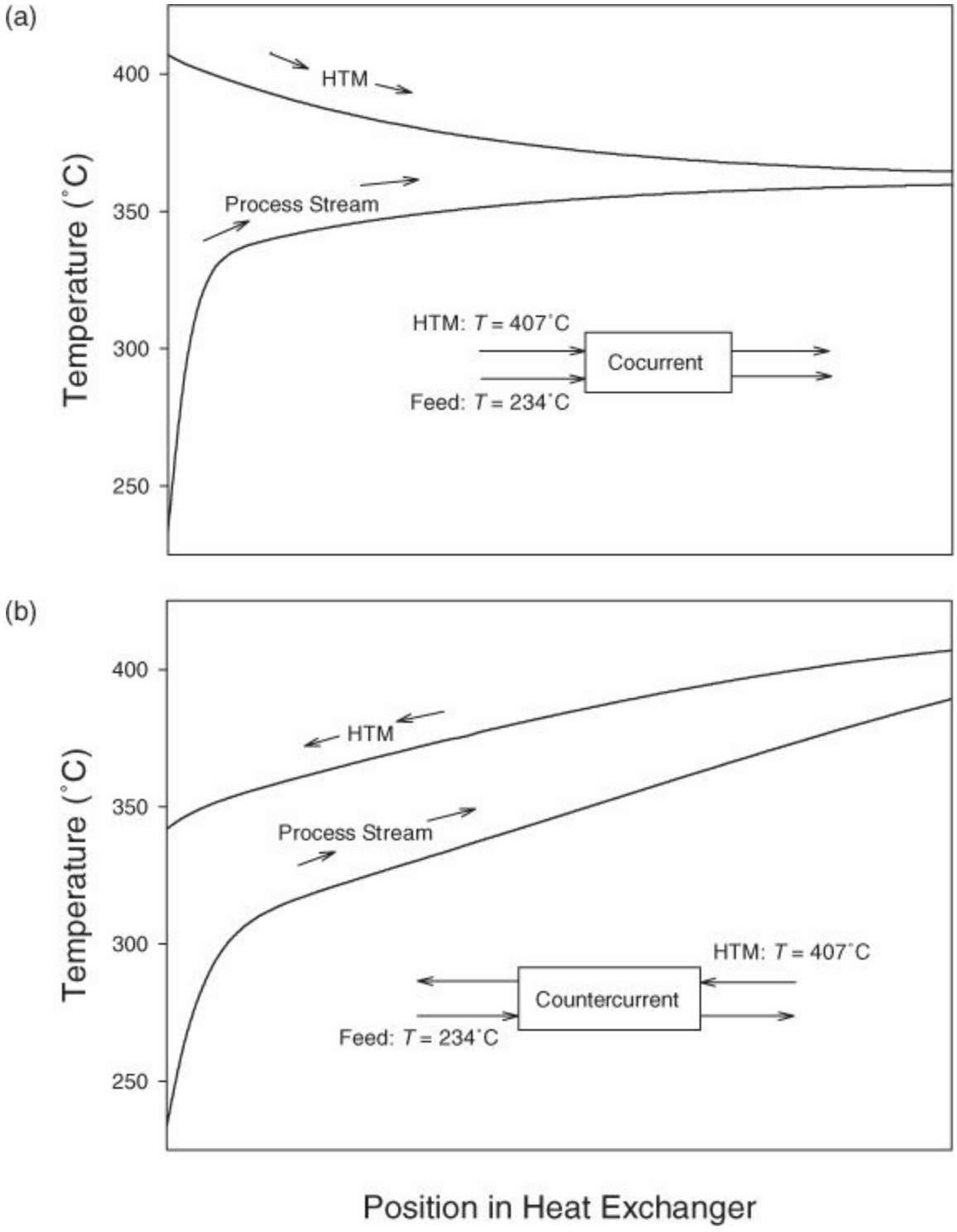


Figure 23.11. Temperature Profiles in Acetone Reactors for Cocurrent and Countercurrent Flow (IPA Conversion of 90%)

Figure 23.11(a) reveals four options that will increase the average heat flux:

1. Increase the temperature of the HTM.
2. Decrease the temperature of the reaction stream.

3. Operate with the HTM introduced countercurrent to the reacting stream.
4. Heat the feed stream to a higher temperature.

An evaluation of these options follows.

Option 1, Increase HTM Temperature: Figure 23.12 presents results obtained for increased acetone production resulting from a change in HTM inlet temperature (flowrate of HTM held constant). Increasing the HTM by 50°C increased acetone production by 48%. This would require a 48% increase in heat duty and a 50°C increase in HTM temperature from the fired heater, H-401.

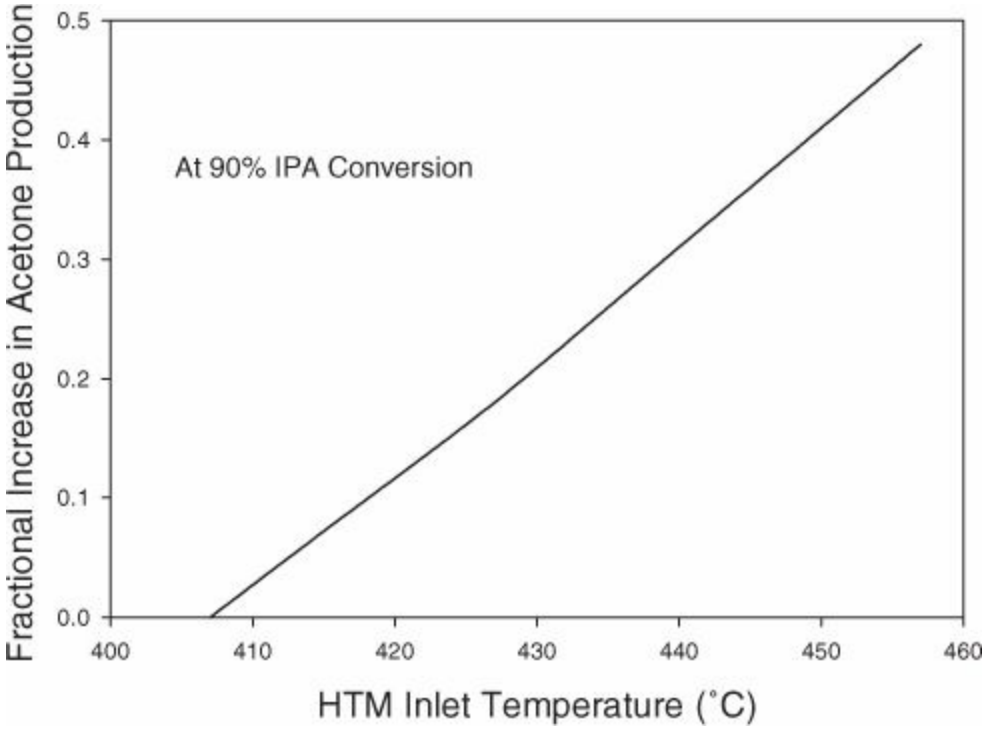


Figure 23.12. Increase in Acetone Production Resulting from Increase in HTM Inlet Temperature (HTM Flow Constant)

Option 2, Decrease Reactor Temperature: Lowering reactor temperatures decreases the reaction rate (lower reaction rate constant, k), reducing acetone production. This option has no merit and is rejected.

Option 3, Countercurrent Flow: Figure 23.11(b) shows the temperature profile obtained by introducing the HTM countercurrent to the reaction stream. Compared with the base case (cocurrent flow), it provides a larger, more constant temperature driving force (and heat flux). This change provides a 13% increase in acetone production. The heat duty of the fired heater, H-401, must be increased by 13% to provide this increase in duty.

Option 4, Heat Feed Stream to Higher Temperature: This provides energy in the form of sensible heat that adds to the energy transferred from the HTM. For an increase in feed temperature of 100°C, the acetone production increases by 14%. This would require an additional fired heater for the reactor feed stream.

This investigation showed there are a number of options that can effect a significant increase in acetone production. A 50% increase in capacity can be obtained from the reactor. All options require an increase in fired heater capacity.

Discussion. It has been shown that there are a number of options that provide increased acetone

production. Except for Option 2, the options provided can be combined. The heat transfer configuration, Option 3, can be combined with an increase in HTM temperature, Option 1. In addition, the reactor feed temperature, Option 4, can be increased. In most situations, there is more than one option to consider to make a desired change in performance.

All options to increase acetone production require an increase in capacity of the fired heater (or addition of a new fired heater). Therefore, the fired heater is likely to represent a bottleneck to increased production. Fired heaters are expensive, and it is not likely that the current heater was oversized enough to provide a 50% increase in heat duty. Until this bottleneck is removed, the additional acetone production required cannot be obtained.

Once the fired heater bottleneck is resolved, the separation system must be able to process the large increase in throughput. It is unlikely that the separation system can process the 50% increase. Therefore, if the fired heater bottleneck is removed, the separation system becomes the bottleneck.

Once a decision is made to eliminate these two bottlenecks (fired heater and separation system), the analysis of reactor behavior could be modified to consider a number of secondary effects. The case study did not consider the effect of increasing reactor flowrates on the heat transfer coefficient (gas-phase resistance dominates). The impact of the increased pressure drop over the reactor was not examined. These options were not necessary to confirm that the reactor is capable of providing a 50% increase in acetone production. The option of increasing the HTM flowrate was not appraised.

Endothermic reactions are inherently safe systems in terms of undergoing an uncontrolled reaction that is characteristic of an exothermic reactions. If the heat source is withdrawn, the temperature of the reactor drops and the rate of reaction decreases.

23.6. Summary

In this chapter, chemical reactor performance was analyzed differently from the way it is usually done in reaction engineering classes. Key qualitative trends were emphasized. This was done in the context of Figure 23.1, which illustrates the interrelationship between product production, reaction kinetics, reactor behavior, and heat transfer limitations. The case studies presented reinforce the interrelationship between these factors.

What You Should Have Learned

- How reactor performance is affected by
  - Stoichiometry (conversion, selectivity, yield)
  - Kinetics (rate of reaction and thermodynamic limitations)
  - Reactor parameters (volume, space time, catalyst, temperature, pressure)
  - Heat transfer

References

1. Zimmerman, C. C., and R. York, “Thermal Demethylation of Toluene,” *Ind. Eng. Chem. Proc. Des. Dev.* 3 (1964): 254–258.
2. Rase, H. F., *Chemical Reactor Design for Process Plants*, Vol. 2: *Case Studies and Design Data* (New York: Wiley-Interscience, 1977), 38.

Short Answer Questions

1. Explain why very high conversions (>99%) are often difficult to achieve in practice, even for plug flow reactors and nonequilibrium constrained reactions.
2. Comment on the following statement: *For an exothermic reaction, if the temperature is increased at constant pressure with a fixed reactor size, the conversion decreases.*
3. It is known that for a certain third-order, gas-phase reaction, the rate of reaction doubles when the temperature goes from 250°C to 270°C. The form of the rate equation is

$$-r_A = k_0 e^{-\left(\frac{E}{RT}\right)} c_A c_B^2$$

   If the rate of reaction is 10 moles/m^{3}s at the base conditions, which are 20 atm pressure and 250°C, and an equal molar flow of A and B are in the feed (no inerts), answer the following questions:

   a. Compared to the base case, by how much does the rate of reaction (at inlet conditions) change if the temperature is increased to 260°C?

   b. Compared to the base case, by how much does the rate of reaction (at inlet conditions) change if the pressure is increased by 15%?

4. For the reactor system shown in Figure P23.4, answer the following:

   a. Is the reaction exothermic or endothermic?

   b. Give two reasons why this reaction is being run at a high temperature.

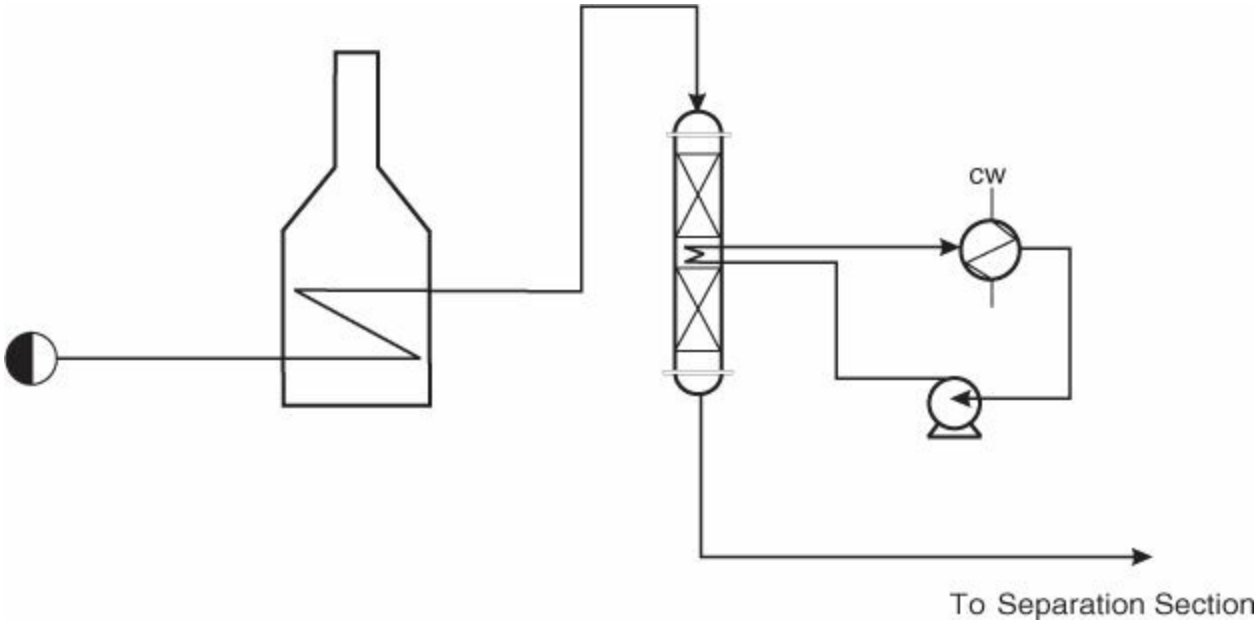


Figure P23.4.

Problems

Note: Information for problems referenced as Appendix C is provided on the accompanying CD.

5. For the hypothetical, endothermic, gas-phase reaction

$$A + B = C$$

   sketch a plot similar to Figure E23.1. Discuss the relationship between equilibrium conversion, temperature, and pressure.

6. For the situation in Example 23.3, if all of the reactions take place, what conditions maximize

the selectivity for P?

7. Examine the reaction network and the reaction kinetics for drying oil production in Appendix B, Section B.4.2. What conditions will maximize the selectivity for drying oil? Sketch concentration profiles for the case when this reaction is run in a packed bed modeled as a PFR.
8. Examine the reaction network and the reaction kinetics for ethylene oxide production in Appendix B, Section B.6.2. What conditions will maximize the selectivity for ethylene oxide? Sketch concentration profiles for the case when this reaction is run in a packed bed modeled as a PFR.
9. Sketch the T-Q diagram for an endothermic reaction in a PFR for
   a. Countercurrent flow of HTM (heat transfer medium)
   b. Cocurrent flow of HTM

   What are the consequences on reactor size of choosing each configuration? Explain your answer by examining the trends (see Chapter 20).
10. In the production of cumene from propylene, the following elementary, vapor-phase, irreversible reaction takes place:

$$\underset{\text{propylene}}{C_3H_6} + \underset{\text{benzene}}{C_6H_6} \xrightarrow{k_1} \underset{\text{cumene}}{C_9H_{12}}$$

The reaction rate is given by

$$r_1 = k_1 c_p c_b \text{ mol/(g cat) sec and } k_1 = 3.5\times10^4 \exp\left(\frac{-12{,}530}{T(K)}\right)$$

The feed to the reactor consists of an equal ratio of benzene and propylene. The reaction takes place in a fluidized bed reactor operating at 300°C and 3 MPa pressure. For this problem, the fluidized bed may be assumed to be a constant-temperature CSTR reactor.

At design conditions, you may assume that the side reaction does not take place to any great extent and the conversion is 68%.

It is desired to scale up production by 25%. All flows to the reactor will increase by 25% at the same feed concentration. Determine the following:

   a. What is the single-pass conversion if the process conditions and amount of catalyst remain unchanged?
   b. What percent change in catalyst would be required to achieve the scale-up assuming that the pressure, temperature, and conversion were held constant?
   c. Estimate how much the temperature would have to be changed (without changes in catalyst amount, operating pressure, or conversion) to achieve the desired scale-up.
   d. By how much would the pressure have to be changed (without changes in catalyst amount, operating temperature, or conversion) to achieve the desired scale-up?

11. Consider a liquid-phase reaction occurring in a constant-volume, isothermal, batch reactor.
   a. For a first-order decomposition, what is the ratio of the time to reach 75% conversion to the time to reach 50% conversion?
   b. For a first-order decomposition, what is the ratio of the time to reach 90% conversion to the time to reach 50% conversion?
   c. Repeat Parts (a) and (b) for a second-order reaction between reactants initially in equimolar

quantities.

d. Explain the results of Parts (a)–(c).

For Problems 23.12–23.26, it is recommended that a process simulator be used.

Problems 23.12–23.16 investigate the performance of the reactor section for a noncatalytic process for the hydrodealkylation of toluene to produce benzene. Reactor R-101 in Figure 23.4(b) operated at the flow conditions shown represents a base case (inlet pressure is 25 bar). Kinetics are given in Table 23.1. Ignore reactor pressure drop. Reactor volume for the base case is 4.76 m^3.

12. Investigate the effect of increasing reactor volume on toluene conversion. Plot the results.
13. Investigate the effect of a variation of hydrogen feed rate (all other parameters held constant at base-case values).
    a. Plot toluene conversion versus percent excess oxygen.
    b. Determine the maximum conversion possible.
14. Investigate a two-reactor system to replace the single adiabatic PFR in the base case. The two-reactor system consists of an adiabatic CSTR followed by an adiabatic PFR. For the base-case toluene conversion (0.75),
    a. Determine the size of the CSTR and PFR that provides the minimum total reactor volume.
    b. Determine the fraction of the total conversion obtained in the CSTR from Part (a).
15. Investigate the effect of increasing the feed rate on reactor performance.
    a. Prepare a performance curve of the toluene conversion versus feed rate.
    b. Prepare a performance curve of benzene generated versus feed rate.
16. Investigate the effect of feed temperature on reactor performance. Prepare a performance curve for toluene conversion versus feed temperature.

Problems 23.17–23.20 investigate the performance of the cumene reactor (fluidized bed), described in Section 23.5.2, that results from replacing the catalyst. The replacement catalyst kinetics are given in Table 23.2. The base case selected is the currently operating reactor (with an active volume of 7.49 m^3). Process output for the base case is given in the flow table in Figure 23.6.

17. a. Derive an equation for the ratio

    η = rate of cumene formation/rate of DIPB formation

    Rewrite the equation in the form $\eta = A/B - 1$.

    b. Present the equation for η given above in terms of the following variables: T, P, k_o, E_{act}, and mole fractions.

    c. Using the equation from Part (b), determine the trend resulting from a change in the following variables. After each item, provide ↑ (increases), ↓ (decreases), ¢ (constant) or ? (cannot be determined).

    (i) Increasing system temperature

    (ii) Increasing system pressure

    (iii) Increasing benzene mole fraction

    (iv) Increasing propylene mole fraction

(v) Increasing propane mole fraction

(vi) Increasing cumene mole fraction

(vii) Increasing DIPB mole fraction

18. Replace the current catalyst with the new catalyst (maintain the same feed rate and conditions) and
    a. Provide a flow table (similar to that in Figure 23.6).
    b. Compare cumene production with the new to the old catalyst.
    c. Compare DIPB production with the new to the old catalyst.
19. Evaluate the effectiveness of the new catalyst at 350°C that results from increasing the reactor volume.
    a. Plot cumene production versus reactor volume.
    b. Plot selectivity (defined as cumene generated/DIPB generated) versus volume.
20. In Figures 23.8 and 23.9, the volumetric flowrate to the reactor was held constant at increased temperatures by reducing the hydrogen in the feed. This altered the feed concentration. Investigate the alternative of reducing the total feed rate (at the same composition) to maintain constant volumetric flowrate.
    a. Plot the cumene production rate versus temperature, and compare to Figure 23.8.
    b. Plot the selectivity (cumene generated/DIPB generated) versus temperature, and compare to Figure 23.9.

Problems 23.21–23.26 investigate the performance of the acetone reactor system. The reaction kinetics are presented in Section 23.5.3. The reactor and internal heat exchanger are fixed. For the base case, the active volume of the reactor is 5.1 m^3 at the operating conditions given in Figure 23.10. Unless otherwise stated, the heat transfer coefficient and reactor pressure drop are to be assumed constant. The feed temperature, pressure, and component concentrations remain constant. For these calculations, assume the utility fluid to be n-heptadecane (at pressures more than 30 bar). At the base case, the utility flow is 58 kmol/h.

21. Reconfigure the heating system to operate in countercurrent fashion. Retain the same utility stream input and IPA conversion (90%).
    a. Determine the change in process feed rate.
    b. Determine the percent change in process feed rate.
22. Increase the utility feed rate by 50%, and maintain the base-case process feed stream.
    a. Determine the conversion obtained.
    b. Determine the percent change in the acetone produced.
23. Increase the utility feed rate by 50%. Retain the IPA conversion of 0.9.
    a. Determine the process feed rate.
    b. Determine the percent change in acetone produced.
24. Increase the utility feed temperature by 50°C. Retain the IPA conversion at 0.9.
    a. Determine the process feed rate.
    b. Determine the percent change in acetone production.

25. Prepare a performance curve for the change in utility flowrate necessary to maintain an IPA conversion of 0.9 at increased process feed rates.

26. Assume the individual film coefficients change according to the relationship

$$h_i \text{ α velocity}^{0.8}$$

a. Estimate the effect of process flow changes on the overall heat transfer coefficient.

b. Determine the process flowrate that provides an IPA conversion of 0.9 resulting from an increase in utility temperature of 50°C.

c. Does the assumption of constant overall heat transfer coefficient result in a higher or lower estimate of the process feed rate? If you worked Problem 23.25, you have this value for comparison.

Chapter 24. Process Troubleshooting and Debottlenecking

What You Will Learn

- What troubleshooting and debottlenecking are
- Strategies for troubleshooting and debottlenecking

Imagine that you are responsible for a chemical process unit. The pressure in a chemical reactor begins to increase. You are concerned about material failure and explosion. What do you do? For a case such as this with potential catastrophic consequences, it may be necessary to shut the process down. However, process shut-down and start-up are very costly, and if a safe alternative were available, you would certainly want to consider it as an option. In another scenario, what would you do if it had been observed that the purity of product from your unit had been decreasing continuously for several days, and customers had begun to complain of poor product quality and have threatened to cancel lucrative contracts?

The situations described above may be classified as **process troubleshooting** problems. Once a plant is built and operating, it is anticipated that it will operate for a number of years (10–30 years). During this time, there will be instances when the plant displays unusual behavior. This unusual behavior may represent a problem or a symptom of a problem that has not yet become apparent. The procedure for identifying the root cause of unusual behavior is part of troubleshooting. The other part is to provide guidance as to what action should be taken to correct the problem or, in the case of a symptom that has not yet resulted in a problem, to prevent a problem from developing. Problems that affect process performance represent financial losses and potential safety hazards, so these problems must be quickly identified and resolved. The key to smooth plant operations is preventive action based on correct diagnosis of early symptoms. Troubleshooting problems associated with process start-up are beyond the scope of this text.

Even during a period of successful operation, the process does not operate at a steady state. Distillation units operate differently in summer than in winter, as well as between night and day, as a result of internal reflux changes resulting from heat losses or gains from the tower. Feed materials fluctuate, the temperature of cooling water changes, catalyst decays, heat exchangers foul, and so on. The control system responds to these changes and alters utility flows to maintain process streams at close to normal operating conditions.

The key to solving troubleshooting problems is to make use of the information regarding the process taken during periods of successful operation. Based on operating experience, the range over which changes can take place without a significant effect on the performance of the process is learned. Consequently, there is no single base case to represent process behavior as there was in Chapter 21. When comparing current operations to normal operations, it is important to determine whether current operation lies within the range of normal operations. The range of normal process operation provides the base case.

Three steps can be identified to troubleshoot a process:

1. **Treat the Symptoms:** In this situation, the observed problem is addressed without investigation of the root cause. If the reactor pressure is increasing, find a way to relieve the

pressure. This is a short-term solution. Because the root cause of the pressure increase has not been identified and addressed, the pressure may increase again. However, the immediate problem (the potential for an explosion) has been avoided, and there is now time to seek the root cause of the problem.

2. **Identify the Cause of the Problem:** Eventually, the cause of the problem should be diagnosed. This is particularly true if the problem recurs or if it is safety related. Because this may take time, the symptoms must continue to be treated.
3. **Fix the Problem:** Ultimately, the problem should be fixed.

Process troubleshooting involves solving open-ended problems for which there are likely to be several possible solutions. It is necessary for the engineer faced with such a problem to consider many identifiable solutions. Failure to consider a sufficient number of possible solutions may result in missing the actual solution.

Now, consider a different situation. It is necessary to determine how much scale-up is possible for the process for which you are responsible. You determine that one process unit can be scaled up only by 10%, whereas all other process units can be scaled up by at least 15%. The process unit that can be scaled up only by 10% is called a bottleneck. Elimination of this bottleneck is called **debottlenecking** and involves determining how to remove obstacles limiting process changes.

To put troubleshooting and debottlenecking problems in context, consider the input/output model shown in Figure 24.1. This model was first introduced in Chapter 19 and was used to define the design and performance problems. The input/output model can also be used to define troubleshooting and debottlenecking problems. Troubleshooting problems involve identification and correction of the change in inputs and/or the process responsible for observed changes in outputs. Debottlenecking problems involve identification and modification of the portion of a process limiting the ability to change inputs or outputs.



Type of Problem	Known	Unknown
Design	inputs and outputs	process
Performance	inputs and process	outputs
Troubleshooting	observed Δoutput	causative Δinputs and/or Δprocess
Debottlenecking	desired Δoutput or Δinput	portion of process limiting magnitude of change

Figure 24.1. Input/Output Relationships for Various Types of Problems

In this chapter, a recommended methodology for attacking process troubleshooting problems is presented. Then five case studies of increasing complexity are presented that will serve to enhance the reader's skills in attacking troubleshooting problems. Finally, an example of a debottlenecking problem is presented.

24.1. Recommended Methodology

When solving complex problems such as troubleshooting and debottlenecking, having a reliable, personal problem-solving strategy is important. Problem-solving strategies are discussed briefly here. More details can be found elsewhere [1].

24.1.1. Elements of Problem-Solving Strategies

Three elements of successful problem-solving strategies are recommended here for attacking process troubleshooting problems (including debottlenecking problems). This is not meant to be an exhaustive list of strategies; it is simply some of the strategies that can be used. The three strategies discussed here are

1. Brainstorming
2. Using known or observed data plus your understanding of equipment behavior
3. Considering the unexpected

Each is considered separately. They can also be combined into a general methodology for solving open-ended problems.

Brainstorming involves generating an extensive list of possible ideas. This need not be a formal process; it can be done informally and rapidly. In fact, the natural response to a troubleshooting

situation is to think immediately and rapidly of several possible causes. If the product is not meeting specifications, think of all of the reasons that can be considered as potential causes, no matter how remote the possibility. Then brainstorm possible solutions. The main rule of brainstorming is that there are no bad ideas. The goal is to generate as many ideas as is possible. After brainstorming, only then is it time to evaluate all items critically to generate the most likely causes and solutions. Although brainstorming is usually a group activity, often it must be done individually. For a large, long-term problem, time can be taken to brainstorm in a group. For an everyday problem, especially an emergency situation, one should train oneself to brainstorm automatically. Brainstorming is a component of most problem-solving strategies.

When brainstorming a troubleshooting problem, consider all ideas, no matter how unusual they may seem.

When troubleshooting a chemical process, an **understanding of equipment behavior** should be used to narrow the list of possibilities. For example, in a staged separation using a mass separating agent, the Kremser equation (see Section 21.3.1) quantifies the relationship between process variables. The most important of these relationships for a variety of unit operations were summarized in Table 20.1. Use of these relationships will be illustrated in the case studies presented later in this chapter.

When there is a problem with process operation, the cause of the problem must be identified. The problem may or may not be located at the unit where poor operation is observed. For example, the output from the separator may be off spec due to lower-quality product exiting the reactor rather than due to poor separator operation. In troubleshooting plant problems, a vast amount of data exist that can be used to help identify the problem. These data would likely include current and historical operating conditions. In addition, the plant P&IDs would show where to look for additional current operating data. Any methodology for troubleshooting must consider this information, and any solution must be consistent with the operating data. Often, solving the problem is facilitated by selection of the data that will lead to identification of the problem.

Although a knowledge of equipment behavior is essential to solving troubleshooting problems, it is important that all alternatives, no matter how **unexpected**, be considered. If the pressure drop in a tray tower is increasing, a knowledge of equipment function suggests that there may be loading or flooding, so an increased liquid or vapor flowrate is a possible cause. However, was the possibility that someone left a toolbox in the downcomer during a recent maintenance shutdown also considered? The lesson here is to expect the unexpected! Consider all possibilities no matter how remote they may seem.

Given the open-ended nature of troubleshooting problems, their solution may best be attacked by creative problem-solving strategies. One such strategy, presented by Fogler and LeBlanc [1], is discussed here in the context of process troubleshooting. (Another similar strategy is presented in Chapter 25.) Their problem-solving strategy involves five steps:

1. Define
2. Generate
3. Decide
4. Implement
5. Evaluate

First, the correct problem must be defined. If the problem is incorrectly defined, it is likely that an incorrect solution will be found. If the product is not meeting specifications, this is the problem. However, if after further investigation it is found that the stream leaving the reactor is not at design conditions but the reactor feed is at design conditions, it may be necessary to redefine the problem to be incorrect reactor performance.

Once the problem is defined, ideas must be generated. This is identical to brainstorming. It is important to generate as many ideas as possible. It is poor problem-solving strategy to focus on one possible solution or to assume that there is only one possible solution. For process troubleshooting, ideas may need to be generated both for the cause of the problem and for remedies to the problem.

Once ideas have been generated, the next step is to decide how to proceed. This is when knowledge of equipment can be used to select the most likely items from the brainstorming list to implement first. The next step is to implement the chosen solution.

Once the chosen solution method is implemented, it is necessary to evaluate the chosen solution. Is it working? If not, why not? Should another solution be implemented? If several solutions have been attempted, none of which appears to be solving the problem, this may be the time to think about whether there is an unexpected solution that can solve the problem.

24.1.2. Application to Troubleshooting Problems

A troubleshooting strategy is given in Table 24.1. It involves five steps. This sequence of steps is shown to parallel the problem-solving strategy of Fogler and LeBlanc discussed in Section 24.1.1.

Table 24.1. Strategy for Troubleshooting Existing Plants

Phase 1	Check out primary suspects. a. Verify the identified problem or symptom. b. Check input to the process. c. If only one unit is involved, check operating conditions of unit. d. Check for fully open or closed control valves.
Phase 2	Identify the unit operation producing the problem or symptom. a. System size is reduced systematically until the unit operation that is the source of the problem or symptom is determined. b. Inputs to each system are checked.
Phase 3	Perform a detailed analysis of unit operation uncovered in Phase 2 to determine and to verify the root cause of the problem or symptom.
Phase 4	Report your diagnosis of the root cause of the problem, and recommend action to remove the problem or symptom.
Phase 5	Report significant observations uncovered during the analysis that may be important to your organization.

Phase 1. Screen the whole process for the most common causes of problems or symptoms of problems in the process. This might involve brainstorming done informally as part of your thought process.

It is important to **define** the correct problem, or to determine whether one even exists. One common situation is false identification of a problem or symptom. An instrument could have been read

incorrectly or could be broken, the analytical analysis (online or in lab) may not be correct, reagents may have been prepared incorrectly, and so on. In this situation, there is no problem with the process; it is a false indication of a problem. Never accept the initial problem identification without verification.

Once it has been determined that a problem really exists, the suspects should be screened. This is the **generate** step. A common cause of problems results from changes in process inputs. The adage "garbage in, garbage out" is universal and applies to chemical processes. Component flows into the process must be verified and compared to those for normal operations. If a problem appears as a result of process inputs, go to Phase 3. If a problem is known to involve a single unit (which may be true only for academic problems), consider possible unit malfunctions (some are listed under Phase 2). In this case, you should also go directly to Phase 3.

A third common cause results from limitations of the control systems on the utility streams used to maintain the temperature and pressure of process streams. If any control valves are found to be fully open or fully closed, there is a high probability that the desired control is not being achieved. All of the utility control valves are not normally shown on the PFD, and it is necessary to review the P&ID. All control valves should be checked. This information is used as input in later phases to identify the cause of the problem observed.

Phase 2. Locate the unit operation that is producing the problem or symptom. This is part of the **decide** step. The process is divided into subsections. If there is no obvious choice for selecting subsections, the process sections identified in the block flow diagram represent a reasonable starting point. Each system analyzed contains the stream identified as having a problem or symptom. Analyze system inputs. This identifies the subsection containing the cause of the problem. The subsection size is reduced, and the inputs are again analyzed. This continues until the unit operation producing the problem is identified. Then the operation of the identified unit should be checked. Ask key questions about each unit. Is there evidence of heat-exchanger fouling? Is the reflux ratio on the distillation column within its normal range? Are the temperature and pressure of the reactor at normal conditions?

Phase 3. Determine the root cause of the problem or symptom by a detailed analysis of the unit operation identified in Phase 1 or 2. This is the remainder of the **decide** step. Normal operation is used as a base case. This is the first place where the utility flows are analyzed. This involves using heuristics (Chapter 11), operating conditions of special concern (Chapter 6), calculation tools, and other material presented in Chapters 19–21.

Phase 4. Present all available evidence that establishes the root cause identified in Phase 3 as valid. Also, present any evidence that may not support the argument. Recommend action to be taken to correct the problem or treat the symptom. This is the **implement** step.

Phase 5. Present an evaluation of any significant observations that resulted from your analysis that could impact this or other processes within your company. This is the **evaluate** step. If you identify process improvements or potential for future problems, you are acting professionally. This is true especially if the suggestions are related to the environment or safety of personnel.

In summary, the cause of a change in output originates with a change in input and/or a change in

process operation. Some possibilities are illustrated in Figure 24.2. This list is not meant to be exhaustive. It illustrates some possible causes for changes in output. The strategy discussed above is illustrated in the problems that follow.

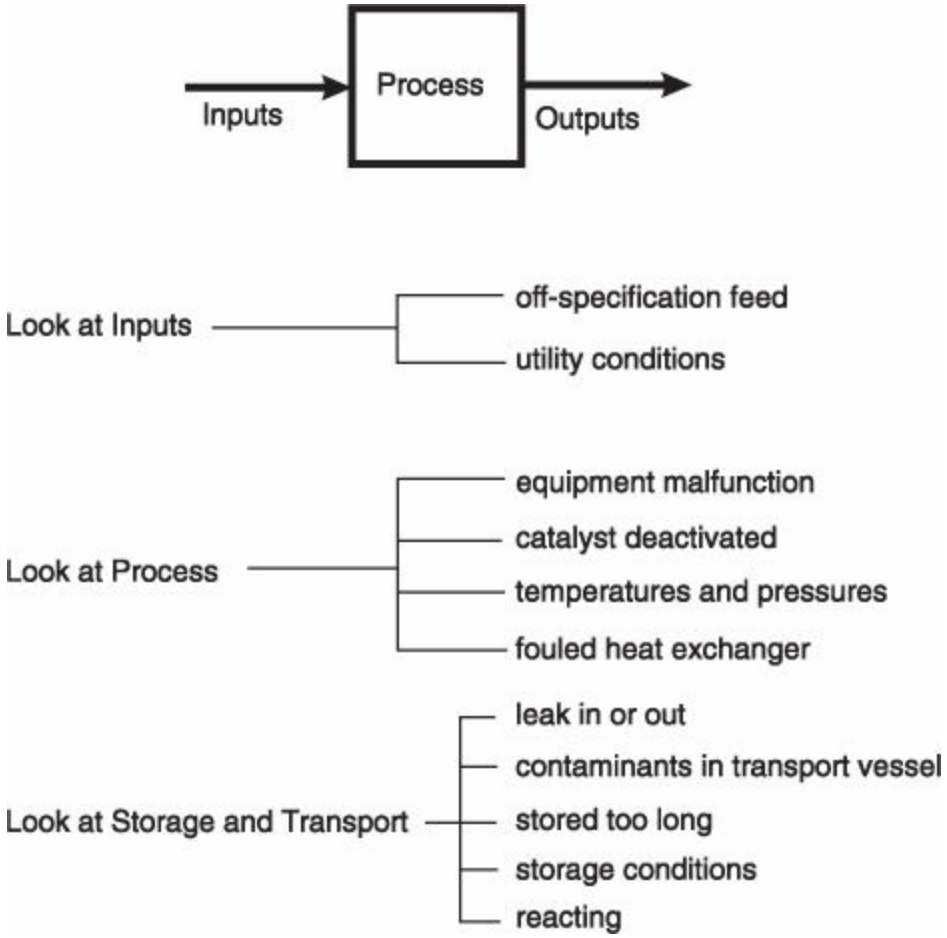


Figure 24.2. Suggestions for Solving Troubleshooting Problems

24.2. Troubleshooting Individual Units

The first two case studies presented involve troubleshooting individual pieces of equipment. Although real troubleshooting situations usually involve an entire process, the necessary skills can be developed on simpler problems such as the two presented in this section.

24.2.1. Troubleshooting a Packed-Bed Absorber

The first troubleshooting problem involves a packed-bed absorber. The absorber has been designed to remove a contaminant from an air purge stream and has been operating for some time as designed. Then it is observed that the outlet air contains more contaminant than it should. A similar problem involving a tray absorber is given at the end of the chapter.

A packed absorber (Figure 24.3) has been designed to reduce the acetone concentration in 40 kmol/h of air from a mole fraction of 0.02 to 0.001. Acetone is absorbed into pure water at 20 kmol/h. Acetone is recovered from the effluent liquid, and the water, which is assumed pure, is recycled to the absorption unit. After a period of successful operation, it is observed that the exit acetone mole fraction in air is now 0.002.

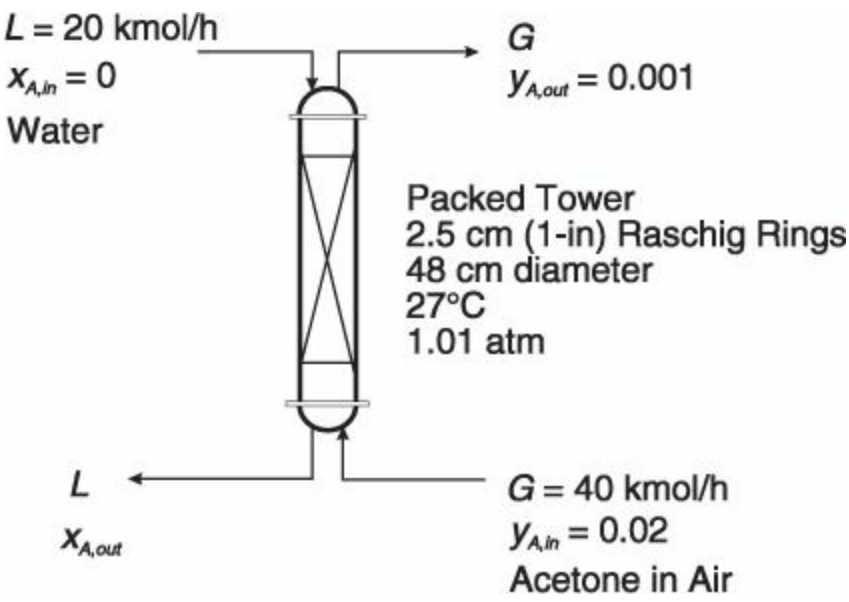


Figure 24.3. Packed Absorber for Troubleshooting Case Study

The column is packed with 2.5 cm (1 in) Raschig rings and has a 48 cm diameter, which was obtained by designing for 75% of flooding. The column is assumed to operate isothermally at 27°C, and the nominal pressure is 1 atm. Raoult's Law is assumed, and the partition coefficient for acetone, $m = y/x = P^*/P$, where $\ln P^* = 10.92 - 3598/T(\mathrm{K})$, has been determined from tabulated data [2]. At 27°C and 1.01 atm, $m = 0.337$.

This problem, which involves dilute solutions, can be analyzed using the Colburn graph, Figure 21.15. On this graph, the interrelationship between the number of transfer units, N_{tOG}, the absorption factor, A ($A = L/mG$), and the mole fraction is defined. The base-case point can be located. The y-axis is at a value of 0.05, and $A = 1.48$. This gives $N_{tOG} = 6.2$. This is shown as point "a" on Figure 24.4.

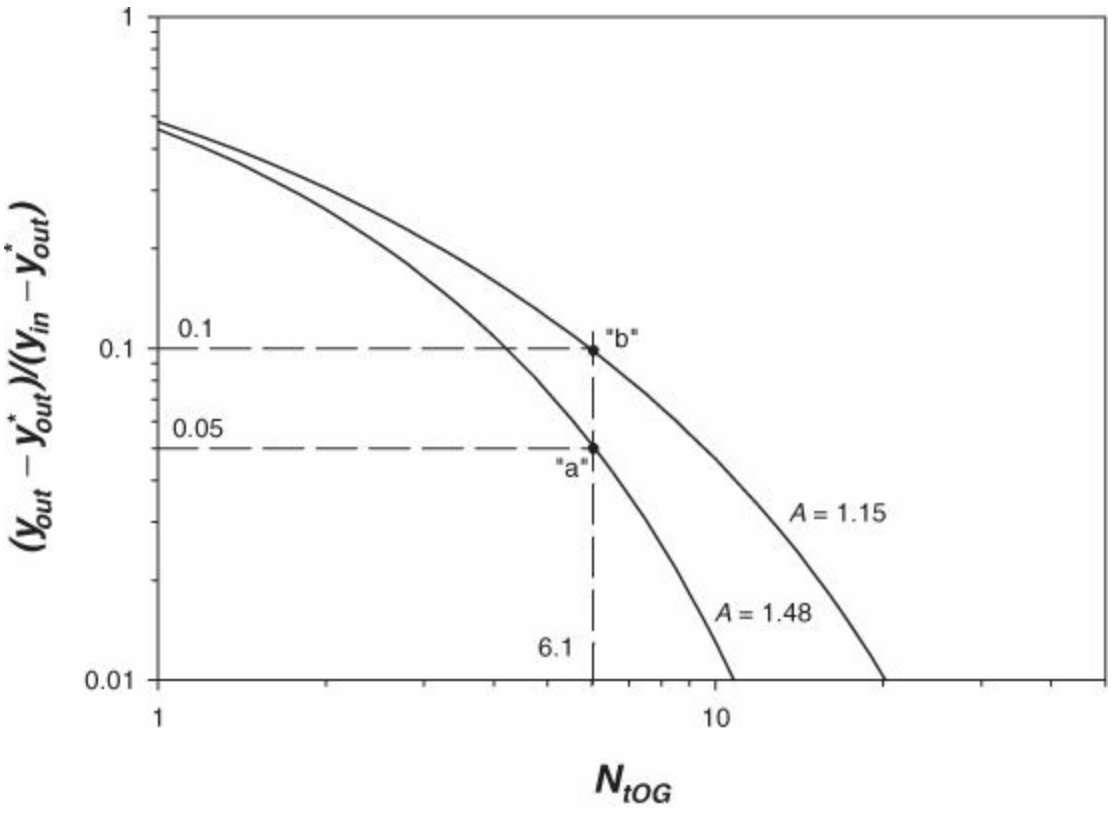


Figure 24.4. Use of Colburn Graph to Solve Example 24.1

The first step is to verify that the acetone concentration has indeed increased. This might involve having an operator or technician make flow and concentration measurements on the effluent stream in question. It is assumed that the increased concentration at the normal flowrate has been verified. The next step in Phase 1 is to check process inputs and process operation (because only one unit is known to be involved) for potential causes for the observed change in output concentration. Changes in input are evaluated first. If the inputs are not found to be the cause of the problem, process operation is then investigated. Example 24.1 shows seven possible causes ("suspects") for the observed change in output concentration.

Example 24.1.

Generate a list of causes for the observed change in absorber output. First, examine input changes, and then examine process operation changes.

The knowledge of packed-bed absorber performance illustrated on the Colburn graph is a good starting point. Any or all of these parameters could be different from design conditions.

Potential input problems include the following:

1. **Increased Flowrate of Gas to Be Treated:** A disturbance in A is a possible cause. Intuitively, if it is the gas rate, G, that has been disturbed, an increased gas rate would be the cause of an increased acetone concentration in the exit gas stream. This would result in a decrease in A.
2. **Decreased Flowrate of Water:** This would also result in a decrease in A.
3. **The Water Does Not Enter Acetone Free:** If the entering water contains acetone, intuitively, less acetone can be absorbed.
4. **There Is More Acetone in the Feed:** If the mole fraction of acetone in the feed were increased, the same fractional removal of acetone from air would result in a higher acetone mole fraction in the exit air stream.

These four items would be checked first to determine whether they are the cause of the faulty absorber performance. If they were not found to be the cause, the process operation would be investigated. Potential process operation problems include the following:

5. **A Decrease in Column Pressure:** Intuitively, a decrease in column pressure favors the vapor phase. Mathematically, because $A = L/mG$, and $m = P^*/P$, a decrease in P increases m, causing a decrease in A.
6. **An Increase in Column Temperature:** Intuitively, an increase in column temperature favors the vapor phase. Mathematically, because P^* increases with temperature, so does m, causing a decrease in A.
7. **There Is Channeling in the Packed Bed:** If there were channeling in the packed bed, not all of the available (and designed for) mass transfer area would be used. This could cause faulty absorber performance.

To reiterate, the process inputs would be checked. If they were not found to be the problem, then process operation would be investigated. The next step would be to check for fully open or closed control valves. In this problem, it is assumed that control valves are not involved. Phase 2 is also not applicable because there is only one unit operation involved in this problem.

Phase 3 involves a detailed analysis of the suspects. In Example 24.1, items 1, 2, 5, and 6 can be represented on the Colburn graph. For these items, diagnosis is that the absorption factor has decreased, which moves the operating point for the column vertically at constant $N_{tOG} = 6.2$ to point "b." The new absorption factor is 1.15. The problem could be in any (or all) of the parameters of the absorption factor. L could have decreased to 17,391 mol/h, or G could have increased to 46,000 mol/h. Alternatively, the value of m could have changed to 0.388, meaning that the temperature of the column increased to about 30°C (30.5°C), or that the column pressure decreased to 0.87 atm. However, because the air stream discharges to the atmosphere, a decrease in column pressure below 1 atm is not possible.

There is an alternative diagnosis, however, which is item 3 in Example 24.1. The operating point can remain fixed in the original position (point "a"), but the outlet acetone concentration in air increased due to the presence of acetone in the water fed to the column. This makes the second term in the numerator and denominator of the y-axis nonzero. Solution for the inlet acetone concentration in water yields a mole fraction of 0.00312.

Thus far, five possible causes for the observed increase in outlet acetone concentration in air have been identified. There are certainly additional possible causes, some of which are associated with equipment operation such as liquid distribution, channeling, and fouling, which could also contribute to the observed performance decrease. One of these is identified as item 6 in Example 24.1.

At this point, there is not enough information given to complete Phase 3 to identify the root cause of the problem. The next step would be to measure the input flows and concentrations, column temperature, column pressure, and column pressure drop (a measure of channeling). This should allow identification and verification of the root cause of the problem.

If the root cause of the reduced performance of the absorber is understood, then possible methods of compensation are straightforward (Phase 4). Here, it is assumed that compensation cannot be achieved by altering the cause of the disturbance; that is, if the cause is an increased gas rate, then the gas rate cannot be lowered. However, in the context of a chemical process, the possibility of reversing the disturbance should be investigated.

If the gas rate is too high, the liquid rate can be increased to compensate. However, flooding could be a problem, especially if both gas and liquid rates are increased. The Colburn graph does not account for flooding, which is specific to a given packed column.

If the liquid rate is too low, it is unlikely that the gas rate can be decreased without scaling down the entire process. A better choice might be to decrease the temperature of the absorber to 22°C, increase the pressure in the absorber to 1.15 atm, or make a combination of changes in temperature and pressure, in order to make the absorption equilibrium more favorable and bring the absorption factor back to a value of 1.48.

If a temperature increase is the problem and altering flowrates is not desirable due to flooding considerations, one possible compensation is to alter the pressure. Another might be to decrease the temperature of the water used to remove the acetone from the air. Increasing the liquid rate moves the column toward flooding, but a small increase should not be a serious problem.

Finally, if the cause of the disturbance is acetone in the water, compensation can be accomplished by decreasing the temperature, increasing the liquid rate, or increasing the pressure. For this situation, the stripping column used to remove scrubbed acetone from the water stream should also be investigated, because the cause of the faulty absorber performance may lie in an adjacent piece of

equipment.

In general, adjusting the temperature or pressure is probably the best method of compensation, because flooding is not an issue. Of course, there can be multiple causes of the disturbance, and compensation can be achieved by adjusting two variables by smaller amounts rather than by adjusting only one variable.

As an example of Phase 5, suppose that the root cause was determined to be an increase in acetone content of the scrubber liquor (water). It is necessary for you to notify anyone else using the same water supply of the acetone contamination. Similarly, suppose that channeling in the absorber was identified as the problem. It is necessary to report the operating conditions that caused the channeling to other parts of the company using the same packing material.

To review, this relatively simple problem illustrates how there can be multiple possible causes and multiple solutions to a troubleshooting problem. The strategy presented here for solving troubleshooting problems was illustrated.

24.2.2. Troubleshooting the Cumene Process Feed Section

This problem deals with the feed section to the cumene process in Appendix C, Figure C.8. This problem is actually part of the problem presented in Appendix C, and the process flowsheet along with calculations associated with the pumps can be found there. The problem is restated here.

A problem has recently arisen regarding the feed pumps to the cumene process. A maintenance check showed that P-802 (propylene feed pump) needed a new bearing, and a new one was installed. Premature bearing failure in this pump, often associated with cavitation, has occurred several times. The latest problem occurred during a recent warm spell, when the ambient temperature reached 110°F. The same maintenance check showed that P-801 (benzene feed pump) was fine. The ambient temperature has now returned to an average of 70°F, and both pumps seem to be working fine. Suggest a diagnosis and a method for compensation for the problem with P-802. In the process description in Appendix C, it is stated that propylene is stored in a tank as a saturated vapor/liquid mixture with liquid drawn from the tank as feed, and that liquid benzene is stored in a tank (most likely with an inert vapor blanket such as nitrogen) at atmospheric pressure.

In this case, the problem is immediately verified; the bearing had to be replaced. A check of the pump input might identify a contaminant that could have caused the bearing to deteriorate. It is assumed that no such contaminant was found. Because the unit operation producing the problem has already been identified, the root cause of the problem must be identified (Phase 3).

An intuitive understanding of pump operation suggests that the primary suspect is cavitation of P-802. This is consistent with the need for replacement of a bearing because cavitation can damage the internals of a pump. This may also be consistent with the recent warm spell, because the available Net Positive Suction Head, $NPSH_A$, often decreases at higher temperatures due to increasing vapor pressure. Recalling the discussion in Section 21.2.4,

$$NPSH_A = P_{inlet} - P^* \qquad (24.1)$$

Because the vapor pressure P^* increases with increasing temperature, it seems logical that the available NPSH decreased during the warm spell, causing cavitation that damaged the pump bearing. Example 24.2 shows the results of an analysis of the propylene feed pump.

Example 24.2.

Calculate the $NPSH_A$ for the propylene feed pump under normal ambient conditions (70°F) and for the warm spell (110°F).

Equation (24.1) can be rewritten as in Section 21.2.4, with an expression for P_{inlet} substituted.

$$NPSH_A = P_{tank} + \Delta P_{static} + \Delta P_{friction} - P^* = P_{tank} + \rho g h - \frac{2\rho f L_{eq} u^2}{D} - P^* \qquad \text{(E24.1)}$$

For the case of propylene being stored as a vapor/liquid mixture, the pressure in the tank is equal to the vapor pressure. As a consequence, $NPSH_A$ does not change with temperature because $P_{tank} = P^*$. Therefore, the $NPSH_A$ = 7 feet of liquid at the **level alarm low** (LAL—the tank level at which an alarm goes off warning of too low a liquid level in the tank) in the tank at all temperatures, as per the calculations shown in Appendix C.

The lesson learned from Example 24.2 is that although a belief in the understanding of how equipment works can help you focus on a solution to a troubleshooting problem, the tendency to focus on the first solution or on only one solution can lead to an erroneous solution.

> **Resist the temptation to focus on only one solution or the first solution that comes to mind.**

The reason why the pump malfunctioned is still not clear. If cavitation were the reason, the $NPSH_A$ expression should be investigated further. It is now known, for this situation, that

$$NPSH_A = \Delta P_{static} + \Delta P_{friction} \qquad (24.2)$$

reasons must be sought why this expression may have decreased in value. There may be reasons for the pump malfunction not associated with the $NPSH_A$. Therefore, five additional possibilities that should be analyzed (Phase 3) for causing the pump malfunction are as follows:

1. The static pressure has decreased. Perhaps the level in the tank has fallen below the low alarm level and the alarm has failed. Therefore, these items should be checked.
2. The frictional pressure has increased. Perhaps the flowrate from the tank has increased, causing an increase in frictional losses. The flowrate monitors and the settings on the control valve after the pump should be checked. This scenario would have additional consequences, because an increased propylene flowrate would have an effect on reactor conversion and possibly on product production rate and purity. Therefore, the flowrate and purity of the reactor effluent should also be checked.
3. The bearing in the pump wore out with age. Just because pump cavitation often causes damage to pump internals such as bearings does not mean that it was the cause of this pump's malfunction. Given the analysis above, it is possible, indeed likely, that the pump malfunction observed here was simply caused by a worn bearing.
4. Mechanical problems in the pump. The bearing could be wearing out prematurely due to poor shaft alignment within the pump.
5. There is a manufacturing defect within the pump. If the pump shaft or other internals were defective (incorrect size, for example), the bearing might wear out prematurely.

The recommended action (Phase 4) will depend upon which (if any) of the five causes of bearing failure listed above is identified to be the problem. If problems are found with the pump (item 4 and/or 5), it would be appropriate for you to notify others in your company using the same pump or similar pumps from the same manufacturer of the problem you have had with your pump.

24.3. Troubleshooting Multiple Units

In this section, two troubleshooting case studies are presented that involve multiple unit operations. One of the lessons of these case studies is that the symptoms of a problem are not necessarily observed at the source of the problem. In these two case studies, only one solution is discussed. Generation of alternative possibilities is the subject of problems at the end of the chapter.

24.3.1. Troubleshooting Off-Specification Acrylic Acid Product

This problem concerns an acrylic acid production process similar to the one in Appendix B, Figure B.9.1. The process flow diagram, stream flows, and equipment specifications are presented there.

At another acrylic acid plant owned by your company, process shutdown for modifications and improvements has recently been completed, and the process has been started up once again. Customers have begun to complain that the acrylic acid product does not appear to be meeting specifications. They have observed that the acrylic acid has a yellowish color, which is different from the clear liquid they had previously received. Their tests also found that the viscosity of the acrylic acid has increased.

The following process modifications were completed during the recent shutdown:

1. A new catalyst that is supposed to minimize side reactions was installed in the reactor. The reactor specifications were not changed.
2. A new solvent is now being used in the extraction unit. It is less expensive than the previous solvent, and the performance of the extraction unit is supposed to be unchanged. No modifications were made to the extraction equipment.
3. As a cost-cutting measure, refrigerated water (entering at 10°C) has been replaced by cooling water (entering at 30°C) in the acrylic acid purification column. The column has 25 actual trays with 2.25-in weirs, a total condenser, and a partial reboiler.

The following operating restrictions are also known: For the new catalyst, the operating range is between 250°C and 350°C and between 1 bar and 5 bar. Once the acrylic acid has been produced and condensed into the liquid phase, the temperature is to be maintained below 90°C to avoid polymerization of the acrylic acid.

The first step is to verify the problem. Assume that you had a technician take a sample of acrylic acid product, and the yellowish color and increased viscosity were both verified. This means that the problem is not in the shipping and storage steps but is within the plant. Therefore, the problem is yours, not the customer's. Further, assume that all process inputs have been checked and found to be within normal operating conditions, and that a check has found no control valves to be fully open or closed.

There are several possible causes for the off-specification acrylic acid product. The most likely causes are changes that may have occurred during shutdown. Perhaps the new catalyst is not

performing as designed. Perhaps the new solvent is contaminating the product. The reactor effluent and the extractor effluent streams should be checked for contamination. Suppose that has been done, and everything has been found to be within normal conditions. Therefore, the most likely cause involves the temperature in the acrylic acid distillation column. In this column, acrylic acid and acetic acid are separated. It will be assumed that this is a simple binary distillation.

There must have been a reason for using refrigerated water in the distillation column prior to the recent shutdown. This can be understood using an analysis similar to the one in Section 22.2. From tabulated data [2], the following vapor pressure expressions can be obtained for acrylic acid and acetic acid:

$$\text{Acrylic acid:} \quad \ln P^* \text{ (mm Hg)} = 19.776 - \frac{5450.06}{T(\text{K})} \tag{24.3}$$

$$\text{Acetic acid:} \quad \ln P^* \text{ (mm Hg)} = 18.829 - \frac{4786.41}{T(\text{K})} \tag{24.4}$$

Because acrylic acid is the heavier component, the bottom of the column must remain below 90°C to avoid undesired acrylic acid polymerization. From Equation (24.3), assuming that pure, saturated acrylic acid leaves the bottom of the column, the pressure at the bottom of the column is 118 mm Hg, which is 5.26 ft of liquid, assuming that liquid, acrylic acid and liquid acetic acid have the same density as liquid water. The pressure drop per tray will be approximated by the height of liquid on the tray. The height of liquid on each tray will be approximated by the weir height. Because there are 25 trays, the pressure drop in the column is

$$25 \text{ trays}[(2.25/12)\text{ft liquid/tray}] = 4.69 \text{ ft liquid}$$

Therefore, the pressure at the top of the column is 5.26 – 4.69 = 0.57 ft liquid = 12.8 mm Hg. From Equation (24.4), assuming pure, saturated acetic acid at the top of the column, $T = 21$°C. Because cooling water enters at 30°C, it is not possible to condense acetic acid at 21°C with cooling water. This is why refrigerated water was used in the original design.

The above discussion suggests that the switch to cooling water could be one reason for the off-specification acrylic acid product. With cooling water available at 30°C, it is not possible for the top of the column to be less than 30°C, which places a lower bound on the top pressure of the column. Because the pressure drop in the column is fixed by the weir height on the trays, there is also a lower bound on bottom pressure in the column, which places a lower bound on the bottom temperature, which is greater than 90°C, thereby promoting polymerization. Apparently, this column has no control room pressure reading (perhaps the instrument is out of order). Therefore, an operator would be sent to measure the pressure at the top of the column.

There is one simple remedy. Refrigerated water should be used in the condenser. If this is not desirable for the long term, the incremental economics of modifying the trays to have lower weirs could be considered, which could happen only at the next plant shutdown. It is also necessary for you to report this problem to any other plants within your company making acrylic acid so that they can avoid (or correct) problems arising from the use of cooling water instead of refrigerated water.

It is observed that rough calculations involving certain reasonable, simplifying assumptions were used to obtain an approximate result very quickly. It is neither necessary nor desirable to do detailed calculations when screening alternatives in a troubleshooting problem.

When screening alternatives, rough calculations using reasonable approximations are

more useful than detailed simulations.

The approximations that were made to facilitate a rapid calculation for the distillation column were that the top and bottoms products were pure and that the height of liquid on the trays equaled the weir height. Although these are not exactly true, detailed calculations would show that these are good approximations.

24.3.2. Troubleshooting Steam Release in Cumene Reactor

This problem involves the reactor in a cumene process similar to the one in Appendix C, Figure C.8. The process flow diagram is presented in Appendix C.

A company has been testing a new cumene catalyst at a facility producing the identical amount of cumene as the one in Appendix C. The new catalyst completely suppresses the undesired DIPB formation reaction. However, the reaction rate for the desired reaction is lower. Therefore, when the new catalyst is used in the existing reactor, a single-pass conversion of only 50% is obtained. This new catalyst, which is less expensive than the previous catalyst, is known to have a higher initial activity that decays rapidly to constant activity. During the initial activity period, a 33% increase in cumene production has been observed. The operating parameters of the benzene distillation column have been altered, the recycle benzene stream has been increased, the DIPB column has been taken off-line, and the plant has been producing cumene successfully.

The reactor for cumene production, which is shown in Figure 24.5, is of the shell-and-tube design, with catalyst in the tubes and boiler feed water vaporized to form high-pressure steam in the shell. The pipe to the steam header is 2-in schedule 40 and contains 32.5 m of equivalent pipe length after the regulating valve. Under normal operating conditions, the pressure drop across the regulating valve is 50 kPa. There is a pressure-relief valve on the shell side of the reactor rated at 4500 kPa. The tubes are completely submerged in the boiler feed water. As part of the test of the new catalyst, the plant has been shut down briefly every three months for the past year, and the catalyst has been replaced so that the spent catalyst could be studied.

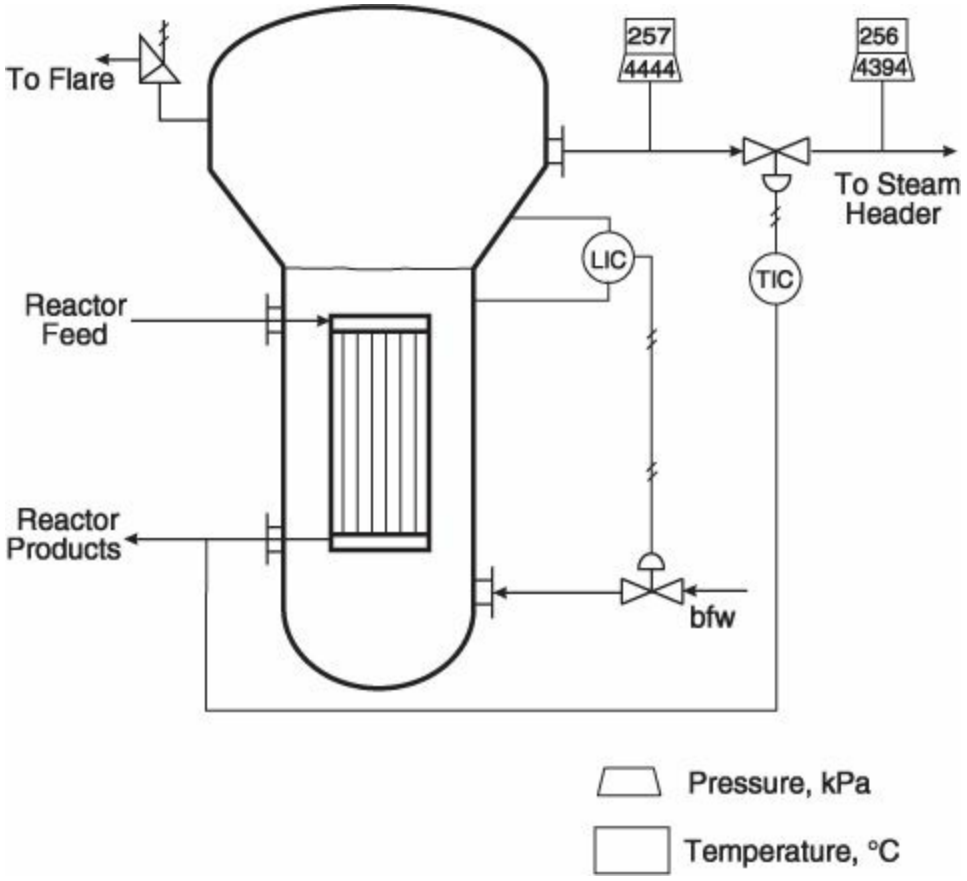


Figure 24.5. Cumene Reactor in Case Study

After start-up subsequent to each shutdown, the pressure-relief valve on the shell side of the reactor has opened periodically for a few days. Because only steam was released and it is not in a part of the plant where anyone could be harmed, the problem was attributed to start-up transients and was ignored. A recent safety audit has resulted in the suggestion that the cause of this problem be identified and corrected.

The problem is verified by the observation of a steam release. Assume that you have checked all process inputs, the operation of all other units, and control valves and you have decided that the problem must be at the reactor. A check of the reactor feed and the boiler feed water input reveals normal conditions. Therefore, the problem must be with reactor operation, which points to the higher-activity catalyst.

First, it is necessary to calculate some operating parameters for the design conditions. Under normal operating conditions, from Appendix C, the heat generated in the reactor is 9800 MJ/h. The amount of steam formed can be calculated.

$$Q = \dot{m}_{stm}[C_p(T_{stm} - T_{bfw}) + \lambda_{stm}] \qquad (24.5)$$

Solving for the mass flow of steam yields

$$\dot{m}_{stm} = \frac{9{,}800{,}000 \text{ kJ/h}}{[4.35 \text{ kJ/kg°C}(256 - 90\text{°C}) + 1700 \text{ kJ/kg}]} = 4046 \text{ kg/h}$$

Here, the heat capacity of water is taken at an average temperature of 173°C, and the temperature of steam formed in the shell corresponds to the pressure in the shell calculated below. Because high-pressure steam is made, the pressure of steam downstream of the reactor is that of high-pressure steam, 4237 kPa. Under design conditions, the pressure of steam in the reactor exceeds this value to account for the pressure drop in the pipe leading to the steam header and across the regulating valve.

The density of the steam varies with the pressure. It will be assumed that the average steam conditions between the reactor shell and the steam header are 255°C and 4300 kPa. At these conditions, the density of steam is about 17.6 kg/m^3. For 2-in schedule-40 pipe ($D = 0.05250$ m), at the given mass flow and density of steam, the velocity in the pipe is 28.3 m/s, so the Reynolds number is

$$\mathrm{Re} = \frac{(0.0525\ \mathrm{m})(28.3\ \mathrm{m/s})(17.6\ \mathrm{kg/m^3})}{1.88 \times 10^{-5}\ \mathrm{kg/m\ s}} = 1.39 \times 10^6$$

For commercial steel pipe, $e/d = 4.6 \times 10^{-5}$ m/0.0525 m = 0.0009. From Figure 20.1, the friction factor $f = 0.009$. Therefore, the pressure drop in the pipe leading to the steam header is

$$\Delta P = \frac{2f\rho L_{eq}u^2}{D} = \frac{2(0.009)(17.6\ \mathrm{kg/m^3})(32.5\ \mathrm{m})(28.3\ \mathrm{m/s})^2}{0.0525\ \mathrm{m}} = 157\ \mathrm{kPa}$$

The pressure in the reactor shell, under normal conditions, is the pressure at the steam header plus the pressure drop in the pipe plus the pressure drop across the valve, which is

$$P_{rxr} = 4237 + 157 + 50 = 4444\ \mathrm{kPa}$$

The situation immediately after catalyst replacement can be analyzed using base-case ratios. If the activity of the new catalyst is higher than that of the old catalyst, then the reaction rate is increased. Because the only reaction involved is for cumene production, 33% more steam is produced. Therefore, the steam velocity in the pipe leading to the steam header is increased by 33%. Because the flow is fully turbulent, the friction factor remains constant, and, assuming unchanged density,

$$\frac{\Delta P_2}{\Delta P_1} = \left(\frac{v_2}{v_1}\right)^2 = 1.33^2 = 1.77 \qquad (24.6)$$

where subscript 2 refers to new conditions and subscript 1 refers to design conditions. Therefore,

$$\Delta P_2 = 157\ \mathrm{kPa}(1.77) = 278\ \mathrm{kPa}$$

If it is assumed that the control system has responded by opening the regulating valve completely, so there is no pressure drop across the valve, then the pressure in the reactor shell is

$$P_{rxr} = 4237 + 278 = 4515\ \mathrm{kPa}$$

which exceeds the rating for the pressure-relief valve, causing it to open and release steam.

Now that the problem has been identified, the next question is how to compensate for this problem. It is likely that necessary changes can be made only during the next shutdown, which is not a problem because there are no releases for most of an operating cycle. One alteration would be to reset the pressure-relief valve to a higher pressure. Caution is warranted here because the 4500 kPa limit was originally chosen for a reason. The pressure ratings for the materials of construction and reactor design should be checked very carefully to determine their limits.

Another simple solution would be to replace the line leading to the steam header with larger-diameter pipe. The next larger size, 2.5-in schedule 40, has a diameter $D = 0.06271$ m. Using a relationship from Table 20.1, a base-case ratio at the original flowrate is

$$\frac{\Delta P_2}{\Delta P_1} = \left(\frac{D_1}{D_2}\right)^5 = \left(\frac{0.05250}{0.06271}\right)^5 = 0.41$$

So the pressure drop, under normal operating conditions with the new pipe, is

$$\Delta P_2 = 157\ \mathrm{kPa}(0.41) = 64.4\ \mathrm{kPa}$$

and the pressure drop with the new pipe with increased catalyst activity is

$$\Delta P_2 = 64.4 \text{ kPa}(1.77) = 114 \text{ kPa}$$

and the pressure in the reactor is

$$P_{rxr} = 4237 + 114 = 4351 \text{ kPa}$$

With the larger-diameter pipe, it is possible for there to be a pressure change across the regulating valve without exceeding the cutoff pressure of the relief valve.

Finally, you should report these results and explanations clearly so that proper modifications can be made in similar plants prior to switching to the new catalyst.

24.4. A Process Troubleshooting Problem

In this section, a troubleshooting problem involving an entire process is presented [3]. It is based on the production of cumene problem presented in Appendix C, Figure C.8. The process flowsheet and stream flow table are included in Appendix C.

Lately, Unit 800 has not been operating within standard conditions. There is a new supplier of propylene; however, the contract guarantees that the new propylene feed will contain less than 5 wt% propane.

Upon examining present operating conditions, the following observations were made:

1. Production of cumene has dropped by about 8%, and the reflux in T-801 was increased by approximately 8% in order to maintain 99 wt% purity. The flows of benzene (Stream 1) and propylene (Stream 2) have remained the same. Pressure in the storage tanks (not shown on the flowsheet) has not changed appreciably when measured at the same ambient temperature.
2. The amount of fuel gas being produced has increased significantly and is estimated to be 78% greater than before. Additionally, it has been observed that the pressure control valve on the fuel gas line (Stream 9) leading from V-802 is now fully open, whereas previously it was controlling the flow.
3. The benzene recycle Stream 11 has increased by about 5%, and the temperature of Stream 3 into P-201 has increased by about 3°C.
4. Production of steam in the reactor has fallen by about 6%.
5. Catalyst in the reactor was changed six months ago, and previous operating history (over the last ten years) indicates that no significant drop in catalyst activity should have occurred over this time period.
6. p-diisopropyl benzene (p-DIPB) production, Stream 14, has dropped by about 20%.

Suggest possible causes and potential remedies for the observed problems.

The reactions are as follows:

$$\underset{\text{propylene}}{C_3H_6} + \underset{\text{benzene}}{C_6H_6} \rightarrow \underset{\text{cumene}}{C_9H_{12}} \qquad (24.7)$$

$$\underset{\text{propylene}}{C_3H_6} + \underset{\text{cumene}}{C_9H_{12}} \rightarrow \underset{\text{p-diisopropyl benzene}}{C_{12}H_{18}} \qquad (24.8)$$

Assume that all of the above symptoms have been verified. The next step would be to check process

inputs, which might reveal off-specification feed. This might immediately identify the problem. A check of the control valves verifies that only the valve in Stream 9 is fully open, as stated in Observation 2. If there were no problems with the feed, the next step would be to check the individual units to determine which ones were not operating within normal limits. As part of Phase 2, analyze the six observations above to determine what they suggest.

An analysis of the six observations above suggests the following:

1. Observation 1 suggests that either less cumene is being produced in the reactor or that significant cumene is being lost as fuel gas. If it is assumed that the feeds are unchanged, these are the only possibilities.
2. Observation 2 suggests that the fuel gas rate has increased significantly. Components of fuel gas could be cumene, unreacted propylene and benzene, propane, and p-DIPB.
3. Observation 3 suggests that additional benzene is being processed in the distillation column. The temperature increase could be due to the increased concentration of benzene relative to propane and propylene at the top of T-801.
4. Observation 4 suggests that less cumene is being formed in the reactor. This is the opposite situation to that in the case study presented in the previous section.
5. Observation 5 suggests that catalyst deactivation should not be a problem. This does not necessarily guarantee that catalyst deactivation is not a problem.
6. Observation 6 suggests that the selectivity for the desired reaction, Equation (24.7), has increased.

Among the possible causes of some of these observations are the following:

1. The propylene feed contains propane impurity in excess of 5 wt%. Even though the new supplier claims that the propylene meets specifications, it is possible that the propylene is off specification. This would be verified in Phase 1. If the propylene feed contains undetected excess propane, it is likely that the feed rate would be unchanged. (This could also be verified.) Therefore, the concentration of propylene in the reactor feed would decrease, thereby decreasing the reaction rate. Conversion in the reactor would then decrease. An examination of Figure 24.6, the approximate reactor profiles, shows that a decrease in reactor conversion would have a larger percentage effect on the p-DIPB, because its concentration is lower. Examination of the kinetics, which are based on the assumption that Equations (24.7) and (24.8) are elementary steps, also supports this diagnosis. If the concentration of propylene is decreased, the rates of Equations (24.7) and (24.8) decrease. This decreases the concentration of cumene in the reactor, which causes the rate of Equation (24.8) to decrease even further, reducing the p-DIPB concentration more than the cumene concentration. If this reactor scenario were true, then there would be additional propane leaving the reactor. This would increase the flow of fuel gas, which is mostly propane and propylene, and increase the recycle, which is mostly benzene. It is seen that this scenario is consistent with all six observations.

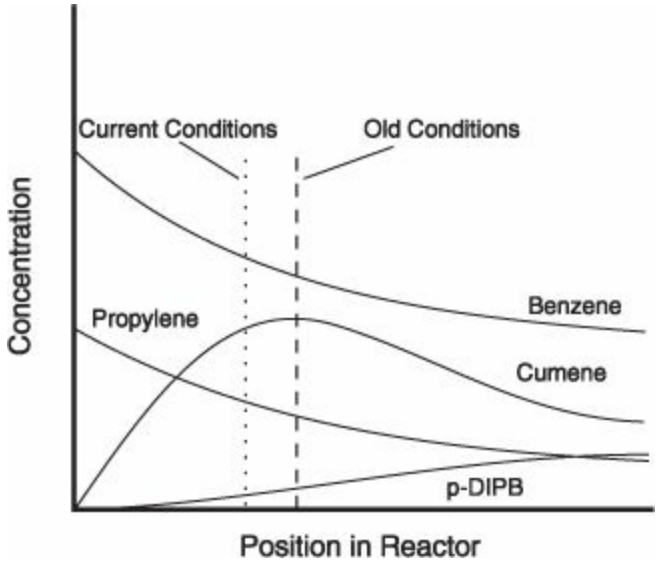


Figure 24.6. Concentration Profiles in Reactor for Case Study

2. The catalyst is defective and has begun to deactivate. This could be checked by analyzing samples of the reactor input and reactor output. If the catalyst is defective and has begun to deactivate, all reaction rates would decrease. This would result in less cumene and p-DIPB and more unreacted benzene and propylene. This scenario is consistent with five of the six observations. Because the possibility of bad catalyst must be acknowledged, this scenario is also possible.
3. Reactor temperature has decreased. This could be checked in the control room, but the possibility of a faulty thermocouple or indicator should also be considered if the "correct" temperature was observed. A decrease in reactor temperature would result in decreased reaction rates. Qualitatively, the results are similar to those for deactivated catalyst in item 2.
4. Reactor pressure has decreased. This could be checked in the control room, but the possibility of a faulty pressure transducer or indicator should also be considered if a "correct" pressure was observed. A decrease in reactor pressure would result in a decrease in all gas-phase concentrations and a decrease in all reaction rates. Qualitatively, the results are similar to items 2 and 3.
5. The flow controllers on Streams 1 and/or 2 have failed. Suppose that the benzene flow were increased or the propylene flow were decreased. The benzene concentration would increase, which would increase the excess benzene and increase the selectivity for the desired reaction. This is consistent with the last observation above. If this were not observed in the control room, the possibility of faulty instrumentation should be considered.
6. The temperature and/or pressure in V-802 is not at specification. This could be checked, but a "correct" reading could be due to faulty instrumentation. If the temperature and/or pressure in the flash vessel were incorrect, the desired separation would not be accomplished. If the temperature were too high and/or the pressure were too low, additional fuel gas would be produced, causing less cumene to leave as product and less benzene in the recycle. If the opposite were true, additional feed to the distillation column would be produced, which could cause flooding in the column and compromise the desired separation.
7. The problem stems from a combination of any or all of the above items. There is no guarantee that the problem has only one cause. Therefore, combinations of the above possibilities should be considered.

An examination of items 1–7 suggests that taking a sample of the fuel gas would identify the root cause of the problem. If there was too much propane in the fuel gas, the problem would be with the feed. If there was too much benzene in the fuel gas, the problem would be reduced conversion in the reactor. If there was too much or too little cumene in the fuel gas, the problem would be that the temperature and/or pressure of the flash was incorrect.

The next question is how to remedy the problem. It is not always necessary to identify the cause of a problem in order to begin to compensate. However, it is necessary to identify the problem to ensure that it does not recur. It is also necessary to be certain that what appears to be a remedy is not itself a problem. For example, if the propylene feed contains excess propane or if the catalyst was deactivated, it would still be necessary to find a way to compensate temporarily until new feed and/or catalyst could be obtained. Also, detailed quantitative solutions may not be necessary as long as the qualitative trends are understood.

In order to suggest remedies, it will be assumed that the cause of the observed process upset is in the process feed and in the reactor (items 1 and 2). Possible remedies include, but are not limited to, the following:

1. **Increase the temperature in the reactor.** Intuitively, this seems like a reasonable possibility. However, Chapters 22 and 23 should be consulted for the limitations associated with increasing reactor temperature. Increasing the reactor feed temperature can be accomplished by increasing the air and natural gas flows to the fired heater, but the reactor operation is limited by heat transfer. Increasing the reaction temperature increases the reaction rate exponentially, so a large temperature increase should not be needed. However, increasing the inlet temperature does not guarantee that the reactor operation will change appreciably. This situation was illustrated in Example 22.1 and is an example of heat transfer limitations of reactor performance, as discussed in Section 23.4. One consequence of increasing reactor temperature is that the temperature of the boiling water used to remove the heat of reaction must increase. This requires an increased steam pressure. It must be determined whether the materials of construction of the reactor can withstand the required pressure increase. The temperature limitations of the catalyst support and of catalyst activity must also be considered. Increasing the temperature high enough to damage the catalyst is an example of the remedy causing another problem.
2. **Increase the pressure on the process side in the reactor**. Increasing the pressure in the reactor can be accomplished by closing the valve after the reactor. The increase in pressure increases the reaction rate by increasing the concentration. The effect is not as significant as for temperature, because temperature increases the reaction rate exponentially.
3. **Increase the flow of propylene feed.** Increasing the propylene feed can be accomplished only by using the spare pump (P-802B) in series or in parallel with the operating pump (P-802A), due to limitations in pumping capacity shown on the pump and system curve plot, which is shown in Appendix C. In principle, the flow of propylene can be increased enough so that the specified cumene production rate is achieved in the reactor. However, it must be determined how each piece of equipment will perform when subjected to the increased capacity and concentration changes caused by this remedy. The required calculations are performance problems like those discussed in Chapters 21 and 22.

There are several lessons to be learned from this process troubleshooting problem. As discussed

earlier in this chapter, it is important not to focus on one possible solution to the exclusion of others. It is important to consider as many alternatives as possible. Several possible causes were presented here for the observed process upsets. Without detailed measurements and/or simulations, which take more time to perform, the other possibilities could not be ruled out. They would cause the same qualitative trends, but different quantitative values for the upset parameters.

It is also important to observe that a problem in the reactor was manifested in process locations far removed from the reactor: the fuel gas, the benzene recycle, the cumene production rate, and the p-DIPB production rate.

The cause of an observed process upset may be located in a different part of the process.

Finally, if the problem was identified to be impure propylene feed or defective catalyst, it would be necessary to report this problem to other plants in your company using the same propylene feed supplier or the same catalyst.

24.5. Debottlenecking Problems

In the course of operating a chemical process, it may become necessary to modify operating conditions. Possible changes include scale-up, scale-down, handling a new feed composition, and so on. A bottleneck is defined as the part of the process that limits the desired change. Troubleshooting the bottleneck is called debottlenecking. Debottlenecking is a sequential process. A bottleneck is identified and removed. The next bottleneck is then identified and removed, and so on. The removal of these bottlenecks does not usually involve a large capital investment.

The performance of a heating loop problem discussed in Section 22.3 was actually a debottlenecking problem. In this problem, described in detail in Appendix C, it is necessary to scale up production of the allyl chloride facility (see Appendix C, Figure C.4) due to an unscheduled shutdown at a similar facility owned by the same company. The problem is to determine the maximum level of scale-up possible for the allyl chloride facility. Therefore, it is necessary to determine the maximum scale-up possible for the reactor. (*Note:* Some conditions in the problem in the appendix are different from those in Section 22.3.)

For the problem in Section 22.3, it was determined that the pump in the Dowtherm A loop could handle only 5% increased flow, which allowed only 2% increased reactor operation. Within the reactor portion of the allyl chloride process, the pump is identified as the bottleneck. From the perspective of the entire process, assuming that all other units can be scaled up by more than 5%, the Dowtherm A loop is the bottleneck. In Section 22.3, it was shown that by operating the two reactor heat-exchange coils in parallel, the reactor could be scaled up by 15%. Altering configuration of the reactor heat-exchange coils is the act of debottlenecking the process. For this problem, it can be shown that additional scale-up in the reactor and Dowtherm A loop is possible by operating the pump and the spare either in series or in parallel (Problem 22.6). Suppose that the maximum scale-up were now found to be 25% (not the correct answer to Problem 22.6). What if one of the distillation columns downstream could handle only 20% increased throughput before flooding? Then the distillation column would become the new bottleneck. You would now focus on methods for debottlenecking the distillation column. If this were possible, then another unit would become the bottleneck, and so forth. Therefore, debottlenecking is a progressive problem in which bottlenecks

are removed from the process one at a time. Eventually, the maximum possible change, where a bottleneck cannot be removed, will be reached. At this point, a decision would have to be made whether a significant capital investment should be made in order to increase further the maximum scale-up. When significant process modifications involving new equipment are required, the procedure is called **retrofitting**.

24.6. Summary

In summary, process troubleshooting problems and debottlenecking problems, such as the ones described here, are very realistic problems in terms of what the process engineer will experience. Unlike comprehensive design problems, the troubleshooting problems rely on simple, approximate calculations along with an intuitive understanding of a chemical process rather than repetitive, complex calculations. In order to solve troubleshooting and debottlenecking problems, it is important to develop both an intuitive feel for chemical processes and the ability to do approximate calculations to complement your ability to do repetitive, detailed calculations.

What You Should Have Learned

- If there is a process upset, it may be traceable to a distant part of the process.
- There are multiple possible causes for a process upset, and all must be considered.
- When debottlenecking a process, identify the most severe bottleneck, and if that portion can be debottlenecked, proceed to the next most severe bottleneck, and so on.

References

1. Fogler, H. S., and S. E. LeBlanc, *Strategies for Creative Problem Solving*, 2nd ed. (Upper Saddle River, NJ: Prentice Hall, 2008), 20.
2. Perry, R. H., D. W. Green, and J. O. Maloney, eds., *Perry's Chemical Engineers' Handbook*, 7th ed. (New York: McGraw-Hill, 1997), 2–61.
3. Shaeiwitz, J. A., and R. Turton, "A Process Troubleshooting Problem," *1996 Annual ASEE Conference Proceedings*, Session 3213.

Problems

1. For the absorber problem in Section 24.2.1, it is necessary to adjust process operation temporarily to handle a 20% increase in gas to be treated.
   a. Can this be accomplished by increasing the liquid rate by 20%?
   b. Suggest at least two additional methods for handling the increase. Be quantitative.
2. A five-equilibrium-stage tray absorber is used for the acetone separation described in Section 24.2.1. It is now observed that the outlet mole fraction of acetone in air is 0.002.
   a. Suggest at least six individual causes for the faulty absorber performance.
   b. For the causes listed in Part (a) that are represented on the Kremser graph, determine the exact value of the parameter (i.e., what flowrate would cause the observed outlet mole fraction?).
   c. For each cause listed in Part (b), suggest at least three compensation methods. Be quantitative.

3. For the situation in Problem 24.2, how would you handle the following temporary process upsets? Be quantitative. Suggest at least three alternatives for each situation.
   a. The gas rate must increase by 10%.
   b. The feed mole fraction of acetone must increase to 0.025.
   c. The outlet mole fraction of acetone in air must be reduced to 0.00075.
4. Suggest additional alternatives for the off-specification acrylic acid in the case study in Section 24.3.1. Analyze the alternatives quantitatively.
5. An acrylic acid facility has been designed to operate successfully using cooling water in the distillation column condenser. However, after a recent warm spell in which the temperature exceeded 100°F for a week, customers complained that the acrylic acid product had the same yellowish color and increased viscosity observed in another plant, as described in Section 24.3.1. Suggest possible causes and remedies for this situation.
6. Suggest additional alternatives for the steam release in the cumene reactor in the case study in Section 24.3.2. Analyze the alternatives quantitatively.
7. During the start-up of a chemical plant, one of the final steps before introducing the process chemicals is a steam-out procedure. Essentially, this step involves filling all the equipment with low-pressure steam and leaving it for a period of time in order to clean the equipment. During one such steam-out, in a plant in Wisconsin, a vessel was accidentally isolated from other equipment and left to stand overnight. Upon inspection the following morning, it was found that this vessel had ruptured.

   The company responsible for the design of the plant claimed that the design was not at fault and cited a similar situation that occurred at a plant in Southern California in which no damage to the vessel was seen to occur.

   From the above information can you explain what happened? What would you suggest be done in the future in order to ensure that this problem does not reoccur?
8. During the hydrogenation of a certain plant-derived oil, the fresh feed is pumped from a vessel to the process unit. The process is illustrated in Figure P24.8(a).

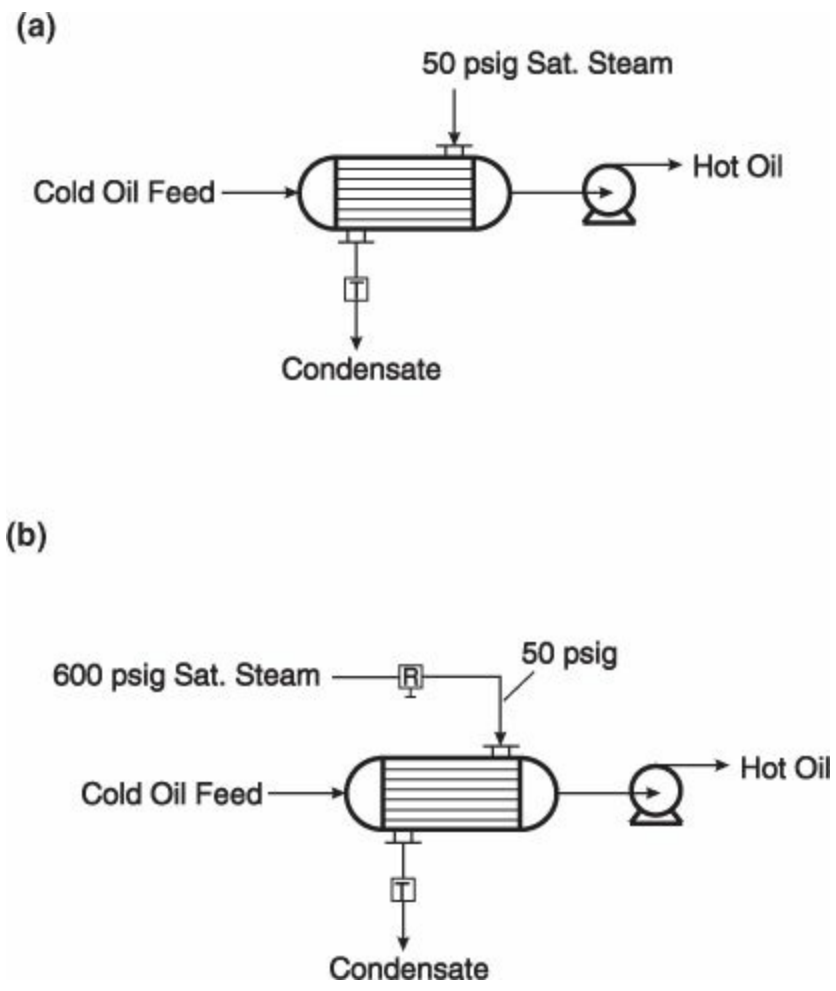


Figure P24.8. Heat-Exchanger Configurations for Problem 24.8

Because the oil is very viscous, it is heated with steam that passes through a heating coil located in the vessel. The present system uses 50 psig saturated steam to heat the oil. Due to unforeseen circumstances, the 50 psig steam supply will be down for maintenance for about a week. It has been suggested that a temporary connection from the high-pressure steam line (600 psig, saturated) be made via a regulator (to reduce the pressure to 50 psig) to supply steam to the steam coil as shown in Figure P24.8(b).

Do you foresee any problems with the recommendation regarding the high-pressure steam? If so, what recommendations do you suggest?

9. During the start-up and operation of a new plant (see Figure P24.9) the pressure-relief/safety valve on top of the steam drum (V-101) of a waste heat boiler (E-101) has opened and low-pressure steam is escaping to the atmosphere through the open valve.

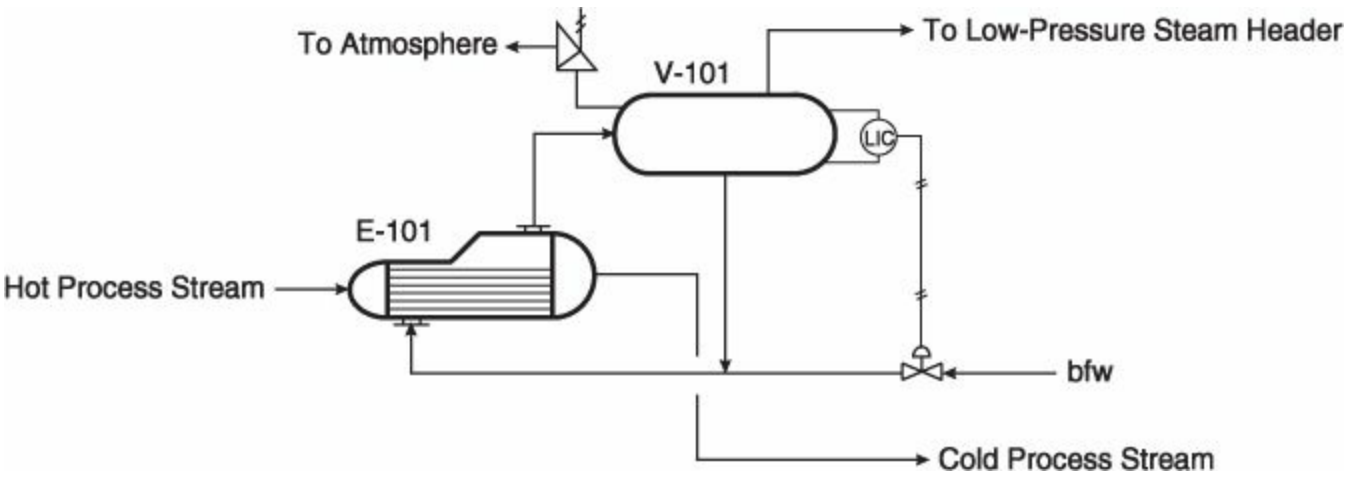


Figure P24.9. PFD for Problem 24.9

Upon questioning the operators from another unit, you discover that similar incidents have occurred during the initial operation of other process units. However, it appears that the situation remedies itself after a few months.

What could be causing this phenomenon to occur? If the situation does not remedy itself, what permanent solution (if any) would you suggest to fix the problem?

10. For the cumene troubleshooting problem in Section 24.4, it has been determined that off-specification propylene will have to be used for the next several months. To assist in handling this feed, prepare the following performance graphs for use in determining what reactor temperature and pressure are required to compensate for increased propane impurity. Determine the maximum possible propane impurity that can be handled in the given temperature or pressure range without loss of cumene production capability.
    a. A plot of cumene production rate versus propane impurity (from 5 wt% to 10 wt%) at pressures from 2700 kPa to 3300 kPa at 400°C and the original propylene feed rate
    b. A plot of cumene production rate versus propane impurity (from 5 wt% to 10 wt%) at temperatures from 300°C to 400°C at 3300 kPa and the original propylene feed rate
11. In the cumene problem in Section 24.4, assume that one possible remedy involves increased benzene recycle with a corresponding decrease in fresh benzene feed. What are some potential consequences on the benzene feed pump, P-201? Support your answer with calculations.
12. You are in charge of a process to manufacture a polymer in which acetone is used as a solvent. The last step is a drying oven in which residual acetone is removed from the polymer into an air stream. The air is fed to the absorber in Example 24.1. All flows, mole fractions, and physical property data in Example 24.1 are assumed to hold.

    It is necessary to scale up polymer production as much as possible. Upstream, there is a spare reactor, dryer, and peripherals, because the plant has been operating below capacity for many years. However, the acetone scrubber was designed and installed recently for the current production capacity. Therefore, it is anticipated that the acetone scrubber will be the process bottleneck. What limit does the acetone scrubber place on scale-up? How would you debottleneck this situation?
13. The phthalic acid production scale-down project (Appendix C, Project 3) involves determining a method for scale-down of phthalic acid production by 50%. The feed section of this process was discussed in Section 22.4.
    a. Identify potential bottlenecks to the 50% scale-down.
    b. Quantify the answer to Part (a); that is, determine the primary bottleneck to 50% scale-down.
    c. Debottleneck your answer to Part (b).
    d. Repeat Parts (b) and (c) until 50% scale-down or a maximum possible scale-down is achieved.
14. For the cumene problem in Section 24.4, it has been determined that the feed is off specification. Until a new propylene supplier can be contracted with, the propylene from the current supplier will have to be used. Tests have shown that this propylene can be expected to have between 5 wt% and 10 wt% propane impurity. It has been decided to try to maintain the design cumene production rate by increasing the propylene feed rate so that a constant, design amount of

propylene enters the reactor. Identify the bottlenecks to the proposed process change. Debottleneck this situation.

15. A saturated liquid is stored in a tank in equilibrium with its vapor. The liquid is pumped to a heat exchanger, where the liquid is vaporized. Frictional losses in the suction line to the pump are negligible; however, frictional losses after the pump are such that the liquid is saturated upon entering the heat exchanger. The heat exchanger vaporizes the saturated liquid to saturated vapor while condensing saturated steam to saturated liquid.

In the base case, the liquid vaporizes at 130°C, and the steam used is passed through a desuperheater to create saturated steam at 155°C from saturated, low-pressure steam at 160°C. It is now necessary to increase the flowrate of the vaporized stream. Pump and system curves are provided in Figures P24.15a and P24.15b. Assume that the pressure entering the vaporizer remains constant.

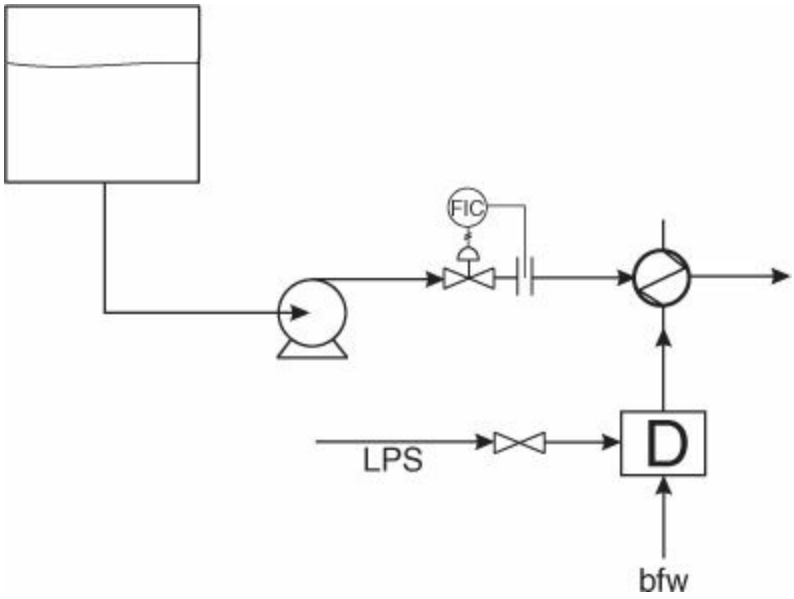


Figure P24.15a. Process Flow Diagram for Problem 24.15

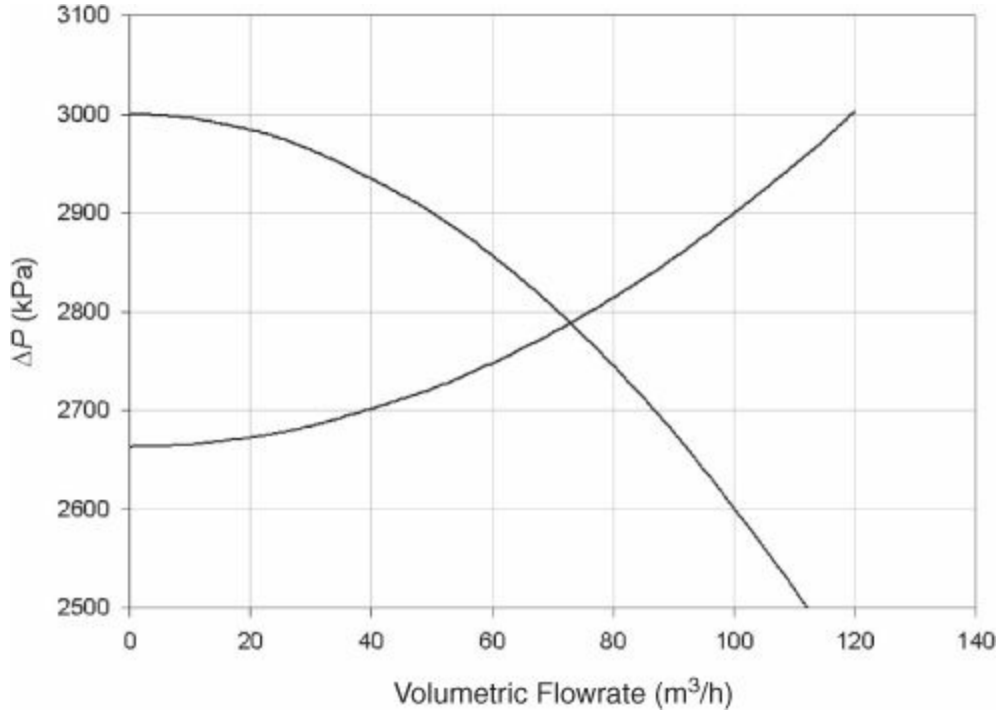


Figure P24.15b. Pump and System Curves for Problem 24.15

a. If the base-case flowrate is 50 m^3/h, identify the bottleneck to process flowrate scale-up.

What is the maximum possible flowrate increase?

b. With scale-up, the frictional losses in the suction line to the pump increase. Is the pump in danger of cavitating? Explain your answer.

For Problems 24.16–24.17, it may be useful to refer to the following document: http://www.che.cemr.wvu.edu/publications/projects/drying_oil/do12.pdf.

16. Refer to the drying oil process in Appendix B. The following problems were encountered after the drying oil facility was started up in early August.

a. Pump P-501 A/B has been noisy since start-up, and the noise (a high-pitched whine) continues to get louder.

b. Problems have been observed in T-501. Column performance has been below specification. Specifically, the flowrate of Dowtherm A through the reboiler, E-502, has had to be increased in order to keep the products at design specifications.

c. It has also been noted recently that production rates have fallen during the graveyard shift (12 p.m. – 8 a.m.). The head of operations believed that this was due to some of the operators not paying attention to the plant during this shift. However, after talking to all concerned, it appears that there might be a problem with the feed of ACO from the storage tank (not shown on the PFD) to the feed vessel, V-501.

d. The pressure-relief valve on E-506 has been open from the start of production, and steam has been venting to the atmosphere. This problem was more severe right after start-up; however, it is still occurring. Suggest causes for these problems, identify the most likely causes, and suggest potential remedies.

17. Refer to the drying oil process in Appendix B. Due to an unfavorable business climate for the product, it is possible that production will have to be cut by 20%. Suggest at least three equipment-related issues that might have to be addressed to implement the production cut.

For Problem 24.18, it may be useful to refer to the following document: http://www.che.cemr.wvu.edu/publications/projects/formalin/formalin12.pdf.

18. Refer to the formalin process in Appendix B.

You have recently joined a chemical company. Among the chemicals that this company produces is methanol, mostly for internal consumption. A major use of internal methanol is to produce formalin, which is a 37 wt% solution of formaldehyde in water. Formaldehyde and urea are used to make urea-formaldehyde resins that are subsequently used as adhesives and binders for particleboard and plywood.

The company recently received a memorandum from a customer who buys this formalin indicating that there are periodic problems, mostly in the summer, with the formalin they are receiving. They claim that the formalin contains unacceptably high amounts of formic acid relative to formaldehyde. It seems that this alters the urea-formaldehyde resin properties such that the particle board and plywood subsequently manufactured do not have the appropriate tensile and load strength. They are threatening legal action unless this problem is rectified immediately.

Storage of formaldehyde/water mixtures is tricky. At high temperatures, undesirable polymerization of formaldehyde is inhibited, but formic acid formation is favored. At low temperatures, acid formation is inhibited, but polymerization is favored. There are stabilizers

that inhibit polymerization, but they are incompatible with resin formation. Methanol, at concentrations between 5 and 15 wt%, can also inhibit polymerizaton, but no separation equipment for methanol currently exists on site, and methanol greater than 1 wt% also causes defective resin production. With ≤ 1 wt% methanol, the storage tank contents must be maintained between 35°C and 45°C.

You have toured the plant, checked the logbooks, spoken to engineers and operators, and have gathered the following information:

- The catalyst is replaced once per year, and for about five days after start-up, a pressure-relief valve in the reactor (R-801) releases.
- During the same time period, bfw consumption in R-801 was not seen to increase beyond normal, day-to-day fluctuations of ±1%, and the reactor outlet temperature was not seen to increase significantly.
- Excess acidity occurs mainly in the summer.
- All existing equipment is made of carbon steel.
- One year ago, an unscheduled, emergency shutdown was required to replace a control system between the tower (T-802) and the subsequent pump (P-803 A/B). Due to availability and time constraints, 1-in schedule-40 pipe was used in place of 1.5-in schedule-40 pipe.
- During hot-weather periods, the inlet temperature of cooling water has been observed to increase by as much as 5°C.
- During these hot-weather periods, the pressure in the distillation column has been observed to increase slightly, but operation over a long period of time shows no leakage or safety problems associated with this change in pressure.
- Pump (P-803 A/B) is located at a height of 5 m below the tower (T-802) exit. There is a total of 30 equivalent meters of pipe, elbows, and valves in the line.
- An inspection of the pressure-relief valve on the reactor (R-801) indicates that it is rated at 1115 kPag. It will open at or above that pressure.
- Over long periods of time after catalyst replacement, the pressure of medium-pressure steam leaving R-801 is 1110 kPag.
- During hot weather, the volume of off gas leaving the absorber increases by 1%. However, the increase in formaldehyde is about 22%, and the increase in water is about 3%.
- Pump (P-803 A/B) constantly makes noise, and each individual pump has been replaced within the last year.

Suggest potential causes for the observed problems, and suggest possible remedies.

19. Delayed coking is an oil refinery process that takes a heavy oil fraction and heats it up to approximately 900°F (480°C) in a furnace. Upon leaving the furnace, the oil is fed to one of two (or more) coking drums, where it is allowed to sit and "cook" for up to 24 hours. During the cooking (coking) process, the oil cracks and gives off a variety of gaseous and liquid products that are processed further. The material remaining in the drums is a solid coke that is subsequently "cut out" of the drum using a very high-pressure water jet. This coke is then shipped out as a salable product. The process is shown in Figure P24.19.

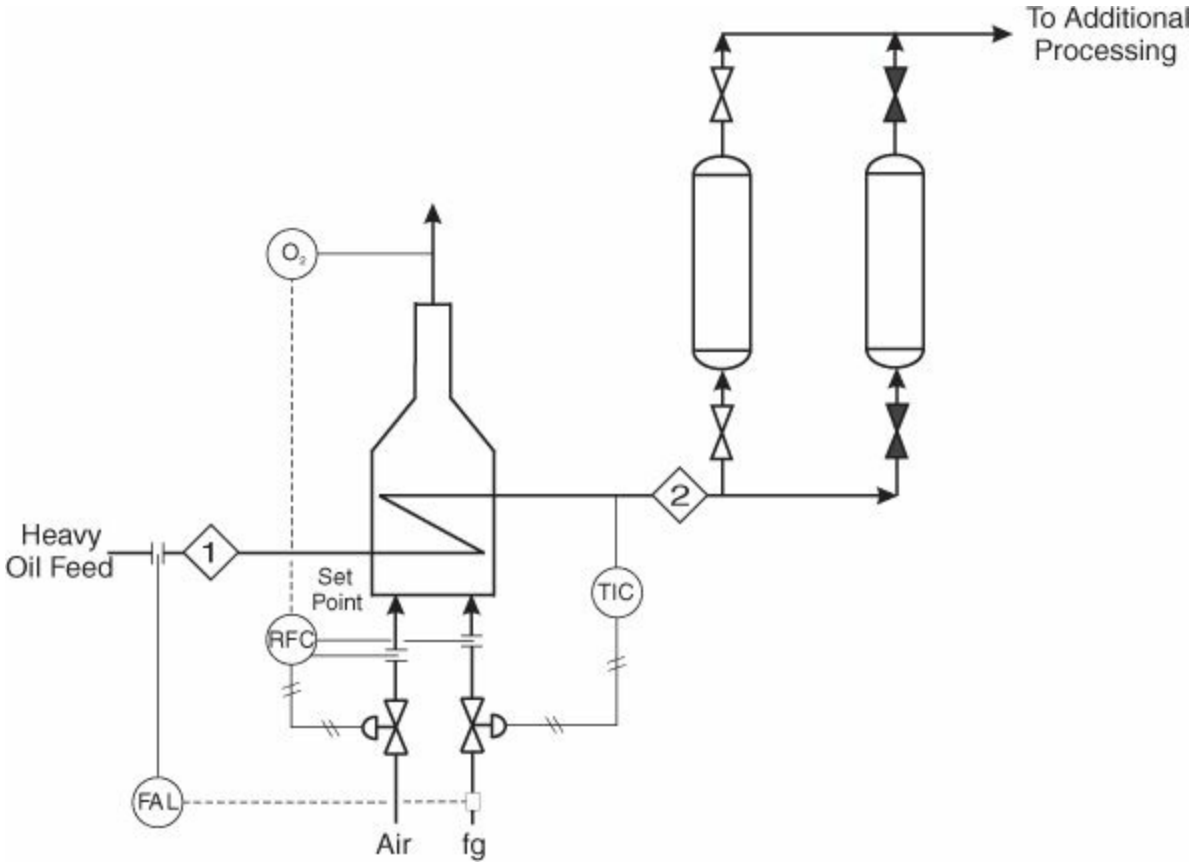


Figure P24.19. PFD for Problem 24.19

The control scheme on the furnace is set to regulate the flow of fuel gas (fg) based on the measured temperature of the exit oil stream (Stream 2). A ratio flow controller adjusts the flowrate of air so that a constant air/fuel ratio is maintained. An oxygen analyzer measures the excess oxygen in the flue gas and adjusts the set point of the ratio controller to maintain the desired air/fuel ratio. A flow alarm is also present to detect a low flow condition in Stream 1 and activates a solenoid shutoff valve to the fuel gas.

A few days ago there was a process upset in which the oil flow to the fired heater was momentarily interrupted. This interruption triggered the shutoff valve, which closed the fuel gas line. The flow of Stream 1 resumed its normal rate after about 30 seconds, at which time the fuel gas solenoid valve opened and the flow of fuel gas resumed. During the upset, the flow of air changed in proportion to the fuel gas flow.

A short time after this process upset, the following conditions were observed. For each scenario given below, give an explanation of what may have happened to cause the observed changes.

a. The flow of fuel gas to the furnace has slowly increased, and the air flowrate has increased proportionally to maintain the same air/fuel ratio. No other changes have been observed. What could be causing the problem? What do you recommend be done?

b. The flow of fuel gas to the furnace has increased, the air flowrate has increased proportionally to maintain the same air/fuel ratio, and the flow of products and coke production rate appear to be slightly lower than before (the upset). What could be causing the problem? What do you recommend be done?

c. The flow of fuel gas to the furnace has increased, the air flowrate has also increased, and the ratio of air/fuel has increased slightly. The flow of products and coke production rate are lower than before (the upset). What could be causing the problem? What do you recommend be done?

20. Study the distillation column in Figure P24.20(a), the stream information in Table P24.20, and the additional information. Use the pump/system curve information in Figure P24.20(b) as needed. It is necessary to scale up the throughput of this column without altering the column pressure.

a. Identify at least four potential bottlenecks to scale-up you can find, estimate the maximum percent scale-up possible for each, and identify the limiting bottleneck. Quantitative calculations are needed to support your result.

b. Suggest one method to debottleneck this problem that might possibly be accomplished without shutting the process down. What problem(s) might arise with this solution?

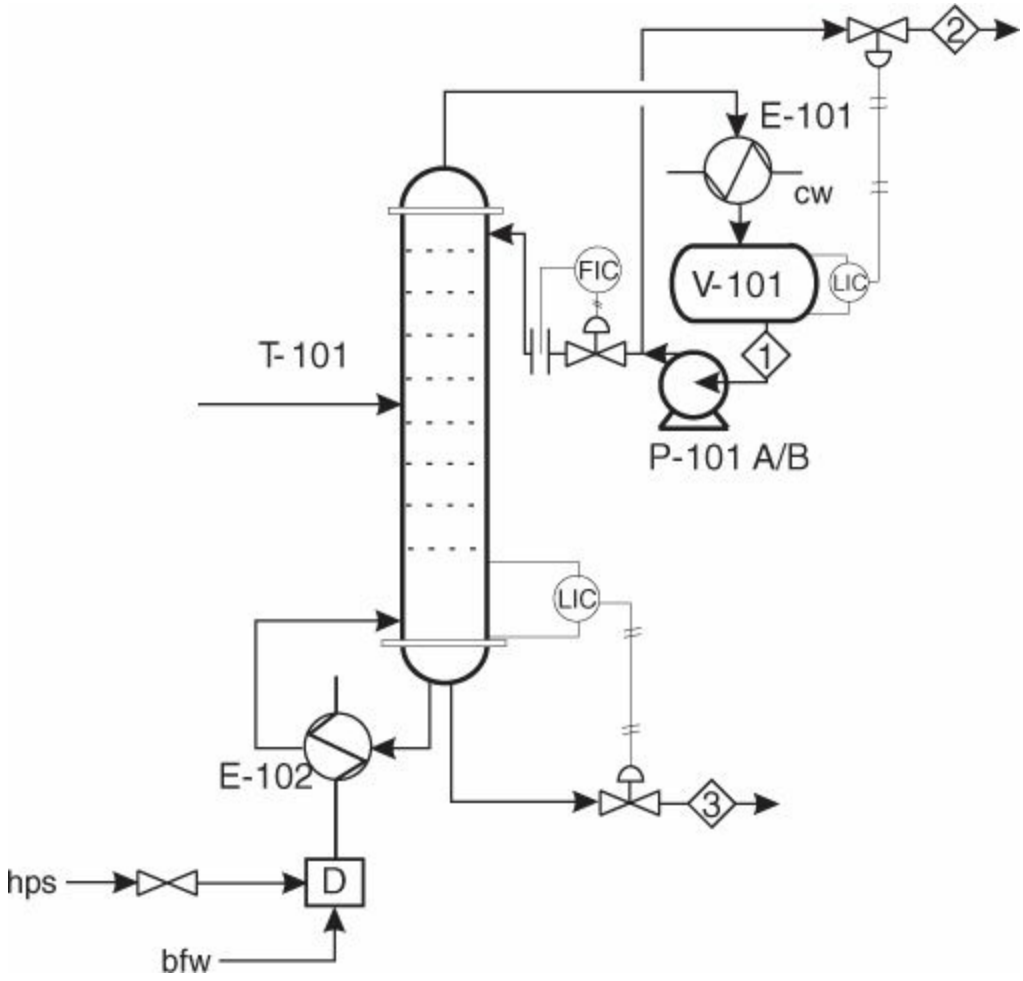


Figure P24.20(a). PFD for Problem 24.20

Table P24.20. Stream Information for Problem 24.20

Stream	1	2	3	cw
Mass flowrate (kg/h)	77,800	55,000	17,470	71,600
Density (kg/m3)	700	700	910	1000
Temperature (°C)	134.4	134.4	155.6	—

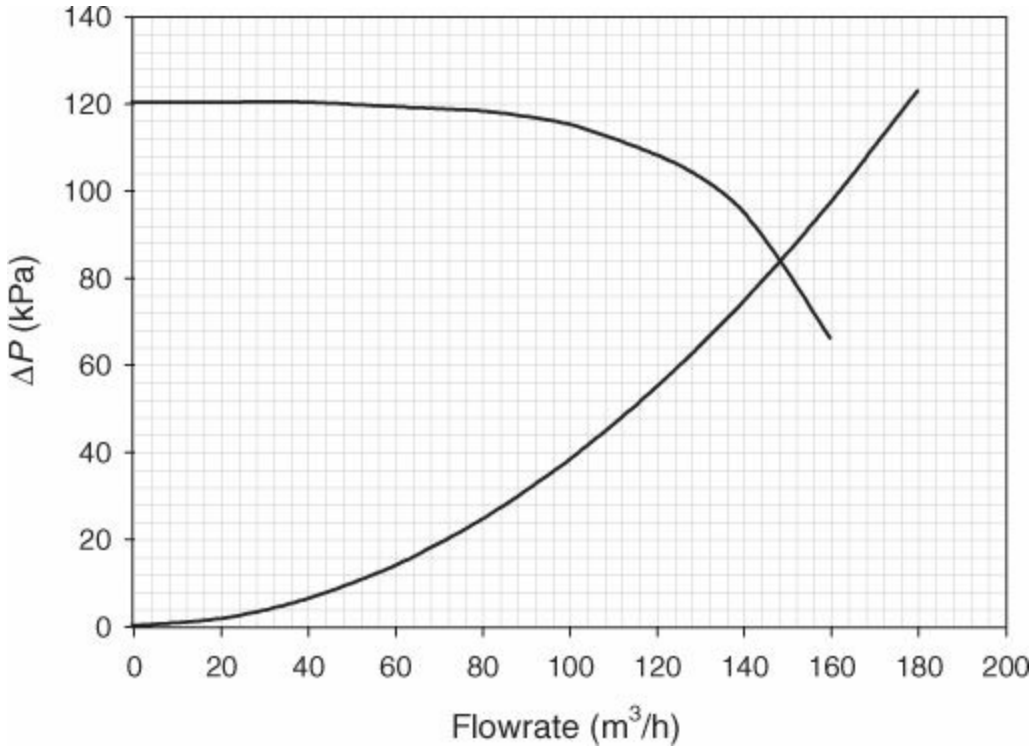


Figure P24.20(b). Pump and System Curve for P-101A/B in Problem 24.20

Additional information:

Cooling water supply lines to E-101 are 4-in schedule 40, $A = 0.0129$ m^2

Pump and system curves provided

P-601 A/B not close to cavitation at normal operating conditions

E-102 uses hps desuperheated to 200°C

Column designed to operate at 70% flooding

Cooling water enters at 30°C and design and maximum return temperature are both 40°C

Assume maximum allowable velocity in pipes and tubes is 3.75 m/s

Equal resistances on each side in E-101

Condensation in shell in E-101

21. The distillate stream from a distillation column (flowrate 35 m^3/h, fluid has density of water) is recycled. The destination of the recycle stream is 3 m below the fluid level in the reflux drum. First, the recycle passes through a pump to supply sufficient head to overcome frictional losses (20 kPa) and reach the pressure of the stream with which it is mixed (250 kPa above distillate stream). Then, it passes through a heat exchanger in which it is heated from 90°C to 120°C using low-pressure steam at 140°C. Assume that all resistance is on the process-stream side of the exchanger (tube side).

It is desired to scale up the entire plant capacity by 15%. It has been determined that the distillation column can be modified to maintain the recycle stream temperature at 90°C. It has also been determined that, with the required changes in the feed section of the process, the temperature of the recycle stream must be between 119°C and 121°C to satisfy liquid-phase reactor inlet conditions after mixing with fresh feed. Figure P24.21 is the pump curve for the pump in the recycle stream.

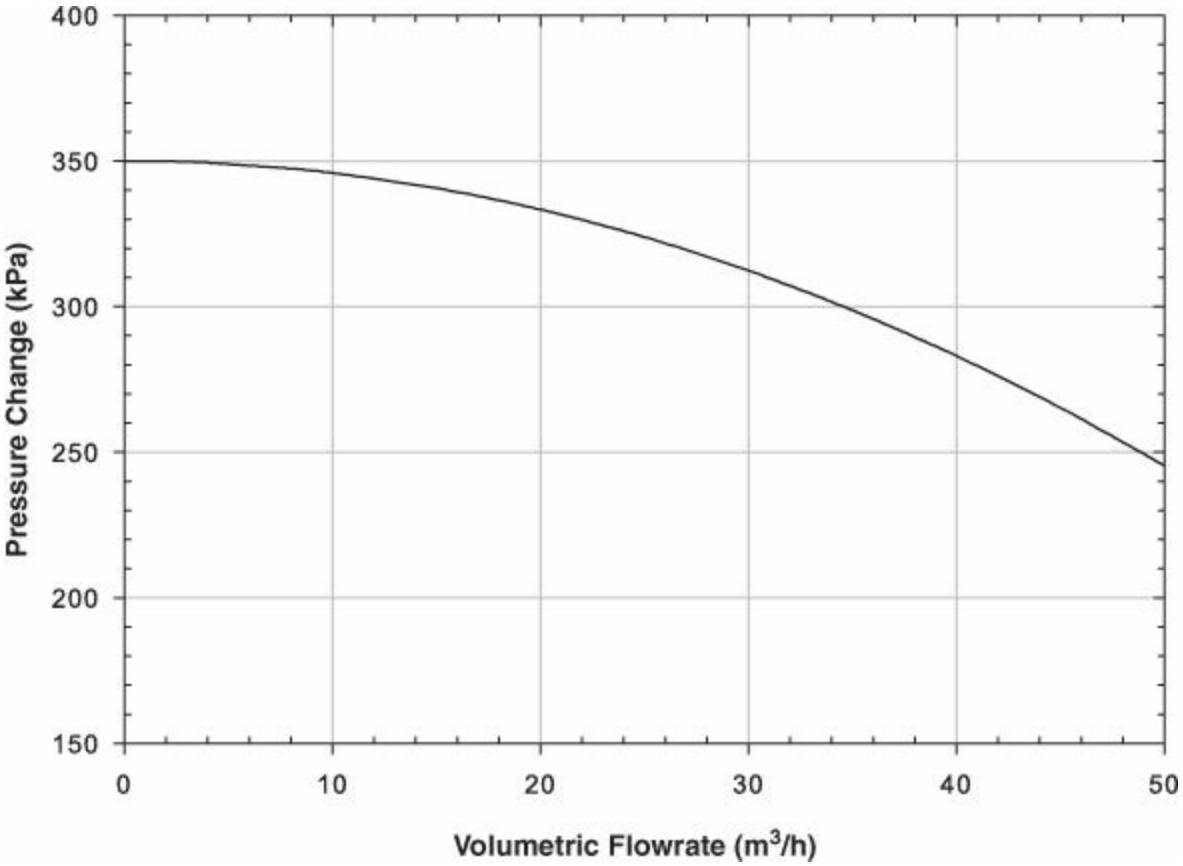


Figure P24.21. Pump Curve for Problem 21

a. Can the temperature criterion be satisfied?

b. Can the flows in this portion of the process be scaled up by 15%?

c. With a scale-up of 15% desired, what feature must be included in this distillation column so that column operation can be modified to maintain the recycle stream at 90°C?

d. It is suggested that because a lower temperature of the recycle stream would reduce the reaction rate, if needed, the pumps in the feed section could be used to increase the reactor pressure, and hence the reaction rate. What is your opinion of this suggestion?

22. The distillate stream from a distillation column (flowrate 35 m^3/h, density of water) is recycled. The destination of the recycle stream is a point 3 m below the fluid level in the reflux drum. First, the recycle passes through a pump to supply sufficient head to overcome frictional losses (20 kPa) and reach the pressure of the stream with which it is mixed (250 kPa above distillate stream). Then, it is heated from 90°C to 120°C using desuperheated low-pressure steam at 140°C. Assume that all resistance is on the process-stream side of the exchanger (tube side).

It is desired to scale up the entire plant capacity. It has been determined that the distillation column can be modified to maintain the recycle stream temperature at 90°C. It has also been determined that, with the required changes in the feed section of the process, the lowest allowable temperature of the recycle stream is 119°C to satisfy liquid-phase reactor inlet conditions after mixing with fresh feed. Figure P24.21 is the pump curve for the pump in the recycle stream.

a. What is the maximum possible scale-up percentage based on the heat exchanger?

b. Can the pump handle the answer in Part (a)?

c. It is suggested that because a lower temperature of the recycle stream would reduce the reaction rate, if needed, the pumps in the feed section could be used to increase the reactor

pressure, and hence the reaction rate. What is your opinion of this suggestion?

Section V: The Impact of Chemical Engineering Design on Society

Throughout this book, the focus has been on the role that a chemical engineer plays in the analysis, synthesis, and design of chemical processes. In this section, that role is put in the context of the profession of chemical engineering, which is defined by the American Institute of Chemical Engineers as "the profession in which a knowledge of mathematics, chemistry, and other natural science gained by study, experience, and practice is applied with judgment to develop economic ways of using materials and energy for the benefit of mankind."

Far from being the "soft" side of engineering, the topics in this section are very much the crucial steps between a design in the mind of the engineer and the realization of a new or improved process or product in the service of humanity. In the past 30 years, the importance of the impact of chemical engineering design on society in terms of how the chemical process industry and chemical engineers are viewed has increased dramatically. No longer is being a "good engineer" defined by one's ability to solve complicated process problems correctly. Instead, a company's reputation and success are often measured in terms of its track record in operating environmentally friendly processes, its ability to find innovative solutions to existing problems, and its ability to develop new products. Chemical engineers are responsible for all these initiatives, and the success of modern engineers is based in large part on their contributions to these areas.

In this section, focus is placed on the engineer's ability to

- Gain the necessary experience and knowledge
- Earn the trust of society
- Ensure that the process and products are safe
- Protect the environment
- Continue to look for new processes that are less harmful to the environment and that pose less risk to society
- Work with other engineers and professionals to bring new chemical-engineering-based products to the marketplace

Chapter 25: Ethics and Professionalism

Engineering problem solving within an ethical framework, legal responsibilities, and professional registration are developed. Ethics case studies and the content of the Fundamentals of Engineering (FE) and Professional Engineering (PE) examinations are included.

Chapter 26: Health, Safety, and the Environment

Methods of analyzing risk are provided, and the basic types of health, safety, and environmental regulations are explained, with references to government databases. Pollution prevention strategies and the assessment of plant safety are introduced through their relationships to **hazard and operability (HAZOP)** studies, the Dow Fire and Explosion Index, and the Dow Chemical Hazards Index.

Chapter 27: Green Engineering

A brief introduction to green engineering design methods—including the pollution prevention hierarchy, green chemistry principles, and flowsheet analysis for pollution prevention—is discussed. Examples of the economics of pollution prevention activities using the profitability methods in Chapter 10 and life cycle analysis are presented. Brief descriptions of environmental risk assessment, analysis of releases, and the software available to do this analysis are given.

Chapter 25. Ethics and Professionalism

What You Will Learn

- There is a subtle difference between morals and ethics.
- One must make one's own ethical decisions.
- There are legal issues that must be considered.

Engineering has been described as "the strategy for causing the best change in a poorly understood or uncertain situation within the available resources" [1]. The realm of ethics and professionalism entails very real, poorly understood problems that are as challenging as any technical problems an engineer will face. This chapter presents heuristics, objective functions (i.e., ways of defining what is *best*), and constraint identification strategies that are especially useful in solving such problems.

As described in Chapter 11, all heuristics are, in the final analysis, fallible and incapable of justification. They are merely plausible aids or directions toward the solution of a problem [1]. Especially for the heuristics described in this chapter, the four characteristics of any heuristic need to be kept in mind:

1. A heuristic does not guarantee a solution.
2. It may contradict other heuristics.
3. It can reduce the time to solve a problem.
4. Its acceptance depends on the immediate context instead of on an absolute standard.

The fact that one cannot precisely follow all ethical heuristics all the time is to be expected, as it is with any set of technical heuristics.

The purpose of this chapter is to help develop strategies to make the best choice when faced with an ethical problem. The set of strategies developed will be different for each reader. A general overview of engineering ethics is presented, and a series of ethics scenarios is introduced. The authors have found that the best way to develop the facility to deal with ethical problems is, after reading the overview, to discuss these scenarios in small groups. Each group presents its solution to the class. Even with seemingly straightforward situations, the solutions can be diverse. A class discussion of the different solutions is followed by a reflection on what was discussed. Then the next problem is addressed. Many such scenarios are given at the end of this chapter and in books and articles [2, 3, 4, 5, 6, 7].

25.1. Ethics

Whenever chemical engineers develop products, design processes and equipment, manage process operations, communicate with other engineers and non-engineers, develop markets and sell products, lead other engineers, interact with clients, represent their firms to the government or to the public—in short, whenever chemical engineers do anything that impacts the lives of anyone—their choices of action are based on ethics. Even when faced with two different equations, one equation is selected, based in part on ethical values. Does the less precise equation include a safety factor that lowers the risk to employer, employees, or the public? Should more time be spend doing more rigorous calculations, costing the firm more money but providing a better answer to the client? How is the

decision made?

In each of these circumstances, engineers apply their own moral standards, mindful of the legal requirements, using their personal code of ethics to make the decision. To help in the development of a personal code of ethics that will provide a framework for making these decisions, first the three types of reasons for ethical behavior are identified:

- Moral
- Legal
- Ethical

Although nearly all people share *some* fundamental moral ideals, each engineer has his or her own distinct set of moral principles. Typically, these principles are shaped by religion, conscience, and especially early childhood family experiences. The basic framework by which one decides what is right and what is wrong is generally very well developed by the time one reads an engineering text. Thus, this text will not take up the moral dimensions of engineering ethics other than to stress the importance of continually reminding oneself to be true to one's moral values as one works through ethical problems.

A few legal aspects of solving ethical problems are covered in Section 25.3, but the full legal consequences of engineering decisions are far beyond the scope of this book. The legal system (which includes government regulations) is a collection of rules of conduct for a society to assist orderly transactions between people. Chemical engineers should seek skilled legal advice whenever these rules, or the consequences for not following them, are unclear.

The aspect of ethical decision making covered here is that commonly referred to as engineering ethics. There are generally accepted codes of conduct for engineers, although, as will become clear, they are too broad to be used alone as prescriptions for engineering choices in difficult situations. **Engineering ethics** is the system of principles and strategies that engineers use to solve complex problems involving other people's lives. It includes aspects of moral principles and legal responsibilities, as well as recognized codes of ethics and generally accepted norms of engineering and business behavior.

25.1.1. Moral Autonomy

Inasmuch as all engineers do not share a single set of moral principles by which to make ethical decisions, it is fully expected that different readers will make different decisions, especially in complex situations. The goal of this chapter is not *uniformity* of decisions by all engineers but *autonomy* of each engineer to make the right decision. In this context, the right decision can be identified by the use of a heuristic. The right decision is one that is

- Consistent with the engineer's moral principles
- Consistent with the generally accepted codes of engineering conduct
- Consistent with obligations that the engineer has accepted
- Consistent with the law
- Consistent with the applicable code of ethics

But, most importantly, *the right decision is one that the engineer can live with.* Of course, it is always possible that one person's decision would not be acceptable to another person.

The ability to make one's own ethical decisions is known as *moral autonomy*.

Moral autonomy does not require that you be able to look back and always be confident that the choice made was the best of all possible choices. Although this is the goal, it is a moving target. Rather, you are exercising **moral autonomy** if you are in control of your decision, if you make the choice based on a reasonable analysis of the potential consequences consistent with your moral, legal, and ethical beliefs, rights, duties, and obligations. If you do not understand your moral principles, if you have no strategy for ethically analyzing a situation, or if you defer your own ethical responsibilities to others, you cannot claim to be exercising moral autonomy.

The goal of this chapter is to help you develop moral autonomy. Previewing the kinds of ethical problems that you are likely to have to resolve is the most powerful tool you can use to learn about and to develop your moral autonomy.

25.1.2. Rehearsal

When learning any new skill, one usually practices or rehearses. To learn to apply the ideal gas law in process calculations, one does end-of-chapter problems in thermodynamics. Understanding the theory behind the ideal gas law is no guarantee that one will be able to solve applied problems. Some people can and some people cannot. But few would argue that one can solve a problem as quickly, as easily, or as correctly the first time as the *n*th time one solves it. Such is the power of rehearsal.

Rehearsal becomes more important when decisions must be made quickly, extremely accurately, or under great stress. And great stress often accompanies ethical problems. Take a look at Example 25.1, for instance.

Example 25.1.

The Falsified Data [2, Reprinted by special permission from *Chemical Engineering*, May 5, 1980, and September 22, 1980, Copyright © 1980 by McGraw-Hill, Inc., New York, NY 10020]

Jay's boss is an acknowledged expert in the field of catalysis. Jay is the leader of a group that has been charged with developing a new catalyst system, and the search has narrowed to two possibilities, Catalyst A and Catalyst B.

The boss is certain that the best choice is A, but directs that tests be run on both, "just for the record." Owing to inexperienced help, the tests take longer than expected, and the results show that B is the preferred material. The engineers question the validity of the tests, but, because of the project's timetable, there is no time to repeat the series. So the boss directs Jay to work the math backward and come up with phony data to substantiate the choice of Catalyst A, a choice that all the engineers in the group, including Jay, fully agree with. Jay writes the report.

In this simple scenario, there is a great deal of stress. If Jay had never thought about what to do in such a situation, it is highly unlikely that he would make a decision that he could live with. It is much more likely that Jay would look back on the event and wish he could go back and make a different choice. Rehearsal provides the opportunity to do just that. The first time the situation is seen, it is best to be in a low-risk environment. If the wrong decision is made, it does not matter. The second time, a better choice can be made.

In early education and in skills training at any level, the goal of rehearsal is to work through a

scenario that is likely to occur in the future and to develop the best response possible. In advanced professional education, and especially in engineering education, the goal of rehearsal is to work through a scenario representative of a broad range of situations that are likely to occur in the future and to develop a strategy for responding to the broad range of problems, many of which cannot be imagined. For ethical decision making, this strategy must be powerful, adaptive, and personal. Throughout your career, new ethical problems will arise. The key is to rehearse frequently, using example and homework problems and conceiving your own representative scenarios.

25.1.3. Reflection in Action

One of the characteristics of successful professionals in a variety of fields is frequent postmortem analysis. This self-imposed study of events that have occurred in one's professional life is called "reflection in action" [8]. After an engineering event has occurred in which ethical decisions were made, one sits down (individually or in a small group) and reviews the case, analyzing the facts, the missing information, the constraints, the unnecessary perceived constraints, the options considered, the options not considered, and the strategy used to arrive at the decision.

As demonstrated in Example 25.2, there are many reasons why reflection in action is so powerful, but the focus here is on two:

- It forces one to analyze the strengths and weaknesses of one's own strategy.
- It provides continual opportunities and encouragement for rehearsal.

Example 25.2.

Reflection on the Falsified Data

Assume that Example 25.1 has occurred. Any standard problem-solving strategy [9] can be used to reconstruct the scenario. Here the McMaster five-step strategy is used [10].

1. **Define:** Was the problem well defined by the participants? Was the real problem that the experimental results were unexpected? Was the real problem that things were now more uncertain than before? There are other possible definitions of the problem, but if one defines the problem as how to deal with obviously flawed data, one may miss the entire point. The problem would thereby be unnecessarily overconstrained. What is the real problem? If the characters had defined the problem better, would they have reached a different conclusion? Would it have been a better conclusion?
2. **Explore:** What alternatives were explored? Are there other alternatives, such as requesting additional time to rerun the experiments, alerting the users of the data to their possible inaccuracy, writing a detailed analysis of the theoretical and experimental discrepancies, debriefing the technician who performed the experiments to determine whether errors in technique could cause the discrepancy? Would a more careful exploration of the alternatives have been helpful in this case? What brainstorming techniques might have been helpful?
3. **Plan:** Did the participants develop an adequate plan? What would (should) you have done differently?
4. **Do It:** Did the participants execute the plan well?
5. **Look Back:** Here is the play within the play. Would it have been helpful if the participants had reflected on past experiences? Would it have been helpful if the participants had projected what

could happen as a consequence of their decision and had analyzed the expected effectiveness of their approach?

Because the outcome of the "Falsified Data" case is unknown, the *Plan* and *Do It* stages cannot yet be fully analyzed. When the full case is reflected upon, the *Plan* and *Do It* stages could be completed.

At the end of any rehearsal or reflection, one (or the group) should develop a list of heuristics to use in future ethical problem solving. These could be the heuristics that had been used effectively (in the case of a reflection) or new heuristics that can be used (in the case of a rehearsal). For Example 25.2, the following heuristics might be identified (use the three blank lines to develop your own heuristics):

- Use a traditional problem-solving strategy for solving ethical problems.
- Consider the possibility that inexperienced people can be right.
- Debrief people fully before assuming facts about their actions.
- Consider what will happen if a specific decision is based on a false assumption.
- Be honest.
- Be concerned about the welfare of your company.
- Be concerned about the welfare of your employees.
- Do not let other people make ethical decisions for you.
-
-
-

25.1.4. Mobile Truth

It is quite natural for people to assume that groups to which they belong are right, and other groups are wrong. This basic response gives rise to loyalty, strong familial pride and duty, willful obedience, and leadership. The strength of collective action depends on this response, which, in terms of ethical decision making in engineering, manifests itself in **mobile truth**.

Assume your AIChE student chapter and the IEEE student chapter are playing volleyball. If the referee makes a difficult call, you are apt to find the call right if it favors your team and wrong if it favors the other. You are not being unethical, but you are perhaps being unreasonable. Similarly, when you start to work for an organization, you begin to develop attitudes toward it that are similar to the bonding that occurs within families, nationalities, and schools. The faster these bonds develop, the faster you will be accepted. The stronger these bonds are, the more loyal you will become. Example 25.3 demonstrates mobile truth.

Example 25.3.

If you work for Company A, which produces polyethylene, you know that Type-A polyethylene is the best. Because you are offered a promotion, higher pay, and desirable relocation, you move to Company B. Almost immediately, Type-B polyethylene becomes the best. It could be because you are such a great chemical engineer, but it is probably because of mobile truth. The world did not change, but your frame of reference and, especially, your loyalty did.

When your affinity to a group clouds your ethical decision making, you are being affected by *mobile truth*.

The point here is to learn to recognize mobile truth and to filter it out of ethical decision making. Obviously, a chemical engineer has ethical duties and obligations to an organization, but one must be ever-vigilant to identify the intrusion of mobile truth into the ethical decision-making process. The point is not just to make the process more "objective" or "fair," but rather to try to see the situation from the point of view of those outside the organization. Here are a few heuristics for avoiding being misled by mobile truth:

- Ask yourself whether your decision would be different if you worked for another part of the company or for another company.
- Imagine that you live just outside the plant fence.
- Imagine that you work for the Environmental Protection Agency.
- Ask for the opinion of someone else in your organization. Explain the situation, suggesting that the facts pertain to a different organization. The response is likely to be less affected by mobile truth.

More heuristics can be developed through rehearsal and reflection.

Related to the concept of mobile truth is the concept of **postrationalization**. Again, it is quite natural and normal for people to try to justify their actions (and the actions of their colleagues and organizations), whether or not they are defensible. Because complex ethical problems can be analyzed and evaluated in so many different ways, it is often easy to fool oneself into thinking that one has acted ethically. But one must keep in mind the frame of reference or point of view of others (outside your organization). If you want to be sure that what you have done or are about to do is ethical, imagine how someone outside the organization would view the decision. If there is a difference, chances are you were post-rationalizing (or prerationalizing).

25.1.5. Nonprofessional Responsibilities

Each chemical engineer has personal responsibilities: to family, to friends, to oneself. These responsibilities, like professional responsibilities, will change dramatically throughout one's life. The obvious example is one's family situation, which is likely to grow and change over a 40-year career. In general, it is easier to make ethical choices when they affect only oneself. Choices that affect one's nuclear family are especially difficult. Some choices might cost you your job, make you a social outcast, compel you to move from your home, even estrange you from your family.

Generally, you can mitigate consequences by

- Thinking early about the effects of your decisions on your family
- Taking into account likely changes in your family situation
- Most importantly, talking with your family about your decision

The choice of when to discuss a professional ethics problem with one's family (and with which members of the family) is certainly a difficult one. Considering what a dramatic effect your decisions can have on your family, it would be wise to consider a hypothetical situation before a real ethical problem arises. Think about various options of whom to tell what and when. Rehearsal can be done with one's family, with a peer group, or by oneself. Whichever you choose, it should make any

potential conflict easier to resolve to everyone's satisfaction.

The crucial impact of ethical decisions on one's family is generally not fully appreciated until one is married or becomes a parent. In using rehearsal to prepare for difficult ethical situations, one should anticipate potential changes in one's family situation that might affect the decision. In a typical senior chemical engineering class, most students are single without children. However, there may be students with a significant range of circumstances. Some might be married without any children; several might be parents. Additionally, some may intend to be the only or the main potential wage earner, whereas others may expect to work or earn less than their husbands or wives. Whenever possible, it is better to form nonhomogeneous groups for rehearsal of ethical scenarios. The addition of a married student to an otherwise single group usually changes the discussion substantially.

While discussing ethical scenarios, financial and other concerns also must be considered. Prospective chemical engineers often say, "I just wouldn't work for a company that would do that," or "I'd quit and get another job before I'd agree to that." But these comments are looked upon as naive by most who have made tough ethical choices, especially whistle-blowers, as is discussed in Section 25.1.8. Often, chemical engineers who no longer have young children or who have saved well for retirement express more willingness to do what they feel is ethically correct. It is unclear whether this expressed willingness translates into action. Some choose to live more frugally, and others choose jobs that require fewer or less difficult ethical choices. Those who become overcommitted—for example, financially—and then feel compelled to make the choice to perform an act that they consider ethically wrong, seldom would claim to be morally autonomous, let alone happy, as seen in Example 25.4.

Example 25.4.

A Question of Integrity [3, Reprinted by special permission from *Chemical Engineering*, March 2, 1987, and September 28, 1987, Copyright © 1987 by McGraw-Hill, Inc., New York, NY 10020]

Under the Toxic Substances Control Act (U.S. Public Law 94-469), all chemicals in general use, or that had been in use, were required to be placed on an inventory list in 1979. Some chemicals were omitted from the initial list through oversight. To produce a chemical not on the list, or a new chemical, a manufacturer must submit a pre-manufacturing marketing notification to the EPA.

(The purpose of notification is to allow EPA 90 days to review a chemical, to ensure that its production, distribution, and use will not be detrimental to human health and the environment. The agency has the authority to place controls as necessary. Heavy penalties can be, and have been, assessed against violators of this regulation.)

Chris supervises a unit that has begun making a "new" chemical (one not on the list) and becomes aware that a premanufacturing notification has not been filed.

If Chris blows the whistle, Chris's career with the company could be over, despite laws to protect whistle-blowers. If Chris does nothing, workers may be exposed to the chemical without safeguards, and be harmed by it. And, if the company is caught, Chris's professional reputation could be stained, especially if it could be shown that the inaction resulted in harm to workers.

Should Chris discuss this ethical problem with her family?

What financial or other hardships might result if she reports the situation?

What obligations does she have to her family in this regard?

What obligations does she have to the community?

What obligations does she have to her employer?

25.1.6. Duties and Obligations

Chemical engineers have certain duties by virtue of their positions, and they acquire other obligations in a number of ways—for example, by accepting assignments, joining professional organizations, and through their family choices. Throughout ethical problem solving, one needs to remind oneself of all of the duties and obligations to which one has agreed.

According to the National Science Foundation, less than 1% of the U.S. population are engineers. Of these, fewer than one in ten are chemical engineers. The American Institute of Chemical Engineers estimates that only 0.05% of U.S. citizens are chemical engineers. Clearly, the vast majority of people are not and do not think like chemical engineers. Few will understand what chemical engineers do, but all will be affected by their actions. Keeping this fact in mind helps to put the awesome responsibilities of chemical engineers in perspective.

One's duties and obligations form the basis for some additional important heuristics in ethical problem solving:

- Remind yourself of relevant duties and obligations that you have accepted.
- Remind yourself of otherwise relevant duties and obligations that you have *not* accepted.
- When accepted duties and obligations are necessarily in conflict, rank these responsibilities.
- If you choose a solution that violates an obligation, discuss the decision with those to whom the obligation was made and determine the consequences.

25.1.7. Codes of Ethics

Codes of ethics are formal obligations that persons accept when they join organizations or when they are allowed to enter a profession. In chemical engineering, there are three main types of codes of ethics: employer, technical society, and government. The employer-based codes of ethics are usually incorporated into the codes of business conduct that one agrees to upon employment with a particular firm. These are covered in Section 25.4. The government-based codes are the professional engineer rules, regulations, and laws that exist in all states and territories of the United States and their counterparts throughout the world. These are covered in Section 25.2.

The most important technical society code for U.S. chemical engineers is the "Code of Ethics" of the American Institute of Chemical Engineers. Similar codes have been adopted by other engineering societies. When you sign your application for membership in AIChE, you agree to abide by this code (Figure 25.1).

AIChE Code of Ethics

(Revised January 17, 2003)

Members of the American Institute of Chemical Engineers shall uphold and advance the integrity, honor and dignity of the engineering profession by: being honest and impartial and serving with fidelity their employers, their clients, and the public; striving to increase the competence and prestige of the engineering profession; and using their knowledge and skill for the enhancement of human welfare. To achieve these goals, members shall

- Hold paramount the safety, health and welfare of the public and protect the environment in performance of their professional duties.
- Formally advise their employers or clients (and consider further disclosure, if warranted) if they perceive that a consequence of their duties will adversely affect the present or future health or safety of their colleagues or the public.
- Accept responsibility for their actions, seek and heed critical review of their work and offer objective criticism of the work of others.
- Issue statements or present information only in an objective and truthful manner.
- Act in professional matters for each employer or client as faithful agents or trustees, avoiding conflicts of interest and never breaching confidentiality.
- Treat fairly and respectfully all colleagues and co-workers, recognizing their unique contributions and capabilities.
- Perform professional services only in areas of their competence.
- Build their professional reputations on the merits of their services.
- Continue their professional development throughout their careers, and provide opportunities for the professional development of those under their supervision.
- Never tolerate harassment.
- Conduct themselves in a fair, honorable and respectful manner.

Figure 25.1. AIChE Code of Ethics (Reprinted with permission of AIChE)

The code can be divided into three parts. The first part identifies to whom the code applies (members of AIChE) and the purpose of the code (to uphold and advance the integrity, honor, and dignity of the engineering profession). Note that this purpose is based on the historical concept that each member of a group (AIChE in this case) has a responsibility to help maintain the "good name" of all members of the group through professional behaviors that tend to increase the trust that society has in the profession. This is a powerful concept in ethics because it acknowledges that the unethical behavior of one member can create trust issues between the society and each member of the profession. Thus, each member has a vested interest in the ethical behavior of all members.

The second part is the list of three goals that identify the duties that chemical engineers have (being honest, impartial, loyal), to whom (employers, clients, the public, the profession), and why (enhancement of human welfare). It also points out that practicing chemical engineering ethically involves improving the profession (striving to increase competence). This section serves at least two important purposes. First, as a chemical engineer reads the goals, he or she realizes the very broad responsibilities to the society that may not be apparent in day-to-day work. A decision made by a chemical engineer might save thousands of lives by providing fertilizer to grow much-needed food, or a decision might kill scores of people in a catastrophic release of toxic materials. These goals are a powerful tool in helping chemical engineers to do the right thing. Second, the list of goals points out quite clearly that not all goals can be met simultaneously all of the time. In fact, one frequently

encounters ethical dilemmas, in which *no* choice is a perfect choice, completely satisfying all of our moral, legal, and ethical responsibilities.

The third part of the code of ethics concerns 11 relatively specific responsibilities that chemical engineers have. Many ethical problems can be attacked by referring to these responsibilities. While reiterating and clarifying the responsibilities of chemical engineers for the safety and health of the society at large, they speak to the responsibilities to clients, employers, employees, and the profession itself. Of particular note are two principles that are sometimes overlooked by beginning engineers. Both refer to the need for continuing education. The seventh principle states that chemical engineers shall "perform professional services only in their areas of competence." It may be obvious that a chemical engineer should not be doing electrical engineering work without having had significant education in the relevant area of electrical engineering, but, even within chemical engineering, there are many areas that are not taught in even the most rigorous B.S.Ch.E. program. Therefore, throughout one's career, one is required by the code to evaluate one's own chemical engineering capabilities continuously and to acquire any needed education (through reading, working with more experienced engineers, consulting experts, or taking courses) before accepting an assignment in any area of chemical engineering. This principle states that the chemical engineer, not some outside governmental agency, must take final responsibility for professional competence. A governmental agency may certify you as a professional engineer after you pass some day-long examinations and a multiyear internship, but you are still the responsible party for your own chemical engineering competence.

The ninth principle states that chemical engineers shall "continue their professional development throughout their careers, and provide opportunities for the professional development of those under their supervision." Many young engineers may think that one's chemical engineering education ends after the B.S., the M.S., or surely after the Ph.D., but the code makes it clear that this is not the case. In the past 40 years, tremendous strides have been made in chemical engineering, and at least as great a change is certainly expected in the next 40 years. Thus, one is required to keep up with the latest advances through such activities as participating in in-house (i.e., within the company) training programs, taking continuing education courses offered by AIChE, universities, and other organizations, reading technical journals, consulting with experts, and so on. The facts that one learns during the B.S. experience are overshadowed by the strategies that one learns to attack problems. And some of the greatest of these problems are to evaluate one's knowledge, to decide what new material needs to be learned, and to develop and implement a plan to acquire that new knowledge.

But why are these principles "ethical" considerations? When one claims to be a chemical engineer, society in general (and employers, clients, and employees in particular) puts trust in that individual. To earn that trust, one must be competent; however, most people do not have the background to judge the competence of a chemical engineer. Therefore, it is an ethical responsibility for the chemical engineer to practice within a scope of competency that can be defined completely only by that chemical engineer. And, as technology expands, a chemical engineer's capability must expand just to maintain a given scope of competency.

In addition to the AIChE code of ethics, two other codes are frequently used in chemical engineering. One is called the "Engineers' Creed":

> *As a professional engineer, I dedicate my professional knowledge and skill to the advancement and betterment of human welfare. I pledge to give the utmost of performance, to participate in none but honest enterprise, to live and work according to*

the laws of man and the highest standards of professional conduct, to place service before profit, honor and standing of the profession before personal advantage, and the public welfare above all other considerations. In humility and with need for divine guidance, I make this pledge.

Some states incorporate this creed into the code of ethics for professional engineers, and some engineering colleges ask engineering graduates to recite this creed at the commencement ceremonies. The Engineers' Creed is a very much more general and "moral" (as opposed to ethical) obligation than is the AIChE code of ethics. The creed can serve as a bonding and an inspirational pledge.

The third common code of ethics is that of the National Society for Professional Engineers (Figure 25.2). This code is more detailed and more specific than is the AIChE code of ethics. It not only includes the canons and principles that are the total of the AIChE Code, but it also prescribes rather specific actions to take in specific circumstances. The NSPE code applies to those who join the organization and to those licensed to practice engineering in states where this code is included in the professional engineers' code. However, it is instructive for any chemical engineer to read the NSPE code periodically, as a reminder of some of the ethical problems that arise in the profession.

National Society of Professional Engineers®

Code of Ethics for Engineers

Preamble

Engineering is an important and learned profession. As members of this profession, engineers are expected to exhibit the highest standards of honesty and integrity. Engineering has a direct and vital impact on the quality of life for all people. Accordingly, the services provided by engineers require honesty, impartiality, fairness, and equity, and must be dedicated to the protection of the public health, safety, and welfare. Engineers must perform under a standard of professional behavior that requires adherence to the highest principles of ethical conduct.

I. Fundamental Canons

Engineers, in the fulfillment of their professional duties, shall:

1. Hold paramount the safety, health, and welfare of the public.
2. Perform services only in areas of their competence.
3. Issue public statements only in an objective and truthful manner.
4. Act for each employer or client as faithful agents or trustees.
5. Avoid deceptive acts.
6. Conduct themselves honorably, responsibly, ethically, and lawfully so as to enhance the honor, reputation, and usefulness of the profession.

II. Rules of Practice

1. Engineers shall hold paramount the safety, health, and welfare of the public.
   a. If engineers' judgment is overruled under circumstances that endanger life or property, they shall notify their employer or client and such other authority as may be appropriate.
   b. Engineers shall approve only those engineering documents that are in conformity with applicable standards.
   c. Engineers shall not reveal facts, data, or information without the prior consent of the client or employer except as authorized or required by law or this Code.
   d. Engineers shall not permit the use of their name or associate in business ventures with any person or firm that they believe is engaged in fraudulent or dishonest enterprise.
   e. Engineers shall not aid or abet the unlawful practice of engineering by a person or firm.
   f. Engineers having knowledge of any alleged violation of this Code shall report thereon to appropriate professional bodies and, when relevant, also to public authorities, and cooperate with the proper authorities in furnishing such information or assistance as may be required.
2. Engineers shall perform services only in the areas of their competence.
   a. Engineers shall undertake assignments only when qualified by education or experience in the specific technical fields involved.
   b. Engineers shall not affix their signatures to any plans or documents dealing with subject matter in which they lack competence, nor to any plan or document not prepared under their direction and control.
   c. Engineers may accept assignments and assume responsibility for coordination of an entire project and sign and seal the engineering documents for the entire project, provided that each technical segment is signed and sealed only by the qualified engineers who prepared the segment.
3. Engineers shall issue public statements only in an objective and truthful manner.
   a. Engineers shall be objective and truthful in professional reports, statements, or testimony. They shall include all relevant and pertinent information in such reports, statements, or testimony, which should bear the date indicating when it was current.
   b. Engineers may express publicly technical opinions that are founded upon knowledge of the facts and competence in the subject matter.
   c. Engineers shall issue no statements, criticisms, or arguments on technical matters that are inspired or paid for by interested parties, unless they have prefaced their comments by explicitly identifying the interested parties on whose behalf they are speaking, and by revealing the existence of any interest the engineers may have in the matters.
4. Engineers shall act for each employer or client as faithful agents or trustees.
   a. Engineers shall disclose all known or potential conflicts of interest that could influence or appear to influence their judgment or the quality of their services.
   b. Engineers shall not accept compensation, financial or otherwise, from more than one party for services on the same project, or for services pertaining to the same project, unless the circumstances are fully disclosed and agreed to by all interested parties.
   c. Engineers shall not solicit or accept financial or other valuable consideration, directly or indirectly, from outside agents in connection with the work for which they are responsible.
   d. Engineers in public service as members, advisors, or employees of a governmental or quasi-governmental body or department shall not participate in decisions with respect to services solicited or provided by them or their organizations in private or public engineering practice.
   e. Engineers shall not solicit or accept a contract from a governmental body on which a principal or officer of their organization serves as a member.
5. Engineers shall avoid deceptive acts.
   a. Engineers shall not falsify their qualifications or permit misrepresentation of their or their associates' qualifications. They shall not misrepresent or exaggerate their responsibility in or for the subject matter of prior assignments. Brochures or other presentations incident to the solicitation of employment shall not misrepresent pertinent facts concerning employers, employees, associates, joint venturers, or past accomplishments.
   b. Engineers shall not offer, give, solicit, or receive, either directly or indirectly, any contribution to influence the award of a contract by public authority, or which may be reasonably construed by the public as having the effect or intent of influencing the awarding of a contract. They shall not offer any gift or other valuable consideration in order to secure work. They shall not pay a commission, percentage, or brokerage fee in order to secure work, except to a bona fide employee or bona fide established commercial or marketing agencies retained by them.

III. Professional Obligations

1. Engineers shall be guided in all their relations by the highest standards of honesty and integrity.
   a. Engineers shall acknowledge their errors and shall not distort or alter the facts.
   b. Engineers shall advise their clients or employers when they believe a project will not be successful.
   c. Engineers shall not accept outside employment to the detriment of their regular work or interest. Before accepting any outside engineering employment, they will notify their employers.
   d. Engineers shall not attempt to attract an engineer from another employer by false or misleading pretenses.
   e. Engineers shall not promote their own interest at the expense of the dignity and integrity of the profession.
2. Engineers shall at all times strive to serve the public interest.
   a. Engineers are encouraged to participate in civic affairs; career guidance for youths; and work for the advancement of the safety, health, and well-being of their community.
   b. Engineers shall not complete, sign, or seal plans and/or specifications that are not in conformity with applicable engineering standards. If the client or employer insists on such unprofessional conduct, they shall notify the proper authorities and withdraw from further service on the project.
   c. Engineers are encouraged to extend public knowledge and appreciation of engineering and its achievements.
   d. Engineers are encouraged to adhere to the principles of sustainable development[3] in order to protect the environment for future generations.

3. Engineers shall avoid all conduct or practice that deceives the public.
   a. Engineers shall avoid the use of statements containing a material misrepresentation of fact or omitting a material fact.
   b. Consistent with the foregoing, engineers may advertise for recruitment of personnel.
   c. Consistent with the foregoing, engineers may prepare articles for the lay or technical press, but such articles shall not imply credit to the author for work performed by others.
4. Engineers shall not disclose, without consent, confidential information concerning the business affairs or technical processes of any present or former client or employer, or public body on which they serve.
   a. Engineers shall not, without the consent of all interested parties, promote or arrange for new employment or practice in connection with a specific project for which the engineer has gained particular and specialized knowledge.
   b. Engineers shall not, without the consent of all interested parties, participate in or represent an adversary interest in connection with a specific project or proceeding in which the engineer has gained particular specialized knowledge on behalf of a former client or employer.
5. Engineers shall not be influenced in their professional duties by conflicting interests.
   a. Engineers shall not accept financial or other considerations, including free engineering designs, from material or equipment suppliers for specifying their product.
   b. Engineers shall not accept commissions or allowances, directly or indirectly, from contractors or other parties dealing with clients or employers of the engineer in connection with work for which the engineer is responsible.
6. Engineers shall not attempt to obtain employment or advancement or professional engagements by untruthfully criticizing other engineers, or by other improper or questionable methods.
   a. Engineers shall not request, propose, or accept a commission on a contingent basis under circumstances in which their judgment may be compromised.
   b. Engineers in salaried positions shall accept part-time engineering work only to the extent consistent with policies of the employer and in accordance with ethical considerations.
   c. Engineers shall not, without consent, use equipment, supplies, laboratory, or office facilities of an employer to carry on outside private practice.
7. Engineers shall not attempt to injure, maliciously or falsely, directly or indirectly, the professional reputation, prospects, practice, or employment of other engineers. Engineers who believe others are guilty of unethical or illegal practice shall present such information to the proper authority for action.
   a. Engineers in private practice shall not review the work of another engineer for the same client, except with the knowledge of such engineer, or unless the connection of such engineer with the work has been terminated.
   b. Engineers in governmental, industrial, or educational employ are entitled to review and evaluate the work of other engineers when so required by their employment duties.
   c. Engineers in sales or industrial employ are entitled to make engineering comparisons of represented products with products of other suppliers.
8. Engineers shall accept personal responsibility for their professional activities, provided, however, that engineers may seek indemnification for services arising out of their practice for other than gross negligence, where the engineer's interests cannot otherwise be protected.
   a. Engineers shall conform with state registration laws in the practice of engineering.
   b. Engineers shall not use association with a nonengineer, a corporation, or partnership as a "cloak" for unethical acts.
9. Engineers shall give credit for engineering work to those to whom credit is due, and will recognize the proprietary interests of others.
   a. Engineers shall, whenever possible, name the person or persons who may be individually responsible for designs, inventions, writings, or other accomplishments.
   b. Engineers using designs supplied by a client recognize that the designs remain the property of the client and may not be duplicated by the engineer for others without express permission.
   c. Engineers, before undertaking work for others in connection with which the engineer may make improvements, plans, designs, inventions, or other records that may justify copyrights or patents, should enter into a positive agreement regarding ownership.
   d. Engineers' designs, data, records, and notes referring exclusively to an employer's work are the employer's property. The employer should indemnify the engineer for use of the information for any purpose other than the original purpose.
   e. Engineers shall continue their professional development throughout their careers and should keep current in their specialty fields by engaging in professional practice, participating in continuing education courses, reading in the technical literature, and attending professional meetings and seminars.

Footnote 1 "Sustainable development" is the challenge of meeting human needs for natural resources, industrial products, energy, food, transportation, shelter, and effective waste management while conserving and protecting environmental quality and the natural resource base essential for future development.

As Revised July 2007

"By order of the United States District Court for the District of Columbia, former Section 11(c) of the NSPE Code of Ethics prohibiting competitive bidding, and all policy statements, opinions, rulings or other guidelines interpreting its scope, have been rescinded as unlawfully interfering with the legal right of engineers, protected under the antitrust laws, to provide price information to prospective clients; accordingly, nothing contained in the NSPE Code of Ethics, policy statements, opinions, rulings or other guidelines prohibits the submission of price quotations or competitive bids for engineering services at any time or in any amount."

Statement by NSPE Executive Committee

In order to correct misunderstandings which have been indicated in some instances since the issuance of the Supreme Court decision and the entry of the Final Judgment, it is noted that in its decision of April 25, 1978, the Supreme Court of the United States declared: "The Sherman Act does not require competitive bidding."

It is further noted that as made clear in the Supreme Court decision:
1. Engineers and firms may individually refuse to bid for engineering services.
2. Clients are not required to seek bids for engineering services.
3. Federal, state, and local laws governing procedures to procure engineering services are not affected, and remain in full force and effect.
4. State societies and local chapters are free to actively and aggressively seek legislation for professional selection and negotiation procedures by public agencies.
5. State registration board rules of professional conduct, including rules prohibiting competitive bidding for engineering services, are not affected and remain in full force and effect. State registration boards with authority to adopt rules of professional conduct may adopt rules governing procedures to obtain engineering services.
6. As noted by the Supreme Court, "nothing in the judgment prevents NSPE and its members from attempting to influence governmental action . . ."

Note: In regard to the question of application of the Code to corporations vis-a-vis real persons, business form or type should not negate nor influence conformance of individuals to the Code. The Code deals with professional services, which services must be performed by real persons. Real persons in turn establish and implement policies within business structures. The Code is clearly written to apply to the Engineer, and it is incumbent on members of NSPE to endeavor to live up to its provisions. This applies to all pertinent sections of the Code.

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Figure 25.2. NSPE Code of Ethics [11] (Reprinted with Permission of NSPE)

25.1.8. Whistle-Blowing [12]

When a chemical engineer notices behavior that is possibly or potentially unethical, the question is, What action should he or she take? As noted in the AIChE and NSPE codes of ethics, there are specific avenues for action in the form of heuristics. For example, the AIChE code requires members to "formally advise their employers or clients (*and consider further disclosure, if warranted*) if they perceive that a consequence of their duties will adversely affect the present or future health or safety of their colleagues or the public." The code also requires chemical engineers to "offer objective criticism of the work of others." The code states that chemical engineers shall "issue statements or present information only in an objective and truthful manner." It is clear that one has the responsibility to tell those who engage one's professional services when there is a problem or potential problem. It is clear that one should be truthful. What is not so clear is what a chemical engineer should do if, after such disclosure, the situation persists.

When is further disclosure "warranted"? What is further disclosure? Does a chemical engineer have a responsibility to disclose further, if warranted? What are the likely consequences of further disclosure? These questions are likely to be the most difficult and most important of one's professional career.

Deciding that further disclosure is warranted and then making that disclosure is called **whistle-blowing**. Most instances of whistle-blowing share the following characteristics:

1. Whistle-blowing rarely results in correction of the specific situation; however, it sometimes changes the prevailing strategy for decision making and thus reduces the chance of a further occurrence.
2. Whistle-blowing often brings about severe personal and professional problems for the whistle-blower.

Given the above characteristics, why would any chemical engineer be a whistle-blower? All three codes of ethics mentioned in Section 25.1.7 require chemical engineers to dedicate their skills to the public welfare, and whistle-blowing has led to improved automobile safety, safer nuclear and chemical plants, better control of toxic wastes, reduced government waste, safety improvements in NASA launches, and other laudable results. Whistle-blowers themselves have stated that they could not stand the stress of nondisclosure, which they viewed as an abdication of their ethical responsibilities. In other words, they could be morally autonomous only by whistle-blowing.

Many laws have been created that protect some whistle-blowers in some circumstances. Federal employees are probably the most protected. There is a specific conduit for an employee, former employee, or applicant for federal employment to make a whistle-blowing disclosure, with the identity of the whistle-blower protected to some extent. And no federal employee may engage in reprisal for whistle-blowing—"take, fail to take, or threaten to take or fail to take a personnel action with respect to any employee or applicant because of any disclosure of information by the employee or applicant that he or she reasonably believes evidences a violation of a law, rule or regulation; gross mismanagement; gross waste of funds; abuse of authority; and substantial and specific danger to public health and safety" (U.S. Code § 2302(b)). Employees in the private sector are protected by other laws and regulations, many of which are summarized on the Department of Labor Web site (www.dol.gov/compliance/laws/comphistleblower.htm). Many whistle-blower laws and regulations exist in other countries and at state and local levels. In each case, there is a limited period (30 days is not uncommon) during which to file a complaint of retaliation. And even though the professional

engineers' code of ethics requires whistle-blowing in some states, protection of the whistle-blower is not ensured. Many states have "employment at will" laws, giving any employer the right to fire an employee for any (or no) reason, and this can make it difficult to prove reprisal. Engineers in private practice (as sole proprietors or partners) may not be protected by many of these laws.

One may go through one's entire chemical engineering career without whistle-blowing, but it is unlikely that one would go through a 40-year career without having to face the question of whether to blow the whistle. Thus, to be able to have the moral autonomy to make the decision, one must consider what one should do.

Before deciding to blow the whistle, one needs to examine four key questions:

1. **What Should One Do to Solve the Problem without Whistle-Blowing?** The assumption here is that a resolution of the problem through normal channels is likely to be more effective, more timely, and less stressful than whistle-blowing would be. The AIChE and NSPE codes require that one attempt these avenues, if they are likely to be successful. Furthermore, most whistle-blowers (successful or not) indicate that whistle-blowing should be a last resort.
2. **Is Whistle-Blowing Likely to Solve the Problem?** One needs to be reasonably certain that there is a problem and that the disclosure outside normal channels will resolve it. Although merely exposing a problem may make one feel virtuous, such action would not be considered whistle-blowing unless the problem were, in the view of the whistle-blower, serious, and unless the disclosure were likely to effect a change for the better.
3. **What Whistle-Blowing Actions Should One Take?** Some whistle-blowing occurs within an organization, the most common being going over one's boss's head. Other whistle-blowing involves disclosures (anonymous or attributed) to the news media. Many levels of action between these two examples are possible. One must consider the action that is most likely to effect the change that one wants, consistent with the risks that one is willing to take. The goal is to change the situation for the better, not just to expose it.
4. **What Are the Potential Consequences to One's Personal and Professional Life?** The consequences of disclosure are often serious. Loss of one's job is a clear possibility. Identification as a whistle-blower can derail or end one's career; finding another job may be very difficult. If the disclosure results in a plant closing, loss of jobs, or financial loss to the company or to other property owners, those affected may be very angry with the whistle-blower. One's family may encounter cruel treatment from those who consider the whistle-blower to be the problem. On the other hand, nondisclosure could result in danger to employees or to the general public, financial damage to shareholders or to taxpayers, or charges of a cover-up. Most whistle-blowers recommend early discussion of any potential whistle-blowing action with one's family. Nearly all wish they had legal protection from retribution. Some of these whistle-blowing issues are demonstrated in Example 25.5.

Example 25.5.

Insider Information [3, Reprinted by special permission from *Chemical Engineering*, March 2, 1987, and September 28, 1987, Copyright © 1987 by McGraw-Hill, Inc., New York, NY 10020]

One day, Lee, a process engineer in an acrylonitrile plant, runs into a former classmate at a technical society luncheon. The friend has recently taken a job as a regional compliance officer for OSHA and reveals, after several drinks, that there will be an unannounced inspection of Lee's plant. In a

telephone conversation a few days later, the friend mentions that the inspection will occur on the following Tuesday.

Lee believes that unsafe practices are too often tolerated in the plant, especially in the way that toxic chemicals are handled. However, although there have been many small spills, no serious accidents have occurred in the plant during the past few years.

What should Lee do? A problem-solving strategy for this scenario is suggested, leaving the details to a class discussion.

1. **Define:** Determine what the problem is and what the ethically desired final outcome should be. Reread the relevant codes of ethics. What are Lee's obligations according to the AIChE code of ethics? According to the NSPE code of ethics? Are there conflicting obligations?
2. **Explore:** Brainstorm for solutions in a small group. Consider internal (within the company) actions, external actions, and nonaction.
3. **Plan:** Rank the possible actions according to their likelihood to bring about the ethically desired result. Determine the most effective order for these actions. Which should be done first? Under what circumstances should you go to the next step? When would you involve your family and others? Remember that internal actions, if effective, are often the faster method to reach the desired solution.
4. **Do It:** Imagine that you followed through with your plan.
5. **Look Back:** Consider the consequences of the proposed actions. Do the likely consequences of the actions change the ranking or the ordering? Predict the final outcome of the action plan. Evaluate the outcome based on your moral, ethical, and legal responsibilities.

25.1.9. Ethical Dilemmas

Some ethical problems can be solved easily. In fact, one does this every day. The goal of this chapter is to help the reader to prepare for the difficult choices, the answers to the *ethical dilemmas*. Some problems (such as the examples in this chapter and the problems at the end) have no "perfect" solution. Whistle-blowing, for example, may satisfy one ethical obligation while violating another. The same can be said of not blowing the whistle. A simple example that many would judge an ethical dilemma is Example 25.6.

Example 25.6.

Initial Employment [6]

Robin is a senior seeking employment. In January, Robin is offered a job by Company X for $5000/month and given 10 days to accept the offer. Robin accepts this offer. Two weeks later, Robin receives an offer of $5500/month and a more exciting position from Company Y. What should Robin do?

At first many may think the answer is obvious. Some will wonder whether this example is even an ethical dilemma. Yet if you ask five people what their responses would be, you are likely to get more than one answer. What are the student's obligations to Company X after accepting employment but before becoming an employee? Some companies have rescinded job offers after they have been accepted. Does this fact change Robin's obligations? Should Robin's family responsibilities affect

the solution?

When faced with an ethical dilemma, *one must necessarily rank one's ethical obligations*. This is perhaps the important heuristic in solving ethical dilemmas, but here are others:

- Rank order your ethical obligations again after brainstorming for solutions.
- Admit that you may not be able to satisfy all of your obligations, but then *try* to satisfy them all.
- Combine the individual actions identified in the brainstorming into action plans. Evaluate each entire plan (rather than individual actions) for its consequences and effectiveness.
- At some point in the decision-making process, involve those who are most affected by the consequences but who are not active participants in the solution (often family, friends, trusted colleagues).

25.1.10. Additional Ethics Heuristics

Many heuristics for the solution of ethical problems have been presented in Section 25.1. A crucial heuristic is *always try to develop new heuristics*. In this vein, more heuristics are offered:

- Acquire all the information you can about the situation. The problem may be more serious than it first appears, or there may be no real problem at all.
- Be honest and open. This is especially important when dealing with those who are predisposed to distrust you.
- Acknowledge the concerns of others, whether or not you share their concerns.
- Remember that one is only as ethical as one can afford to be. One can enhance one's ability to afford to do the right thing by knowing the consequences and by balancing the responsibilities that one accepts with the rest of one's life.

For other heuristics and for cases to use for rehearsal, please see the references listed at the end of this chapter and the Internet-based resources given in the following section.

25.1.11. Other Resources

There are a myriad of resources on engineering ethics. The following are a few of the most helpful.

Center for Engineering, Ethics and Society. This center, founded in 2007, incorporates the Online Ethics Center (www.onlineethics.org), which has many engineering ethics resources, including the following:

- **Ethics Cases:** More than 470 engineering ethics cases that have been developed by organizations (such as NSPE), universities, and others can be accessed through this Web site, as well as dozens of essays on engineering ethics. These include famous accidents with significant engineering ethics issues, such as Three-Mile Island and the space shuttle *Challenger*.
- **Moral Exemplars:** These are accounts of engineers and scientists showing leadership in very difficult and important ethical situations.
- **Ethics Codes and Guidelines:** There are links to several dozen engineering and science codes of ethics, both in the United States and in other countries.
- **Educational Resources:** This section of the Web site provides typical assignments, syllabi, strategies for exploring professional ethics, and assessment procedures.

Engineering Ethics at TAMU. This Web site at http://ethics.tamu.edu was developed at Texas A&M

University through a National Science Foundation grant and provides the ethics case studies mentioned above, as well as links to current news media articles on real ethics issues.

National Institute for Engineering Ethics (NIEE). This Web site (http://www.niee.org) is maintained by the Murdough Center for Engineering Professionalism at Texas Tech University. This institute was initially created by NSPE, and it developed and distributes the excellent engineering ethics videos titled "Gilbane Gold" (1989), "Incident at Morales" (2003), and "Henry's Daughters" (2010). Additional study materials are available for each. The NSPE ethics cases since 1976 are also available, as is the *Ethics Resource Guide*, an extensive bibliography of 400 books, articles, and videos on engineering ethics. Additional resources available through this Web site include the following:

- **Applied Ethics in Professional Practice Case of the Month.** Each month, a new ethics case is presented. One can respond with a suggested action, and the results of these responses are available on the site the next month.
- **Ethics Resource Guide.** An extensive bibliography of 400 books, articles, and videos on engineering ethics is given.
- **NAFTA Ethics.** This is a report describing the efforts under the North American Free Trade Agreement to develop a code of ethics for engineering throughout Canada, Mexico, and the United States. The "Principles of Ethical Conduct in Engineering Practice under the North American Free Trade Agreement" are presented. These principles include the aspects of the AIChE code of ethics and go further in two specific areas. The NAFTA principles specifically recognize the responsibility of all engineers to strive for efficient use and conservation of the world's resources and energy and to examine the environmental impact of their actions. It also specifies that whistle-blowing (although that term is not used) is a responsibility of all engineers and that the order of disclosure should be to employer, client, public agencies, and the public.

American Chemical Society. This technical society is for chemists and chemical engineers, although chemists outnumber chemical engineers by a wide margin. The ACS "Chemical Professional's Code of Conduct" is given in Figure 25.3. This code is "for the guidance of Society members" and is not a formal agreement when one accepts membership, as is the case for AIChE. It also focuses more on scientific integrity and less on professional responsibility to the public than do the engineering codes of ethics.

Chemical Professional's Code of Conduct

The American Chemical Society expects its members to adhere to the highest ethical standards. Indeed, the Federal Charter of the Society (1937) explicitly lists among its objectives "the improvement of the qualifications and usefulness of chemists through high standards of professional ethics, education and attainments..." The chemical professional has obligations to the public, to colleagues, and to science.

"The Chemist's Creed," was approved by the ACS Council in 1965. The principles of The Chemist's Code of Conduct were prepared by the Council Committee on Professional Relations, approved by the Council (March 16, 1994), and replaced "The Chemist's Creed." They were adopted by the Board of Directors (June 3, 1994) for the guidance of Society members in various professional dealings, especially those involving conflicts of interest. The Chemist's Code of Conduct was updated and replaced by The Chemical Professional's Code of Conduct to better reflect the changing times and current trends of the Society. It was approved by Council on March 28, 2007 and adopted by the Board of Directors on June 2, 2007.

Their Responsibilities:

- ***The Public***
  Chemical professionals have a responsibility to serve the public interest and safety and to further advance the knowledge of science. They should actively be concerned with the health and safety of co-workers, consumers and the community. Public comments on scientific matters should be made with care and accuracy, without unsubstantiated, exaggerated, or premature statements.
- ***The Science of Chemistry***
  Chemical professionals should seek to advance chemical science, understand the limitations of their knowledge, and respect the truth. They should ensure that their scientific contributions, and those of their collaborators, are thorough, accurate, and unbiased in design, implementation, and presentation.
- ***The Profession***
  Chemical professionals should strive to remain current with developments in their field, share ideas and information, keep accurate and complete laboratory records, maintain integrity in all conduct and publications, and give due credit to the contributions of others. Conflicts of interest and scientific misconduct, such as fabrication, falsification, and plagiarism, are incompatible with this Code.
- ***Their Employer***
  Chemical professionals should promote and protect the legitimate interests of their employers, perform work honestly and competently, fulfill obligations, and safeguard proprietary and confidential business information.
- ***Their Employees***
  Chemical professionals, as employers, should treat subordinates with respect for their professionalism and concern for their well-being, without bias. Employers should provide them with a safe, congenial working environment, fair compensation, opportunities for advancement, and proper acknowledgment of their scientific contributions.
- ***Students***
  Chemical professionals should regard the tutelage of students as a trust conferred by society for the promotion of the students' learning and professional development. Each student should be treated fairly, respectfully, and without exploitation.
- ***Associates***
  Chemical professionals should treat associates with respect, regardless of the level of their formal education, encourage them, learn with them, share ideas honestly, and give credit for their contributions.
- ***Their Clients***
  Chemical professionals should serve clients faithfully and incorruptibly, respect confidentiality, advise honestly, and charge fairly.
- ***The Environment***
  Chemical professionals should strive to understand and anticipate the environmental consequences of their work. They have a responsibility to minimize pollution and to protect the environment.

Figure 25.3. Chemical Professional's Code of Conduct (Reprinted with Permis-sion of the American Chemical Society)

National Society of Professional Engineers. The Web site of NSPE (http://www.nspe.org) contains one of the most extensive collections of items related to engineering ethics. There are 500 cases (1958–2010) from the Board of Ethical Review, a list of articles, books, Web sites, and the following videos:

- **"Henry's Daughters":** This 32-minute video involves ethical complications when a father consults for a company that is in direct competition with another company employing his daughter. The winner of the competition is to be decided by a Department of Transportation team led by his other daughter. A study guide, script, presentation handout, and suggested assignment can be downloaded from the NIEE Web site. Produced in 2010, with subtitles in 13 languages.
- **"Gilbane Gold":** This 24-minute video presents an excellent case study involving a chemical/environmental engineer, an electrical engineer, a manager, a mechanical/industrial engineer, a public agency, two engineering consultants, and the news media. A study guide, PowerPoint presentation, and the script can be downloaded free from the NIEE Web site. Produced in 1989.
- "**Incident at Morales":** This 36-minute DVD presents a complex case involving a new chemical product, moving production from the United States to Mexico, environmental, technical, safety, and financial concerns, and the need to make decisions quickly. A study guide, PowerPoint presentation, and the script can be downloaded free from the NIEE Web site. Produced in 2003, rereleased in 2005 with subtitles in 13 languages.
- "**Ethics Test":** This 25-item, true-false examination is an excellent way to examine one's knowledge of the NSPE code of ethics. Answers, with section references, are provided.

25.2. Professional Registration

To be recognized as a chemical engineer and to offer such services to the public, one must be a licensed (registered) professional engineer. Each state (and other U.S. jurisdictions) has its own Board of Professional Engineers and its own regulations on licensure and practice. However, engineers registered in one state can generally become registered in any other state: one needs only to certify the experience, testing, and other requirements to the new state and pay a fee.

Although the professional engineer laws bar those not registered from offering their engineering services to the public, most states have a "corporate exemption." This exemption excludes from the licensure requirement engineers who offer their engineering services only to their employer and not to any outside firm or individual. If the firm offers engineering services, a licensed professional engineer must still sign, seal, and take responsibility for all such services. Stretched to the limit, this would mean that only the chief engineer of the firm would need to be a professional engineer. However, because the seal of the professional engineer on the engineering report or drawing certifies that the details of work have been checked by that engineer, in practice, all principal engineers in the firm need to be licensed. In the language of the law, anyone in "responsible charge" of engineering work must be licensed.

There are many reasons to become a licensed professional engineer, even though many chemical engineers historically have not been.

1. One cannot be in "responsible charge" of engineering work that will be offered to other firms or to the public (or indeed call oneself an "engineer" in some states) without a PE license. Effectively, this means that chemical engineers who work for engineering design or engineering and construction firms need to be licensed early in their careers. Chemical engineers in many other kinds of firms will need to be licensed before they can rise above a certain technical level. And one cannot be a consultant or an expert witness without a license.
2. The corporate exemption described above is under review in many states and could be eliminated. This is a serious career concern, because most states have already eliminated the "grandfather clauses" that previously allowed someone with many years of significant experience in the field to be granted a PE license without the normal examinations. If the corporate exemption is rescinded, the status of engineers who are licensed will be enhanced, whereas other engineers will need to study for and pass the examinations and to document the appropriate years of engineering experience just to retain their status.
3. In the past, many states exempted their own government employees from PE requirements; however, there is a strong move to eliminate all such exemptions. In fact, many states now *require* all government employees who have the word *engineer* in their job title to be PEs. There is also a move to require engineering design professors to be registered, which is already the case in 11 states.
4. Professional engineer registration is an indication to potential employers, as well as to the general public, of one's competence in the field.

There are two steps to becoming registered: engineer-in-training and professional engineer.

25.2.1. Engineer-in-Training

The first level of certification is as an engineer-in-training (EIT). As an EIT (also known as an engineering intern), one may begin to acquire engineering experience as an employee, but one may not offer services as an engineer directly to the public (or to firms other than one's employer). To obtain EIT certification, one must take and pass the Fundamentals of Engineering (FE) exam, sometimes referred to as the EIT exam. This is an eight-hour, closed-book, multiple-choice examination on a wide range of technical subjects typically covered in engineering programs. The exam is given twice a year on a Saturday (in October and in April), on the same day in all U.S. jurisdictions.

To sit for the FE exam, one must have completed or be about to complete a B.S. in an engineering field from a department that is accredited by ABET. Most U.S. chemical engineering departments are so accredited, and an increasing number of programs outside the U.S. are becoming accredited by ABET. Some states still allow a person with a nonengineering degree (or a nonaccredited engineering degree) to take the exam after acquiring substantial experience. Applicants with engineering degrees from other countries can sit for the exam if ABET certifies that the curriculum they followed is "substantially equivalent" to a U.S. ABET-accredited program. All applicants must pay a fee to the state board, and references must be provided to certify that one is of good character. The address of the State Board for Professional Engineers can be obtained from any chemical engineering department or on the Internet at http://www.ncees.org.

The examination is best taken while one is still an undergraduate. Some states allow one to take the examination only during the last semester before graduation, and some allow it to be taken any time during the senior year or earlier. The examination is written by the National Council of Examiners for Engineering and Surveying (NCEES, Clemson, SC 29633, http://www.ncees.org), from whom sample

examinations and study materials can be obtained. A 260-page *FE Supplied-Reference Handbook* is provided at the examination. Applicants cannot bring any materials to the examination except a calculator that meets certain requirements. The *FE Supplied-Reference Handbook* is available for free downloading from the NCEES Web site, and it should be studied extensively before the examination date.

The morning session of the FE exam consists of 120 multiple-choice questions (four choices per question) on general engineering, math, and science topics, as shown in Table 25.1. Each correct answer is worth 1 point, and no points are deducted for wrong answers. Therefore, all questions should be answered.

Table 25.1. Subject Categories for the Morning Session of the FE exam

Subject	Average Number of Questions	Typical Preparation Courses in Chemical Engineering Curriculum
Chemistry	10.8	General chemistry
Computers	8.4	Introduction to programming (any structured language) plus spreadsheets
Electricity and Magnetism	10.8	Introduction to circuit theory or general physics plus AC power, Op amps, complex algebra
Engineering Economics	9.6	Section 2 of this book
Engineering Probability & Statistics	8.4	Introduction to probability and statistics
Ethics and Business Practices	8.4	Chapter 25 of this book and the Code of Professional Conduct given in the *FE Supplied-Reference Handbook*
Fluid Mechanics	8.4	Fluid mechanics or introduction to transport phenomena
Material Properties	8.4	Introduction to materials science
Mathematics	18.0	Multivariate calculus, differential equations, linear algebra, analytic geometry
Strength of Materials	8.4	Strength of materials
Engineering Mechanics	12.0	Statics and dynamics, general physics
Thermodynamics, Heat Transfer	8.4	Physical chemistry plus cycles or general engineering thermodynamics

The afternoon session of the FE exam consists of 60 multiple-choice questions (four choices per question) on the specific engineering field chosen. There are separate afternoon exams for chemical, civil, electrical, environmental, industrial, and mechanical engineering. There is also an "other disciplines" afternoon exam, with more difficult questions in most of the same subjects as in the morning section. Table 25.2 shows the breakdown of topics for the afternoon chemical engineering exam. Each correct answer is worth 2 points, and no points are deducted for wrong answers. As in the morning section, all questions should be answered.

Table 25.2. Subject Categories for the Chemical Engineering (Afternoon) Session of the FE exam

Subject	Average Number of Questions
Chemistry	6
Chemical Reaction Engineering	6
Chemical Engineering Thermodynamics	6
Computers in Chemical Engineering	3
Fluid Dynamics (including pumps and packed beds)	6
Heat Transfer (including heat-exchanger design)	6
Mass Transfer (including unit operations)	6
Material/Energy Balances	9
Process Control	3
Process Design and Economic Optimization	6
Safety, Health, and Environmental	3

Over the years, the definitions of these subject categories have changed. The latest information is always available on the NCEES Web site.

Many engineering schools provide refresher courses for the morning session during the six weeks or so before the exam date. In addition to this refresher or in case no such opportunity is available, a good strategy for preparing for the examination is the following:

1. At least six weeks before the exam, form a study group of people who are planning to take the FE exam on the same day.
2. Study all the chapters of the *FE Supplied-Reference Handbook*. There are two reasons to do this. First, this is the only reference material available during the exam. Second, it shows the level of depth, breadth, and detail that is involved in the examination questions. Note that most of what is in the civil engineering chapter is not relevant to the morning or the ChE afternoon sessions, but about half of the electrical and computer engineering chapter is basic electricity and magnetism that is found on the morning session of the exam. In the environmental engineering chapter, the session on dispersion modeling is included in the afternoon ChE exam. In the industrial engineering chapter, be sure to study the statistical quality control and the ANOVA sections. And in the mechanical engineering chapter, study the fluid mechanics and heat transfer sections. Become familiar with the location of the material in the book and the use of the table of contents and the index. If any parts of these chapters are unfamiliar, study those topics using prior course notes, textbooks, and FE study books. This part of the preparation should take about two weeks.
3. If any of the topics covered in the chapters are unfamiliar because they were not covered in your curriculum, consult the course instructor for appropriate introductory textbooks and study guides. The group should study these topics together. In most cases, this should take about a week.
4. Purchase sample exams either through the NCEES Web site or through one of the many commercially available FE study books. The study group will need approximately 240 morning questions and 60 afternoon chemical engineering questions.
5. Randomly choose 15 morning questions for each member of the study group. Each member

takes one exam in 30 minutes, using only the *FE Supplied-Reference Handbook* and an approved calculator (see the NCEES Web site). After the exam is taken, look at the correct answers and then share experiences among the group members, in terms of both test-taking strategy and the questions themselves. Then do the same for the afternoon ChE examination, using 8 questions in 32 minutes.

6. After studying the topics of the questions answered incorrectly in Step 5, a quarter-scale or half-scale version of the exam should be attempted, about a week later. Again, the experiences of all group members should be shared.
7. After studying any topics related to questions answered incorrectly on this exam, a final, full-length practice exam should be taken under real FE exam conditions. In all of these postexam study sessions, it is important to study the general topic area of concern, and not just the specific question.
8. On the night before the exam, a good night's rest is essential. On the day of the exam, arrival at the exam site early is a must.

Scores on the FE examination are reported to the state board eight to ten weeks after the test date. Shortly after that, the results are usually released to the applicant by the state board. A diagnostic report is often sent to those who fail. The nominal passing score is approximately 168 points. However, the NCEES recalibrates the passing score after the examination date because some examinations turn out to be slightly more or less difficult than anticipated. The procedure used to perform this recalibration is standard across nearly all standardized tests. It involves experimental questions and a procedure called equating. The bottom line is, if one routinely scores more than 168 out of 240 points on full-scale practice FE exams, one is probably ready to take the real exam. At the spring 2010 examination, 87% of all applicants taking the chemical engineering afternoon session of the FE exam for the first time passed, higher than in any other field. Only 46% of applicants retaking the chemical engineering exam passed. These are also the typical passing rates for the last four years. Rules for retaking the exam vary from state to state.

Many engineers who take the FE exam after they graduate wish they had taken it earlier. The examination is geared toward the material covered in B.S. engineering programs, and many engineers become more specialized during their careers. Those engineers would require more preparation for the FE examination. Also, the designation of engineer-in-training on one's credentials certainly makes a candidate more attractive to a potential employer. Finally, the next step in the registration process requires specific engineering experience, and many states count only experience that is gained after registration as an engineer-in-training. Thus, if one decides to become a PE at a later date, one may have to wait four years more to become registered. Significant opportunities may be lost in the meantime.

25.2.2. Registered Professional Engineer

After becoming an engineer-in-training, one must acquire considerable engineering experience before one can take the Principles and Practice examination (often called the PE exam). In most states, four years of responsible work must be certified by engineers for whom the applicant has worked or engineers who have reviewed the applicant's work in detail and can attest to its quality. Generally, only registered professional engineers may certify experience. Character references are also required.

The Chemical Engineering Principles and Practice exam is an eight-hour, open-book, multiple-choice

examination. There are 40 questions in the morning session and 40 questions in the afternoon session. Each correct answer is worth 1 point. As with the FE exam, each question has four possible answers, and there is no deduction for incorrect answers. A separate exam is given for each field of engineering. The Chemical Engineering exam is given twice a year (April and October) on the Friday just before the date the FE exam is given. The nominal passing score is approximately 48 points; however, as with the FE exam, recalibration to ensure uniform difficulty in passing the examination is performed. On the April 2011 Chemical Engineering PE exam, 78% of applicants taking the exam for the first time passed. Only 31% of those retaking the exam passed. The results are sent to the state board eight to ten weeks after the exam is taken and are sent to the applicant by the state board after that.

The difficulty of questions on the PE exam is roughly equivalent to that of the questions on a final exam in the respective course. The questions are design oriented. The topics covered are shown in Table 25.3. Note that thermodynamics questions are included in both the mass and the energy balances subjects and in the mass transfer subject. Preparing for the PE exam generally takes more effort than preparing for the FE exam. Full-length, hard-copy practice exams are available from NCEES and various publishers. Many applicants also take a refresher course, available through AIChE local sections and commercial services. In addition to the national Chemical Engineering PE exam, most states require a short law exam on the legal requirements for engineering practice in that state.

Table 25.3. Subject Categories for the Chemical Engineering PE Exam

Subject	Average Number of Questions
Mass/Energy Balances and Thermodynamics	18
Heat Transfer	13
Fluids	13
Mass Transfer	11
Kinetics	9
Plant Design and Operation	16

To renew a PE license, one must demonstrate continuing professional competency by documenting 15 professional development hours (PDHs) per year, although some states allow averaging over two years. Typical activities that can count (under specific rules) for PDHs are taking a course, attending seminars, publishing articles or books, and receiving a patent.

A PE license can be revoked by the state board for violation of the engineering code of ethics for that state. Such revocation becomes a matter of public record.

25.3. Legal Liability [13]

Chemical engineers often encounter legal liability for their work. Legal advice cannot be provided in this book, but some of the situations in which a chemical engineer should seek legal counsel are noted. Perhaps the best advice is to take a short course in legal issues for engineers early in your career and seek the advice of a licensed attorney if there are any doubts about your legal rights, obligations, or liabilities.

When applying for registration as an engineer-in-training or a professional engineer, each person is given a copy of the appropriate state laws and regulations and he or she is required to certify that these are understood. These should be studied in detail. Beyond these specific licensing requirements, a chemical engineer must deal with government regulations, contracts, and issues of civil and even criminal liability.

For example, throughout a chemical engineering career, one will deal with government agencies such as the Environmental Protection Agency (EPA), Occupational Safety and Health Administration (OSHA), Department of Transportation (DOT), and others. Federal and state laws give these agencies authority to regulate industry and commerce by enacting various regulations. For federal agencies, these regulations are first published in the *Federal Register* and then periodically cataloged in the *Code of Federal Regulations* (CFR). These documents are available in most large libraries and in all law libraries as well as online (http://www.gpo.gov/fdsys). It is worthwhile to look at some of these regulations while you are still in school, to become aware of the scope, detail, and format of these documents. The regulations cover, for example, maximum concentrations for wastewater discharges, approved process safety procedures, and requirements for transportation of hazardous materials. They are generally written by technically trained professionals (often engineers), although the wording will have been checked by the legal staff. Thus, it is expected that competent chemical engineers can and will read, understand, and follow these regulations.

Sometimes the engineer's responsibilities are greater than they might first appear. For example, OSHA sets maximum permissible employee exposure levels for many substances, but adherence to these may not be enough, because the **general duty clause** of the OSHA Act of 1970 has been interpreted as requiring an employer to avoid exposing employees to any hazards that are known or that *should be known* to the employer. If a substance is known to cause harmful effects (e.g., such a study has been published or the company has proprietary knowledge of such effects), the employer must control employee exposure even though OSHA has no standard for that substance.

Contracts are another form of legally binding document, in which two or more parties agree to accept one or more obligations. Before signing any written contract or agreeing to any oral contract, one should understand one's obligations and what consideration (e.g., payment) is promised in return from the other party. Upon obtaining employment, one may be asked to sign an employment contract in which consideration (salary) is offered in return for certain chemical engineering services to the firm, and for adherence to specific codes of conduct (see Section 25.4). If any aspect of a contract is unclear, one should obtain legal counsel. If one is signing the contract on behalf of the firm, the firm's attorney is consulted. If one is signing as an individual, a private attorney is consulted. Whenever there is any indication that either party may not live up to its obligations, appropriate counsel should be consulted.

Beyond the legal issues of contracts, civil legal actions (known as **torts**) sometimes involve engineers. These suits are brought when some action or lack of action by the defendant is alleged to have caused injury (physical, financial, or emotional) to the plaintiff. Both compensatory damages (to pay for correction of the injury) and punitive damages (to punish the party that did the injury) can be recovered by the plaintiff. Again, good advice here is to consult legal counsel whenever such circumstances arise or are anticipated to arise.

Finally, engineers can face criminal prosecution for actions such as falsifying records submitted to federal regulatory agencies or willfully subjecting employees to hazardous environments. Although such actions are rare, the penalties are severe.

25.4. Business Codes of Conduct [14, 15]

Most firms have formal codes of conduct that must be adhered to as a condition of employment. Often one is asked to sign these on the first day of work. As with any contract, it is important to read and to understand all of the details and to then fulfill all of the obligations undertaken. If an employee does not adhere to the code, he or she may be fired.

In consideration for employment, a chemical engineer (or any employee) accepts what are called **fiduciary responsibilities**. This means that trust has been placed in the engineer to act faithfully for the good of the firm. This is a general legal principle and is covered in the AIChE code of ethics.

Related to fiduciary responsibilities is the avoidance of conflicts of interest. The focus here is to avoid circumstances where you have, or appear to have, contradictory obligations. For example, if you own stock in a valve manufacturer, it would be a conflict of interest if you were to order valves from that company for your present employer, if there were another supplier of equal-quality valves at a lower price. In general—and especially in government service, where the regulations are quite strict—one must avoid not only actual conflicts of interest but also apparent conflicts of interest. The test is that, if a reasonable person could reasonably assume there to be a conflict of interest, one has an apparent conflict of interest.

It is assumed that much information about employees will become known to the company. In a typical business code of conduct, one agrees to keep personnel information confidential. That is, one agrees not to release such information to anyone outside the firm and to release it only to those within the firm who have a clear need to know. Strict adherence to such an agreement is essential.

In the business code of conduct or in a proprietary secrecy or patent agreement, the employee agrees that certain knowledge gained and discoveries made through employment are the property of the firm and may not be divulged to others. It is crucial that engineers read and understand this agreement in detail before signing. Much of the value of a firm resides in **proprietary** knowledge, that is, knowledge that is not shared with others. Breaching a secrecy agreement can be very costly to a firm, and the engineer could be in serious legal trouble. Similarly, a firm hires a chemical engineer to do work that often results in patentable discoveries. If such discoveries are made on company time, with company property, or with proprietary knowledge, the patent agreement will require disclosure to the firm and assignment of patent rights to the firm. If one does make discoveries completely outside the realm of employment, one should keep extremely careful and complete notes to avoid patent ownership difficulties.

If the firm has significant international operations, the code of conduct generally covers the conduct of employees representing the firm abroad. Because business customs vary widely from country to country, this can be an especially important subject. Before leaving the country on assignment, it is crucial to obtain as complete knowledge as possible both about the customs and laws of the other country and about any changes in business procedure that are authorized by the firm. The U.S. government forbids representatives of U.S. corporations from engaging in certain business practices, even if they are customary in that country.

A final aspect of business conduct that must be considered, and that might be included in the code of conduct, is employee relations. Specific guidelines for hiring and firing of employees must be followed to avoid legal difficulties. Whenever you are in a position to hire or fire, you must be proactive to learn the appropriate company procedures. There are specific legal requirements about what information you cannot request from job applicants and what information you can use to make

employment decisions. Also, most business codes of conduct include requirements to avoid any discriminatory or harassing behavior. Good advice here, as mentioned above regarding conflicts of interest, is to avoid even the appearance of discrimination or sexual harassment.

25.5. Summary

In this chapter, the role of ethics in the chemical engineering profession was explained and strategies were provided for making ethical decisions. The framework for registration of professional engineers in the United States was also described, including strategies for preparing for the licensing examination.

What You Should Have Learned

- Morality relates to beliefs; ethics relates to behavior.
- Moral autonomy is the ability to make one's own ethical decisions.
- Legality and legal obligations may supersede ethics.
- The AIChE and NSPE have codes of ethics.

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Problems

1. **Proprietary Information** [6]: I am a senior. Last summer, I had an excellent job designing a new type of heat exchanger that the company was developing. When I returned to school, my professor asked me to use my knowledge on a design project, and to explain heat-exchanger design to other seniors in the design group. I really feel that I have something exciting to share with my fellow classmates. Is it ethical for me to share my experiences with my colleagues?
2. **Medical School** [6]: I am a senior in chemical engineering, but I plan to go to medical school next year. I have not been accepted yet. I want a good summer job, and yet, if my application for medical school is turned down, I would want the job to be permanent. Jobs are hard to get, and the interviewers with whom I have talked so far will offer me permanent employment but not summer employment. I have three interviews left. What do I tell these interviewers?
3. **Sophomore** [6]: I am a sophomore. None of my classmates has a summer job. Jobs are hard to get, and I need money to pay for school next year. I have been offered a well-paying job with lots of engineering experience to work on the production of propellants/explosives for antipersonnel mines. Personally, I strongly believe that this product should not be manufactured. Should I accept the job? Should I tell the company of my personal beliefs?
4. **Not a Hazard as Defined** [3, Reprinted by special permission from *Chemical Engineering*, March 2, 1987, and September 28, 1987, Copyright © 1987 by McGraw-Hill, Inc., New York, NY 10020]: In a unit where grain is steeped, sulfur dioxide is added directly to grain and water. Operators have long complained about sulfur dioxide fumes, citing runny noses, teary eyes, coughing, and headaches. The concentration has been checked many times and has always measured lower than OSHA specifications. Management's stance has always been, "Don't spend money to fix something if it isn't broken." A few employees have quit, citing allergies and other medical problems. Operators in the area have requested an engineering study to remedy the situation. Chris is given the job of investigating whether the exhaust fan should be replaced with an expensive ventilation system. What are Chris's obligations? Can they all be met? What creative strategies can you suggest to Chris to deal with this situation?

5. **Improving a Reaction** [5, Reprinted with permission of AIChE]: Look up this article, and write a one-page response to the case. Then look up the reader responses. Write a one-page reflection on the case.
6. **The Falsified Data Strike Back** [2, Reprinted by special permission from *Chemical Engineering*, May 5, 1980, and September 22, 1980, Copyright © 1980 by McGraw-Hill, Inc., New York, NY 10020]: In the case described in Section 25.1.2, Jay has written the report to suit the boss, and the company has gone ahead with an ambitious commercialization program for Catalyst A. Jay has been put in charge of the pilot plant where development work is being done on the project. To allay personal doubts, Jay runs some clandestine tests on the two catalysts. To Jay's astonishment and dismay, the tests determine that even though Catalyst A works better under most conditions (as everyone had expected), at the operating conditions specified in the firm's process design, Catalyst B is indeed considerably superior. What should Jay do?
7. Contact the Board of Registration for Professional Engineers in your area. Determine what code of ethics is required and what are the specific requirements for registration.
8. In a small group (approximately four students), obtain examples of codes of conduct from different companies and compare their features.
9. Develop five heuristics (not mentioned in this chapter) for ethical problem solving.
10. Develop a scenario of an ethical dilemma, and, in a small group, use a problem-solving strategy to analyze it.
11. Find the Process Safety Management regulation in the *Code of Federal Regulations* (29CFR1900.119), and write a two-page synopsis of it.
12. View the (24-minute) video "Gilbane Gold," National Society for Professional Engineers, 1989. Evaluate the actions taken by the plant manager, the production engineer, the environmental engineer, and the two consulting engineers. Write a group report detailing this evaluation and referring to sections of the NSPE code of ethics where appropriate.
13. View the (two-hour) movie *Acceptable Risks*, ABC-TV productions, 1986. Evaluate the actions taken by the headquarters management, the plant manager, the production engineer, and the maintenance engineer. Write a group report detailing this evaluation and referring to sections of the AIChE code of ethics where appropriate.
14. Study the student code of conduct (sometimes referred to as the honor code, the definition of academic dishonesty, or the students' rights and responsibilities) at your institution. Develop a hypothetical (but plausible) case concerning engineering students. Present the case to the class for a 30-minute discussion.
15. The NCEES Rules of Professional Conduct (in the *FE Supplied-Reference Handbook*) was developed as a model code to be accepted by or modified by the individual state boards of professional engineers. Compare it with the AIChE code of ethics and with the NSPE code of ethics.

Chapter 26. Health, Safety, and the Environment

What You Will Learn

- The basics of health, environment, and safety

One goal of chemical engineering is to produce goods and services that enhance the quality of life. Chemical engineers have been at the forefront of efforts to improve health (e.g., pharmaceuticals), safety (e.g., shatterproof polymer glasses), and the environment (e.g., catalytic converters). Moreover, throughout the product life cycle, chemical engineers are concerned with potential harm to the health and safety of people and damage to the environment. This chapter focuses on assessment of these potential dangers. Chapter 27 focuses on proactive strategies to avoid them.

Although many of the chemical processing industries regard improvements of health, safety, and the environment (HSE) as one general function, the U.S. government has separated the field into distinct categories, based on the varying rights afforded to different classes and for historical purposes. The health and safety of employees, for example, is regulated by the Occupational Safety and Health Administration (OSHA), whereas the health of nonemployees and the environment are regulated by the Environmental Protection Agency (EPA). Other activities are regulated by the Department of Transportation (DOT) or the Department of Energy (DOE), among other agencies.

An exact description of applicable laws, rules, and regulations would be out of date before any textbook could be printed; rather, this chapter describes the types of regulations that are relevant to chemical engineering and provides guidance on where to find the current (and proposed) regulations. The focus is on the general concepts and strategies of risk assessment and reduction that transcend the details of regulations.

26.1. Risk Assessment

There are many ways to view risks to a person's health or safety. Some people will knowingly accept tremendous risk (such as in rock climbing or smoking), some expose themselves to risk perhaps without knowing (such as by sunbathing), and some refuse to be exposed at all to certain risks (such as extremely low concentrations of pesticides in food). Generally, people are much more accepting of risks that they choose (voluntary exposures) than to risks that are forced upon them (involuntary exposures). Also, people are generally much more accepting of risks that they understand than they are of risks that they do not understand. For example, the population at large tends to accept that human activity often degrades rivers and lakes with biological and chemical pollution, but they do not accept any measurable radioactive emissions from power plants.

26.1.1. Accident Statistics

Engineers quantify risks to provide a rational basis for deciding what activities should be undertaken and which risks are worth the benefits provided. These decisions are frequently made by nonengineers; thus, it is essential that the measures that engineers use be understandable to the public. For this reason, several measures have been established.

The **OSHA incidence rate** is the number of injuries and illnesses per 200,000 hours of exposure. Any injury or work-related illness that results in a "lost workday" is counted in the ratio. Thus, minor

injuries that can be treated with first aid are not counted, but counted injuries range all the way to death. The 200,000 hours is roughly equivalent to 100 worker years. The OSHA incidence rate illustrates two features of risk measures: the details of the accident are not included, and these measures can be used for non-work-related exposures.

The **fatal accident rate (FAR)** is the number of fatalities per 10^8 hours of exposure. Only fatalities are counted, and the 100,000,000 hours is roughly equivalent to 1000 worker lifetimes. Although only deaths are counted, in many fields there is a strong correlation between numbers of injuries and numbers of deaths. Thus, the reasonable presumption is that a decrease in the FAR will also decrease the OSHA incidence rate.

For some exposures, the available data are insufficient to determine the total time of exposure. For these cases, the **fatality rate** can be used. This measure is the number of fatalities per year divided by the total population at risk. For example, the exposure of individual smokers is extremely variable because of differences in type of cigarette, number of inhalations per cigarette, and so on. However, one can determine the fatality rate (~0.005), which gives a rough estimate of the chance that a smoker will die this year from smoking-related causes of 0.5%.

Table 26.1 shows some representative numbers of these three risk measurements. One of the possibly surprising observations is that the chemical process industries are relatively safe (for workers) compared with many other industries. There are many reasons for this, ranging from the high level of remote sensing and operation, which separates workers from the most dangerous parts of the plant, to the historical concern for the hazards of industrial chemicals. Regardless of the reasons, chemical engineers continue to try to improve the safety of chemical plants.

Table 26.1. Comparison of Three Risk Measurements [1]

Activity	OSHA Incident Rate (Injuries and Deaths per 200,000 h)	Fatal Accident Rate (Deaths per 100,000,000 h)	Fatality Rate (Deaths per Person per Year)
Working in chemical industry	0.49	4	
Staying at home		3	
Working in steel industry	1.54	8	
Working in construction	3.88	67	
Traveling by car		57	170×10^{-6}
Rock climbing		4000	40×10^{-6}
Smoking (1 pack per day)			5000×10^{-6}
Being struck by lightning			0.1×10^{-6}

Another observation is that there are differences in relative rankings if one uses the different risk measurements. Perhaps most striking is that the FAR for employees of the chemical industry is only slightly higher than the FAR for people staying in their homes. However, this is a potentially misleading comparison. The portion of the population that works is on average more healthy than the portion that does not. Also, most people take risks at home that they would not be allowed to take at work. Finally, a worker is probably more tired and prone to accidents at home after a hard day at work.

The main use of these statistics is not to compare one activity with another (unless they can be

substituted for one another) but to monitor improvements to the health and safety of workers and others achieved by process modifications.

26.1.2. Worst-Case Scenarios

Another measure of risk is to imagine the worst possible consequence of an operation. Such a study is called a **worst-case-scenario** study, and it is required by some government agencies. These studies have some drawbacks, but they can be very useful in identifying ways to avoid serious accidents. A related strategy that is routinely used throughout the industry for identifying potential hazards is called HAZOP and is discussed in Section 26.4.

The development of worst-case scenarios is certainly subjective, but government agencies and organizations develop guidelines for this task. For example, there is certainly a chance that an asteroid will impact Earth directly in the middle of the chemical plant. Should this be the worst-case scenario? Most people would argue that this takes the worst-case scenario study beyond reason, but there are no clear-cut rules. The subjective rules that have been developed contain definitions such as the worst accident that might reasonably be assumed possible over the life of the facility. Different people would define "possible" (or "probable") in different ways. Is sabotage by an employee possible? Is the simultaneous failure of three independent safety systems probable? Certainly the events of September 11, 2001, have indicated that a terrorist-attack scenario is not impossible. Sometimes probabilities of occurrence can be estimated, but often they cannot.

By EPA definition (40CFR68.3), "*Worst-case release* means the release of the largest quantity of a regulated substance from a vessel or process line failure that results in the greatest distance to an endpoint defined in § 68.22(a)." This end point is a specified concentration of a toxic substance, an overpressure of 1 psi for explosions, a radiant heat flux of 5 kW/m^2 for 40 seconds for a fire, or the lower flammability limit for a flammable substance, whichever is appropriate. Thus, the worst case is defined by the size of the area adversely affected by the release. There are also definitions of how much of the material in a tank (often 100%) should be considered over what period of time (often 10 minutes) in the scenario.

All this is to say that worst-case-scenario analyses can be extremely helpful, but they are difficult to perform and potentially difficult to understand. They are most useful when specific guidelines are followed and when they are used to enhance safety by developing safeguards against the accident scenarios developed. For the risk management plan described in Section 26.2.2, worst-case-scenario analyses are required by regulation.

These guidelines are constantly changing, so they are not described in detail here. The most current guidelines should be obtained from the EPA, OSHA, or other agencies.

26.1.3. The Role of the Chemical Engineer

As the professional with the best knowledge of the risks of a chemical processing operation, the chemical engineer has a responsibility to communicate those risks to employers, employees, clients, and the public.

It can be very difficult to explain FARs in deaths per 10^8 hours to the general, nontechnical public. However, the consequences of failure to explain rationally and honestly to the public the risks and the steps taken to reduce those risks are tremendous. The ethical role of the chemical engineer in this

communication is discussed in Chapter 25. Beyond those responsibilities, the damage from poor communication can destroy an industry. For example, the nuclear power industry in the United States has been destroyed in large part by the failure to communicate risks to the general public in a way that it could understand. When even relatively minor accidents occur, many feel that they were misled by engineers who seemed to have said that there were no risks, no chance of an accident.

26.2. Regulations and Agencies

Rules and regulations arise both from governmental agencies and from nongovernmental organizations (such as AIChE). These rules and regulations change constantly, and the most up-to-date rules should always be determined. The following sections describe the kinds of rules and regulations promulgated (put into effect by formal public announcement) by various organizations. The actual agency should be contacted directly for the latest rules.

Federal government rules and regulations are published in the *Federal Register* (FR), which is issued daily. Notices of proposed or pending regulations are also given in the FR. Annually, the regulations of a specific type are collated and published in the *Code of Federal Regulations* (CFR). Both the FR and the CFR are available in large libraries and in all law libraries, as well as on the Internet. In Table 26.2 the Internet addresses for the FR and CFR as of the date this book is written are provided. Because Internet addresses change frequently, the use of a search engine to find new URLs is suggested if the links given here are broken. However, note that only server addresses ending in ".gov" are official U.S. government Web sites.

Table 26.2. Internet Addresses for Federal Agencies

Code of Federal Regulations (CFR)	http://www.gpo.gov/fdsys
Federal Register (FR) and U.S. Code	http://www.gpo.gov/fdsys
DOT regulations (FR and 49 CFR)	http://www.phmsa.dot.gov/hazmat/regs
EPA regulations (FR and 40 CFR)	http://www.epa.gov/lawsregs
MSHA regulations (FR and 30 CFR)	http://www.msha.gov/regsinfo.htm
NIOSH databases	http://www.cdc.gov/niosh/database.html
OSHA regulations (FR and 29 CFR)	http://www.osha.gov

In addition to the direct government sources, numerous private firms collate federal regulations (more quickly than does the government), and they sell their compendia, often tailored to the needs of the customer.

State and local government regulations are also available in hard copy and increasingly in online form. However, it is best to contact these agencies directly to be sure that one has all the relevant regulations. Nongovernmental organizations can be contacted directly for their rules. *However, sources of information on the Internet are notoriously inaccurate and out of date.* Unless it is an official government Web site (with the date of the latest update), beware.

26.2.1. OSHA and NIOSH

In general, the Occupational Safety and Health Administration promulgates regulations having to do with worker safety and health in industries other than mining (Mine Safety and Health Administration, MSHA, serves a similar role there). The National Institute for Occupational Safety and Health (NIOSH) is a federal research organization that provides information to employees, employers, and

OSHA to help assess health and safety risks. Regulations are not promulgated by NIOSH, although it does certify various analytical techniques and equipment (such as respirators).

One major law and five major regulations in this area are the OSHA Act [2], Hazard Communication (29CFR1910.1200), Air Contaminants (29CFR1910.1000), Occupational Exposure to Hazardous Chemicals in Laboratories (29CFR1910.1450), Hazardous Waste Operations and Emergency Response (26CFR1901.120), and Process Safety Management of Highly Hazardous Chemicals (29CFR1910.119).

OSHA Act and Air Contaminants Standard. The original act of Congress that set up OSHA, the Occupational Safety and Health Act of 1970 [2], specified certain regulations and standards and required OSHA to promulgate others. Perhaps of most importance is the so-called **general duty clause** of the OSHA Act stating that "each employer shall furnish to each of his employees employment and a place of employment which are free from recognized hazards that are causing or are likely to cause death or serious physical harm to his employees" [Reference 2, Section 5.a.1]. This clause has been interpreted to mean that an employer must avoid exposing employees to hazards that *should have been known* to the employer, whether or not that hazard is specifically regulated by OSHA. Thus, the responsibility of researching the literature to see whether anyone has identified a hazard is placed on the employer. Most chemical engineers are employees, and yet they often represent the employer and therefore assume the responsibilities under the general duty clause.

To search for published data on chemical hazards, a good place to start is the Integrated Risk Information System (IRIS), the Hazardous Substances Data Bank (HSDB), and other databases at http://www.toxnet.nlm.nih.gov.

Some specific regulations ensued from the OSHA Act, notably for the chemical industry exposure limits for certain substances in breathing air for employees (29CFR1910.1000 Air Contaminants). These limits are called **permissible exposure limits (PEL)** and are often given in parts per million (by volume). Related limits are updated yearly by the American Conference of Governmental and Industrial Hygienists (ACGIH, a nongovernmental association) and are called **threshold limit values (TLV)** [3]. In fact, the original OSHA regulations merely made these TLVs the official government limits. NIOSH also publishes **recommended exposure limits (REL)**, but these are not legally binding regulations. Each of these exposure limits is based on the assumption that a typical worker can be exposed to that concentration of the substance for eight hours a day, five days a week, for a working lifetime, without ill effects. These assumptions are often based on sketchy data extrapolated from animal studies. All these limits (PEL, TLV, REL) are given in the convenient *NIOSH Pocket Guide to Chemical Hazards* [4], available in printed form from NIOSH for a small charge or available free as an HTML or PDF download from the NIOSH Web site. Respirator requirements and a description of the health effects of exposure are also given.

The exposure limits are based on a **time-weighted average (TWA)** over an eight-hour shift, which means that higher concentrations are allowable, as long as the average over the shift is not greater than the PEL. When even short-term exposure to higher levels is harmful, there is a separate **short-term exposure limit (STEL)**, which is a 15-minute time-weighted average concentration that must never be exceeded, or an OSHA **ceiling concentration**, which is an instantaneous concentration that must never be exceeded. Also, maximum concentrations from which one could escape within 30 minutes without experiencing escape-impairing or irreversible health effects are identified as **immediately dangerous to life and health (IDLH)** concentrations. The IDLH limit is used under

conditions in which a respirator is normally used. In the event of a respirator failure, the employee might not be able to escape if the concentration is greater than the IDLH. These limits are also given in the NIOSH handbook [4].

Hazard Communication Standard. This regulation is also known as the **Worker Right to Know** or simply **HazCom**. The reference is 29CFR1910.1200. It requires that the employer train all employees so that the employees understand the hazards of the substances that they are handling or are exposed to or potentially exposed to. It is explicitly stated that the employer has not met this standard merely by giving the employee the hazard information orally or in written form. The employer must make sure that the employee *understands* the hazards; thus, much effort in training goes into satisfying this requirement. Two very obvious results and requirements of this regulation are proper labeling of containers and availability of **material safety data sheets (MSDS)**. Table 26.3 lists typical major sections of an MSDS, but the precise format of an MSDS is not presently defined by regulation, although some of the minimum requirements are, and these are also listed in Table 26.3. The MSDS must list the substances, their known hazards, and procedures for proper handling of the material and for proper actions in an emergency. Although only hazardous materials must have these MSDSs, they are available for almost all substances and mixtures in commerce. They are available directly from the supplier or manufacturer or on the Internet. It is recommended to use the Internet only as a preliminary source for MSDSs. One should get an MSDS directly from more than one manufacturer if possible, because errors in MSDSs do occur and because different MSDSs will contain different data.

Table 26.3. Typical Sections of a Material Safety Data Sheet (MSDS)

1. Material and manufacturer identification
2. Hazardous ingredients/identity information
3. Physical/Chemical characteristics
4. Fire and explosion hazard data
5. Reactivity data
6. Health hazard data
7. Precautions for safe handling and use
8. Control measures
From OSHA Form 1218-0072.

Unfortunately, often MSDSs are difficult to read quickly. They are filled with much useful information, but they are often several pages long. In addition, different chemical suppliers use different formats. (OSHA now recommends the ANSI 16-section format.) They must be studied extensively *before* any hazardous situation is encountered. A group of international agencies (UN Environment Programme, International Labour Office, and the World Health Organization in cooperation with NIOSH and the European Community) has developed a simpler, standard, two-page data card that can be understood quickly and used in an emergency. In addition to the required MSDSs, the ready availability of this **international chemical safety card** wherever a hazardous material is used, stored, or transported is highly recommended. They can be found at http://www.cdc.gov/niosh/ipcs/ipcscard.html.

On June 1, 2007, the European Community put into force a new regulation called **Registration,**

Evaluation, Authorisation and Restriction of Chemicals (REACH). Although it specifically applies to manufacturers within the European Union and manufacturers that import into the EU, it is becoming the de facto worldwide standard for regulation of chemical products. All firms that handle one metric tonne or more per year of any chemical product or produce any chemical product that is new to commerce are covered. For many existing chemical products, new data have been measured to determine hazards more accurately. Substances that are high-volume, mutagenic, or very toxic to aquatic organisms have already been fully phased in. Other low-volume substances will be phased in through May 2018. Details of the regulation are available at http://echa.europa.eu.

Minimum Requirements for MSDS (29CFR1910.1200[g]). An MSDS is required for each "hazardous chemical," including those specifically listed in 29CFR1910 (subpart Z), any material assigned a TLV, or any material determined to be cancer causing, corrosive, toxic, an irritant, a sensitizer, or one that has damaging effects on specific body organs. There are numerous facts that may be given in an MSDS; however, the minimum information required is listed below.

1. Written in English.
2. Identity used on label.
3. Chemical name and common name of all ingredients that are hazardous and that are present in ≥1%concentration or that could be released in harmful concentrations.
4. Chemical name and common name of all ingredients that are carcinogens and that are present in ≥0.1%concentration or that could be released in harmful concentrations.
5. Physical and chemical characteristics of the hazardous chemical (such as vapor pressure, flash point).
6. Physical hazards of the hazardous chemical, including the potential for fire, explosion, and reactivity.
7. Health hazards of the hazardous chemical, including signs and symptoms of exposure, and any medical conditions that are generally recognized as being aggravated by exposure to the chemical.
8. Primary routes of entry.
9. OSHA permissible exposure limit, ACGIH TLV, and any other exposure limit used or recommended by the chemical manufacturer, importer, or employer.
10. Whether the hazardous chemical is listed in the National Toxicology Program (NTP) *Annual Report on Carcinogens* (latest edition) or has been found to be a potential carcinogen in the International Agency for Research on Cancer (IARC) Monographs (latest editions), or by OSHA.
11. Any generally applicable precautions for safe handling and use that are known to the chemical manufacturer, importer, or employer preparing the MSDS, including appropriate hygienic practices, protective measures during repair and maintenance of contaminated equipment, and procedures for cleanup of spills and leaks.
12. Any generally applicable control measures that are known to the chemical manufacturer, importer, or employer preparing the MSDS, such as appropriate engineering controls, work practices, or personal protective equipment.
13. Emergency and first aid procedures.
14. Date of preparation of the MSDS or the last change to it.

15. Name, address, and telephone number of the chemical manufacturer, importer, employer, or other responsible party preparing or distributing the material safety data sheet that can provide additional information on the hazardous chemical and appropriate emergency procedures, if necessary.

Process Safety Management of Highly Hazardous Chemicals (29CFR1910.119). This OSHA regulation applies to essentially all of the chemical processing industries and requires action in 13 different types of activities as shown in Table 26.4. Note, however, that transportation of hazardous materials is regulated by the U.S. Department of Transportation under 49CFR100 through 49CFR185 (http://www.phmsa.dot.gov/hazmat/regs). Similarly, the safe operation of chemical laboratories is regulated by OSHA through 29CFR1910.1450, which recognizes that laboratories and production facilities present different kinds of hazards.

Table 26.4. Process Safety Management of Highly Hazardous Chemicals (29CFR1910.119)

1. Employee participation
2. Process safety information
3. Process hazards analysis
4. Operating procedures
5. Training
6. Contractors
7. Pre-start-up safety review
8. Mechanical integrity
9. Hot work permit
10. Management of change
11. Incident investigation
12. Emergency planning and response
13. Compliance safety audit

When OSHA promulgated the Process Safety Management Regulation in 1992, it used the already existing rules of the American Institute of Chemical Engineers' *Guidelines for Technical Management of Chemical Process Safety* [5] and the American Petroleum Institute's Recommended Practices 750 [6] as guides. In fact, as is often the case, OSHA essentially gave the force of law to these voluntary nongovernmental standards.

Process safety management (PSM) embraces nearly the entire safety enterprise of a chemical process organization. It requires employee training, written operating procedures, specific quality in the engineering design of components and systems, very specific procedures for some activities, investigation and reporting of accidents that do occur, and an internal audit of the safety enterprise of the company. Following is a description of each of the 13 components.

1. **Employee Participation:** The employer must actively involve the employees in the development and implementation of the safety program. Employees are more likely to understand the hazards and to follow the established safety procedures when they are involved early and continuously in the development of the safety program. This item was added to the

earlier API and AIChE standards.

2. **Process Safety Information:** The employer must research the materials, process, and operation to determine the potential hazards and keep in an immediately accessible form all safety information. This includes all MSDSs, as well as information on the process itself, such as up-to-date process flow diagrams and P&IDs.
3. **Process Hazards Analysis:** Before a process is started up and periodically thereafter (typically every three to five years or whenever significant modifications are made), a detailed study must be made of the process to determine potential hazards and to correct them. There are several approved procedures, and an organization can opt to use an alternative procedure if it can be shown to be as effective. In fact, most of the chemical processing industry uses the HAZOP technique, which is described in Section 26.4. This technique is a modified brainstorming process in which potential hazards are identified, their consequences are determined, and an action to deal with the hazard is identified.
4. **Operating Procedures:** Written operating procedures must be available to operators, and any deviations in the plant operation from these procedures must be noted. These procedures must include start-up, shutdown, and emergency response to process upset.
5. **Training:** The employer must train all employees in the hazards present and the procedures for mitigating them.
6. **Contractors:** The employer is responsible for the safe conduct of any contractors. Although each contractor is responsible for the safe conduct of the contractor's employees, the owner or operator of the plant who enters into a contract with the contractor remains liable for the safe operation of the contractor. This is an OSHA addition to the earlier API and AIChE standards.
7. **Pre-start-up Safety Review:** The regulation specifically requires that there be a review of the safety aspects of the process before any processing occurs on the site. The review must be documented, and any deviations of the plant as built from the design specifications must be addressed.
8. **Mechanical Integrity:** Vessels and other equipment must meet existing codes and be inspected during manufacture and after installation. Appropriate procedures for maintenance must be developed and followed.
9. **Hot Work Permit:** This is a very specific procedure by which a wide range of people in the plant are notified before **hot work,** such as welding, can occur. Many chemical plants use flammable materials, and everyone in the area needs to be informed so that no flammable vapors are released during the operation.
10. **Management of Change:** During accident investigations in the chemical process industries, it has often been found that severe incidents (involving deaths and massive destruction) occurred because equipment, processes, or procedures were changed from the original design without careful study of the consequences. Thus, the OSHA regulation requires companies to have in place a system by which any modification is reviewed by all of the appropriate people. For example, any change in the reactor design must be reviewed not only by the design engineer but also by the process engineer who can evaluate how the overall process is affected. The maintenance leader must also make sure that the modification does not adversely affect the maintenance schedule or the ability of workers to get to or to maintain the equipment.

11. **Incident Investigation:** When there is a hazardous process upset, it must be investigated and a written report must be developed indicating the details of the incident, the probable cause, and the steps taken to avoid future incidents.
12. **Emergency Planning and Response:** There must be a written plan, and employees must be trained to respond to possible emergency situations.
13. **Compliance Safety Audit:** Periodically, all of the elements of the safety system (including items 1–12 above) must be audited to make sure that the approved procedures are being followed and that they are effective.

One item that is included in the industry codes but not in the PSM regulation is the entry of workers into **confined spaces**. This situation—in which the environment of the space or the difficulty of egress from the space could create a hazard—is encountered frequently in the chemical process industries. OSHA regulation 29CFR1910.146 covers the required permitting procedures to ensure that workers are protected in confined spaces.

26.2.2. Environmental Protection Agency (EPA)

The role of the EPA is to protect the environment from the effects of human activity. Although this is a very broad role, in the context of the chemical processing industries it usually relates to emissions of harmful or potentially harmful materials from the plant site to the outside by air or by water. There are three classes of such emissions: (1) planned emissions, (2) fugitive emissions, and (3) emergency emissions. This section describes some of the present regulations for these classes of emissions. There are many more regulations that are not mentioned here. In any facility, one must keep constantly aware of new and modified regulations through research, use of an environmental compliance consulting firm, or communication with the local, state, and federal environmental protection agencies.

Planned Emissions. Any process plant will have emissions. These may be harmful to the environment, benign, or, in rare cases, beneficial. In any case, a permit is usually required before construction or operation of the plant. Significant modifications to the plant (especially if they change the design emissions) will likely require a modification to the permit or a new permit.

These emissions permits are normally obtained through the state environmental protection agency, but federal regulations must be met. In some regions, states, or localities, the requirements for the permit may be significantly more stringent than the federal EPA regulations. One must contact the local agencies. However, searching the EPA databases described in Section 26.2 can provide a good preliminary overview.

Permits frequently require an extensive **environmental impact statement (EIS)** detailing the present environment and any potential disturbances that the planned activity could produce. For process plants, these EISs are typically written by a team of chemical engineers, biologists, and others, and they deal not only with planned emissions but also with potential process upsets and emergencies. In this regard, the worst-case scenario mentioned in Section 26.1.2 is used.

Permitting is based on assessment of potential degradation of the environment, and thus both the level of emissions from the plant and the present level of contamination in the local environment are considered. There are National Ambient Air Quality Standards (NAAQS) for a few materials and National Emissions Standards for Hazardous Air Pollutants (NESHAP) and New Source

Performance Standards (NSPS) for these and others. Major sources (defined as those plants that emit more than some annual threshold quantity such as 25 tons of hazardous air pollutants) must meet the most stringent emissions criteria and require more permits. Similar standards are applied for water quality and for discharges into the water. Many of these regulations are based on the Clean Air Act and Clean Water Act, among others.

Beyond the effects on the environment after emissions are fully dispersed in the air or the water, there can be acute, short-term effects on nearby populations. Often chemical engineers perform dispersion studies to determine the range and longevity of the plume of harmful materials that flows from the point of discharge into the air or water.

The focus of the Clean Air Act Amendments of 1990, Title I, is the release of **volatile organic compounds (VOCs)**, which are precursors to the photochemical production of ozone (smog), especially in areas that have not attained NAAQS. The definition of a VOC is any organic compound with an appreciable vapor pressure at 25°C that participates in atmospheric photochemical reactions. It does not include methane, ethane, and a number of other substances listed in 40CFR51.100(s). **Hazardous air pollutants (HAP)** are also regulated through Title III of the act.

An important part of planned emissions are so-called **fugitive emissions**. These are losses from seals in rotating equipment (e.g., pumps, agitators, compressors), losses through connections between equipment (e.g., piping connections, valves), and other losses that result from incomplete isolation of the interior of the process from the atmosphere (e.g., tanks). Although substantial progress has been made over the last two decades to reduce fugitive emissions through improved equipment design, fugitive emissions are still substantial and are, in some cases, the major source of all emissions from a process plant.

Emergency Releases. Process upsets can create catastrophic releases of hazardous materials, and regulations require that there be an effective plan to deal with these occurrences and that the consequences for affected populations not be too serious. As mentioned earlier, worst-case scenarios and dispersion modeling are used to make this assessment.

One such regulation is the Emergency Planning and Community Right to Know Act (EPCRA) of 1986, also known as SARA, Title III. This regulation requires plants to provide the local community with information about potentially hazardous or toxic materials or processes. Further, the plant must work with the local community to develop effective emergency procedures that will be implemented automatically in the event of an accident. A local emergency planning committee is formed of members of the local government, emergency response organizations, and plant personnel. Also, releases of certain hazardous substances must be reported to the EPA and a compilation of these releases made available to the public through the Toxic Release Inventory System.

The EPA provides querying and mapping functions for its databases through the EPA Envirofacts System at http://www.epa.gov/enviro/facts/qmr.html. Included are the Toxic Release Inventory and databases on Superfund sites, drinking water, water discharge, hazardous waste, UV index, and air releases.

Through the DOT, regulations require all over-the-road transport vehicles to carry a manifest of hazardous materials that is immediately available to all emergency personnel in the event of an accident. Also, the DOT and the U.S. Coast Guard regulate the conditions under which hazardous cargo can be transported. For example, these regulations frequently require stabilizing additives to

prevent runaway polymerization.

The National Response Center (1-800-424-8802) is operated by the U.S. Coast Guard "to serve as the sole national point of contact for reporting all oil, chemical, radiological, biological, and etiological discharges into the environment anywhere in the United States and its territories." When a call is received, the information is relayed to the National Response Team as well as to various government agencies that maintain incident databases.

Many other EPA regulations that are beyond the scope of this book impact the operation of chemical processing facilities, including the Resource Conservation and Recovery Act (RCRA); the Comprehensive Environmental Response, Compensation, and Liability Act known as Superfund (CERCLA); the Superfund Amendments and Reauthorization Act (SARA); and the Toxic Substances Control Act (TSCA).

EPA Risk Management Program. The Clean Air Act Amendments of 1990 also "require the owner or operator of stationary sources at which a regulated substance is present to prepare and implement a Risk Management Plan (RMP) and provide emergency response in order to protect human health and the environment" [40 CFR 68]. The final rule was implemented in 1999. As with the OSHA Act, there is a general duty clause in this regulation specifying that owners and operators of plants have "a general duty . . . to identify hazards which may result from such releases using appropriate hazard assessment techniques, to design and maintain a safe facility taking such steps as necessary to prevent releases, and to minimize the consequences of accidental releases which do occur" [Reference 7, Section 112(r)(1)]. The RMPs must be registered with the EPA, they must be made public, and they must be periodically updated. The risk management program, which includes as a subset the risk management plan, must include three elements:

- Hazard assessment
- Prevention
- Emergency response

This program is coordinated with OSHA's process safety management (PSM). In fact, compliance with the PSM standard is considered equivalent to the prevention part of the RMP. The following overview of the risk management program pertains to all plants covered under the PSM standard, which includes most plants in the chemical process industries.

The **hazard assessment** must include a worst-case analysis, an analysis of non-worst-case accidental releases, and a five-year accident history. The **worst-case release scenario** is defined by the EPA [40 CFR 68] as

> *the release of the largest quantity of a regulated substance from a vessel or process line failure, including administrative controls and passive mitigation that limit the total quantity involved or the release rate. For most gases, the worst-case release scenario assumes that the quantity is released in 10 minutes. For liquids, the scenario assumes an instantaneous spill; the release rate to the air is the volatilization rate from a pool 1 cm deep unless passive mitigation systems contain the substance in a smaller area. For flammables, the worst case assumes an instantaneous release and a vapor cloud explosion.*

The EPA rule specifies default values of wind speed, atmospheric stability class, and other parameters for the development of the offsite consequence analysis of worst-case scenarios. It also

specifies the end point for the consequence analysis, based on the calculated concentration of toxic materials, the overpressure (1 psi) from vapor cloud explosions, and the radiant heat exposure for flammable releases (5 kW/m^2 for 40 seconds).

The prevention program is identical to the PSM standard, except that the emergency planning and response item is covered under a separate category in the RMP.

The emergency response program portion of the risk management plan is coordinated with other federal regulations. For example, compliance with the OSHA Hazardous Waste and Emergency Operations (HAZWOPER) rule (29 CFR 1910.120), the emergency planning and response portion of the PSM standard, and EPCRA will satisfy this requirement in the RMP regulation.

The RMP must designate a qualified person or position with overall responsibility for the program, as well as show the lines of authority or responsibility for implementation of the plan.

Overall, then, the only additional RMP requirement for plants already covered by the OSHA process safety management regulation is the hazard assessment (including offsite consequence analyses of worst-case and non-worst-case accidental release scenarios). This hazard assessment must not be confused with the process hazard analysis (PHA). The hazard assessment is a study of what will happen in the event of an accidental release and usually includes, for example, air dispersion simulations. The PHA (e.g., HAZOP) studies the hazards present in the process and seeks to minimize them through redesign or modifications to operating procedures.

26.2.3. Nongovernmental Organizations

Many professional societies and industry associations develop voluntary standards, and these are often accepted by government agencies and thereby are given the force of law. Examples of such organizations and their standards are as follows:

- American Petroleum Institute (API), Recommended Practices 750
- American Institute of Chemical Engineers (AIChE)
  - Center for Chemical Process Safety (CCPS)
  - Design Institute for Emergency Relief Systems (DIERS)
- American National Standards Institute (ANSI)
- American Society for Testing and Materials (ASTM)
- National Fire Protection Association (NFPA), fire diamond
- American Conference of Governmental Industrial Hygienists (ACGIH), TLVs
- American Chemistry Council, Responsible Care program
- Synthetic Organic Chemicals Manufacturers Association (SOCMA)
- American Society of Mechanical Engineers (ASME), boiler and pressure vessel code

The Responsible Care program is a chemical industry initiative started in 1988. All the members of the American Chemistry Council (about 160 companies) as well as several other industry organizations in the United States and in 50 other countries agree to operate according to this health, safey, and environment code. The details are given on the ACC Web site (http://www.americanchemistry.com). Its key areas include

1. Environmental impact
2. Employee, product, and process safety

3. Energy
4. Chemical industry security
5. Product stewardship: managing product safety and public communications
6. Accountability through management system certification
7. Contribution to the economy

26.3. Fires and Explosions

The most common hazards on many chemical plant sites are fires and explosions. Whenever a fuel, an oxidizer, and an ignition source are present, such a hazard exists. Detailed analyses of these hazards and their consequences are covered in other books [1, 8]. Here, the terminology of the field is introduced.

26.3.1. Terminology

Combustion is the very rapid oxidation of a fuel. Most fuels oxidize slowly at room temperature. As a fuel is heated, it oxidizes more rapidly. If the heating source is removed, the fuel cools, and its oxidation returns to its normal rate for room temperature.

However, if a certain temperature (the **auto-ignition temperature**) is exceeded, the heat liberated by the oxidation is sufficient to sustain the temperature, even if the external heating source is removed. Thus, above the auto-ignition temperature, the reaction zone will expand into other areas having appropriate mixtures of fuel and oxygen. The minimum energy required to heat a small region to the auto-ignition temperature is called the **ignition energy** and is often exceedingly small.

A gaseous mixture of fuel and air will ignite only if it is within certain concentration limits. The **lower flammability** (or **explosive**) **limit** (LFL or LEL) is the minimum concentration of fuel that will support combustion and is somewhat below the stoichiometric concentration. The maximum concentration of fuel that will support combustion is called the **upper flammability** (or **explosive**) **limit** (UFL or UEL). Above the UFL, the mixture is too "rich"—that is, it does not contain enough oxygen. These two limits (UFL and LFL) straddle the stoichiometric concentration for complete combustion of the fuel. It is because of the convenient upper flammability limit of gasoline that this fuel is not more dangerous than it is. (See Problem 26.8.) Any mixture within the flammability limits should be avoided or very carefully controlled.

The **flash point** of a liquid is the temperature at which the vapor in equilibrium with the standard atmosphere above a pool of the liquid is at the LFL. Thus, a low flash point indicates a potential flammability problem if the liquid is spilled. Diesel fuel, for example, is much safer than is gasoline because diesel has a higher flash point. Regulations for transportation and use of gasoline are therefore much more stringent than they are for diesel. Flash point can be measured by the open-cup or the closed-cup method. In the **open-cup** method, an open container of the liquid is heated while a flare-up of the vapor is intentionally attempted with an ignition source. The temperature at which flare-up occurs is the flash point. In the **closed-cup** method, the liquid is placed in a closed container and allowed to come to equilibrium with air at standard pressure. Ignition is attempted at increasing temperatures. Although the open-cup and closed-cup flash points for many materials are very close, materials that vaporize slowly and disperse in the atmosphere quickly can have much higher open-cup flash points than their closed-cup flash points. Although the MSDS will give the flash point, one must notice which type of flash point is being reported.

Explosions are very rapid combustions in which the pressure waves formed propagate the combustion. The combustion creates a local pressure increase, which heats the flammable mixture to its auto-ignition temperature. This secondary combustion causes the pressure wave to propagate through the mixture. This traveling pressure pulse is called a **shock wave**. Often, a strong wind accompanies the shock wave. The combination of shock wave and wind, called a **blast wave**, causes much of the damage from explosions. When the shock wave speed is less than the speed of sound in the ambient atmosphere, the explosion is called a **deflagration**. When the speed is greater than the speed of sound, the explosion is called a **detonation**. Detonations can cause considerably more damage from the combination of blast wave, overpressure, and concussion. The damage from an overpressure of only 1 psi on structures can be extensive. Such a pressure differential on a typical door, for example, would result in considerably more than one ton of pressure on the door—enough to break most locks.

Of special concern when flammable gaseous mixtures (or dispersions of combustible dusts in air) are present is the so-called **vapor cloud explosion (VCE)**. If there is a natural gas leak, for example, the cloud (mostly methane) will spread and mix with air. The cloud, parts of which are within the flammable limits, can be quite large. If it ignites, the deflagration will cause a shock wave perpendicular to the ground that can cause great damage, often flattening buildings. When a liquid stored above its ambient boiling point suddenly comes in contact with the atmosphere (through a rupture in the tank, for example), the rapid release and expansion of the vapor can cause a massive shock wave. This phenomenon is called a **boiling-liquid expanding-vapor explosion (BLEVE)**. The failure of a steam drum, for example, can cause a BLEVE. When the BLEVE is of a flammable substance, the resulting cloud can explode. This combination of BLEVE and VCE is one of the most destructive forces in chemical plant accidents. The classic example is a propane tank that ruptures when it becomes overheated in a normal fire (a BLEVE). The propane is stored as a liquid under pressure. As the tremendous quantity of propane that vaporizes mixes rapidly with the atmosphere, it creates a massive VCE.

Runaway reactions are confined, exothermic reactions that go from their normal operating temperatures to greater than the ignition temperature; that is, they liberate more heat than can be dissipated. Thus, the temperature increases, increasing the reaction rate. Although there may be a steady state at a higher temperature (as there is in combustion), often the limits of mechanical integrity of the reaction vessel are reached before that point, causing catastrophic failure of the vessel. Such a failure can cause direct injuries, release toxic material, cause a fire, or lead to a BLEVE and/or a VCE.

To reduce the chance of a runaway condition during process upsets, the temperature difference between the reacting mixture and the cooling medium should be kept small. This may seem counterintuitive. However, consider a case where the temperature driving force is 1°C. If the temperature of the reacting mixture increases by 1°C during a process upset, the driving force for cooling has doubled! If the heat-exchange system had been designed for a 10°C driving force, that same upset would result in only a 10% increase in cooling. In systems with a chance of runaway, increased heat transfer area is the cost of an inherently safer system.

A common scenario for an accident involving an exothermic reaction is the **loss of coolant accident (LOCA)**. Unless the cooling system is backed up to the extent that it is essentially 100% reliable, one must consider this scenario in designing the vessels and the pressure-relief systems.

26.3.2. Pressure-Relief Systems

During a severe process upset, the pressure and/or temperature limits of integrity for vessels can be approached. To avoid an uncontrolled, catastrophic release of the contents or the destruction of the vessel, **pressure-relief systems** are installed. Usually, these are relief valves on vessels or process lines that open automatically at a certain pressure. Downstream, they are connected to **flares** (for flammable or toxic materials), **scrubbers** (for toxic materials), or a **stack** directed away from workers (for materials such as steam that present physical hazards). The design of the pressure-relief system is especially important, because the worst-case scenario must be considered, which is sometimes the simultaneous failure of multiple relief systems, as was the case for the Bhopal tragedy in 1984.

The design of such systems is complicated by several factors. The devices are designed to operate under unsteady conditions. Therefore, a dynamic simulation is required. Also, the flow through the relief system may be single-phase or two-phase flow. For two-phase flow, not only are the calculations more difficult, but also more factors affect the pressure drop, such as whether the line is horizontal or vertical.

In addition to the relief valves (which are called **safety valves**, **relief valves**, **pressure-relief valves**, or **pop valves** depending on service), rupture disks are used to open the process to the discharge system. **Rupture disks** are specially manufactured disks that are installed in a line, similar to the metal blanks used between flanges to close a line permanently. However, the disks are designed to fail rapidly at a set pressure. Ideally, the rupture disk allows no flow when the pressure is less than the set pressure, and it ruptures immediately, offering no resistance to flow, when the pressure hits the set point.

26.4. Process Hazard Analysis

Under the "Process Hazard Analysis" requirement of the Process Safety Management of Highly Hazardous Chemicals regulation (29 CFR 1910.119), employers must complete such an analysis of all covered processes using one or more of the following techniques:

- What-If
- Checklist
- What-If/checklist
- Failure mode and effects analysis (FMEA)
- Fault-tree analysis (FTA)
- Hazards and operability study (HAZOP)

or "an appropriate equivalent methodology." The OSHA regulation specifically refers to the AIChE Center for Chemical Process Safety for details of process hazard analysis methods [9], which is an excellent source for details of these techniques.

The **what-if** technique involves a group of engineers and others going through the flowsheet and operating procedures methodically and considering what would happen if something were not as expected. For example, What if the reactor were not at the specified temperature? The answers to these hypothetical situations can uncover potential problems. This process hazard analysis technique is normally used only for simple, small-scale processes, such as laboratory experiments. For more complicated processes, the more rigorous HAZOP technique is used. This technique, which is

described in the next section, is a formalized version of what-if.

Checklists have been developed by various companies for their specific processes. These lists can include hundreds of items [1, 9]. Checklists are very specific and focused; they do not typically lead to the identification of safety problems that have never been encountered. Therefore, checklists (which are focused on areas of known concern) are often used in combination with what-if techniques (which are focused on thinking "outside the box").

The **FMEA** was invented by NASA in the 1960s. The underlying principle is that failures of individual components cannot be avoided, but these component failures must not cause a catastrophic failure of the system. Therefore, the analysis begins by identifying the various ways that each individual component can fail (a failure mode). Then the effect of these failures (individually and in combination) is studied. FMEA is thus a bottom-up approach that leads to identification of critical combinations of component failures that can cause some catastrophic failure. The result is usually an attempt to improve the reliability of specific components or to design protective redundancy into the system. In principle, FMEA requires the prediction and consideration of all failure modes of all components—a very large task for a complex system.

FTA is based on the premise that many of the component failure modes that would be studied in the FMEA technique would not contribute to any system failure. FTA is a top-down analysis of the system failures. First, the catastrophic system failures to be avoided are identified. Then contributing failures of subsystems and individual components are considered. FTA is widely used in the nuclear power industry, where catastrophic system failures are clearly defined.

In both the FTA and FMEA analyses, large logic diagrams are created to show the connections between low-level failures and higher-level failures. If a combination of failures is required to create a higher-level failure, the connection is denoted as an **AND gate**. If any one of several failures can create a high-level failure, the connection is denoted as an **OR gate**. There can be many levels of failures, dozens of systems failures, and several failure modes for each of thousands of components. This logic diagram leads directly to the probability of system failure if the reliability of the individual components is known.

26.4.1. HAZOP

The most widely used process hazards analysis technique in the chemical process industries is HAZOP. Unlike FTA and FMEA, the **HAZOP** technique is an outside-the-box technique. It is a modified brainstorming technique for identifying and resolving process hazards by considering seemingly unusual occurrences. Although it is a bottom-up technique, it is more efficient than the FMEA because it involves early dismissal of component failure modes that are of no consequence to system operation and focuses early on the more probable failure scenarios. A HAZOP is especially useful in identifying human factors that can contribute to system failures. For example, a HAZOP based on a sabotage scenario could consider failure modes not apt to be uncovered by the FMEA.

HAZOP consists of asking questions about possible deviations that could occur in the process (or part of a process) under consideration. A HAZOP is always done in a group, and the regulation requires that the team have "expertise in engineering and process operations," have "experience and knowledge specific to the process being evaluated," and be "knowledgeable" about the HAZOP methodology. As with any brainstorming process, the ideas and suggestions can come very quickly, and there must be an identified **scribe** ready with appropriate software to capture them. Various

software packages are available to speed this process and to offer additional triggers in the brainstorming process.

The first step in a HAZOP is to identify the normal operating condition or purpose of the process or unit. This is called the **intention**. Next, a **guide word** is used to identify a possible **deviation** in the process. For example, the intention may be to keep the temperature in a vessel constant. The guide words are

- None, no, *or* not
- More of
- Less of
- More than *or* As well as
- Part of
- Reverse
- Other than

In the example here, there may be no coolant flow. Once such a possible deviation is identified, the team notes any possible *causes* of the deviation. If there are any safety *consequences* of the deviation, those are noted. Suppose the coolant flow ceased because of a pump failure. The consequence may be a runaway reaction. The *action* to be taken is assigned by the HAZOP team. In this case, the action might be assigning the process engineer to investigate a backup pumping system. The team then goes on to the next possible deviation, until all reasonable deviations have been considered. The team does not solve the safety problem during the HAZOP; its job is to identify the problem and to assign its resolution to a specific person. An example of part of a HAZOP for the feed heater (H-101) of the hydrodealkylation of toluene process (Figure 1.5) is shown in Table 26.5. Several features of a HAZOP are shown. Several of the items are dismissed for "no probable cause." Others are redundant. A few are outside-the-box deviations that could lead to important safeguards for rare events. Also, the result of the HAZOP is a list of action items. These action items are not themselves decisions to change the process. They are decisions to study potential changes.

Table 26.5. HAZOP for the Feed Heater of the Hydrodealkylation (HDA) Process

Process Unit: H-101, Feed Heater, Figure 1.3

Intention: To provide feed to the reactor (Stream 6) at 600°C

Guide Word	Deviation	Cause	Consequence	Action
No	No flow (Stream 4)	Blockage in line	Fluid in H-101 overheats	Consider an interlock on fuel gas flow.
⇓	No O_2 in combustion products	Rich fuel:air mixture	Unburned fuel and CO in combustion products	None. O_2 analyzer with self-checking circuit controls ratio reliably.
⇓	⇓	O_2 analyzer malfunction	Potentially rich fuel:air mixture	⇓
⇓	No flow (Stream 6)	Heat tubes burst	Explosion	Interlock with sudden pressure drop alarm and shutdown.
⇓	No benzene in Stream 6	C-101 not working	Hydrogen:toluene ratio off to R-101 and loss of hydrogen to fuel gas	Maintain spare compressor C-101.
⇓	No fuel gas flow	Supply pipe rupture	Cold shot to R-101, quenching reaction	Interlock with process shutdown.
⇓	No flame	Momentary loss of fuel gas	Explosive mixture	Automatic flame detection with reignition cycle.
More of	More flow in Stream 4	Surge of C-101	Unstable operation	Alarm.
⇓	Higher temperature	Sudden reduction in Stream 6 flowrate	Reactor overheats	Consider an interlock on fuel gas flow.
⇓	Higher pressure	Dowstream blockage	Tube failure	Pressure-relief system on tubes.
⇓	Higher temperature in heater	Increased temperature of Stream 4	Flame becomes erratic	Robust demister design.
⇓	⇓	Loss of furnace control	Higher temperature in Stream 6	Interlock on furnace controls.
⇓	Higher concentration of O_2 in exhaust	Lean fuel:air ratio	Waste of fuel	
⇓	⇓	No flame	Explosive mixture	Automatic flame detection with reignition cycle.
Less of	Lower temperature	Flameout	Cold shot to R-101, quenching reaction	Include automatic flame detection with reignition cycle.
⇓	Less flow in Stream 6 than in Stream 4	Heat tubes burst	Explosion	Interlock with differential flow alarm and shutdown.
⇓	Less pressure in tubes	Burst pipe downstream	Explosive and toxic release	Alarm on low pressure or low flow.
⇓	Fuel gas flow	Process upset	Cold shot to R-101	Automatic supervisory control of plant.
⇓	Less atmospheric pressure	Storm	No consequence	
⇓	⇓	Tornado	Destruction of plant	Monitor severe weather.
As well as	Liquid drops in fuel gas	Failure of V-101 demister	Flame becomes erratic	Robust demister design.

⇓	⇓	Failure of V-103 demister	⇓	⇓
⇓	Water in fuel gas	No probable cause		
⇓	Benzene in fuel gas	Unlike overflow of V-102		
Part of	Low toluene in Stream 6	P-101 not working	No reaction in R-101	Install low-flow alarm on Stream 2.
⇓	Low benzene in Stream 6	C-101 not working	Hydrogen:toluene ratio off to R-101 and loss of hydrogen to fuel gas	Maintain spare compressor C-101.
Reverse	Decrease in Stream 6 temperature through H-101	No probable cause		
⇓	Reversal of flow (from Stream 6 to 4)	No probable cause		
Other than	Impurities in Stream 6	Impurities in feed or overheating in tubes	Impurities in product and/or catalyst deactivation	Monitor concentrations and H-101 temperatures.
⇓	Toluene in Stream 4 replaced by other hydrocarbon	Wrong connection to TK-101 by sabotage	Explosion and loss of product	Redundant management controls on storage facilities.
⇓	Fuel gas replaced by liquid fuel	Wrong connection during plant modification	Explosion	Better management of change procedures.

The OSHA process safety management regulation requires that the actions assigned be taken in a timely manner and that all process hazard analyses be updated at least every five years.

26.4.2. Dow Fire & Explosion Index and Chemical Exposure Index

The Dow Fire & Explosion Index was developed by Dow Chemical in the 1960s and is today used by many companies to identify high-risk systems. It is a form of process hazards analysis that focuses on fires or explosions, but it also goes beyond the identification of these hazards to quantifying the probable loss from a resulting fire or explosion.

The format of this index is similar in many ways to an income tax form, as seen in Figures 26.1 and 26.2, which are for a fictitious reactor in a polymer plant (provided by Dow Chemical, Inc., May 1998, at a workshop for faculty). The details of these procedures are given in the official guide, available from AIChE [10].

FIRE & EXPLOSION INDEX

AREA/COUNTRY	DIVISION	LOCATION	DATE
North America	North Central	Your State	05/18/98

SITE	MANUFACTURING UNIT	PROCESS UNIT
No Loss	My Polymer	Reactor

PREPARED BY:	APPROVED BY: (Superintendent)	BUILDING
Pat Smith	Robin Doe	A-103

REVIEWED BY: (Management)	REVIEWED BY: (Technology Center)	REVIEWED BY: (Safety & Loss Prevention)
Jo Big	Chris Wright	Lee Safe

MATERIALS IN PROCESS UNIT
Cyclohexane, Isopentane, DFI, Isoprene, Strene, Butadiene, IPA, Phosphoric Acid

STATE OF OPERATION	BASIC MATERIAL(S) FOR MATERIAL FACTOR
___DESIGN ___STARTUP _X_NORMAL OPERATION ___SHUTDOWN	Butadiene

Material Factor (See Table 1 or Appendices A or B) Note requirements when unit temperature over 140°F (60°C)			24
1. General Process Hazards		**Penalty Factor Range**	**Penalty Factor Used(1)**
Base Factor		1.00	1.00
A. Exothermic Chemical Reactions		0.30 to 1.25	0.50
B. Endothermic processes		0.20 to 0.40	
C. Material Handling and Transfer		0.25 to 1.05	
D. Enclosed or Indoor Process Units		0.25 to 0.90	
E. Access		0.20 to 0.35	
F. Drainage and Spill Control	_____ gal or cu.m.	0.25 to 0.50	0.25
General Process Hazards Factor (F_1)			1.75
2. Special Process Hazards			
Base Factor		1.00	1.00
A. Toxic Material(s)	$N_H = 2$	0.20 to 0.80	0.40
B. Sub-Atmospheric Pressure (<500 mm Hg)		0.50	
C. Operation In or Near Flammable Range	___ Inerted ___ Not Inerted		
1. Tank Farms Storage Flammable Liquids		0.50	
2. Process Upset or Purge Failure		0.30	0.30
3. Always in Flammable Range		0.80	
D. Dust Explosion (See Table 3)		0.25 to 2.00	
E. Pressure (See Figure 2)	Operating Pressure 15 psig ~~or kPa gauge~~ Relief Setting 90 psig ~~or kPa gauge~~		0.06
F. Low Temperature		0.20 to 0.30	
G. Quantity of Flammable/Unstable Material:	Quantity 59.6K lb ~~or kg~~ H_c = 19.0K BTU/lb ~~or kcal/kg~~		
1. Liquids or Gases in Process (See Figure 3)	1.132 x 10^9 BTU		1.56
2. Liquids or Gases in Storage (See Figure 4)			
3. Combustible Solids in Storage, Dust in Process (See Figure 5)			
H. Corrosion and Erosion		0.10 to 0.75	0.10
I. Leakage--Joints and Packing		0.10 to 1.50	0.10
J. Use of Fired Equipment (See Figure 6)			
K. Hot Oil Heat Exchange System (See Table 5)		0.15 to 1.15	
L. Rotating Equipment		0.50	0.50
Special Process Hazards Factor (F_2)			4.02
Process Unit Hazards Factor (F_1 x F_2) = F_3			7.04
Fire and Explosion Index (F_3 x MF = F&EI)			169

(1) For no penalty use 0.00.

Figure 26.1. Dow Fire & Explosion Index (Form reproduced with permission of the American Institute of Chemical Engineers. Copyright © 1994 AIChE. All rights reserved. Example used by permission of SACHE (www.aiche.org/sache), a component of the Center for Chemical Process Safety providing instructional materials to member chemical engineering departments throughout the world.)

LOSS CONTROL CREDIT FACTORS

1. Process Control Credit Factor (C_1)

Feature	Credit Factor Range	Credit Factor Used(2)	Feature	Credit Factor Range	Credit Factor Used(2)
a. Emergency Power	0.98	0.98	f. Inert Gas	0.94 to 0.96	0.96
b. Cooling	0.97 to 0.99	0.97	g. Operating Instructions/Procedures	0.91 to 0.99	0.91
c. Explosion Control	0.84 to 0.98	1.00	h. Reactive Chemical Review	0.91 to 0.98	1.00
d. Emergency Shutdown	0.96 to 0.99	0.96	I. Other Process Hazard Analysis	0.91 to 0.98	0.94
e. Computer Control	0.93 to 0.99	0.93			

C_1 Value(3) **0.70**

2. Material Isolation Credit Factor (C_2)

Feature	Credit Factor Range	Credit Factor Used(2)	Feature	Credit Factor Range	Credit Factor Used(2)
a. Remote Control Valves	0.96 to 0.98	0.96	c. Drainage	0.91 to 0.97	0.91
b. Dump/Blowdown	0.96 to 0.98	1.00	d. Interlock	0.98	0.98

C_2 Value(3) **0.86**

3. Fire Protection Credit Factor (C_3)

Feature	Credit Factor Range	Credit Factor Used(2)	Feature	Credit Factor Range	Credit Factor Used(2)
a. Leak Detection	0.94 to 0.98	0.94	f. Water Curtains	0.97 to 0.98	1.00
b. Structural Steel	0.95 to 0.98	1.00	g. Foam	0.92 to 0.97	1.00
c. Fire Water Supply	0.94 to 0.97	0.94	h. Hand Extinguishers/Monitors	0.93 to 0.98	1.00
d. Special Systems	0.91	1.00	I. Cable Protection	0.94 to 0.98	1.00
e. Sprinkler Systems	0.74 to 0.97	0.97			

C_3 Value(3) **0.86**

Loss Control Credit Factor = C_1 x C_2 xC_3(3) = **0.51** (Enter on line 7 below)

PROCESS UNIT RISK ANALYSIS SUMMARY

1. Fire & Explosion Index (F&EI) (See Front)	169		
2. Radius of Exposure (Fig. 7)	142	ft ~~or m~~	
3. Area of Exposure	63,192	ft^2 ~~or m^2~~	
4. Value of Area of Exposure		$MM	5.00
5. Damage Factor (Fig. 8)	0.88		
6. Base Maximum Probable Property Damage -- (Base MPPD [4 x 5]		$MM	4.38
7. Loss Control Credit Factor (See Above)	0.51		
8. Actual Maximum Probable Property Damage -- (Actual MPPD) [6 x 7]		$MM	2.24
9. Maximum Probable Days Outage (MPDO) (Fig. 9)	30	days	
10.Business Interruption -- (BI)		$MM	4.74

(2) For no credit factor enter 1.00. (3) Product of all factors used.

Refer to *Fire & Explosion Index Hazard Classification Guide* for details.

Figure 26.2. Loss Control Credit Factors (Form reproduced with permission of the American Institute of Chemical Engineers. Copyright © 1994 AIChE. All rights reserved. Example used by permission of SACHE (www.aiche.org/sache), a component of the Center for Chemical Process Safety providing instructional materials to member chemical engineering departments throughout the world.)

First, a specific process unit is selected. The components in the unit have the greatest impact on the hazard, so a "material factor" is determined. This factor is a measure of the energy released during a fire or explosion involving a specific material and varies from 1 (e.g., for sulfur dioxide) to 40 (e.g., for nitromethane). Material factors for 328 materials (substances or defined mixtures) are given in the

official guide, as well as procedures for determining the factor for any other material based on flammability and reactivity. In the case of the hypothetical example, the reactor contains several materials, but the material factor for butadiene is the highest, so it is used as the base.

Various corrections are made for type of reaction, facility, and materials handling to arrive at a **general process hazards factor**. In the case of Figure 26.1, there is a polymerization (exothermic) penalty, and there is a **drainage and spill control** penalty because there is only a 20-minute supply of fire water available.

Then a **special process hazards** factor is calculated based on extreme process conditions, storage of large quantities of hazardous materials, corrosion and erosion, fired equipment, and so on. In the example, there is a toxic penalty of 0.4 for butadiene. The operation is nitrogen padded but operates in the flammable range, so a penalty of 0.3 applies. There is a 0.06 penalty based on high-pressure operation with the specified relief setting. The flammable material penalty is based on the total heat of combustion for all materials in the unit (not only the butadiene). Corrosion has been estimated at less than 0.127 mm/y, and minor leakage at pumps occurs, which lead to the respective penalties. There is an agitator, which accounts for the rotating equipment penalty.

From these three hazards indicators (materials factor, general process hazards factor, and special process hazards factor), the Fire & Explosion Index (F&EI) is calculated, 169 in the example. Table 26.6 shows the qualitative level of hazard for various values of the F&EI. This example is in the "severe" hazard class. Although the F&EI is useful in identifying process units where hazardous conditions exist, it does not estimate the damage that might result from such an event.

Table 26.6. Dow Fire & Explosion Index [10]

Fire & Explosion Index	Qualitative Hazard Level
1–60	Light
61–96	Moderate
97–127	Intermediate
128–158	Heavy
159–	Severe

The second part of the analysis (Figure 26.2) involves estimating the probable damage if the hazard leads to a catastrophic event. The damage from a fire or explosion depends on the area affected by the event, the value of the equipment destroyed, and the loss of production while the equipment damage is being repaired. All three of these are estimated by detailed algorithms described in the guide. Three categories of mitigating factors are considered: process control, material isolation, and fire protection. Typical values are used in the example. These allow the calculation of a **loss control credit factor**, which is used to correct the damage estimates.

The final part of the analysis (bottom of Figure 26.2) is the calculation of probable loss of property and loss of business if a fire or explosion were to occur. The area likely to be damaged is estimated from the F&EI. The value of the equipment in this area ($5 million in the example) is used to estimate the likely property loss, which is a function of loss control credits. The business interruption loss is estimated based on (1) probable days of outage and (2) annual fixed costs plus before-tax profit.

The Dow Chemical Hazards Index is a somewhat similar index that provides an estimate of the hazard from accidental atmospheric release of toxic substances. A central factor in this analysis is the

CEI, which is proportional to the square root of the ratio (toxic release flowrate):(threshold limit value). The details are available in the official guide [11].

A Dow "risk analysis package" consists of the analyses developed with the Dow F&EI and the Dow Chemical Exposure Index plus reports of loss prevention measures. This risk analysis package is used by industrial insurance carriers to predict the likelihood and size of loss from catastrophic events.

26.5. Chemical Safety and Hazard Investigation Board

The Clear Air Act Amendments of 1990 (Reference 7, Section 112[r][6]) created the Chemical Safety and Hazard Investigation Board to "investigate, determine and report to the public in writing the fact, conditions and circumstances and the cause or probable cause of any accidental release resulting in fatality, serious injury or substantial property damages." The board is an independent scientific investigatory agency with no regulatory or enforcement duties. This board investigates chemical accidents, but it does not investigate all such accidents. Investigations are prioritized according to the likelihood that they would reduce further such accidents, either through enhanced knowledge of the causes or through stimulating a regulatory agency to consider further actions. Although the board was authorized in 1990, it was not funded until 1998. Since that time, it has produced numerous investigation reports, which are available on its Web site (http://www.csb.gov).

As with other governmental safety and accident investigation boards, the Chemical Safety and Hazard Investigation Board seeks to determine root causes of accidents, with a focus on avoiding future accidents and not on assigning blame.

26.6. Inherently Safe Design

Although safety controls can be added to existing processes, a more effective and efficient strategy is called **inherently safe design** [12]. The idea is to streamline the process to eliminate hazards, even if there is a major process upset. This strategy is based on a hierarchy of six approaches to process plant safety:

1. **Substitution:** One avoids using or producing hazardous materials on the plant site. If the hazardous material is an intermediate product, for example, alternative chemical reaction pathways might be used. In other words, the most inherently safe strategy is to avoid the use of hazardous materials.
2. **Intensification:** One attempts to use less of the hazardous materials. In terms of a hazardous intermediate, the two processes could be more closely coupled, reducing or eliminating the inventory of the intermediate. The inventories of hazardous feeds or products can be reduced by enhanced scheduling techniques such as **just-in-time (JIT)** manufacturing [13].
3. **Attenuation:** Reducing, or attenuating, the hazards of materials can often be effected by lowering the temperature or adding stabilizing additives. Any attempt to use materials under less hazardous conditions inherently reduces the potential consequences of a leak.
4. **Containment:** If the hazardous materials cannot be eliminated, they at least should be stored in vessels with mechanical integrity beyond any reasonably expected temperature or pressure excursion. This is an old but effective strategy to avoid leaks. However, it is not as inherently safe as substitution, intensification, or attenuation.
5. **Control:** If a leak of hazardous material does occur, there should be safety systems that reduce

the effects. For example, chemical facilities often have emergency isolation of the site from the normal storm sewers, and large tanks for flammable liquids are surrounded by dikes that prevent any leaks from spreading to other areas of the plant. Scrubbing systems and relief systems in general are in this category. They are essential, because they allow a controlled, safe release of hazardous materials, rather than an uncontrolled, catastrophic release from a vessel rupture.

6. **Survival:** If leaks of hazardous materials do occur and they are not contained or controlled, the personnel (and the equipment) must be protected. This lowest level of the hierarchy includes firefighting, gas masks, and so on. Although essential to the total safety of the plant, the greater the reliance on survival of leaks rather than elimination of leaks, the less inherently safe the facility.

26.7. Summary

This chapter described the overall framework of health, safety, and environmental activities in the chemical process industries. The specific regulations change constantly, and the cognizant agencies must be consulted for the current rules.

26.8. Glossary

ACC: American Chemistry Council

ACGIH: American Congress of Governmental Industrial Hygienists

AIChE: American Institute of Chemical Engineers

ANSI: American National Standards Institute

API: American Petroleum Institute

ASME: American Society of Mechanical Engineers

ASTM: American Society for Testing and Materials

BLEVE: boiling-liquid expanding-vapor explosion

CAA: Clean Air Act

CCPS: Center for Chemical Process Safety

CERCLA: Comprehensive Environmental Response, Compensation, and Liability Act

CFR: *Code of Federal Regulations*

CMA: Chemical Manufacturers' Association; former name of the American Chemistry Council

DIERS: Design Institute for Emergency Relief Systems

DOT: Department of Transportation

EIS: environmental impact study (or statement)

EPA: Environmental Protection Agency

EPCRA: Emergency Planning and Community Right to Know Act, also known as SARA, Title III

F&EI: Dow Fire & Explosion Index

FAR: fatal accident rate

FMEA: failure modes and effects analysis
FR: *Federal Register*
FTA: fault-tree analysis
HAP: hazardous air pollutant
HAZOP: hazard and operability study
IDLH: immediately dangerous to life and health
LEL: lower explosive limit
LFL: lower flammability limit
LOCA: loss of coolant accident
MSDS: material safety data sheet
MSHA: Mine Safety and Health Agency
NAAQS: National Ambient Air Quality Standards
NESHAP: National Emissions Standards for Hazardous Air Pollutants
NFPA: National Fire Protection Association
NIOSH: National Institute for Occupational Health
NIOSHTIC: NIOSH Technical Information Center
NSPS: New Source Performance Standards
OSHA: Occupational Safety and Health Agency
PEL: permissible exposure limit
PHA: process hazard analysis
PSM: process safety management
RCRA: Resource Conservation and Recovery Act
REL: recommended exposure limit
RMP: risk management program (or plan)
SARA: Superfund Amendments and Reauthorization Act
SOCMA: Synthetic Organic Chemical Manufacturers' Association
STEL: short-term exposure limit
TLV: threshold limit values
TSCA: Toxic Substances Control Act
TWA: time-weighted average
UEL: upper explosive limit
UFL: upper flammability limit
VCE: vapor cloud explosion
VOC: volatile organic compound

What You Should Have Learned

- There are numerous federal agencies regulating the chemical process industry.
- Process safety management involves numerous activities aimed at creating an environment that anticipates potential safety problems and corrects them before incidents occur.
- A HAZOP is a procedure by which potential process hazards are identified, and by which strategies to prevent incidents are built into the design.

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Problems

1. You work for a chemical company with 30,000 employees. If your company has a typical safety record for the chemical industry, what is your best estimate of how many of your employees
   a. Will succumb to a fatal accident while on the job this year?
   b. Will be injured but not killed on the job?

2. Locate the nearest steam plant on campus.
   a. Develop two possible accident scenarios that should be considered when searching for worst-case scenarios.
   b. List the safeguards that have been built into the system to mitigate some (or all) of these effects.
3. Find an MSDS for each of the components listed in the HDA process.
4. Summarize all regulations (safety, environmental, transportation) that you can find for benzene.
5. Assume that the unit operations lab in your department must meet the process safety management standard. Choose two of the 13 components of PSM, and write a critical analysis of these aspects of lab operation.
6. Some paints have a closed-cup flash point near room temperature, whereas they have no measurable open-cup flash point.
   a. Explain this apparent paradox.
   b. Which is the more useful flash point when using a paint?
7. Assume gasoline to be 87 vol% iso-octane (2,2,4 tri-methyl pentane) and 13 vol% n-heptane. At room temperature, the air above a pool of gasoline will become saturated.
   a. Is the air-gasoline mixture within its flammable limits?
   b. Could there be any location where the mixture will be within its flammable limits? Explain.
8. Perform a HAZOP on R-101 of the HDA process. Be sure to perform the analysis in a team.
9. Benzene in gasoline is now limited by regulation to a maximum of 0.62 vol%. Is the benzene concentration in the air above a pool of gasoline greater than or less than the PEL? Show the effect of temperature.
10. Calculate the Dow Fire & Explosion Index for the HDA Reactor 101. Compare this with the F&EI for tank TK-101.
11. Use the various resources from this chapter to find health, safety, and environmental information about a chemical process plant in your area.
12. Obtain an environmental impact study for a facility in your area. Prepare a synopsis and lead a class discussion.

Chapter 27. Green Engineering

What You Will Learn

- There are design processes that minimize pollution.

Green engineering can be defined as engineering for the environment. In terms of chemical engineering and chemical process design, green engineering means design for reduction of emissions, design to eliminate particularly hazardous chemicals, design to minimize the use of natural resources, and design to minimize energy usage.

Several books have been published on green engineering and pollution prevention [1, 2, 3]; therefore, only a summary of the bare essentials is possible in one chapter. The reader desiring a more in-depth treatment should consult these references.

In this chapter, environmental regulations, particularly the Pollution Prevention Act of 1990, are reviewed. Methods for understanding and estimating the behavior of chemicals in the environment are surveyed. Then the concept of green chemistry is defined and discussed briefly. Next, methods for pollution prevention at every stage of a design are discussed. The economics of pollution prevention are discussed. Finally, life cycle analysis, a study of the environmental consequences of manufacturing, using, and disposing of a product, is introduced.

There are several Web-based resources for pollution prevention and green engineering. The Environmental Protection Agency (EPA) Web site (http://www.epa.gov) is one, as is its green engineering program Web site (http://www.epa.gov/oppt/greenengineering).

27.1. Environmental Regulations

The Pollution Prevention Act of 1990 has one major requirement. Companies are required to report on their pollution prevention activities. It establishes a waste management hierarchy, which, from most to least desirable, is as follows:

1. **Source Reduction:** Source reduction means that the process is modified so that less waste and/or less-hazardous waste is generated. The best way to accomplish this is by modification of the chemistry in the reactor. If hazardous waste is not made, there is no chance of its becoming a pollutant.
2. **In-Process Recycle:** This is the recycle of unreacted feed so that it will not become a waste product. It has already been established several places in this book that this is also sound economic policy, because raw materials are almost always the largest operating cost in a chemical process. Therefore, in-process recycle, along with other pollution prevention concepts, has economic as well as environmental advantages.
3. **On-Site Recycle:** An example of on-site recycle is to convert waste generated in a reactor to a useful product in another reactor.
4. **Off-Site Recycle:** Off-site recycle is the separation of waste, the transfer of the waste off-site, followed by its conversion to a useful product at another facility. The definition of another facility may include a different part of the same chemical plant.
5. **Waste Treatment:** Waste treatment involves separation of waste generated in the process

followed by treatment to make it less hazardous.

6. **Secure Disposal:** Secure disposal involves separation of waste generated in the process followed by disposing of it in a secure facility such as a landfill.
7. **Release to Environment:** Here, waste generated in the process is separated and released to the environment.

Although items 1–6 could each be considered pollution prevention in its own way, the Pollution Prevention Act of 1990 defines only the first two as being pollution prevention. However, most engineers consider anything that converts waste into a useful product to be pollution prevention.

The hierarchy is clear. The top priority is not to produce waste or to minimize the production of waste, which is understood to be a difficult task. If waste products are made, they should be converted to useful products. If this cannot occur, they should be rendered less hazardous. Only as last resorts should there be disposal to a landfill (which could ultimately become a release to the environment) or direct release to the environment.

There are other laws regulating different aspects of the environment. As a whole, they are the lower bounds for environmental protection and human safety for the chemical industry. Many companies go beyond these minima (see, for example, "Responsible Care," in Section 26.2.3). Nine current, major laws are summarized in Table 27.1, and many of these laws have subsequent amendments. The text of all of these laws is available at http://www.epa.gov/lawsregs/laws/index.html.

Table 27.1. Summary of Environmental Laws

Law	Year	Summary
Occupational Safety and Health Act (OSH Act)	1970	Created OSHA; provides regulations protecting worker safety on the job; requires development of MSDS sheets, training of employees on safe handling of chemicals.
Clean Air Act (CAA)	1970	Establishes air quality standards for criteria pollutants; defines criteria pollutants as CO, Pb, NO_x, SO_2, ozone, and particulates.
Clean Water Act (CWA)	1972	Requires permits for all discharges; permit holders must monitor discharges.
Federal Insecticide, Fungicide, and Rodenticide Act (FIFRA)	1947 (amended 1972)	Requires that pesticides be registered with EPA. Manufacturer must prove product efficacy and that it is not harmful to humans.
Toxic Substances Control Act (TSCA)	1976	Chemical manufacturers must report processing information for all chemicals; premanufacturing notices required for all new chemicals.
Resource Conservation and Recovery Act (RCRA)	1976	Requires maintenance of records of hazardous waste generated and its ultimate fate; those transporting such waste also must maintain similar records.
Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA)	1980	Amended by the Superfund Amendments and Reauthorization Act (SARA) of 1986; defines "Superfund" sites; parties responsible for cleanup identified; assigns economic liability for cleanup; makes such liability retroactive.
Emergency Planning and Community Right to Know Act (EPCRA)	1986	Before this act, it was common for the community not to know what went on in a chemical plant; requires facilities to work with local agencies to develop plans for dealing with accidental release; also requires reporting of waste stored, transferred off-site, and released.
Pollution Prevention Act (PPA)	1990	Establishes pollution prevention hierarchy; only mandated provision is to report pollution prevention activities.

27.2. Environmental Fate of Chemicals

Methods have been developed to estimate the fate of chemicals if they have been released to the environment. This is done by defining properties of a molecule that are a measure of the molecule's behavior in the environment. These estimation techniques are based on group contribution methods used to estimate thermodynamic properties [4]. In group contribution methods, a physical property is estimated by breaking the molecule down into its component parts—for example, the number of carbons, the number of alcohol (or ether, ester, etc.) groups, and so on. There are correction factors quite often for branching, aromatic structure, and so on, and there are also methods based on counting the number and type of bonds. The physical property is estimated by adding the contributions of all component parts of the molecule. Most of the group contribution values have been obtained empirically by correlating measured values with a molecule's group structure. These methods are

beyond the scope of this textbook, and the interested reader can find more detailed descriptions elsewhere [1]. Software (EPIWIN Suite—downloadable at http://www.epa.gov/oppt/exposure/pubs/episuite.htm) has been developed that does the group contribution calculations for any molecule [1].

In pollution prevention, the properties calculated by group contribution methods are estimates of how a molecule behaves in the environment. These properties are best used for comparison between molecules. Table 27.2 lists selected properties that can be estimated using group contribution methods that have been used to estimate environmental fate.

Table 27.2. Physical Properties That Influence Environmental Phase Partitioning [2]

Property	Definition	Significance in Estimating Environmental Fate and Risks
Melting point (T_m)	Temperature at which solid and liquid co-exist at equilibrium	Sometimes used as a correlating parameter in estimating other properties for compounds that are solids at ambient or near-ambient conditions
Boiling point (T_b)	Temperature at which the vapor pressure of a compound equals atmospheric pressure; normal boiling point	Characterizes the partitioning between gas and liquid phases; frequently used as a correlating variable in estimating other properties
Vapor pressure (P^*)	Partial pressure exerted by a vapor when the vapor is in equilibrium with its liquid	Characterizes the partitioning between gas and liquid phases
Henry's Law constant (H)	Equilibrium ratio of the concentration of a compound in the gas phase to the concentration of the compound in a dilute aqueous solution (sometimes reported as atm-m^3/mol)	Characterizes the partitioning between gas and aqueous phases
Octanol-water partition coefficient (K_{ow})	Equilibrium ratio of the concentration of a compound in octanol to the concentration of the compound in water	Characterizes the partitioning between hydrophilic and hydrophobic phases in the environment and the human body; frequently used as a correlating variable in estimating other properties
Water solubility (S)	Equilibrium solubility in mol/L	Characterizes the partitioning between hydrophilic and hydrophobic phases in the environment
Soil sorption coefficient (K_{oc})	Equilibrium ratio of the mass of a compound adsorbed per unit weight of organic carbon in a soil (in µg/g organic carbon) to the concentration of the compound in a liquid phase (in µg/mL)	Characterizes the partitioning between solid and liquid phases in soil, which in turn determines mobility in soils; frequently estimated based on octanol-water partition coefficient, and water solubility
Bioconcentration factor (BCF)	Ratio of a chemical's concentration in the tissue of an aquatic organism to its concentration in water (reported as L/kg)	Characterizes the magnification of concentrations through the food chain

Example 27.1 illustrates the use of one of these properties to estimate environmental fate.

Example 27.1.

Methyl tertiary butyl ether (MTBE, CH_3-O-$C(CH_3)_3$) is an oxygenated gasoline additive. Oxygenated gasoline additives are mandated by law to reduce air pollution. Oxygenated fuel additives burn cleaner—for example, producing CO_2 rather than CO. However, because there is inevitably some leakage from underground gasoline tanks, the potential exists for the components of gasoline to enter the water table, ultimately contaminating drinking water. This is a problem for water treatment facilities, and it is an even more significant problem for those using well water.

For this calculation, gasoline is assumed to be 2,2,4-trimethyl pentane ($CH_3C(CH_3)_2$

$CH_2CH(CH_3)CH_3$) (also known as isooctane). The table summarizes several of the properties of these two compounds, calculated using the EPI Suite software.

Property	MTBE	Gasoline
Boiling point (°C)	47.04	81.44
$\log_{10}$ of octanol/water partition coefficient	1.43	4.09
Water solubility (mg/L)	1.98×10^4	9.91
Henry's Law coefficient in water (atm m^3/mol)	2.02×10^{-3}	3.01
$\log_{10}$ soil sorption coefficient	0.721	2.44

The observation is that MTBE has much higher water solubility than gasoline and a much lower soil sorption coefficient. Therefore, MTBE in leaking from underground tanks preferentially enters groundwater, whereas gasoline leaking from underground tanks preferentially adsorbs to the soil.

27.3. Green Chemistry

When a chemical is manufactured, a raw material is used. In the chemical industry, this raw material can usually be traced back to a depletable natural resource such as crude oil. Furthermore, when a chemical is manufactured, there are usually side reactions that produce undesired contaminants, which become hazardous waste if they cannot be converted to useful products. The processes illustrated in this book generally ignore all except the most important undesired contaminants; however, in real applications, there are usually trace amounts of several undesired contaminants that must be separated and eventually treated. Another possible source of waste is the need to use hazardous solvents or catalysts to promote a reaction.

Three issues in green chemistry are a search for the following:

- Alternative feedstocks
- Green solvents
- New synthesis pathways

One component of green chemistry is to use alternative feedstocks that either improve the environmental performance of a process or that do not deplete nonrenewable resources as much as the traditional process. For example, it has been suggested that adipic acid, a feedstock for nylon, can be manufactured from glucose, a renewable resource, by using a microbial biocatalyst [5]. The traditional method uses benzene, a known carcinogen, which can trace its origin back to nonrenewable fossil fuels such as oil and coal.

Green solvents are another component of green chemistry. In principle, the group contribution methods described in Section 27.2 could be used to design a solvent providing the desired performance and having properties that are less toxic to humans and less hazardous to the environment. The applicability of such a solvent would also depend on how it is manufactured. If the only way to make a green solvent is by a process more hazardous than the process that uses the original solvent, then there is no advantage to using the green solvent. The expense of the green solvent is also an issue.

The use of new synthesis pathways that avoid hazardous intermediates and/or hazardous by-products is also a component of green chemistry. For example, an elimination reaction (AB → A + B), where

A is the desired product and B is a waste product, is less desirable than an addition reaction (A + B → C) because no waste products are made. Another example is the elimination of unwanted side reactions, such as the production of p-diisopropyl benzene in the cumene process shown on the CD-ROM accompanying this book. New synthesis pathways will most likely be obtained only by development of new catalysts.

Clearly, green chemistry is in its infancy. The concepts are clear, but the implementation is years away. Example 27.2 relates to green chemistry.

Example 27.2.

Phosgene ($COCl_2$) is one of the most toxic chemicals known. It was used as mustard gas in World War I. Currently, phosgene is used as a raw material in the manufacture of pesticides and urethanes. It has been suggested that dimethyl carbonate (DMC, CH_3-O-(C=O)-O-CH_3) can serve as a reactant in many of the same processes that use phosgene [6]. This is an example of an alternative feedstock.

However, the traditional method for manufacturing DMC is from phosgene and methanol.

Phosgene manufacture $CO + Cl_2 \rightarrow COCl_2$

DMC manufacture $COCl_2 + 2CH_3OH \rightarrow CH_3\text{-O-(C=O)-O-}CH_3 + 2HCl$

Patents have been issued on a process to manufacture DMC directly from CO and O_2 [7]. The reaction is

$$CO + O_2 + 2CH_3OH \rightarrow CH_3\text{-O-(C=O)-O-}CH_3 + H_2O$$

This new process illustrates two of the principles of green chemistry listed above. First of all, DMC is manufactured without using the hazardous phosgene feed. In fact, the phosgene is not even produced in the new pathway. Second, the DMC can be a raw material substitution for phosgene in the manufacture of pesticides and urethanes. Furthermore, the first principle of waste management hierarchy is demonstrated in that the by-product HCl is not produced (although, if market conditions were appropriate, the HCl produced could be purified and sold as a commodity).

27.4. Pollution Prevention During Process Design

The most important issues when trying to prevent pollution during process design are to try to minimize generation of waste products in the reactor, to try to design separation systems for maximum recovery and minimum energy usage, to minimize effluent streams containing waste, and to minimize leaks, particularly during storage and transfer operations.

Because raw materials are almost always the largest operating cost, their efficient use is necessary for economical process operation. As every chemical engineer learned in the material and energy balances class, unreacted raw materials are separated and recycled. This is also green engineering. If the raw materials were not recycled, their fate would either be subsequent reaction (the same effect as recycle), emission, or, for organic chemicals, combustion to produce energy. Clearly, emission is undesirable, from both an economic and a green engineering perspective. Combustion is also undesirable from both perspectives. From a green engineering viewpoint, combustion generates carbon dioxide, a greenhouse gas, and possibly trace amounts of other pollutants. From an economic viewpoint, using a valuable chemical for fuel is a bad idea. Where supplies are available, natural gas is commonly used as fuel to produce energy (for process steam, for example). Any chemical more

valuable than methane is a poor choice as a fuel. In general, the more carbons in an organic chemical, the higher its value. Therefore, in terms of raw material usage, green engineering and economics coincide (or have similar goals).

Heat integration is another example in which green engineering and economics coincide. Fuel must be burned to create a heat source. It was shown in Section 8.3.2 that there are electricity costs associated with producing cooling water. Most electricity is obtained from burning fossil fuels. Therefore, the production of both heating and cooling utilities produces carbon dioxide, and both increase manufacturing costs. Heat integration can be implemented to minimize utility (e.g., cooling water, steam) usage (MUMNE method; see Chapter 15), so heat integration is both green engineering and economically beneficial.

It was mentioned previously that most chemical reactions produce undesired side products. Research in green chemistry aims to find catalysts and/or reaction pathways that reduce or eliminate these undesired side products. However, until this research bears fruit, the chemical engineer must try to reduce production of undesired side products. This requires maximizing selectivity for the desired product. Maximizing selectivity is also sound process economics, because it minimizes the fraction of raw materials not converted to the desired product. Methods for maximizing selectivity include optimizing the reactor temperature, optimizing the ratio of reactants, and optimizing the method of delivery of reactants to the reactor. Some of these methods are discussed in Chapter 23, and a more detailed discussion is available elsewhere [8].

Separation processes contribute to the problem of waste management because no separation is perfect. There are always trace contaminants in any "pure" stream. The goal in pollution prevention is to minimize these trace contaminants. For example, if absorption is used, a low-volatility solvent should be chosen to minimize contamination of the effluent gas stream. Distillation does not introduce additional contaminants, but it requires heating and cooling, both of which produce carbon dioxide and increase manufacturing costs. Therefore, distillation sequences should be designed for optimum energy usage. If solvents are required (e.g., absorption, extraction), they must be recovered. Organic solvents are expensive, so their recycle is tantamount to recycle of raw materials; if they were not recycled they would be burned at great expense and with carbon dioxide emission. In some processes (ethylene oxide, formalin—see Appendix B) water is used as a solvent. Water can even be used as an inert in a reactor (styrene—see Appendix B). Water that comes in contact with organics must be sent to wastewater treatment, which is expensive and consumes energy. Therefore, recycle of all solvents, including water, is both green engineering and economically beneficial. Solvent recycle is a simple example of mass integration, which is discussed in Chapter 15.

One potential source of pollution that does not typically receive much attention is the emissions generated during the loading and unloading of storage tanks. Consider the following scenario: A storage tank contains a somewhat volatile liquid. Therefore, there will be vapor in equilibrium above the liquid. The tank is to be filled by pumping liquid into the bottom of the tank. Where does the vapor go as the liquid level rises? An unsatisfactory solution to this problem is to vent the vapor to the atmosphere. A greener solution is to collect the vapor as it leaves the tank and recycle it to the tanker truck or rail car providing the liquid to fill the tank. This is commonly done when filling underground gasoline tanks. In some areas, gasoline pumps used to fill passenger cars have this capability. Emissions during normal tank operation (not during loading) are also a pollution prevention issue. Different types of tanks have different problems. A fixed-roof tank has the problem described above during loading and also must have a vent to prevent overpressurization when, for example, the

ambient temperature increases. Placing a separator on the vent can minimize emissions, as can a vapor recompression/cooling system. A floating-roof tank, in which the roof floats on top of the liquid, minimizes the vapor problem described above, but it creates the problem of thin films of liquid remaining on the inside vertical surface of the tank, which is exposed to the atmosphere when the liquid level in the tank decreases. The inevitable result is that storage tanks leak to the atmosphere, and the best that can be done is to minimize these leaks. Additional methods for minimizing these leaks can be found [1, 3]. TANKS software can be used to estimate losses from tanks, and it is available for download at http://www.epa.gov/ttnchie1/software/tanks/.

The problem of leaking equipment is not unique to storage tanks. Flanges and valves also leak. Reflux drums and reactors usually have relief valves, and they also might leak. These are called **fugitive emissions** and occur because of leaks in valves, pumps, flanges, and so on. Fugitive emissions are especially prevalent in moving equipment (e.g., pumps and valves), where there must be a seal between the process side and the outside that allows movement of a shaft. Typically, these seals are made of a packing material that offers a tortuous, high-pressure-drop path between the inside and outside. Some leakage occurs, and often, for liquid systems, the small leakage provides lubrication for the shaft. For such a packing seal, the lower the fugitive emissions, the higher the frictional losses from the shaft rotation.

As plants are designed for lower "stack" emissions, the fugitive emissions are increasingly the dominant emission type. Thus, the emissions from thousands of valves, pumps, flanges, and so on must be estimated and reported. There are several procedures to make these estimates [9], from crude assumptions that all valves leak at the same rate to experiments in which working valves are bagged in plastic and the fugitive emission rate directly measured. Fugitive emissions *can* be measured for existing plants, but they *must* be estimated for new plants in the design stage. The Clean Air Act defines a plant to be a "major source" if it emits 25 ton/y of any combination of hazardous air pollutants or 10 ton/y of any single hazardous air pollutant. Plants defined as major sources can get permits to operate only by demonstrating **best available control technology (BACT)**, which is tantamount to a negotiation with the EPA. The estimates for fugitive emissions virtually guarantee that any new chemical plant in the design stage will be considered to be a major source. Once a plant is constructed, careful monitoring is needed to ensure that fugitive emissions are minimized.

27.5. Analysis of a PFD for Pollution Performance and Environmental Performance

After a process design has been conceptualized and a preliminary PFD developed, further analysis is possible to reduce pollution. The PFD should be studied to make certain that all possible recycle opportunities have been exploited. For processes with multiple streams containing the same solute, mass integration is possible using the method of mass-exchange networks (MENs) described in Chapter 15. More detail on the MEN method and other methods for analysis to maximize solute recovery is available [10]. Example 27.3 demonstrates this type of analysis of a PFD.

Example 27.3.

Examine the PFD for the styrene process in Appendix B, Project B.3. Suggest methods for pollution prevention.

One of the most obvious methods is to maximize the selectivity for styrene in the reactor. The

ethylbenzene is already being recycled; however, minimizing the amount of ethylbenzene in the benzene/toluene effluent stream is both sound economics and pollution prevention. The fate of the benzene/toluene stream is also important. Because ethylbenzene is made from benzene, the benzene can be separated and returned to the ethylbenzene plant, which is almost always at the same facility. This is sound pollution prevention, although it might not qualify as pollution prevention according to the Pollution Prevention Act, because it does not constitute in-process recycle.

Another possibility is to recycle the wastewater stream to make the low-pressure steam used in the feed. On the surface, this appears to be a good idea for pollution prevention. However, there is a problem. There will certainly be trace amounts of organics in the wastewater stream. In a fired heater, the temperature is so high that the tubes in which the process stream flows are undoubtedly glowing red hot. These high temperatures can cause the organics to carbonize, that is, form carbon deposits on the tubes, with hydrogen gas being released into the process stream. The hydrogen gas is not a problem because it is made in the reactor, and there are already provisions in the process for its separation. However, the carbon deposits will foul the fired heater tubes, reducing the heat transfer performance. Therefore, if recycling the wastewater stream is desired, a separation step such as carbon adsorption should be included to remove the trace organics from that stream.

Finally, there are models that permit analysis of the fate of chemicals in the atmosphere that might be released from a chemical process. The most popular model is the Mackay Level III model [1, 11]. In this model, air, water, soil, and sediment are considered to be separate, well-mixed compartments in equilibrium with each other. Additional inputs and outputs are allowed to model air flow, river flow, and so on, for certain of these compartments. The equilibrium between compartments is modeled using fugacity. Therefore, for an emission into, for example, air, by knowing the physical properties of the chemicals involved (calculated from the group contribution method described in Section 27.2), the ultimate fate of all chemicals emitted can be predicted.

27.6. An Example of the Economics of Pollution Prevention

The economics of pollution prevention can be analyzed using the incremental economic analysis discussed in Chapter 10. First, assume that pollution prevention activities require an additional capital investment. This incremental capital investment can be that required for modifications to an existing plant or the incremental capital investment required to include pollution prevention technology in a new design. The incremental net present value is

$$INPV = -PC + YS(P/A,i,n) \qquad (10.4)$$

This means that the incremental net present value for the pollution prevention improvement, *INPV*, can be calculated from the incremental project cost: the additional capital investment needed for pollution prevention technology, *PC*, and the yearly savings resulting from the pollution prevention improvement, *YS*. The question is how to estimate *YS*.

As an example, consider the Love Canal near Buffalo, New York [12]. Hooker Chemical Company followed all existing regulations when burying toxic waste drums in a clay dome. Years later, the local municipality decided, against the strong objections of Hooker, to build homes and a school near that disposal site. During construction, the clay dome was disturbed, and the toxic chemicals began to leak. However, this leak was not discovered until health problems were observed years later. Subsequently, CERCLA (see Table 27.1) was enacted. Despite having followed all existing regulations at the time and having repeatedly warned the municipality not to disturb the site, it was

Hooker, and not the municipality or any of the construction companies, that was held liable for the cleanup and for civil actions. This is an example of the meaning of "retroactive liability" in CERCLA.

The lesson from this true story is that it is not always possible to predict the yearly savings from pollution prevention improvements with any certainty. This is one motivation for the Monte-Carlo uncertainty analysis discussed in Chapter 10, because this method allows these types of uncertainties to be factored into an economic analysis. Although it may look as if there are no yearly savings, estimating future liability with any certainty is difficult, if not impossible. Because the government has already established a precedent that it will change the rules and impose retroactive liability, a company doing business legally today may find itself liable for damages from laws not yet enacted. The conclusion is that pollution prevention activities are not only good environmental policy but also probably excellent long-term economic policy.

27.7. Life Cycle Analysis

A **life cycle analysis** or **life cycle assessment (LCA)** is a detailed technical study of the "environmental consequences of a product, production process, package, or activity (done) holistically, across its entire life cycle" [13]. The time frame of such an analysis is often termed "cradle-to-grave."

The first step in any life cycle analysis is to define the boundaries of the analysis. If a vessel is used in the process, are the manufacture and possible disposal of the vessel within the boundaries? Is the production of the steel for the vessel included? Should the environmental effects of the mining of the iron ore be included? Or should the analysis begin with the on-site installation of the equipment? The choice of boundaries defines the scope of the analysis. A broader scope requires greater effort but leads to a more complete understanding of the environmental impact of a process.

The remainder of the LCA consists of three stages:

1. **Inventory Analysis:** This is a quantitative study of the material and energy inputs and the air, water, and solid waste outputs of the entire life of the product or process.
2. **Impact Analysis:** The environmental consequences of both the inputs and the outputs of the inventory analysis are enumerated in this part of the LCA.
3. **Improvement Analysis:** The opportunities for improving the environmental consequences through modifications to the product or process are included in this section.

The life cycle itself can be divided into five stages [3]:

1. Raw materials acquisition
2. Material (of construction) manufacture
3. Product manufacture
4. Product use and reuse
5. Product and equipment disposal

Some models combine material manufacture and product manufacture into one stage [2]. At every stage in the life cycle, energy and material inputs are considered, as well as waste emissions. Therefore, a very "clean" process to manufacture a chemical may be considered less desirable, from an LCA standpoint, if a raw material (or a raw material for a raw material) is manufactured using a process that is very energy intensive or that produces large amounts of waste.

Simple life cycle analyses are available [14]. They are most useful when parallel LCAs are done on competing products or processes, because they allow one to evaluate objectively the overall environmental impact of the choices. In this case, it is especially important that all parallel LCAs use the same boundaries. Example 27.4 demonstrates a very simplified life cycle analysis.

Example 27.4.

Consider polyethylene, which can be made into plastic wrap (e.g., Glad Wrap) or plastic containers such as milk jugs. You work in a manufacturing facility that produces a variety of polyethylenes (e.g., low density and high density). Trace the life cycle of the products of your facility qualitatively.

Polyethylene is manufactured from very pure ethylene. Ethylene is a by-product of oil refining, and hence the ultimate source of polyethylene is a fossil fuel natural resource. Therefore, all of the energy and waste disposal issues associated with oil refining (and even with oil production) are part of the polyethylene life cycle. Ethylene is usually purified from other light hydrocarbons; therefore, their fate is also part of this life cycle. This is usually not a problem, because methane can be used as a fuel and propane and propylene also have uses and are not disposed of. In preliminary separation steps, ethylene and ethane are in the same stream, but ultimately, they must be separated from each other. Because ethane and ethylene are close boilers and high-purity ethylene is needed, their separation by distillation is difficult, requiring large columns with large reflux ratios. The large reflux ratios increase the energy consumption, so this is also part of the polyethylene life cycle.

The ultimate fate of the plastic wrap and plastic containers is also part of the polyethylene life cycle. If used containers are recycled and refilled, this is a beneficial part of the life cycle. If either the containers or the wrap could be collected and remanufactured into new containers or wrap, this would also be part of the life cycle. If the containers, for example, could be converted back into ethylene as part of a recycling program, this would also be part of the life cycle. If the polyethylene, in whatever form, ends up in a landfill, where it does not degrade, this is the ultimate part of the life cycle.

Clearly, a quantitative life cycle analysis can easily become very involved. This example is simplified and does not include all aspects of the life cycle. For example, the materials used to manufacture the process equipment were not considered to be within the system boundaries. You can imagine how complex a life cycle analysis can get if all aspects are included.

27.8. Summary

Green engineering is important because it is the right thing to do from an environmental standpoint, because it is likely to be good long-term economic policy, and because of the realities of the political climate involved in regulation of the chemical industry. This chapter has provided only a flavor of green engineering or pollution prevention. It was designed to give the reader a perspective on the issues associated with pollution prevention. It should be considered as a beginning, not an end. Further study is necessary to understand how to apply the principles introduced in this chapter to an actual chemical process design.

What You Should Have Learned

- Pollution prevention can be built into a process design.

- Key issues include
  - The environmental fate of released chemicals
  - Avoiding harmful chemicals and waste chemicals
    - Increasing selectivity
    - Choosing better reaction pathways
  - Avoiding emissions

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Problems

For the following processes in Appendix B, suggest modifications that would make the process greener:

1. The ethylbenzene process
2. The styrene process
3. The maleic anhydride process
4. The ethylene oxide process
5. The formalin process
6. The ethylbenzene process
7. The DME process
8. The acetone process

Section VI: Interpersonal and Communication Skills

A chemical engineer is very much a member of a tiny technical elite of modern society. In the United States, less than 1% of the population is trained in engineering and sciences. Chemical engineers account for only 0.05% of the population, and yet they design and manage the plants that produce such essential goods as pharmaceuticals, plastics, paper, fertilizers and pesticides, fuels, synthetic fabrics, and clean water. Chemical engineers use jargon and perform calculations that are, at best, mysterious to most people. Their success depends not only on performing the calculations correctly but also on convincing the public that they can add value to the quality of life. In addition, to communicate clearly with the public as a whole, chemical engineers work most often as part of a team of professionals. The interaction and communication between team members are absolutely crucial to the success of any given project.

The following chapters deal with the issues of team building and effective communications.

Chapter 28: Teamwork

The essential elements of team building and teamwork are described. The choice of group members, initial organization determination, roles within and outside the group, group management, team building, team member roles and responsibilities, and team self-evaluation are described. References to the most accessible team-building literature and examples of problems typically encountered by poorly functioning teams are included.

Chapter 29: Written and Oral Communication

Through a focus on audience analysis, strategies for improving the effectiveness of both written and oral presentations are explained. Commonly accepted (but frequently broken) formatting rules for figures and tables are covered, as are hints to effective use of communication software (available on the accompanying CD).

Chapter 30: A Report-Writing Case Study

Following a sample student design report, this chapter offers models of both strong and weak written communication in several formats: memoranda, visual aids, and short design reports. A checklist of common errors is provided (available on the accompanying CD).

Chapter 28. Teamwork

What You Will Learn

- Teamwork is essential in all fields of endeavor, including the chemical process industry.

Chemical engineers work both with and for other chemical engineers, other types of engineers, scientists, and nontechnical people—often all at the same time. In short, chemical engineers do not work alone.

Teamwork is not just working with or for other people; it is working together as a unit to accomplish goals in a way that each member of the team accomplishes more than that person could accomplish alone. The concept of teams and teamwork is an old and powerful one.

Some would say that teamwork cannot be learned or that it is easy. In this chapter, both of these misconceptions are addressed.

Developing the skill set for effective teamwork is an essential part of being a chemical engineer. As with the rest of engineering, although it is not easy, it can be learned.

28.1. Groups

A team is a subset of a group. Therefore, this chapter starts by addressing groups and group work.

Any collection of people working on a common project can be considered a group. Two students working together in the chemistry laboratory course compose a group. Five students working on a design project are a group. A chemical engineer, a civil engineer, and a project manager working to get a water treatment plant on line act as a group. In each of these examples, and in myriad others inside and outside the engineering world, collections of people form groups to get a job done. One certainly hopes that the group is more *effective* than any of the people working alone. However, that could not justify the existence of the group (although some groups only barely meet this criterion). To be an effective group, the group output should be better than the total output from all the individuals working alone. The concept that explains this increased *efficiency* is called **synergy**. It is related to the concept of economy of scale discussed in Chapter 7.

When people form groups, various organizational behaviors occur. Some of these behaviors are productive, some are nonproductive, and some are counterproductive. However, none of these organizational behaviors is unchangeable. Section 28.1.3 describes some of the organizational behaviors of groups and provides strategies to improve the efficiency and effectiveness of the group. The next two sections discuss characteristics of effective groups and offer a general strategy for improving group work.

28.1.1. Characteristics of Effective Groups

An effective group produces an output that is better than the total of outputs from the individual group members working alone. There are three important keys to achieving this effectiveness:

1. Task differentiation

2. Work environment
3. Coordination

Task Differentiation. In any group, members do different tasks. However, imagine a group in which each member did the same job, and then someone chose the best result to go forward. The group would be terribly inefficient. In fact, such a group would not even satisfy the first criterion of a group: that the group be *more effective* than any of the people working alone. In this example, the output of the group is only as good as the output of a single person working alone. However, this example suggests one of the keys to effective task differentiation:

Each job should be done by the group member who can do it best.

This is a heuristic. As with all heuristics, it cannot always be applied (nor should it), but it is a very helpful guide. For this heuristic, it is very important that the special abilities of each group member, vis-à-vis the project tasks, be known. Of course, a single group member might be best at a large proportion of the tasks, and that would lead to unequal workload, which would be a problem. Therefore, a second heuristic is used:

Each group member should contribute equally to the group outcome.

The overall group outcome should be the best that it can be (i.e., it should be optimized). This heuristic typically overrides the previous two heuristics for highly effective groups. It could easily be that the best outcome occurs when one (or a few) members do more than their share of work and/or when individual tasks are done by members who are not experts in that task. As in all of engineering, optimization is important.

Other aspects of task differentiation may be important. For example, it may be optimal to train a member to do a task that another already does well. It may be helpful to have more than one member do the same task and then compare answers. (This is a classic error-checking strategy.)

Too much task differentiation can create problems. The project outcome should never be dependent on any one person. For example, if a group member becomes sick, someone must be able to step in and do the job. This can be accomplished in two ways. Either all tasks have assigned backups (understudies), or all members develop and maintain competencies in a broad range of tasks. The former is a quick fix. The latter is more stable and leads to greater flexibility.

Work Environment. People are more productive when the environment that they work in is safe, supportive, and challenging. It is incumbent on all group members to create and maintain this environment.

Safety in this context often refers to the safety of one's job. One of the most damaging events in a work environment is notice that someone is being reassigned or even fired. People work best when they feel somewhat safe, but they also need to be challenged.

When the job is demanding, one tends to rise to the occasion. Clearly, then, there is an anxiety level, between safe and overly demanding, that optimizes one's performance. Because this optimum anxiety level is affected by many factors, it is difficult to predict. To be a good group member, one needs to know one's own optimum anxiety level and to give feedback to the group when one is outside the

optimal range.

The supportive aspect of the group work environment refers to help that other group members give when one's efforts for the group do not meet expectations. Group members who are supported are much more likely to stretch for greater productivity or to be more creative. Both of these activities give rise to both higher overall outcomes and higher numbers of failures. Without a supportive environment, people take the easy path, which leads to few failures but only mediocre success.

There are many heuristics to help group members improve the work environment and thereby increase group effectiveness. Here are some:

- Tell the group when you are unable to meet expectations.
- Be constructive and accept constructive criticism.
- Assume that negative feedback was meant to help you improve.
- Give positive reinforcement to group members.
- Provide assistance to group members in achieving their professional goals.
- Give credit to other group members when talking with group members and when talking with those outside the group.
- Thank group members for taking risks.
- Accept group responsibility for failures.
- Avoid competition within the group.
- Focus competition outside the group.
- Offer assistance when group members have nonwork problems.
- Try to obtain support for the group, not for individual group members.
- Immediately cover for a group member who is having trouble.

Coordination. Synergy requires a coordinated effort by the group members. This coordination involves breaking down the project into components, assigning these components to group members, ensuring communication of results, and assembling the results into the final product. As in any problem solving, these steps are taken many times and often out of the order just described. An essential aspect of coordination is flexibility. If a project component is initially assigned to what turns out to be the wrong group member, it must be reassigned, without prejudice. If the chosen communication scheme breaks down, it must be changed. Example 28.1 describes such a scenario.

Example 28.1.

In a typical design assignment, there are many aspects of the problem: problem definition, alternatives generation, research, communication with the client, technical analysis, economic analysis, error checking, report generation, presentation to the client, and others. Coordination in such a project might initially involve meeting together to discuss the problem, choosing a leader, determining a schedule, and specifying a division of duties. These activities are generally serial to the flow of the project. Then various aspects of the research can be done in parallel. One group member studies the given flowsheet and puts it on the process simulator. Another member researches processes commonly used for the application. Another member meets with the client to gather any additional information. Still another studies the economics of the process and identifies opportunities. Then the

group convenes to share the information, to verify the problem statement in light of the information obtained, and to brainstorm alternatives. Members then go off to work on their assigned tasks, with frequent communication with the other group members. Then the group reassembles to plan the final output and the format for delivery to the client.

Obviously, many other steps are taken by the group, but, in each step, coordination is important. If two group members do the same job, effort is wasted (although, as noted in the previous section, this situation may provide some error checking). If something remains undone because it is not explicitly in any one member's "job description," the project may not get done on time. It may not get done at all. Here are some heuristics for group coordination:

- Always know what everyone else's assignment is.
- Share information when it conceivably could be relevant to the work of another group member.
- Ask the group, "Are we missing anything?"
- When a gap in assignments is noticed, inform the group and offer a modification to solve the coordination problem.
- Role-play the client/group interaction.
- When information is shared, make sure you understand, even if it is not directly within the sphere of your assignment.
- Focus on your assignment as a *contribution* to the group effort, not as a *division* of what is and is not your responsibility.
- Be flexible.

28.1.2. Assessing and Improving the Effectiveness of a Group

Throughout any engineering activity, self-assessment is important. For a calculational homework problem, checking the answer before submission is standard procedure. On an examination, it can mean the difference between a good grade and a poor one. Group work is assessed in a similar way. The final answers (e.g., the details of the final report) must be checked by the entire group. Beyond that, the effectiveness of the group itself must be assessed repeatedly. For this assessment, the form in Figure 28.1 can be used. This form was developed by Dr. C. J. Coronella at University of Nevada, Reno (2001). An on-line team-formation and assessment tool is available at www.catme.org.

Group Assessment

Name

Please enter a score from 0 (worst) to 10 (best) in each row, for yourself and for your team members. If you enter uniform scores across the board, I know you haven't taken this assessment seriously. A 10 should be an unusual score.

Enter your initials in the first column and those of the members of your group in the remaining columns.	(me)				
Leadership 10 Very strong leader, provided direction, inspired and encouraged others 5 Willing follower, took directions easily 0 Frustrated the group, blocked progress, criticized others					
Cooperation 10 Worked readily with others, outstanding contributor, anticipated requests 5 Cooperated with occasional prompting 0 Rarely contributed or cooperated, worked alone, had to be coerced					
Initiative 10 Produced good ideas which helped others, "went the extra mile" 5 Accepted other's ideas and improved on them 0 Criticized other's ideas, never contributed original ideas					
Attitude 10 Positive, enthusiastic, encouraging others to work better 5 Neutral, worked with the group without either enthusiasm or grumbling 0 Negative, complained about the project, worked unwillingly					
Effort 10 Worked hard on assigned tasks, independently and cooperatively 5 Worked reasonably hard, also socialized a lot. Occasional prodding needed. 0 Didn't contribute much at all, tasks were unsatisfactory.					
Preparation and conduct of Lab work 10 Enthusiastic, came prepared to meetings and to lab. 5 Came to all meetings, somewhat prepared. Often helpful. 0 Missed lab, was unprepared, we'd have accomplished more without him or her.					
Writing of report 10 Enthusiastic, contributed substantially to production 5 Contributed everything that was asked. Work needed revision 0 Didn't contribute to the production					
Preparation and delivery of presentation 10 Enthusiastic, contributed substantially to production 5 Contributed everything that was asked. Work needed revision 0 Didn't contribute.					
Computation 10 Helped others to understand and use computer tools 5 Good, but not incredible, use of computers 0 Uninterested or unable to use computer tools effectively					
Grade You have **100** points to divide among your team members. Distribute the points in an equitable manner, where each score reflects effort and contribution, (which aren't always the same.)					
Assessment of the group 10 Best group I've ever worked with; the project was fun as a result 5 Group sometimes worked well together, with occasional problems 0 Worst group I've ever worked with (or not); this was a miserable experience					
∑ Who in your group took most of the leadership for this last assignment? ∑ Is your group functioning better, worse, or just differently than at the beginning of the semester? Explain. C. J. Coronella, © 2001.					

Figure 28.1. Group Assessment Form (Used by permission of Dr. C. J. Coronella, University of Nevada, Reno, copyright 2001)

The assessment is short and therefore can be used at frequent intervals. The form should be used after the first meeting, halfway through the project, and at the end of the project. In addition, it should be used at least every week for longer projects. At this stage, some of the items on the form may not yet apply. Note that the form is parallel to many of the heuristics given above. Immediately after the group members fill out the form, a summary of all the forms should be shared with all. A discussion should immediately follow about the results, with the only goal being to make changes to improve the working of the group. All group members have a vested interest in improving the group effectiveness.

Each member should try to take the feedback as constructive. The group result will be better, the group members will be less stressed, and the positive contributions of each member will be clear to all, as seen in Example 28.2.

Example 28.2.

By using the form in Figure 28.1, the group finds that Jo believes that the other group members are putting in little effort. Robin thinks that effort was fairly consistent across the group but that the attitude of Sam and Lee was negative. Chris received low scores in leadership from everyone except Sam. After discussion of these results, it was determined (and accepted by all group members) that Chris needed to be more positive about group successes in group meetings. All of the group members began to understand the effect of morale on the effectiveness of the group. Jo found out that Robin, Sam, and Pat actually spent much effort in researching process alternatives that did not end up providing improvements. Because these alternatives were not part of the ongoing design work, Jo was unaware of this essential effort. It was decided that roles for and results from all group members would be discussed in the group meetings.

Sometimes major problems occur in groups that make them highly ineffective and inefficient, such as withdrawal of a group member from the communal effort or competition for credit between group members. To be resolved, these problems must come to the attention of the group. If the matter is very personal, the group leader may need to deal with it directly. Otherwise, the group as a whole can seek to solve the problem, but only after the problem is identified through assessment. The following section describes typical group problems and offers often successful solutions.

28.1.3. Organizational Behaviors and Strategies

Throughout the group work, behaviors of members of the group will sometimes be conducive to group effectiveness and sometimes not. The following are some typical organizational behaviors. For more complete lists and strategies, see [1, 2, 3].

Friction. The group is like an engineering system, and the unappreciated dissipation of otherwise useful energy is friction. This friction comes from a variety of sources and must be reduced or eliminated as quickly as possible so that the energies of the group members are focused on the project. Here are some examples:

- **Apparently Unequal Work Distribution:** Members of the group who believe they have more to do than others operate at lower efficiency. They have a responsibility to mention this perception to the group leader, who has the responsibility either to explain why the distribution is fair or to equalize the workload if it is unfair. Maintaining silence about this situation increases stress. Sharing perceptions with only a subset of the group makes the matter worse and harder to correct.
- **Low Motivation, Low Morale:** People work harder when they are motivated. More important, they also work smarter. For example, motivated group members fill gaps between individual assignments when they notice them. Group members can become demotivated when they do not feel that their work is that important, when they do not care whether the group succeeds, when they are overwhelmed by group and nongroup pressures, and so on. Individual group members should try to be aware of their own low motivation; however, it is often more noticeable to other

group members. In either case, this is a problem to be solved with the help of the group. The group leader should talk with the individual involved, try to determine the underlying cause of the low motivation, and make reassignments or offer other help. The extent to which the entire group is involved depends on whether the members have already sensed the problem. If so, the resolution should be described to them. A related source of friction is low morale. Groups work best when they have an emotional stake in the group result. If good group work increases one's sense of well-being, one works harder and smarter. High morale can be maintained by frequent positive feedback to all group members, individually and jointly. Giving credit to group members whenever it might be deserved is a good policy.

- **Lack of Concurrence with Group Decisions:** This is especially troublesome with groups in which the members are inexperienced in effective group work. First, the opinions of the members need to be aired. Then the group leader should lead a discussion of how the various options will advance the group project. If there are multiple options that appear to advance the group work nearly equally, the group leader makes the decision. The group leader should explain the value of continuing with the project, rather than worrying about the decision. The leader also has responsibility to explain the process by which decisions are made so that all the group members can accept the decision and move on, even if they do not believe the decision to be the best one.
- **Overlapping or Gapping Work Assignments:** All group members have the responsibility to do their assigned work and to fill in the noticeable gaps in assignments between group members. If these gaps are too great, they require reassignment of work. The group leader should be alert to this possibility at all times, and the group members must inform the leader when gaps appear. Some overlap between work assignments should be expected and appreciated. Group members should try not to take offense when another member is assigned some of the same work.
- **Uncomfortable Group Interactions:** Some people may be uncomfortable interacting with other group members for any number of reasons. Although much less common today, one historical example is the discomfort that some men have felt while working for a woman. Another common problem in undergraduate design groups is the existence of cliques and "outsiders." These types of friction can be the most disruptive to group work, and they must be dealt with directly and quickly. Group interactions must be based on trust, respect, and responsibility. Reminding all group members of this principle of group work may mitigate the friction. However, in the context of a course design group, faculty help should be requested if needed.
- **Assigning Blame:** Sometimes, a decision made by the group is later found to be a bad one. Unfortunately, too often this leads to one group member blaming another, which results in decreased efficiency for all. When problems arise, it is best to view them as group problems. "It's not his fault or her fault; it's our fault." This viewpoint encourages a group solution that will be more durable than any individual's solution.
- **Disengagement:** For maximum effectiveness and efficiency, all group members must be engaged in the group work process. When a group member is disengaged, often the first symptom is a statement such as, "Just give me my work assignment and let me go." The group members should offer encouragement by indicating the value of the individual's work to the group result and by explaining that the group needs to work as a unit to avoid extra effort. Disengagement often follows from low motivation and/or low morale.

Leadership. The most important thing about the leadership of the group is that there be an identified

leader. Leaderless groups waste time discussing unimportant decisions, and all decisions seem to be temporary—open to additional time-consuming discussions at a later date. The role of the leader is to focus discussion, develop the structure of the group, pace the group members, and make decisions that advance the group and are acceptable to the group members. It is extremely important that all group members accept that the leader has these responsibilities to avoid friction from control issues. In response, the goal of the leader should be to improve the effectiveness of the group effort; the goal should not be to exert control. If the leader is flexible and yet consistent in decision making, friction can be minimized and more group member time will be spent effectively on task. Effective leaders ask for feedback on their leadership and use that feedback to improve. Some first-time leaders make too many plans without group input and make too many demands without sufficient explicit appreciation of the work done by the group members. Effective leaders guide their groups to develop plans that all group members appreciate and find that their group members are eager to do even more than what is assigned. Every group leader should read a complete book about developing the many unique skills required [4].

Organization. In a small group, the organizational structure is simple—only the leader and everyone else. For larger groups (ten or more) a three- (or more) tiered structure may be required. However, such a structure necessarily reduces the ratio of "workers" to "management," which is apt to reduce group effectiveness. Therefore, the temptation to create multiple levels of organization should be resisted. If two group members research patents, there is no need to identify which person is "in charge" of patents. In large groups, the subgroups are best organized according to capabilities rather than according to fixed tasks. For example, a subgroup might be formed of five people who have the capability to find information in the literature and to analyze its value. The task assigned to this subgroup would vary during a design assignment, from patent searching, to alternatives research, to economic research. However, some of the members of this subgroup may be needed in another subgroup halfway through the project to work on process simulation. Thus, the organizational structure should be focused on both flexibility and capability (not task) functionality.

Choosing Group Members. Two types of characteristics are important in choosing group members. Obviously, the group needs members who are competent in certain technical fields—for example, chemical engineers, chemists, and mechanical engineers. The technical expertise may need to be more specific, such as catalysis, simulation, thermodynamics, and so on. However, beyond their technical (or task-oriented) expertise, group members must have complementary process-oriented skills. "Process" here means the group process, or how group members interact. Many engineering students are currently evaluated by the Myers-Briggs Type Indicator (MBTI) or another tool designed to give feedback on one's preferred style of learning and interacting with others on intellectual tasks. A well-constructed group will contain members with a breadth of learning and working styles. For example, a group of only introverts may ignore the concerns of the client, and a group of only intuitive members may fail to recommend much-needed experimental work in the final report. Crucial to the success of a group with a spectrum of styles is respect for all styles by all members of the group. Therefore, the best strategy for selecting group members depends on the sophistication of the members. If they already understand and value learning styles other than their own, the broad-spectrum approach is appropriate. If the concept of learning styles is new to the group (or the group leader!), it is better to choose a more coherent group—people who generally approach problem solving in a similar (but not identical) way. However, the latter approach will nearly always reduce the creativity of the group,

even as it reduces friction. It should be used only until the group members can get to a learning styles workshop, which is available through most universities, technical societies, and large corporations.

One indicator of different styles that is always available in a course is grade-point average. Students with straight A's are different from students who earn B's or C's—and this difference often has more to do with learning styles and working styles than anything else. Therefore, it is advisable to choose group members so that the group is heterogeneous on this metric also. Grouping all *A* students together in one group and all *B* students in another is an ineffective strategy that has led to numerous group failures.

Another consideration in choosing group members is friendship. Groups based on friendship are frequently unsuccessful on technical projects. In any reasonably complex project, there will be disagreements as to the best route to the final report. Friends may take these disagreements personally, in a way that people who view their relationship as purely professional may not. Professional relationships based on respect allow a more direct and honest dialogue, whereas personal relationships involve the added dimension of predicting the emotional response and modifying communication based on that prediction. In addition, other group members may hold back communication if they perceive themselves to be outside a clique of other group members. All these concerns have led to dysfunctional groups in design courses, with resulting poor project performance. Overall, it is easier to be efficient and effective working with a colleague than with a friend.

An extreme case of this type of dysfunctional group behavior can occur when there are prior, current, or potential romantic relationships between group members. It is best to avoid such conflicts in choosing group members. The more high performing the group, the more damaging romantic complications can be. When conflicts of this type arise, they can become intense and lead to low morale, disengagement from group activity, and polarization of the entire group.

Throughout one's career, one works in groups with a wide variety of people. Sometimes another group member will be one's polar opposite. For example, one member prefers to take in all the information, think about it, and give a solution without detailing the steps. Another prefers to go step-by-step and always keeps a neat calculations notebook. Group members need to interact on a basis of respect for each other's unique styles. Interactions based on respect and professionalism make use of this diversity to enhance creativity, to improve communication with a wide variety of clients, and to help all group members develop a broader array of capabilities.

When groups are chosen by someone outside the group (a professor in a course or a manager in industry), one hopes that the above heuristics are used. Whether they are or not, self-selection of group members is the exception; outside selection is the norm.

Roles and Responsibilities. The glue that holds the group together, as well as the lubricant that reduces the friction, is the clear understanding of roles and responsibilities of group members. The leader has the role of making decisions based on the best input from the group; however, this entails a responsibility to make those decisions even when it becomes unpopular to do so. Another leader responsibility is to monitor the group process continually to keep everyone on track, to make sure that nothing falls between the cracks, and to reduce unproductive tensions between group members proactively if possible (but retroactively if necessary).

Each group member should know all group members' roles on the project. If a role is unclear, it is the responsibility of the group member to obtain clarification from the leader. All group members have

the responsibility for the final project results, jointly and severally. If the report is poor, it reflects poorly on all group members; if the report is good, all receive credit. If any one group member is unaware of the group results, it casts doubt on the entire group effort.

Mobile Truth, Groupthink, Mob Effect. Earlier, group friction was described. Although this characterization covers most disruptive problems encountered by groups, another problem is "mobile truth" and related issues. As described in Chapter 25, when your affinity to a group clouds your ethical decision making, you are being affected by mobile truth. However, related situations arise frequently in group work that do not seem exactly like ethical problems. For example, group cohesion can lead to an autocatalytic agreement on group design decisions once they are proposed. If a tray column is chosen over a packed column by one group member, other group members may suspend their own judgment to add their vote. As more members agree, it becomes less likely that *any* other group member will disagree. The disturbing fact is that the same scenario could describe the same group, with the same available data, if the first person chose the packed column over the tray column. Thus, a random suggestion becomes the group choice without sufficient analysis. This phenomenon, known as **groupthink**, is well known to observers of groups but is often difficult for groups to see themselves. All group members must guard against it. One heuristic is to ask whether there is a better way whenever all the group members appear to be in agreement. It is potentially disastrous to know that you are right (by unanimous agreement!) when you are clearly (to those outside the group) wrong.

28.2. Group Evolution

As groups develop, they go through stages. A widely used categorization of these stages devised by Tuckman [5] is used in this section. As with problem-solving strategies, the order of the stages is the typical case, but active groups of experienced group members tend to recycle back to earlier stages to optimize the group work.

28.2.1. Forming

The first stage is **group formation**. This stage may include the actual choosing of the group members, but often the members are chosen by someone external to the group. The group members get to know each other, including their technical abilities and preferred working styles. They share contact information to allow sharing of results outside normally scheduled group meetings. The leader is identified by the group members or externally, and the leader establishes an organizational structure. Rules and procedures for the group work are established. The charter or mission of the group is established. A **charter** is a statement of scope, task, and responsibility determined externally and given to the group. A **mission** is the same type of statement, but it is developed by the group itself as is common in what are referred to as self-directed work teams. These teams are given more autonomy, along with the responsibility to plan and manage their performance. They are expected to self-assess both their task results and group process activities. Example 28.3 is an example of forming.

Example 28.3.

A group of six students in a design class is formed to design a portable fuel cell that can compete with existing gasoline-fueled generators for electrical power in remote locations. They introduce each other and share e-mail addresses and cell phone numbers. The members describe the way they do their engineering homework and study for exams as a low-key way to share their working styles. They

discuss the charter presented to them by the course instructor. The group leader (chosen by the course instructor) sets up procedures, assigns tasks, and schedules daily meetings.

28.2.2. Storming

Creating a well-functioning group often requires a period of **storming** or flailing about. Group members test one another. They become aware of differences between themselves and focus on them as barriers to success. They disagree and debate issues—sometimes very minor issues. They question the mission of the group or the meaning of the problem posed to the group. They question the leadership and organizational structure developed in the forming stage. Although this is a normal stage in the development of the group, it can derail the entire project. Therefore, experienced group members recognize that reining in the discord is essential after the storming becomes counterproductive. The ability to guide this stage requires practice and self-reflection after each such situation. One heuristic for beginners: Just before the discord starts to digress into personal rather than professional attacks, point out that *storming* is going on and that it is time to move on to the next stage, as shown in Example 28.4.

Example 28.4.

The group begins to complain about the wording of the charter, and they openly question why Chris was chosen as leader by the course instructor. Jo asks why they must meet every day; Lee wants to meet whenever the need arises. Robin wants to go to the course instructor to settle all these issues, but Sam thinks the group should function on its own. Pat says, “Let’s just stop this storming and get on with it.”

28.2.3. Norming

Norms are rules and procedures (some stated, some not) that guide group interactions. During this stage, norms are developed and accepted by the group members. The diversity of backgrounds, viewpoints, and experiences of the group members is accepted. Disagreement between group members on technical issues and on group process issues is accepted, but the group moves on. Individuals take on and accept their assigned roles and develop a sense of shared responsibility for the group effort. At this stage, detailed scheduling may be most effective. The group develops a Gantt chart or a PERT chart, if the project is complex enough to benefit (most are). The Gantt chart is a matrix of tasks (rows) versus time (columns). An open bar in the appropriate row going from the start of effort on the task to its conclusion is shown on the schedule. The bar is filled in proportion to the completed results of the task. At any time, the Gantt chart thus indicates which tasks are ahead of schedule and which are behind schedule. Various notations are made to show linkages between tasks, milestones, and slack time, but this is all beyond the scope of this text. Please see the excellent article by Dewar [6] for a clear and very useful description of this technique, which is the most common scheduling technique in engineering. The **critical path method (CPM)** and the **PERT technique (program evaluation and review technique)** can be used to determine the set of activities that must be performed in series without delays to minimize the total project time. These incorporate a flowsheet to show linkages between tasks and are especially useful for complex projects. See the excellent description by Smith [7], which also includes helpful software for the CPM. The PERT technique also allows for including uncertainty in the projected time required for individual tasks.

Example 28.5 is an example of a scheduling meeting.

Example 28.5.

Chris has read an article about Gantt charts and organizes a meeting to create one. It has been decided that all group meetings must have an agenda, so Chris provides one. At the meeting, Lee has many suggestions of tasks, but Jo is nearly silent. Once Lee stops talking, Jo asks, "Do we really need to do task number 7? It doesn't seem to be linked to our overall goal." Robin believes that task 7 is essential, Pat and Sam are not sure, and a short discussion ensues. Finally, the entire group realizes that they need to link each task to the goal and that the diversity of opinions just witnessed helped them to reach a better solution. It is decided that, at each meeting, one group member will be assigned to observe discussions and to indicate when enough time has been spent on that issue. If a consensus has not been reached, Chris will make a decision. It is decided that communication with the course instructor will be primarily through Pat, who will report all such communication at each meeting.

The Gantt chart created by the group is given in Figure E28.5, updated for four weeks after this meeting. Note that the group is a week behind in research and technical analysis but a week ahead in economic analysis. It becomes clear from this diagram that the effort on economic analysis should be redirected immediately to research and technical analysis to catch up, especially because a client meeting occurs next week.

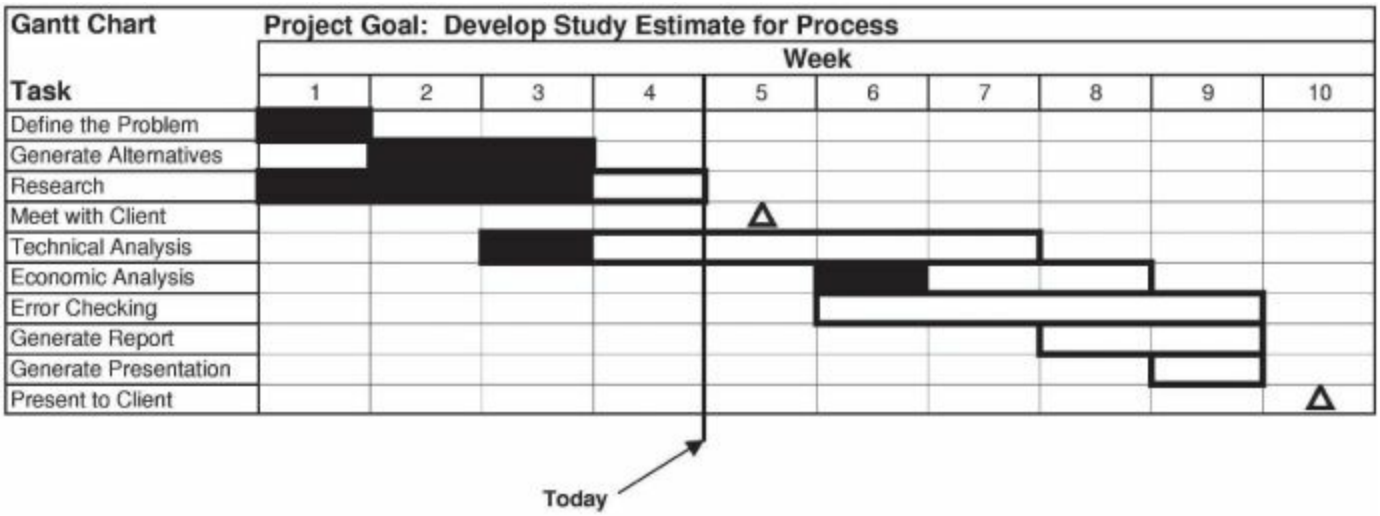


Figure E28.5. Gantt Chart for Example 28.5

28.2.4. Performing

During the **performing** stage, most of the group on-task work is done. The preceding stages allow the development of the group processing that is essential to the smooth functioning of the group on the task. There is agreement on the project schedule, assigned tasks, and leadership. Results are shared with the group, and the project progresses to its conclusion. Diversity of analyses, conclusions, and recommendations by different group members is regarded as an advantage in developing creative solutions, optimizing group processes, and assessing the group results. The performing stage is the goal of the earlier stages, and results-oriented professionals such as engineers often try to jump right into this stage, without valuing the earlier stages. Although experienced group members can shorten the time in the earlier stages, they especially understand the need for developing an effective group culture, which is the goal of the forming, storming, and norming stages. It is essential for all groups to spend time and exert effort to develop this culture.

28.3. Teams and Teamwork

A team is the ultimate group. As people become comfortable in group work, when they become efficient in group processing, and when they can maximize the effectiveness of the group to develop the best group result, their groups become teams. Thus, two characteristics that differentiate groups and teams are morale and task performance [2].

28.3.1. When Groups Become Teams

The process of developing a team from a group is called **team building**. There are many specific procedures for team building used in countless short courses. A characteristic of most team members is that each has attended one or more such short courses or workshops. The best general advice to generate team skills is to attend such a workshop. These workshops are available through most universities and corporations, as well as through technical organizations (such as AIChE, SWE, or Tau Beta Pi). It is not necessary (nor even necessarily preferable) for all members of a team to have attended the same workshop; diversity of team-building approaches can enhance the activity. Before or after attending such a workshop, one can hone team-building skills by using heuristics such as the following:

- Actively and consciously follow the four stages of group development.
- Find common ground with each team member.
- Find value in each team member's contribution.
- Create a team identity.
- Appreciate diversity as a trigger in brainstorming, as a facilitator in filling gaps, and as a mirror to simulate the response of the client.
- Accept all criticism as constructive.
- Present all criticism in a constructive way.
- Read through a chapter on teamwork while thinking about the working of your team. Choose one or two aspects of teamwork to work on as you work on the present task.
- Joke with team members. Show concern when other team members are having trouble.
- Scan the team for team members who may feel left out. Actively bring them into the core of the teamwork.
- Share your analyses and opinions, but strive for the best decisions for the team, not for yourself.
- Have and show concern for the development of other team members.
- Ask frequently, "Are we a team yet?"

When everyone in the group not only wants to but also works to improve the performance of every *other* member of the group, a team has been created.

28.3.2. Unique Characteristics of Teams

Teams can be identified (internally and externally) by several key characteristics. These improve morale, effectiveness, efficiency, and stability. Some of these are as follows:

- **Concern for Each Other:** Team members help each other on their assignments in such a way that both team members become better problem solvers. A team member in difficulty asks for

help, and other team members automatically provide it. The helping team member tries to teach the other how to avoid the difficulty in the future. When there is a crisis for one team member (professional or personal), the other team members immediately step in to help.

- **Leaving No One Behind:** In teams, all team members are assigned essential tasks, tasks that if not done properly will negatively impact the team result. A goal (shared and individual) of team members is to help each team member improve. All team members share in the successes and failures of the team. Individual team members are not blamed for failures; the team reflects on the failure and develops procedures to avoid it in the future. Team members congratulate each other (within the team and outside the team) all the time.
- **Constructive Criticism:** Team members feel comfortable discussing each other's performance. They reflect on team activities and discuss ways for all team members to improve. There is more criticism and self-reflection in a team than in other groups, but there are few hurt feelings.
- **Consensus, Not Voting:** Voting is an impersonal attempt to involve all group members in a decision. Although a decision is made, the procedure creates two (or more) subgroups that have identified their differences. **Consensus building** is a process designed to produce a result by having team members (1) identify common ground and (2) actively keep the best interests of the team (rather than the individual) in mind. Consensus building is definitely not a vote followed by the "losers" giving in to the majority, and it is not a way to find the "least objectionable" or "least common denominator" solution. Consensus building begins with a discussion to determine the features of a solution that are acceptable to all team members. Then the solution is built by identifying divergent ideas and parsing them all (as a team) according to which is best for the team result, without concern for whose ideas they were or how a decision will affect the individual team member. A common misconception is that consensus means that all members believe the decision reached to be the best one. Rather, consensus means that all members consent to the decision. Some may still think that it is not best, but all agree to accept the decision as the group decision and move on. Groups vote. Teams build consensus. Consensus generally results in better decisions and maintains team cohesiveness so that the team can move on without delay.
- **Trust:** Team members share information freely because they have high levels of trust in the team and all its members. This enhanced information flow speeds the teamwork, and it avoids "missing something" along the way. This trust also makes it easier for team members to accept decisions made by individual team members.
- **Sacrifice:** Team members work to advance the team toward its goals. This often means working longer or harder when team progress or the inability of other team members requires it. Team members check their egos at the door. They recognize that a good team result will reflect on them, that helping other team members will improve their own productivity, and that they can depend on other team members to help them.
- **Leadership:** In a high-functioning team, most or all of the team members have the capability to be the leader. They all accept the leader chosen, they try to help the leader improve leadership skills, and they accept the leader's decisions. When decisions are made between alternatives that are nearly equally good, the leader makes those decisions. In other cases, consensus building is led by the leader. The leader is the outside contact for the team, but the leader always gives credit to the entire team.

- **Automatic Compromise:** Team members often have divergent views. As soon as a team member judges another's view as more beneficial to the team, the team member automatically compromises. Team members compromise; group members negotiate. Compromising is essentially acknowledging another's view as better than one's own. Negotiation is coming to an agreement by surrendering one's position to reach a central position. One irrational result of negotiating is that the final position is influenced by the original position. If one artificially hardens one's initial position, the final outcome will tend to be closer to one's views. Thus, negotiation favors exaggeration of differences, which itself causes group friction.
- **Doing More than Is Expected:** Group members never say, "That's not my job." Team members never think it. Team members always tend toward doing more than their assignment. This decreases the chance that the team result will be adversely affected by errors in planning or work assignments.
- **Time on Task:** Of the time spent, teams generally spend more time on task because they do not waste time complaining or trying to promote themselves over other team members.

28.4. Misconceptions

Teamwork and team building are recognized as essential components in engineering. In fact, they are required of all accredited degree-granting engineering programs in the United States. As stated at the beginning of this chapter, chemical engineers work in teams (or groups) in all aspects of their work. This fact is sometimes misinterpreted in a way that leads to dysfunctional behaviors. Two of the main misconceptions arising in chemical engineering courses are addressed in this section.

28.4.1. Team Exams

"If engineers always work in teams, isn't the most appropriate engineering examination a team exam?" No. Examinations test the ability of an engineering student to do the work of a team member. This is clearly an essential skill for an engineer, and it cannot be evaluated by giving a typical engineering examination to students working as a group. The value of such an examination would be to evaluate the *group*, but not the individual group member.

In practice, there is often only one engineer on a team. When there are multiple engineers, often there is only one chemical engineer. Without development of and evaluation of individual engineering abilities, the chemical engineer would be unprepared to work in a group, let alone on a team.

An extremely effective strategy for developing teamwork skills is to study in a team and be evaluated as an individual.

28.4.2. Overreliance on Team Members

In a group, there will be members of varying expertise and ability. As noted earlier, task differentiation is a characteristic of group work, but no group output should be totally dependent on any one member. A common misconception is that individual members can focus only on a narrow field of expertise because other group members will do the rest. Without task overlap, flexibility, and member backups, a slight disturbance can destroy the group momentum. A chemical engineering student may mistakenly conclude that an understanding of thermodynamics or differential equations is unnecessary because other group members can be relied on. The fallacy of this argument becomes clear when it is remembered that there may be only one engineer in the group. On a team, broad and deep knowledge and understanding of basic engineering concepts are even more essential because a

team member is expected to fill in for another team member—even for a nonengineer. Thus, teamwork requires a broader and higher level of individual abilities, not a narrower or lower level.

28.5. Learning in Teams

Teamwork can occur explicitly as a part of a course, in which case it is called **cooperative** or **collaborative learning**. The team can be formed outside the course structure but with the goal of improving the performance of all team members, in which case it is called a **study group**. In either case, the functioning of the group will be enhanced as it advances toward being a team, as described in Section 28.3.

Learning to be an engineer is a challenging, time-consuming, and complex project—the ideal situation for teamwork.

High achievers and low achievers both improve their learning when they study in teams. In fact, study groups function better for all members when there is a diversity of learners in the group. Although some study groups are formed for specific courses and then disbanded, a more effective scheme is to develop a study group across courses for students in the same curriculum.

The following heuristics apply especially to teams set up with learning as the goal:

- State as a goal that each team member will understand all the material, not that the "team" will understand the material.
- Accept all approaches offered by any team member that lead to a correct answer or help to explain the material.
- Realize that explaining information already understood to another team member will enhance learning for both people.
- Congratulate all team members when everyone understands the material.
- Celebrate high exam scores by any member of the team.
- If a team member does poorly on an exam, make it a team goal to improve that team member's learning.
- Verify learning of each team member for a given learning objective.
- Allow each team member time to do the problem individually. Then compare problem-solving strategies as well as answers.
- Plan "time on task" for the entire team, and share contact information so that individual team members can get assistance when doing assignments alone.
- Test each member of the team; that is, the team assesses individual performance.

Instructors often examine teams by choosing which team member will answer any given question. Because each member is responsible for understanding all of the material studied by the team, all team members receive the grade earned by the single team member chosen. This strategy is consistent with the basis for team learning, and it reinforces the concept that a learning team can claim success only when all team members have acquired the individual knowledge and understanding to be successful.

28.6. Other Reading

In this section, several excellent teamwork resources are listed. Each is easily accessible and can provide more in-depth information and ideas than possible in this chapter. A good team resource library should include each of the references.

Teamwork from Start to Finish [1] by Fran Rees is a fun read (200 pages, paperback) that allows the reader to develop a sense of teamwork quickly. Although it does not go into depth in the various aspects of teamwork, it is an excellent foundation that can be read at leisure. This book (and the other references) is typical of the best teamwork literature. The style is not dense as in a typical engineering textbook. It is meant for a general audience and especially for the standard one-day workshop on teamwork that nearly all U.S. engineers are sent to by their employers.

Although *Problem-Based Learning* [2] by Donald Woods is focused on using teams in learning, its scope includes everything from building a team to being an effective chairperson and from coping creatively with conflict to self-assessment. It has a wealth of essential information on teamwork, and an annotated subject index where one can find definitions of terms as well as key page numbers. Dr. Woods is a chemical engineering professor at McMaster University. His engineering viewpoint is obvious from the directness of his explanations of what works and from his many tables, forms, figures, and mind maps. There are problems at the end of each chapter to help the reader process and internalize the information presented.

Kimball Fisher and colleagues present the 100 most common problems that teams encounter and several suggested solutions for each in *Tips for Teams* [3]. This is one of the most popular and accessible of the books that offer advice on how to avoid and to correct conflicts in teamwork.

Although all of these resource books have sections or chapters on leadership skills, anyone who ever wants to be a team leader should read at least one book focused on developing these specific skills. *Leading Self-Directed Work Teams* [4] by Kimball Fisher is an excellent choice.

Every team needs a plan, and the most common planning technique is the Gantt chart. The lively and short article by Jeff Dewar [6] demonstrates the technique and shows why it is so powerful. It is all the reference needed to develop and use Gantt charts.

Teamwork and Project Management [7] by Karl Smith of the University of Minnesota teaches engineering students to work effectively and efficiently in project teams. Case studies of student work demonstrate the various aspects of project work, including the project life cycle, project scoping, monitoring, documentation, and scheduling. The explanation of the critical path method is excellent, as are the chapters on teamwork skills.

The Team Handbook [8] by Peter Scholtes and colleagues is considered by many in industry as a teamwork bible. It has been used in one-day and two-day workshops by companies since the late 1980s, and its format is geared to that application. It is about 200 pages and spiral-bound, with plenty of blank space on every page for notes. The many forms, lists, and guidelines are meant to be used in a team setting to identify problems, understand group behaviors, and move the group toward effective teamwork. The viewpoint of the authors is a common management strategy, continuous quality improvement, that demands teamwork.

Donald Woods has been a world leader in problem solving for decades. Many of the resource materials from his McMaster Problem Solving (MPS) program are available from him through the Web [9]. A particularly useful module is No. 28 on evaluating group skills.

The U.S. National Aeronautics and Space Administration (NASA) provides a library Web site with lists of articles, books, and Internet resources on a wide range of topics. Two of the lists dealing with

teamwork are listed along with their URLs [10]. These are excellent bibliographies.

H. Scott Fogler and Steven LeBlanc's *Strategies for Creative Problem Solving* [11] provides a wide array of exercises for use in team building. Through focusing on the stages of problem solving and the various proven heuristics for implementing them, these authors provide teamwork strategies that can be implemented immediately.

28.7. Summary

Good engineers are team animals. One of their finely honed *individual* skills is the ability to be an excellent *team* member.

In this introductory chapter about teamwork, the features of groups that make them effective and efficient were introduced. Heuristics were given to enhance teamwork by reducing the friction that can build in groups. The four stages of group evolution were described and examples given. The concept of a team as the ultimate group was presented, and misconceptions about individual responsibility versus team responsibility were discussed. Beyond this chapter, there is a wealth of literature on the subject. Some of the most useful resources were described.

What You Should Have Learned

- Teamwork is essential in the chemical process industry.
- Characteristics of effective teams include the following:
  - Members do different tasks, but total compartmentalization is avoided.
  - The work environment is supportive.
  - Members work on tasks appropriate to their skills.
- Characteristics of teams that should be avoided include
  - Unequal work distribution
  - Not having a leader or coordinator
  - Assigning blame for errors or incorrect team decisions

References

1. Rees, F., *Teamwork from Start to Finish: 10 Steps to Results* (San Francisco: Jossey-Bass, 1997).
2. Woods, D. R., *Problem-Based Learning: How to Gain the Most from PBL* (Hamilton, Ontario, Canada: McMaster University Bookstore, 1994).
3. Fisher, K., W. Belgard, and S. Rayner, *Tips for Teams: A Ready Reference for Solving Common Team Problems* (New York: McGraw-Hill, 1995).
4. Fisher, K., *Leading Self-Directed Work Teams: A Guide to Developing New Team Leadership Skills*, 2nd ed. (New York: McGraw-Hill, 1999).
5. Tuckman, B. W., "Development Sequence in Small Groups," *Psychological Bulletin* 63 (1965): 384.
6. Dewar, J. D., "If You Don't Know Where You're Going, How Will You Know When You Get There?" *CHEMTECH* 19, no. 4 (1989): 214–217.

7. Smith, K. A., *Teamwork and Project Management*, 3rd ed. (New York: McGraw-Hill, 2007).
8. Scholtes, P. R., B. L. Joiner, and B. J. Streibel, *The Team Handbook*, 3rd ed. (Madison, WI: Oriel, 2003).
9. Woods, D. R., *Group Skills*, available at http://www.chemeng.mcmaster.ca/innov1.htm as MPS-28, 1998.
10. NASA Headquarters Library Bibliographies, *Interpersonal Relations and Group Dynamics*, 2007 (http://www.hq.nasa.gov/office/hqlibrary/ppm/ppm29.htm), and *Teams and Teamwork*, 2007 (http://www.hq.nasa.gov/office/hqlibrary/ppm/ppm5.htm).
11. Fogler, H. S., and S. E. LeBlanc, *Strategies for Creative Problem Solving*, 2nd ed. (Upper Saddle River, NJ: Prentice Hall, 2008).

Problems

These problems are not like normal homework problems to be done after just reading the chapter. Instead, they are assignments that should be done in the context of an actual group activity to improve group process. Although a group of four or five students is envisioned, the exercises will work with somewhat larger or smaller groups. They are often used during class sessions so that the instructor can provide immediate feedback.

1. In turn, each group member describes the last homework assignment submitted, sharing the strategy used to solve the problem. The assignment chosen should have been done individually. After each member's strategy has been described, the group should discuss the value in each strategy. The goal is not to rank the strategies but to develop respect for each strategy through constructive discussion. After the discussion, the group answers the question, "What have we learned from this exercise?"
2. Each group member describes the most valuable course taken so far and why that course was so valuable. Then the group brainstorms criteria for determining the value of a course. After developing a list of 20 criteria in two minutes, the group creates a set of three criteria to use in assessing courses by developing a consensus rather than voting.
3. As a group, develop a set of norms for a study group. Address such issues as who will be the leader, when and where the group should meet, how much preparation is expected of each member before each meeting, the agenda for a typical meeting, and how the success of the group will be assessed.
4. Within the context of a group design project, meet to discuss and plan task differentiation. When the plan is complete, answer the following questions:
   a. What happens if one of the group members becomes ill and cannot complete the assigned task? (In turns, do this for each member.)
   b. For which tasks is there overlap? Why?
   c. What percent of the effort is being done by each group member?
5. For the last group project completed, each group member fills out the form in Figure 28.1. One group member then collates the responses in a spreadsheet, and the group discusses how the group performed on the project. Finally, the group prepares a list of ways to improve the group work in future projects.
6. Repeat Problem 28.1 for the last examination taken. Be sure to discuss timing as well as

problem-solving strategies used.

7. Each group member describes an example of friction in a prior group situation, and the group does the following:
   a. Determines which of the categories of friction from Section 28.1.3 best describes the example.
   b. Develops a suggestion for how the situation could have been handled better.
8. For your most productive group experience, analyze whether it was a "team," using the characteristics of teams given in Section 28.3.2.
9. Each group member chooses several chapters of references [1], [3], [4], or [7]. Read them and report to the group how the strategies presented can help improve group effectiveness and efficiency.
10. Choose the most difficult course you are likely to face next semester, and create a Gantt chart for succeeding in it. (If you are finishing this semester, choose finding a job or making the best impression in the job you have already chosen.)

Appendix A. Cost Equations and Curves for the CAPCOST Program

The purpose of this appendix is to present the equations and figures that describe the relationships used in the capital equipment-costing program CAPCOST introduced in Chapter 7 and used throughout the text. The program is based on the module factor approach to costing that was originally introduced by Guthrie [1, 2] and modified by Ulrich [3].

A.1. Purchased Equipment Costs

All the data for the purchased cost of equipment for the second edition of this book were obtained from a survey of equipment manufacturers during the period May to September of 2001, so an average value of the CEPCI of 397 over this period should be used when accounting for inflation.

Additional process equipment has been added to the third edition and is listed below:

- Conveyors
- Crystallizers
- Dryers
- Dust Collectors
- Filters
- Mixers
- Reactors
- Screens

The purchased costs for these types of equipment were obtained in 2003, but the costs given here have been normalized to 2001. For this new equipment, bare module factors were not available, nor were pressure factors or materials of construction factors. In general, these units are generally bought as a package, and installation in the plant is not expensive. The bare module factors for these units are taken to be the field installation factors given by Guthrie [1, 2].

Data for the purchased cost of the equipment, at ambient operating pressure and using carbon steel construction, C^o_p, were fitted to the following equation:

$$\log_{10} C^o_p = K_1 + K_2 \log_{10}(A) + K_3[\log_{10}(A)]^2 \qquad \text{(A.1)}$$

where A is the capacity or size parameter for the equipment. The data for K_1, K_2, and K_3, along with the maximum and minimum values used in the correlation, are given in Table A.1. These data are also presented in the form of graphs in Figures A.1–A.17. It should be noted that in these figures, the data are plotted as C^o_p/A as a function of size attribute A. This form of the graph clearly illustrates the decreasing cost per unit of capacity as the size of the equipment increases.

Table A.1. Equipment Cost Data to Be Used with Equation (A.1)

Equipment Type	Equipment Description	K_1	K_2	K_3	Capacity, Units	Min Size	Max Size
Blenders	Kneader	5.0141	0.5867	0.3224	Volume, m^2	0.14	3
	Ribbon	4.1366	0.5072	0.0070	Volume, m^2	0.7	11
	Rotary	4.1366	0.5072	0.0070	Volume, m^2	0.7	11
Centrifuges	Auto batch separator	4.7681	0.9740	0.0240	Diameter, m	0.5	1.7
	Centrifugal separator	4.3612	0.8764	–0.0049	Diameter, m	0.5	1
	Oscillating screen	4.8600	0.3340	0.1063	Diameter, m	0.5	1.1
	Solid bowl w/o motor	4.9697	1.1689	0.0038	Diameter, m	0.3	2
Compressors	Centrifugal, axial, and reciprocating	2.2897	1.3604	−0.1027	Fluid power, kW	450	3000
	Rotary	5.0355	−1.8002	0.8253	Fluid power, kW	18	950
Conveyors	Apron	3.9255	0.5039	0.1506	Area, m^2	1.0	15
	Belt	4.0637	0.2584	0.1550	Area, m^2	0.5	325
	Pneumatic	4.6616	0.3205	0.0638	Area, m^2	0.75	65
	Screw	3.6062	0.2659	0.1982	Area, m^2	0.5	30
Crystallizers	Batch	4.5097	0.1731	0.1344	Volume, m^3	1.5	30
Drives	Gas turbine	−21.7702	13.2175	−1.5279	Shaft power, kW	7500	23,000
	Intern comb. engine	2.7635	0.8574	−0.0098	Shaft power, kW	10	10,000
	Steam turbine	2.6259	1.4398	−0.1776	Shaft power, kW	70	7500
	Electric—explosion-proof	2.4604	1.4191	−0.1798	Shaft power, kW	75	2600
	Electric—totally enclosed	1.9560	1.7142	−0.2282	Shaft power, kW	75	2600
	Electric—open/drip-proof	2.9508	1.0688	−0.1315	Shaft power, kW	75	2600
Dryers	Drum	4.5472	0.2731	0.1340	Area, m^2	0.5	50
	Rotary, gas fired	3.5645	1.1118	–0.0777	Area, m^2	5	100
	Tray	3.6951	0.5442	–0.1248	Area, m^2	1.8	20
Dust Collectors	Baghouse	4.5007	0.4182	0.0813	Volume, m^3	0.08	350
	Cyclone scrubbers	3.6298	0.5009	0.0411	Volume, m^3	0.06	200
	Electrostatic precipitator	3.6298	0.5009	0.0411	Volume, m^3	0.06	200
	Venturi scrubber	3.6298	0.5009	0.0411	Volume, m^3	0.06	200
Evaporators	Forced circulation (pumped)	5.0238	0.3475	0.0703	Area, m^2	5	1000

	Falling film	3.9119	0.8627	−0.0088	Area, m^2	50	500
	Agitated film (scraped wall)	5.0000	0.1490	−0.0134	Area, m^2	0.5	5
	Short tube	5.2366	−0.6572	0.3500	Area, m^2	10	100
	Long tube	4.6420	0.3698	0.0025	Area, m^2	100	10,000
Fans	Centrifugal radial	3.5391	−0.3533	0.4477	Gas flowrate, m^3/s	1	100
	Backward curve	3.3471	−0.0734	0.3090	Gas flowrate, m^3/s	1	100
	Axial vane	3.1761	−0.1373	0.3414	Gas flowrate, m^3/s	1	100
	Axial tube	3.0414	−0.3375	0.4722	Gas flowrate, m^3/s	1	100
Filters	Bent	5.1055	0.4999	0.0001	Area, m^2	0.9	115
	Cartridge	3.2107	0.7597	0.0027	Area, m^2	15	200
	Disc and drum	4.8123	0.2858	0.0420	Area, m^2	0.9	300
	Gravity	4.2756	0.3520	0.0714	Area, m^2	0.5	80
	Leaf	3.8187	0.6235	0.0176	Area, m^2	0.6	235
	Pan	4.8123	0.2858	0.0420	Area, m^2	0.9	300
	Plate and frame	4.2756	0.3520	0.0714	Area, m^2	0.5	80
	Table	5.1055	0.4999	0.0001	Area, m^2	0.9	115
	Tube	5.1055	0.4999	0.0001	Area, m^2	0.9	115
Furnaces	Reformer furnace	3.0680	0.6597	0.0194	Duty, kW	3000	100,000
	Pyrolysis furnace	2.3859	0.9721	−0.0206	Duty, kW	3000	100,000
	Nonreactive fired heater	7.3488	−1.1666	0.2028	Duty, kW	1000	100,000
Heat exchangers	Scraped wall	3.7803	0.8569	0.0349	Area, m^2	2	20
	Teflon tube	3.8062	0.8924	−0.1671	Area, m^2	1	10
	Bayonet	4.2768	−0.0495	0.1431	Area, m^2	10	1000
	Floating head	4.8306	−0.8509	0.3187	Area, m^2	10	1000
	Fixed tube	4.3247	−0.3030	0.1634	Area, m^2	10	1000
	U-tube	4.1884	−0.2503	0.1974	Area, m^2	10	1000
	Kettle reboiler	4.4646	−0.5277	0.3955	Area, m^2	10	100
	Double pipe	3.3444	0.2745	−0.0472	Area, m^2	1	10
	Multiple pipe	2.7652	0.7282	0.0783	Area, m^2	10	100
	Flat plate	4.6656	−0.1557	0.1547	Area, m^2	10	1000
	Spiral plate	4.6561	−0.2947	0.2207	Area, m^2	1	100

	Air cooler	4.0336	0.2341	0.0497	Area, m^2	10	10,000
	Spiral tube	3.9912	0.0668	0.2430	Area, m^2	1	100
Heaters	Diphenyl heater	2.2628	0.8581	0.0003	Duty, kW	650	10,750
	Molten salt heater	1.1979	1.4782	−0.0958	Duty, kW	650	10,750
	Hot water heater	2.0829	0.9074	−0.0243	Duty, kW	650	10,750
	Steam boiler	6.9617	−1.4800	0.3161	Duty, kW	1200	9400
Mixers	Impeller	3.8511	0.7009	–0.0003	Power, kW	5	150
	Propeller	4.3207	0.0359	0.1346	Power, kW	5	500
	Turbine	3.4092	0.4896	0.0030	Power, kW	5	150
Packing	Loose (for towers)	2.4493	0.9744	0.0055	Volume, m^3	0.03	628
Process vessels	Horizontal	3.5565	0.3776	0.0905	Volume, m^3	0.1	628
	Vertical	3.4974	0.4485	0.1074	Volume, m^3	0.3	520
Pumps	Reciprocating	3.8696	0.3161	0.1220	Shaft power, kW	0.1	200
	Positive displacement	3.4771	0.1350	0.1438	Shaft power, kW	1	100
	Centrifugal	3.3892	0.0536	0.1538	Shaft power, kW	1	300
Reactors	Autoclave	4.5587	0.2986	0.0020	Volume, m^3	1	15
	Fermenter	4.1052	0.5320	–0.0005	Volume, m^3	0.1	35
	Inoculum tank	3.7957	0.4593	0.0160	Volume, m^3	0.07	1
	Jacketed agitated	4.1052	0.5320	–0.0005	Volume, m^3	0.1	35
	Jacketed nonagitated	3.3496	0.7235	0.0025	Volume, m^3	5	45
	Mixer/settler	4.7116	0.4479	0.0004	Volume, m^3	0.04	60
Screens	DSM	3.8050	0.5856	0.2120	Area, m^2	0.3	6
	Rotary	4.0485	0.1118	0.3260	Area, m^2	0.3	15
	Stationary	3.8219	1.0368	–0.6050	Area, m^2	2	11
	Vibrating	4.0485	0.1118	0.3260	Area, m^2	0.3	15
Tanks	API—fixed roof	4.8509	−0.3973	0.1445	Volume, m^3	90	30,000
	API—floating roof	5.9567	−0.7585	0.1749	Volume, m^3	1000	40,000
Towers	Tray and packed	3.4974	0.4485	0.1074	Volume, m^3	0.3	520
Trays	Sieve	2.9949	0.4465	0.3961	Area, m^2	0.07	12.30
	Valve	3.3322	0.4838	0.3434	Area, m^2	0.70	10.50
	Demisters	3.2353	0.4838	0.3434	Area, m^2	0.70	10.50
Turbines	Axial gas turbines	2.7051	1.4398	–0.1776	Fluid power, kW	100	4000
	Radial gas/liquid expanders	2.2476	1.4965	–0.1618	Fluid power, kW	100	1500
Vaporizers	Internal coils/jackets	4.0000	0.4321	0.1700	Volume, m^3	1	100
	Jacketed vessels	3.8751	0.3328	0.1901	Volume, m^3	1	100

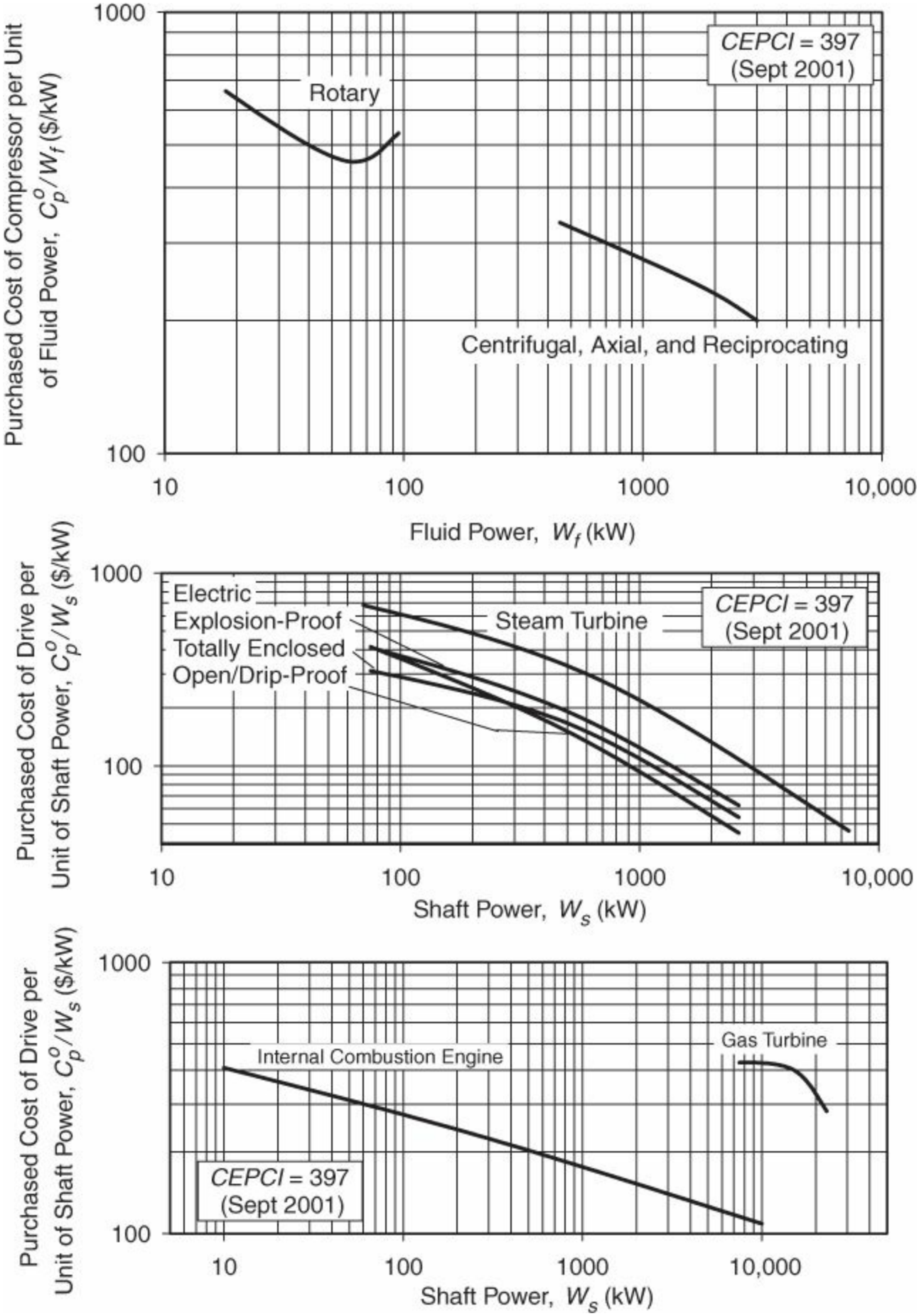


Figure A.1. Purchased Costs for Compressors and Drives (Cost Data for Compressors and Drives Taken from R-Books Software by Richardson Engineering Services, Inc. [4])

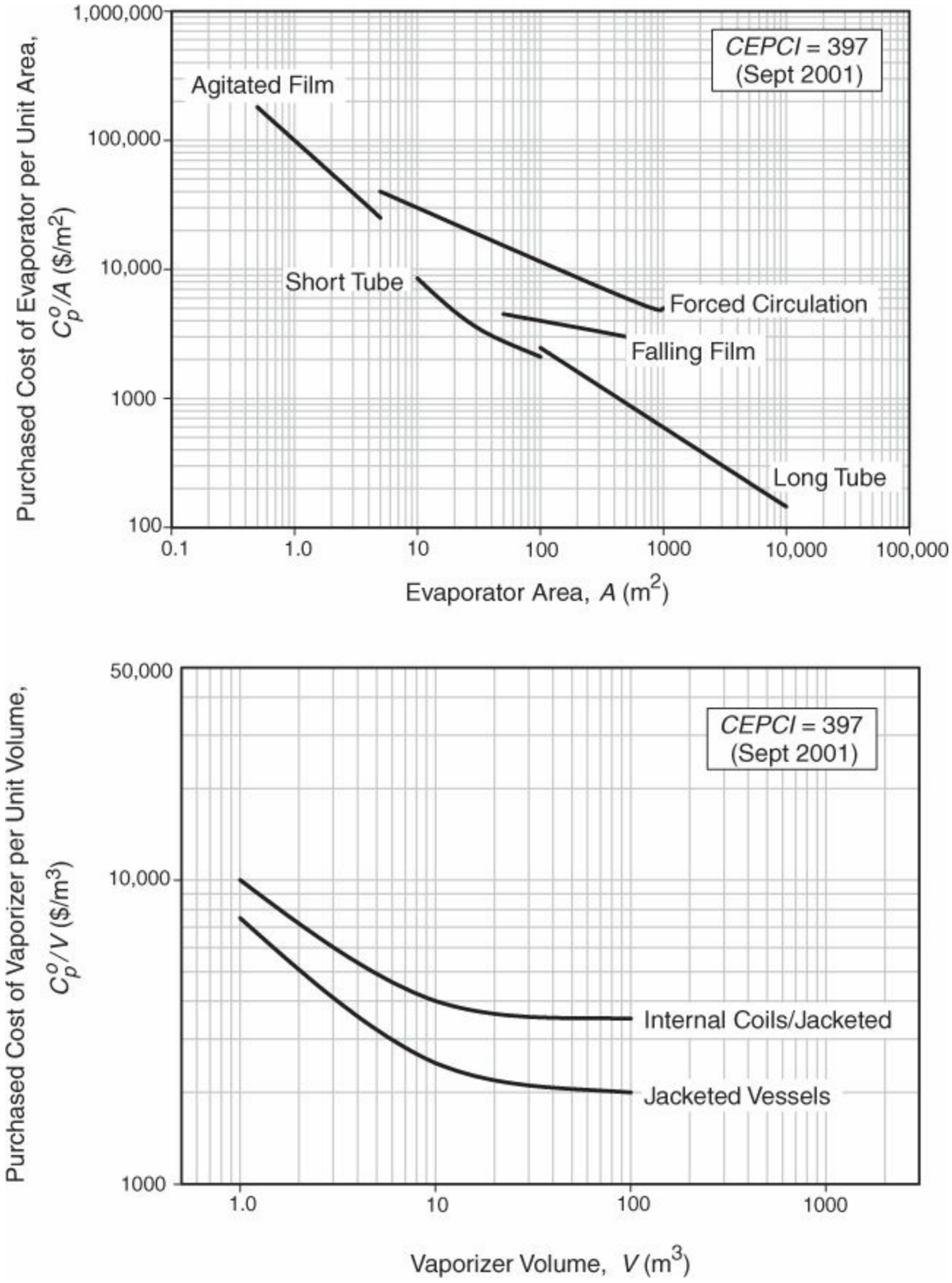


Figure A.2. Purchased Costs for Evaporators and Vaporizers

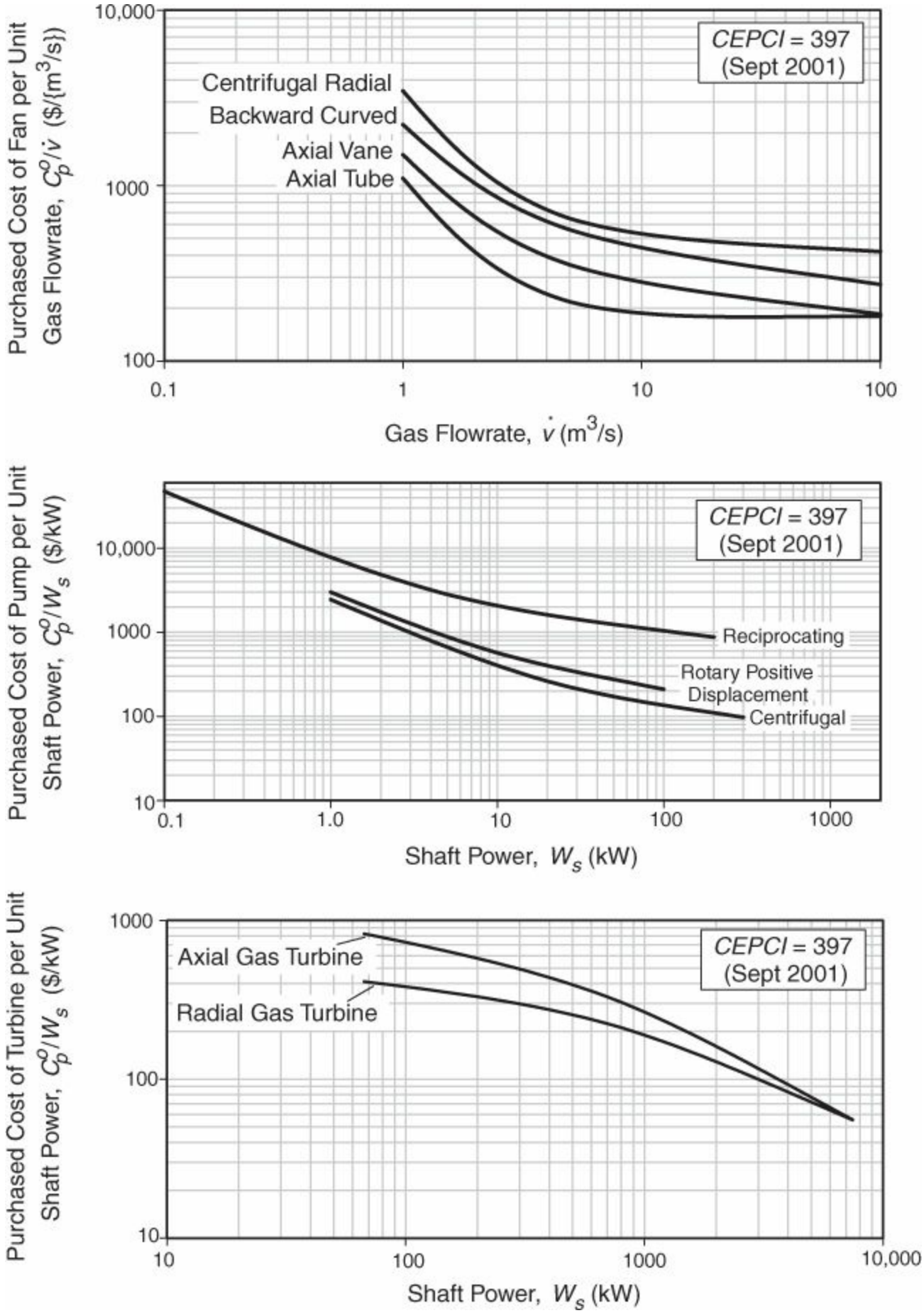
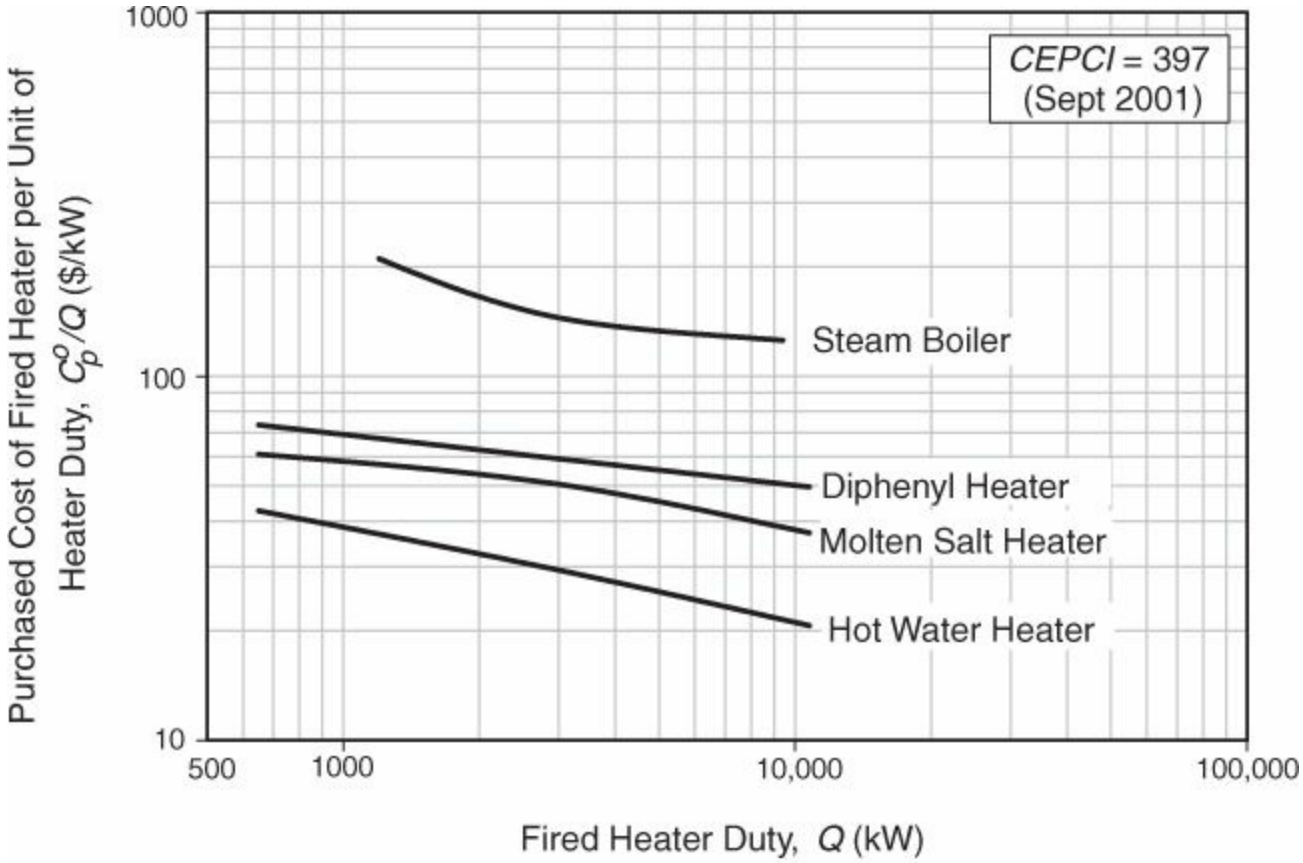


Figure A.3. Purchased Costs for Fans, Pumps, and Power Recovery Equipment (Cost Data for Fans Taken from R-Books Software by Richardson Engineering Services, Inc. [4])



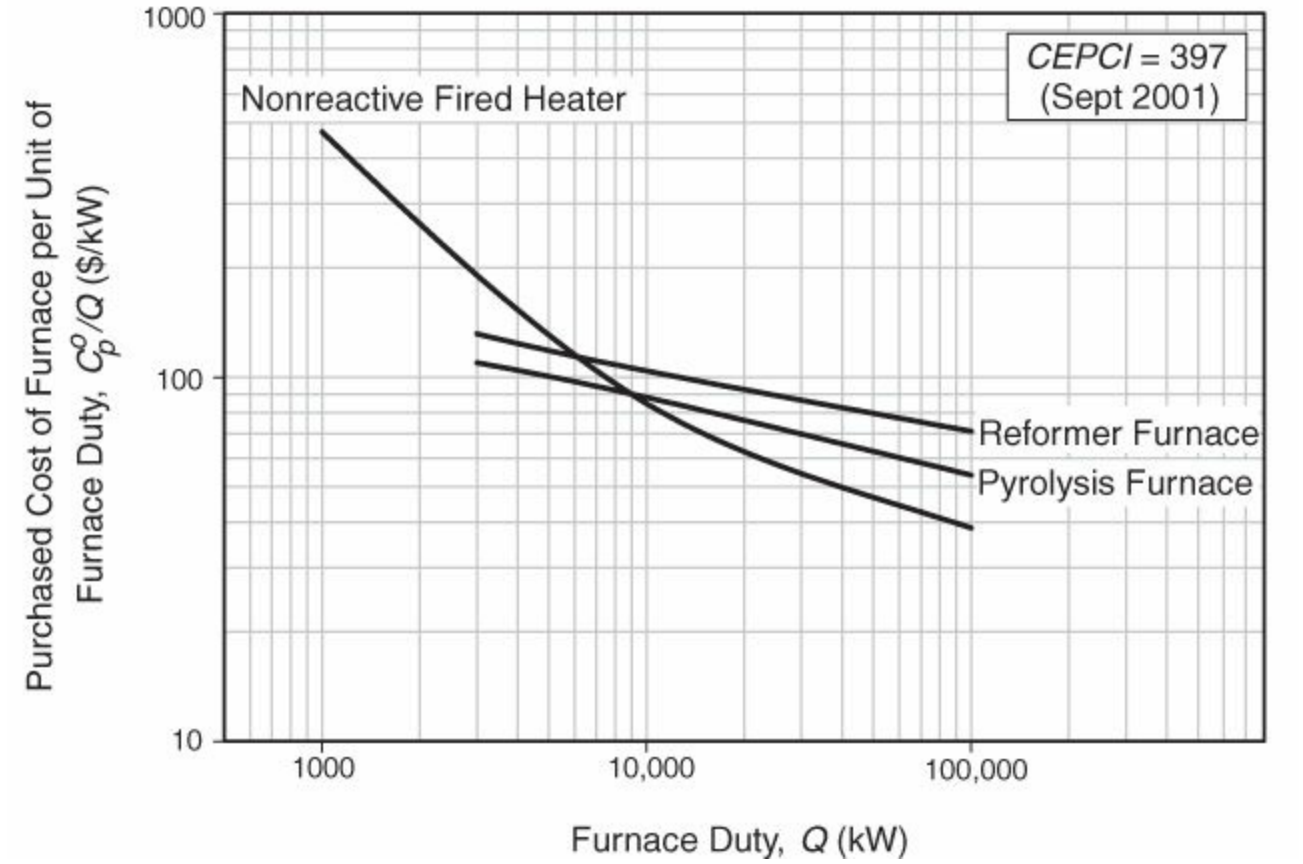


Figure A.4. Purchased Costs for Fired Heaters and Furnaces

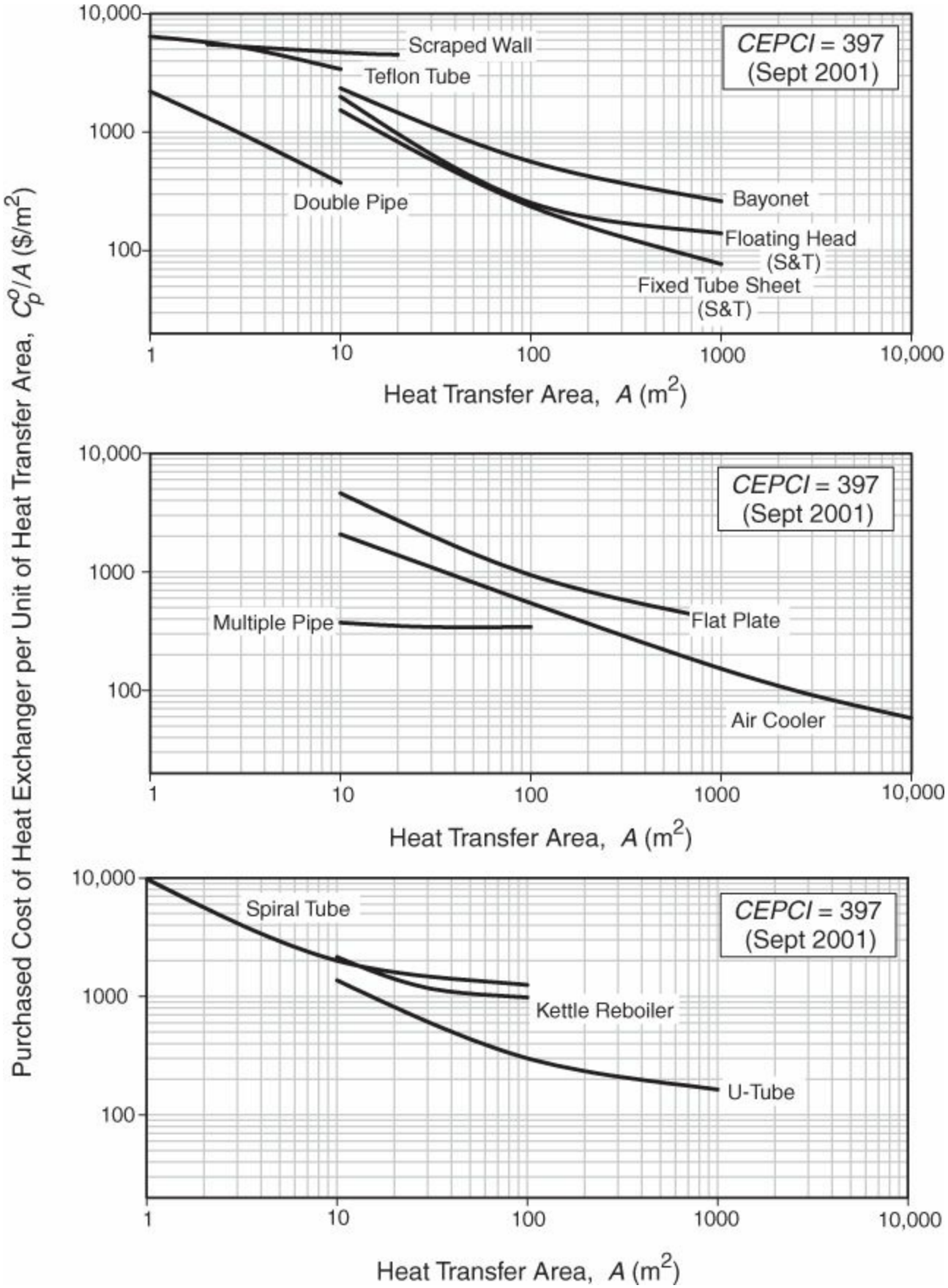
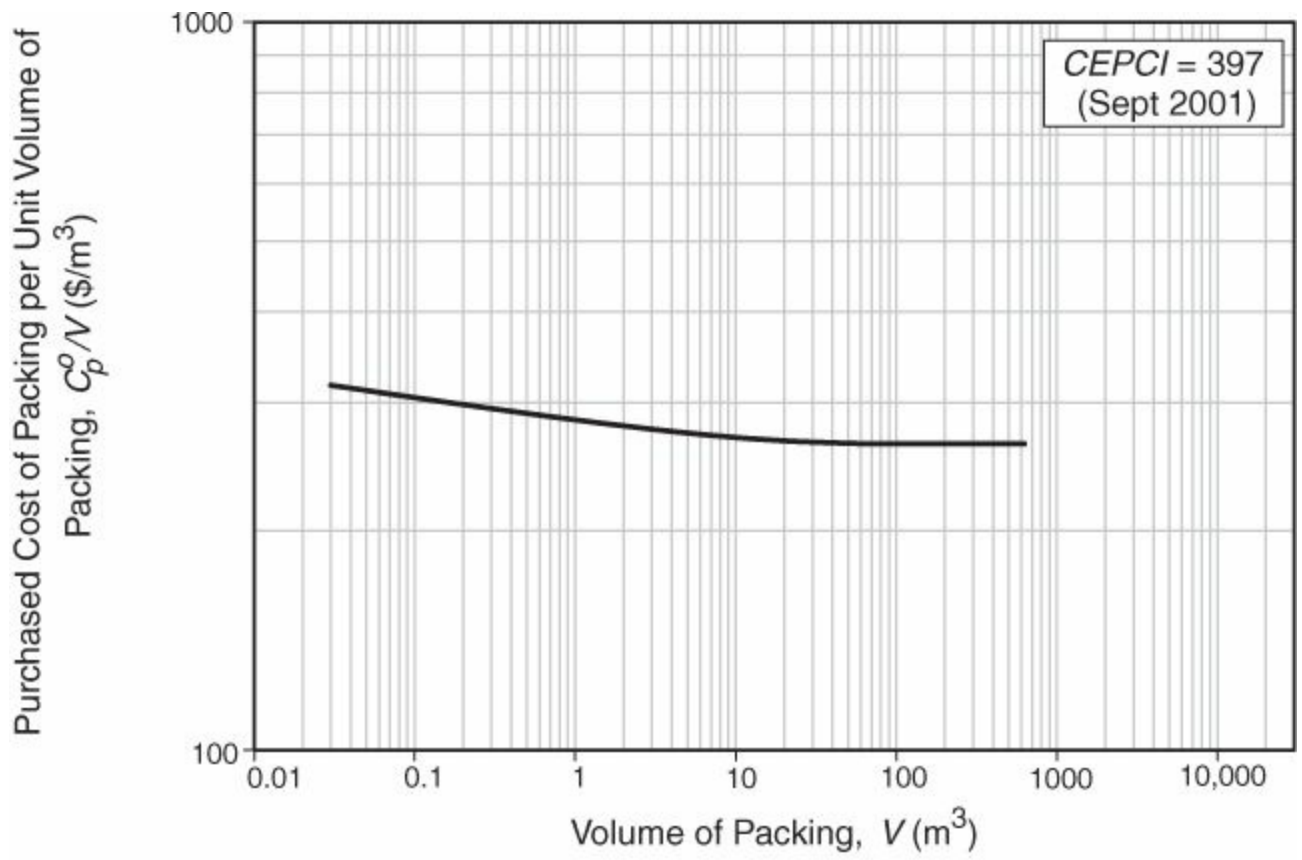


Figure A.5. Purchased Costs for Heat Exchangers



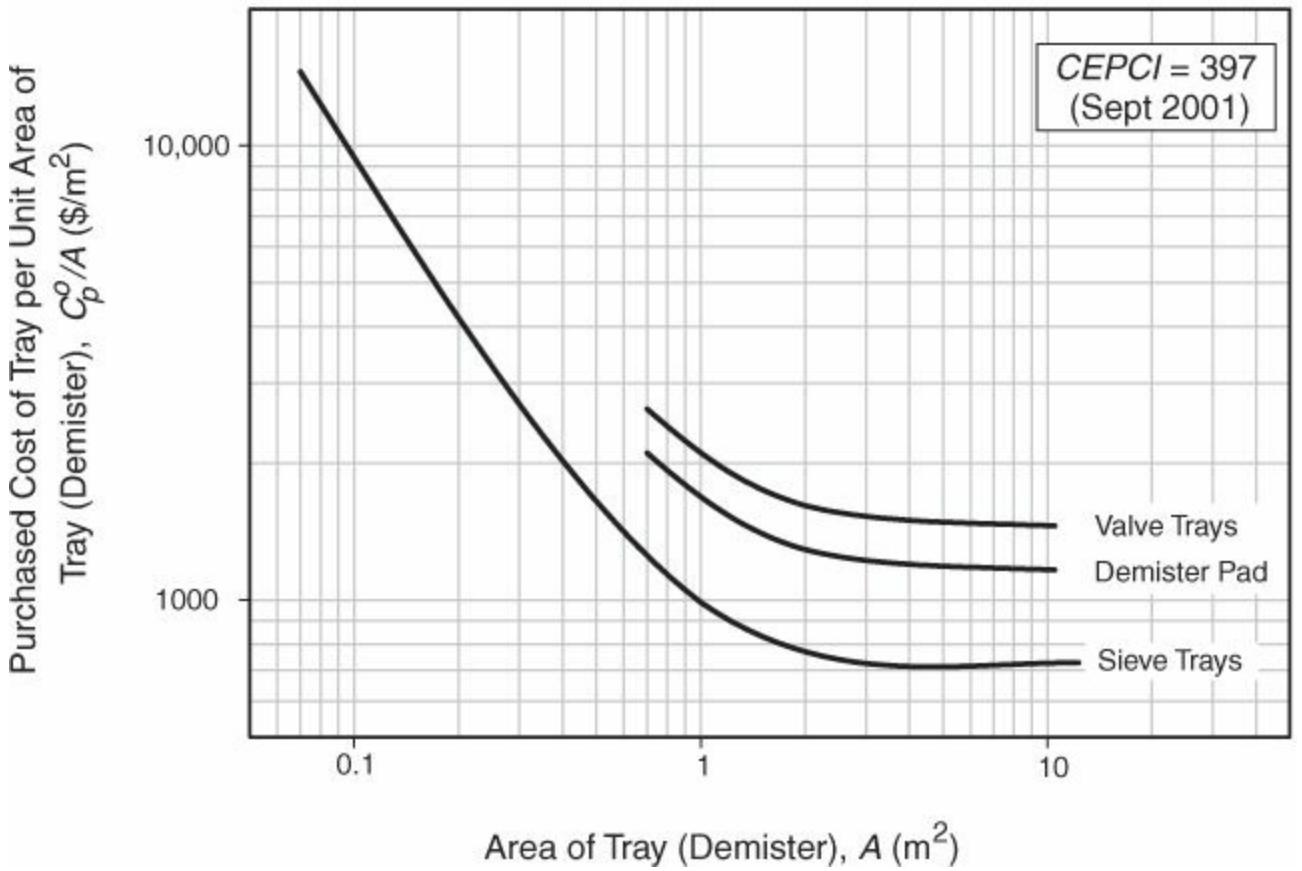


Figure A.6. Purchased Costs for Packing, Trays, and Demisters

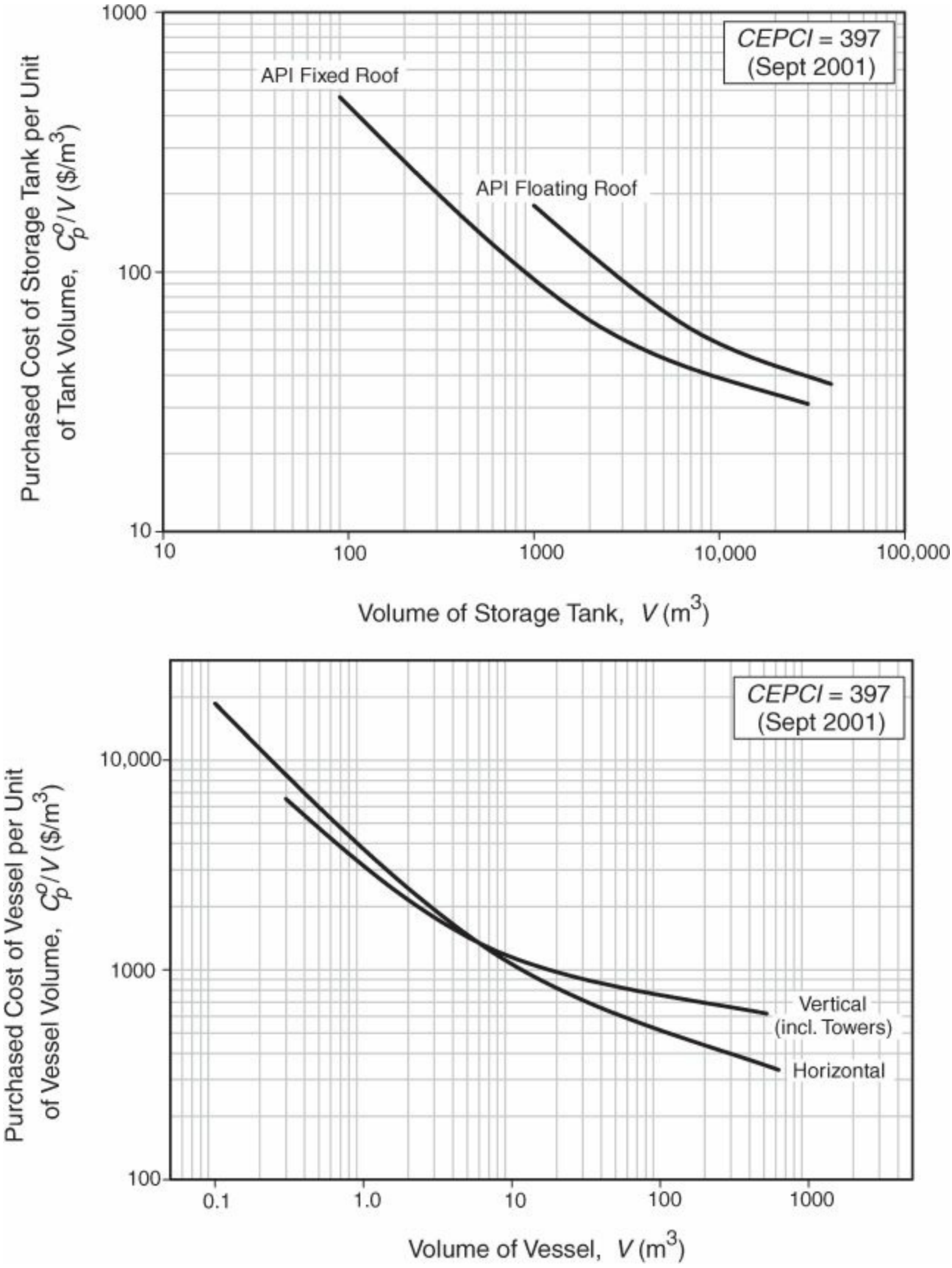


Figure A.7. Purchased Costs for Storage Tank and Process Vessels (Data for Storage Tanks Taken from R-Books Software by Richardson Engineering Services, Inc. [4])

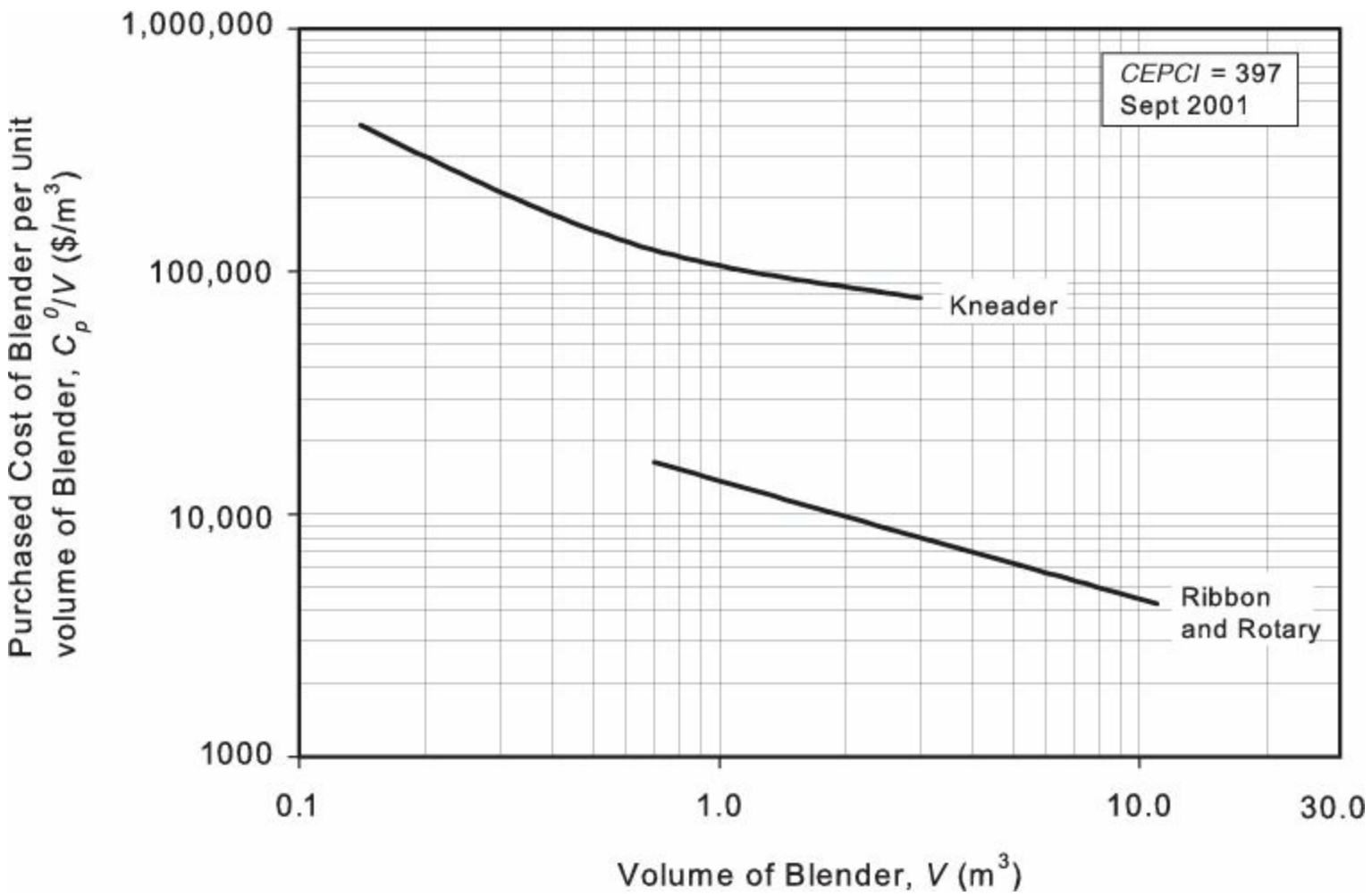


Figure A.8. Purchased Costs for Blenders

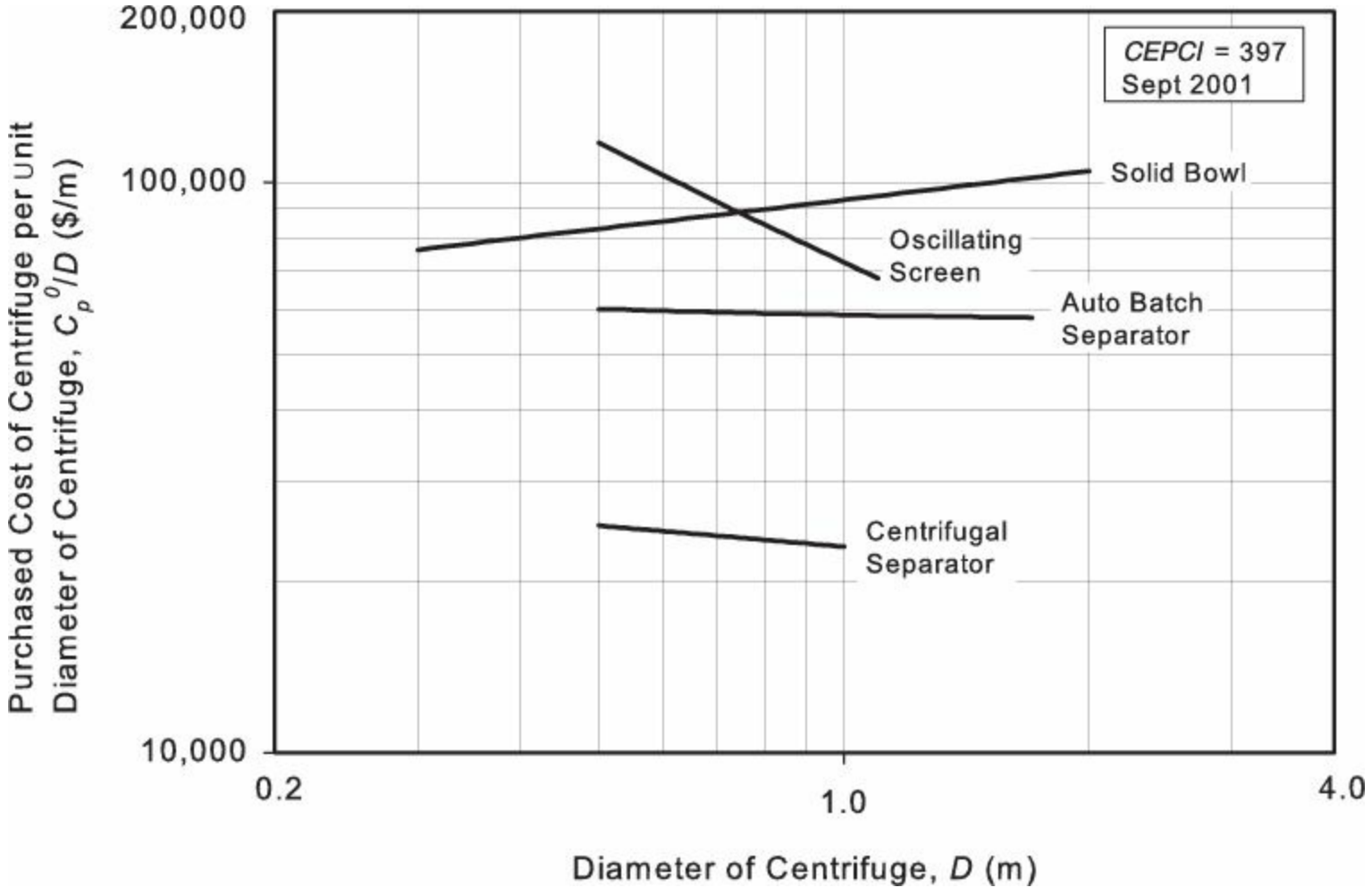


Figure A.9. Purchased Costs for Centrifuges

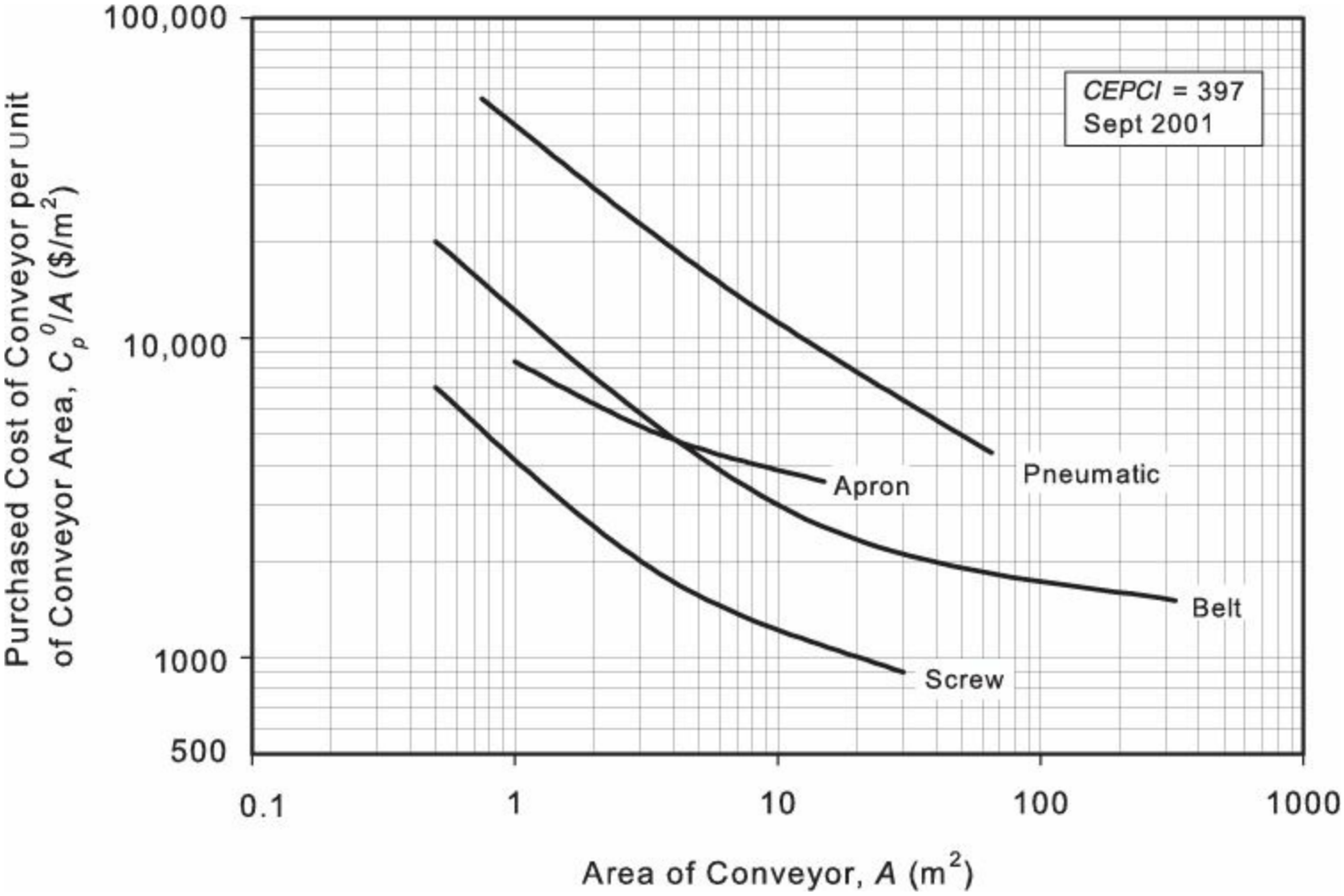


Figure A.10. Purchased Costs for Conveyors

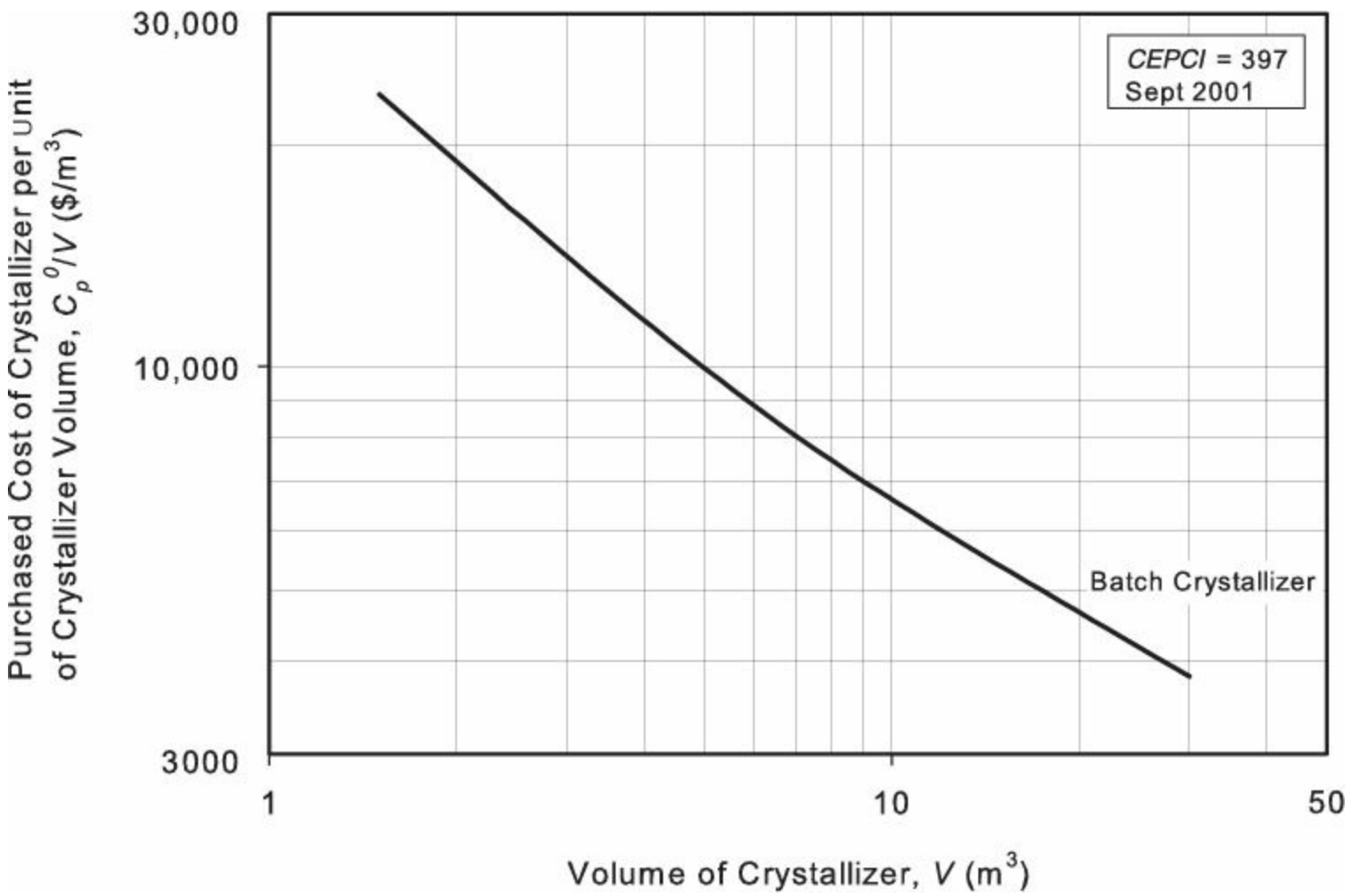


Figure A.11. Purchased Costs for Crystallizers

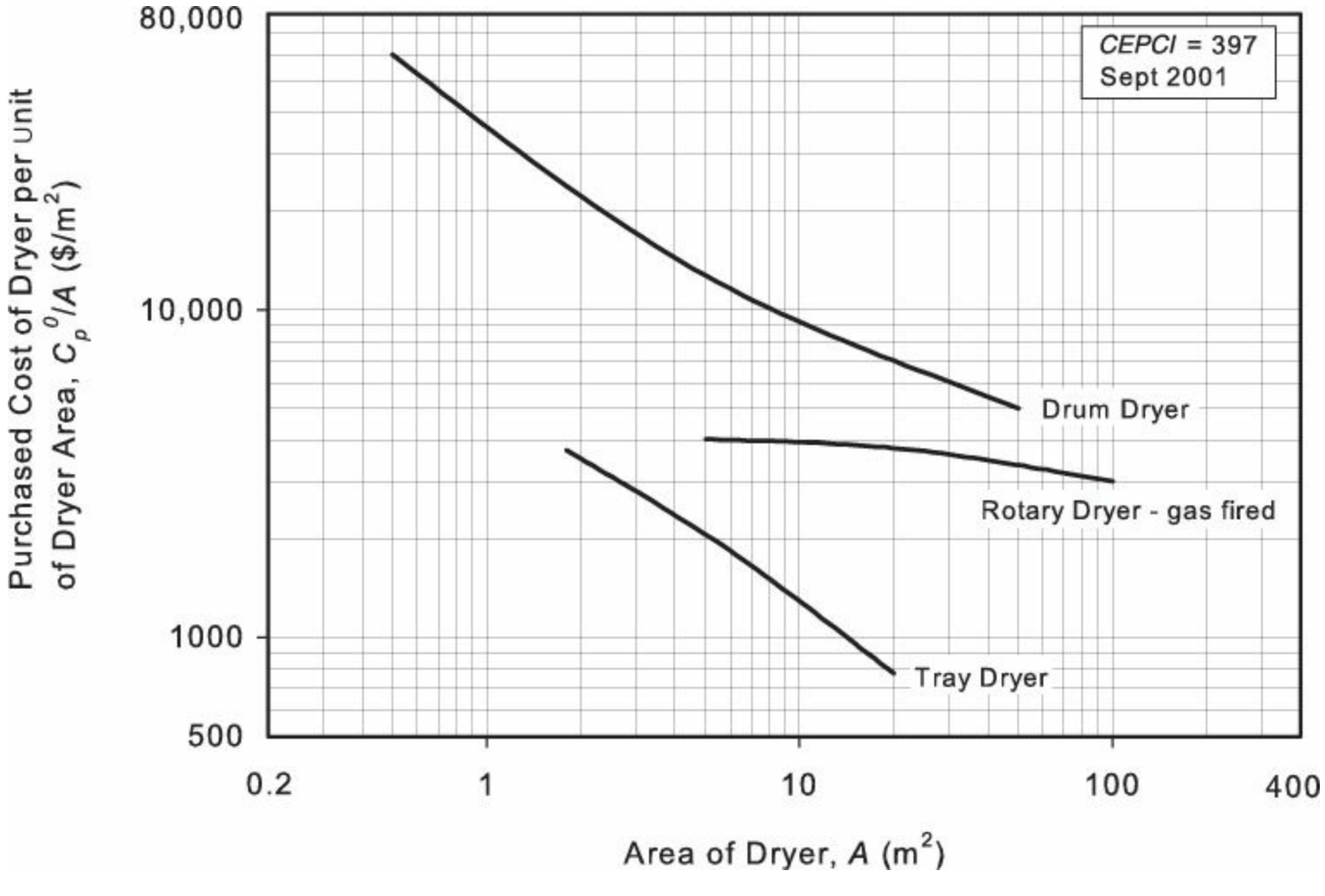


Figure A.12. Purchased Costs for Dryers

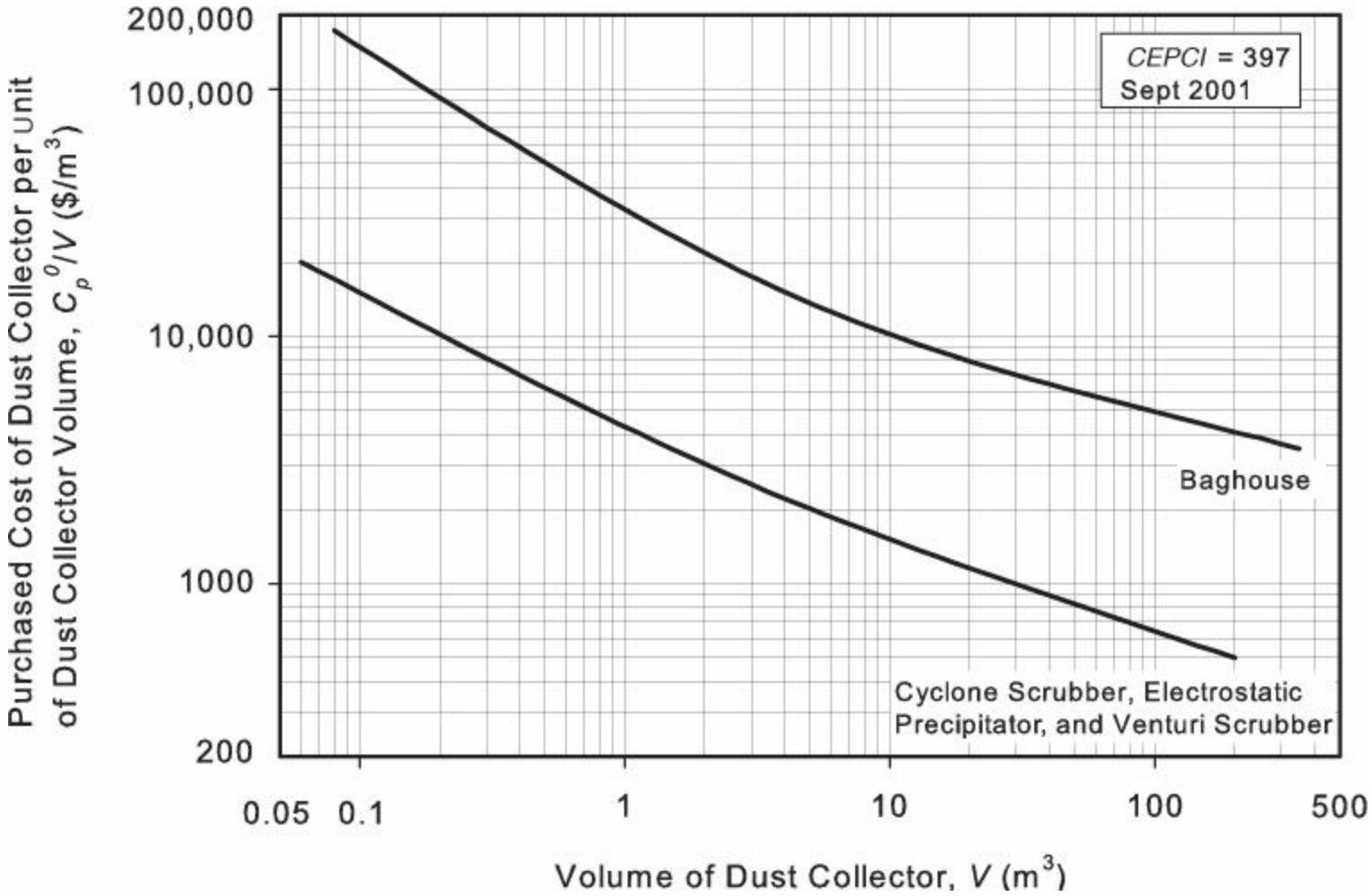


Figure A.13. Purchased Costs for Dust Collectors

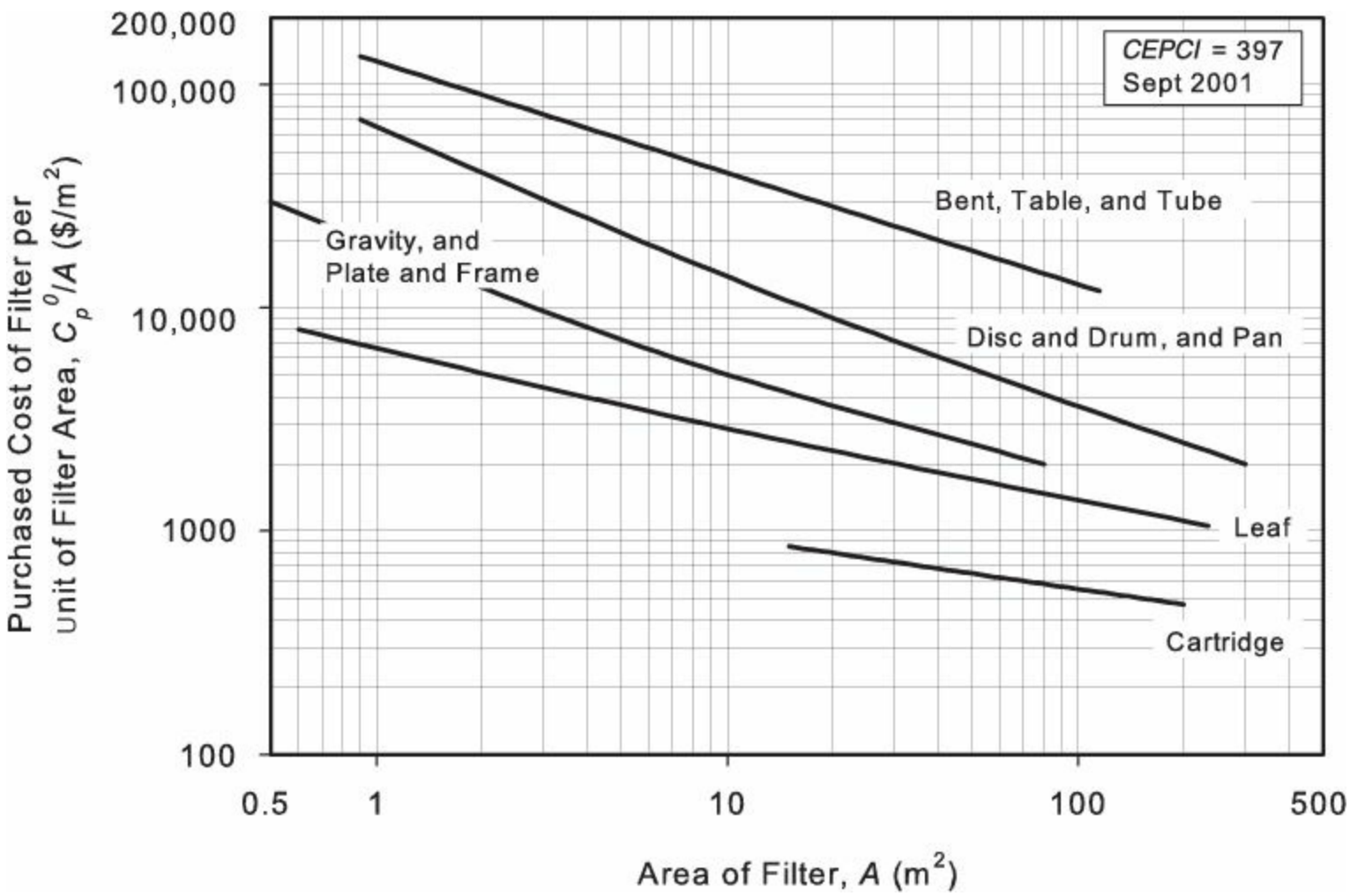


Figure A.14. Purchased Costs for Filters

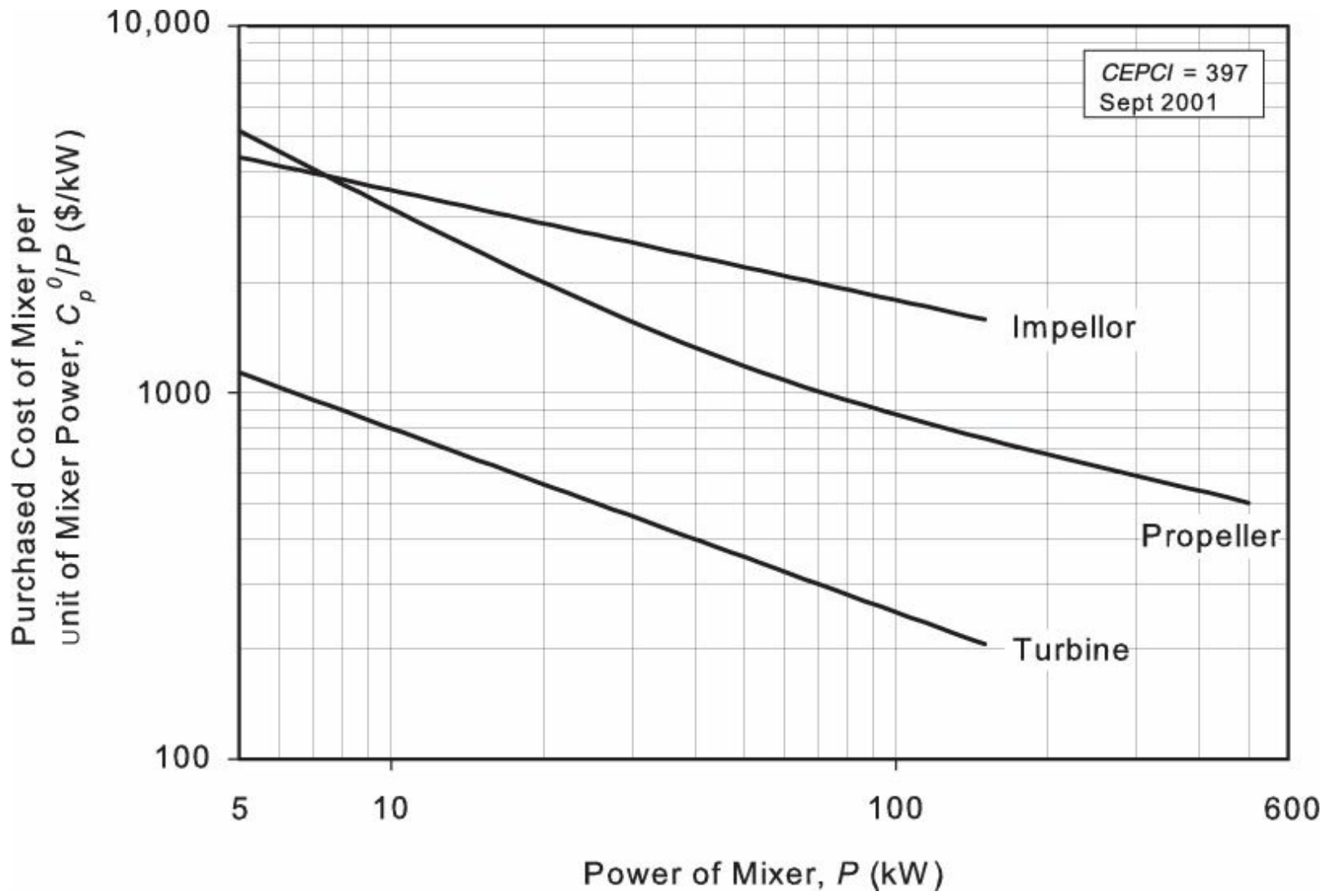


Figure A.15. Purchased Costs for Mixers

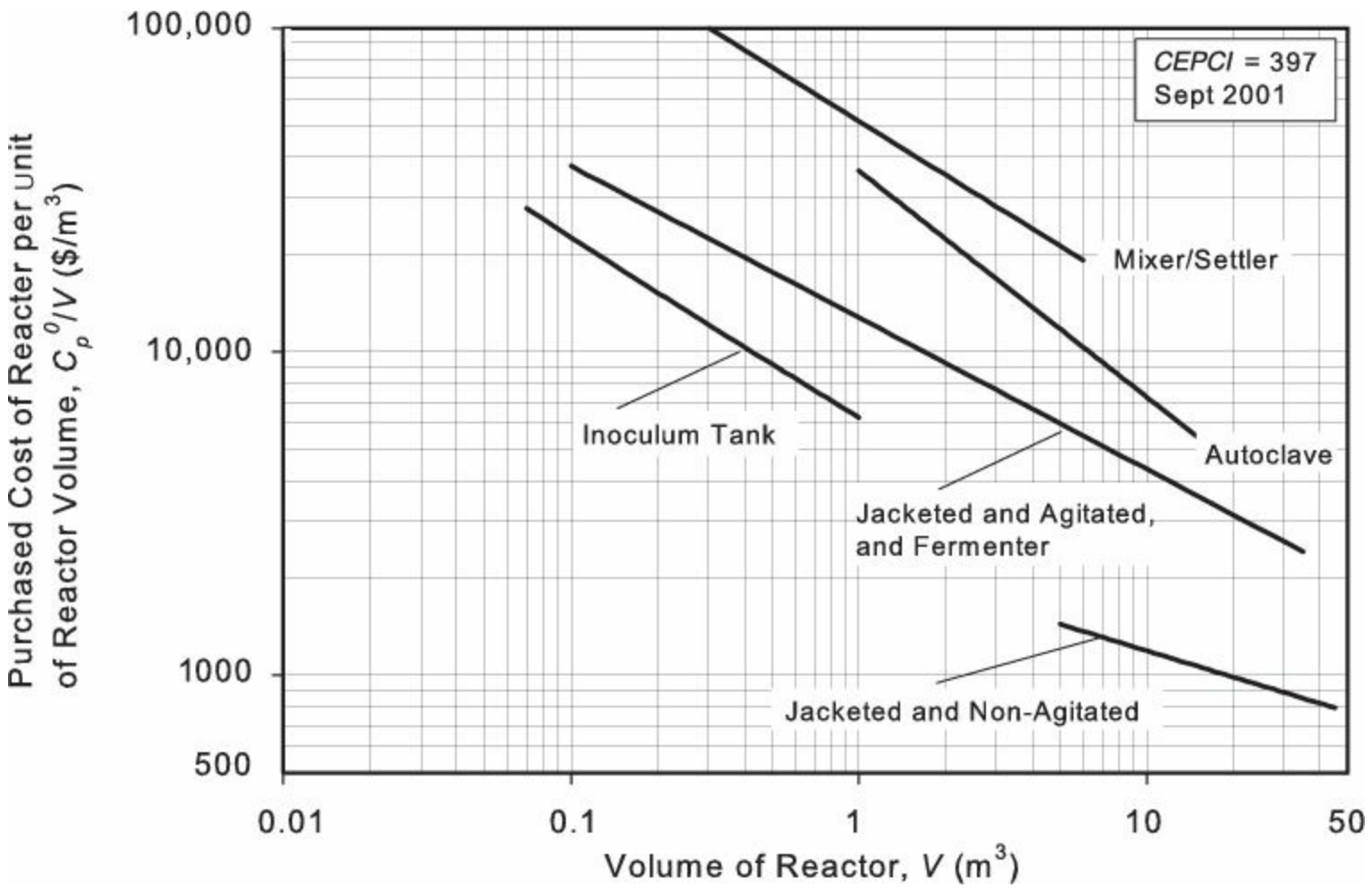


Figure A.16. Purchased Costs for Reactors

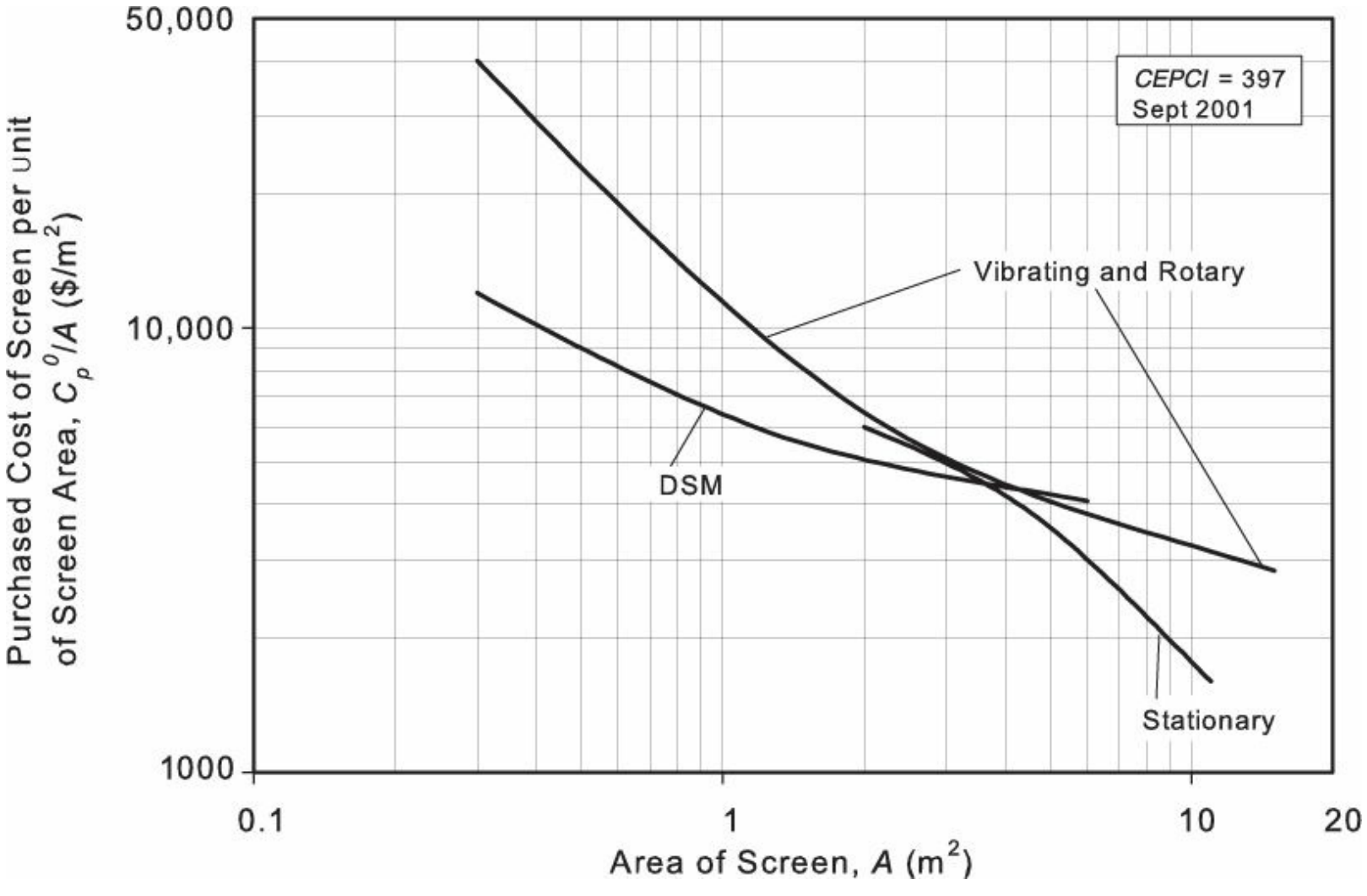


Figure A.17. Purchased Costs for Screens

Data from the R-Books software, marketed by Richardson Engineering Services, Inc. [4], were used as a basis for several of the graphs and correlations; acknowledgment is given in the appropriate figures.

A.2. Pressure Factors

As was pointed out in Chapter 7, the costs of equipment increase with increasing operating pressure. In this section, the method of accounting for changes in operating pressure through the use of pressure factors is covered.

A.2.1. Pressure Factors for Process Vessels

The pressure factor for horizontal and vertical process (pressurized) vessels of diameter D meters and operating at a pressure of P barg is based on the ASME code for pressure vessel design [5]. At base material conditions using a maximum allowable stress for carbon steel, S, of 944 bar, a weld efficiency, E, of 0.9, a minimum allowable vessel thickness of 0.0063 m (1/4 inch), and a corrosion allowance, CA, of 0.00315 m (1/8 inch) gives the following expression:

$$F_{P,vessel} = \frac{\dfrac{(P+1)D}{2[850 - 0.6(P+1)]} + 0.00315}{0.0063} \quad \text{for } t_{vessel} > 0.0063 \text{ m} \qquad \text{(A.2)}$$

If $F_{P,\ vessel}$ is less than 1 (corresponding to $t_{vessel} < 0.0063$ m), then $F_{P,\ vessel} = 1$. For pressures less than –0.5 barg, $F_{P,\ vessel} = 1.25$. It should be noted that Equation (A.2) is strictly true for the case when the thickness of the vessel wall is less than ¼ D; for vessels in the range $D = 0.3$ to 4.0 m, this occurs at pressures of approximately 320 barg.

A.2.2. Pressure Factors for Other Process Equipment

The pressure factors, F_P, for the remaining process equipment are given by the following general form:

$$\log_{10} F_P = C_1 + C_2 \log_{10} P + C_3 (\log_{10} P)^2 \qquad \text{(A.3)}$$

The units of pressure, P, are bar gauge or barg (1 bar = 0.0 barg) unless stated otherwise. The pressure factors are always greater than unity. The values of constants in Equation (A.3) for different equipment are given in Table A.2, and also shown are the ranges of pressures over which the correlations are valid. The values for the constants given in Table A.2 were regressed from data in Guthrie [1, 2] and Ulrich [3]. Extrapolation outside this range of pressures should be done with extreme caution. Some equipment does not have pressure ratings and therefore has values of C_1–C_3 equal to zero. If cost estimates are required for these units at high pressures and the equipment cost is affected by pressure, then the correlations should again be used with caution.

Table A.2. Pressure Factors for Process Equipment (Correlated from Data in Guthrie [1, 2], and Ulrich [3])

Equipment Type	Equipment Description	C_1	C_2	C_3	Pressure Range (barg)
Compressors	Centrifugal, axial, rotary, and reciprocating	0	0	0	–
Drives	Gas turbine	0	0	0	–
	Intern. comb. engine	0	0	0	–
	Steam turbine	0	0	0	–
	Electric—explosion-proof	0	0	0	–
	Electric—totally enclosed	0	0	0	–
	Electric—open/drip-proof	0	0	0	–
Evaporators	Forced circulation (pumped), falling film, agitated film (scraped wall), short tube, and long tube	0	0	0	P<10
		0.1578	−0.2992	0.1413	10<P<150
Fans*	Centrifugal radial, and centrifugal backward curve	0	0	0	ΔP<1kPa
		0	0.20899	−0.0328	1<ΔP<16kPa
	Axial vane and axial tube	0	0	0	ΔP<1kPa
		0	0.20899	−0.0328	1<ΔP<4kPa
Furnaces	Reformer furnace	0	0	0	P<10
		0.1405	−0.2698	0.1293	10<P<200
	Pyrolysis furnace	0	0	0	P<10
		0.1017	−0.1957	0.09403	10<P<200
	Nonreactive fired heater	0	0	0	P<10
		0.1347	−0.2368	0.1021	10<P<200
Heat exchangers	Scraped wall	0	0	0	P<40
		0.6072	−0.9120	0.3327	40<P<100
		13.1467	−12.6574	3.0705	100<P<300
	Teflon tube	0	0	0	P<15
	Bayonet, fixed tube sheet, floating head, kettle reboiler, and U-tube (both shell and tube)	0	0	0	P<5
		0.03881	−0.11272	0.08183	5<P<140
	Bayonet, fixed tube sheet, floating head, kettle reboiler, and U-tube (tube only)	0	0	0	P<5
		−0.00164	−0.00627	0.0123	5<P<140
	Double pipe and multiple pipe	0	0	0	P<40
		0.6072	−0.9120	0.3327	40<P<100
		13.1467	−12.6574	3.0705	100<P<300
	Flat plate and spiral plate	0	0	0	P<19
	Air cooler	0	0	0	P<10
		−0.1250	0.15361	−0.02861	10<P<100
	Spiral tube (both shell and tube)	0	0	0	P<150
		−0.4045	0.1859	0	150<P<400
	Spiral tube (tube only)	0	0	0	P<150
		−0.2115	0.09717	0	150<P<400
Heaters	Diphenyl heater, molten salt heater, and hot water heater	0	0	0	P<2
		−0.01633	0.056875	−0.00876	2<P<200
	Steam boiler	0	0	0	P<20
		2.594072	−4.23476	1.722404	20<P<40
Packing	Loose (for towers)	0	0	0	–
Process vessels	Horizontal and vertical			†	
Pumps	Reciprocating	0	0	0	P<10
		-0.245382	0.259016	−0.01363	10<P<100
	Positive displacement	0	0	0	P<10
		−0.245382	0.259016	−0.01363	10<P<100
	Centrifugal	0	0	0	P<10
		−0.3935	0.3957	−0.00226	10<P<100

Tanks	API—fixed roof	0	0	0	P<0.07
	API—floating roof	0	0	0	P<0.07
Towers	Tray and packed			†	
Trays	Sieve	0	0	0	–
	Valve	0	0	0	–
	Demisters	0	0	0	–
Turbines	Axial gas turbines	0	0	0	–
	Radial gas/liquid expanders	0	0	0	–
Vaporizers	Internal coils/jackets and jacket vessels	0	0	0	P<5
		−0.16742	0.13428	0.15058	5<P<320

*Pressure factors for fans are written in terms of the pressure rise across the fan, ΔP, where ΔP is measured in kPa.
†See Equation (A.2).

A.3. Material Factors And Bare Module Factors

As was pointed out in Chapter 7, the costs of equipment change with changes in the material of construction. In this section, the method of accounting for different materials of construction is covered.

A.3.1. Bare Module and Material Factors for Heat Exchangers, Process Vessels, and Pumps

The material factors, F_M, for heat exchangers, process vessels, and pumps are given in Figure A.18, with the appropriate identification number listed in Table A.3. The bare module factors for this equipment are given by the following equation:

Table A.3. Identification Numbers for Material Factors for Heat Exchangers, Process Vessels, and Pumps to Be Used with Figure A.18

Identification Number	Equipment Type	Equipment Description	Material of Construction
1	Heat exchanger	Double pipe, multiple pipe,	CS-shell/CS-tube
2		fixed tube sheet, floating head,	CS-shell/Cu-tube
3		U-tube, bayonet, kettle reboiler, scraped	Cu-shell/Cu-tube
4		wall, and spiral tube	CS-shell/SS-tube
5			SS-shell/SS-tube
6			CS-shell/Ni alloy tube
7			Ni alloy, shell/Ni alloy-tube
8			CS-shell/Ti-tube
9			Ti-shell/Ti-tube
10		Air cooler	CS tube
11		Air cooler	Al tube
12		Air cooler	SS tube
13		Flat plate and spiral plate	CS (in contact with fluid)
14		Flat plate and spiral plate	Cu (in contact with fluid)
15		Flat plate and spiral plate	SS (in contact with fluid)
16		Flat plate and spiral plate	Ni alloy (in contact with fluid)
17		Flat plate and spiral plate	Ti (in contact with fluid)
18	Process vessels	Horizontal, vertical (including towers)	CS
19		Horizontal, vertical (including towers)	SS clad
20		Horizontal, vertical (including towers)	SS
21		Horizontal, vertical (including towers)	Ni alloy clad
22		Horizontal, vertical (including towers)	Ni alloy
23		Horizontal, vertical (including towers)	Ti clad
24		Horizontal, vertical (including towers)	Ti
25	Pumps	Reciprocating	Cast iron
26		Reciprocating	Carbon steel
27		Reciprocating	Cu alloy
28		Reciprocating	SS
29		Reciprocating	Ni alloy
30		Reciprocating	Ti
31		Positive displacement	Cast iron
32		Positive displacement	Carbon steel
33		Positive displacement	Cu alloy
34		Positive displacement	SS
35		Positive displacement	Ni alloy
36		Positive displacement	Ti
37		Centrifugal	Cast iron
38		Centrifugal	Carbon steel
39		Centrifugal	SS
40		Centrifugal	Ni alloy

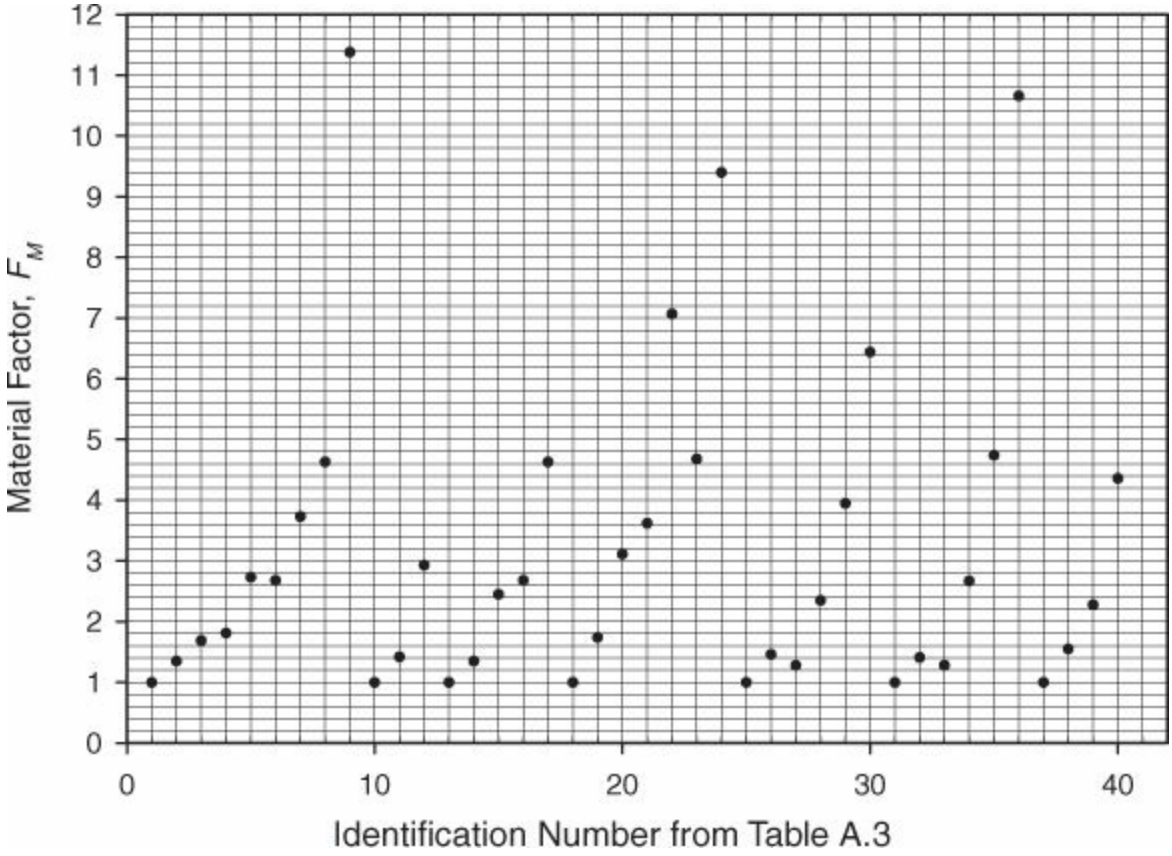


Figure A.18. Material Factors for Equipment in Table A.3 (Averaged Data from References [1, 2, 3, 6, 7, and 8])

$$C_{BM} = C_p^o F_{BM} = C_p^o (B_1 + B_2 F_M F_P) \qquad \text{(A.4)}$$

The values of the constants B_1 and B_2 are given in Table A.4. The bare module cost for ambient pressure and carbon steel construction, $C°_{BM}$, and the bare module factor for the equipment at these conditions, $F°_{BM}$, are found by setting F_M and F_P equal to unity. The data given in Tables A.3 and A.4 and Figure A.18 are average values from the following references: Guthrie [1, 2], Ulrich [3], Navarrete [6], Perry et al. [7], and Peters and Timmerhaus [8].

Table A.4. Constants for Bare Module Factor to Be Used in Equation (A.4) (Correlated from Data in Guthrie [1, 2] and Ulrich [3])

Equipment Type	Equipment Description	B_1	B_2
Heat exchangers	Double pipe, multiple pipe, scraped wall, and spiral tube	1.74	1.55
	Fixed tube sheet, floating head, U-tube, bayonet, kettle reboiler, and Teflon tube	1.63	1.66
	Air cooler, spiral plate, and flat plate	0.96	1.21
Process vessels	Horizontal	1.49	1.52
	Vertical (including towers)	2.25	1.82
Pumps	Reciprocating	1.89	1.35
	Positive displacement	1.89	1.35
	Centrifugal	1.89	1.35

A.3.2. Bare Module and Material Factors for the Remaining Process Equipment

For the remaining equipment, the bare module costs are related to the material and pressure factors by

equations different from Equation (A.4). The form of these equations is given in Table A.5. The bare module factors that correspond to the equations in Table A.5 are given in Figure A.19 using the identification numbers listed in Table A.6. Again, the data used to construct Figure A.19 are compiled from average values taken from Guthrie [1, 2], Ulrich [3], Navarrete [6], Perry et al. [7], and Peters and Timmerhaus [8]. In addition, bare module factors for the equipment added to the third edition of the book (conveyors, crystallizers, dryers, dust collectors, filters, mixers, reactors, and screens) are given separately in Table A.7.

Table A.5. Equations for Bare Module Cost for Equipment Not Covered by Tables A.3 and A.4

Equipment Type	Equation for Bare Module Cost
Compressors and blowers without drives	$C_{BM} = C_p^o F_{BM}$
Drives for compressors and blowers	$C_{BM} = C_p^o F_{BM}$
Evaporators and vaporizers	$C_{BM} = C_p^o F_{BM} F_P$
Fans with electric drives	$C_{BM} = C_p^o F_{BM} F_P$
Fired heaters and furnaces	$C_{BM} = C_p^o F_{BM} F_P F_T$ F_T is the superheat correction factor for steam boilers ($F_T = 1$ for other heaters and furnaces) and is given by $F_T = 1 + 0.00184\Delta T - 0.00000335(\Delta T)^2$ where ΔT is the amount of superheat in °C.
Power recovery equipment	$C_{BM} = C_p^o F_{BM}$
Sieve trays, valve trays, and demister pads	$C_{BM} = C_p^o N F_{BM} F_q$ where N is the number of trays and F_q is a quantity factor for trays only given by $\log_{10} F_q = 0.4771 + 0.08516 \log_{10} N - 0.3473 (\log_{10} N)^2$ for N<20 $F_q = 1$ for N≥20
Tower packing	$C_{BM} = C_p^o F_{BM}$

Table A.6. Identification of Material Factors for Equipment Listed in Table A.5 to Be Used with Figure A.19

Identification Number	Equipment Type	Equipment Description	Material of Construction
1	Compressors/blowers	Centrifugal compressor or blower	CS
2		Centrifugal compressor or blower	SS
3		Centrifugal compressor or blower	Ni alloy
4		Axial compressor or blower	CS
5		Axial compressor or blower	SS
6		Axial compressor or blower	Ni alloy
7		Rotary compressor or blower	CS
8		Rotary compressor or blower	SS
9		Rotary compressor or blower	Ni alloy
10		Reciprocating compressor or blower	CS
11		Reciprocating compressor or blower	SS
12		Reciprocating compressor or blower	Ni alloy
13	Drives for compressors and blowers	Electric—explosion-proof	—
14		Electric—totally enclosed	—
15		Electric—open/drip-proof	—
16		Gas turbine	—
17		Steam turbine	—
18		Internal combustion engine	—
19	Evaporators and vaporizers	Evaporator—forced circ, short or long tube	CS
20		Evaporator—forced circ, short or long tube	Cu alloy
21		Evaporator—forced circ, short or long tube	SS
22		Evaporator—forced circ, short or long tube	Ni alloy
23		Evaporator—forced circ, short or long tube	Ti
24		Evaporator—falling film, scraped wall	CS
25		Evaporator—falling film, scraped wall	Cu alloy
26		Evaporator—falling film, scraped wall	SS
27		Evaporator—falling film, scraped wall	Ni alloy
28		Evaporator—falling film, scraped wall	Ti

29		Vaporizer—jacketed vessel	CS
30		Vaporizer—jacketed vessel	Cu
31		Vaporizer—jacketed vessel	Glass lined/SS coils
32		Vaporizer—jacketed vessel	Glass lined/Ni coils
33		Vaporizer—jacketed vessel	SS
34		Vaporizer—jacketed vessel	SS clad
35		Vaporizer—jacketed vessel	Ni alloy
36		Vaporizer—jacketed vessel	Ni alloy clad
37		Vaporizer—jacketed vessel	Ti
38		Vaporizer—jacketed vessel	Ti clad
39		Vaporizer—jacketed vessel + internal coil	CS
40		Vaporizer—jacketed vessel + internal coil	Cu
41		Vaporizer—jacketed vessel + internal coil	Glass lined/SS coils
42		Vaporizer—jacketed vessel + internal coil	Glass lined/Ni coils
43		Vaporizer—jacketed vessel + internal coil	SS
44		Vaporizer—jacketed vessel + internal coil	SS clad
45		Vaporizer—jacketed vessel + internal coil	Ni alloy
46		Vaporizer—jacketed vessel + internal coil	Ni alloy clad
47		Vaporizer—jacketed vessel + internal coil	Ti
48		Vaporizer—jacketed vessel + internal coil	Ti clad
49	Fans	Fan with electric drive	CS
50		Fan with electric drive	Fiberglass
51		Fan with electric drive	SS
52		Fan with electric drive	Ni alloy
53	Fired heaters and furnaces	Tube for furnaces and nonreactive process heater	CS
54		Tube for furnaces and nonreactive process heater	Alloy steel
55		Tube for furnaces and nonreactive process heater	SS
56		Thermal fluid heater—hot water, molten salt, or diphenyl-based oil	—
57	Power recovery equipment	Turbines	CS
58		Turbines	SS
59		Turbines	Ni alloy
60	Trays and demister pads	Sieve and valve trays	CS
61		Sieve and valve trays	SS
62		Sieve and valve trays	Ni alloy
63		Demister pad	SS
64		Demister pad	Fluorocarbon
65		Demister pad	Ni alloy
66	Tower packing	Packing	Metal (304SS)
67		Packing	Polyethylene
68		Packing	Ceramic

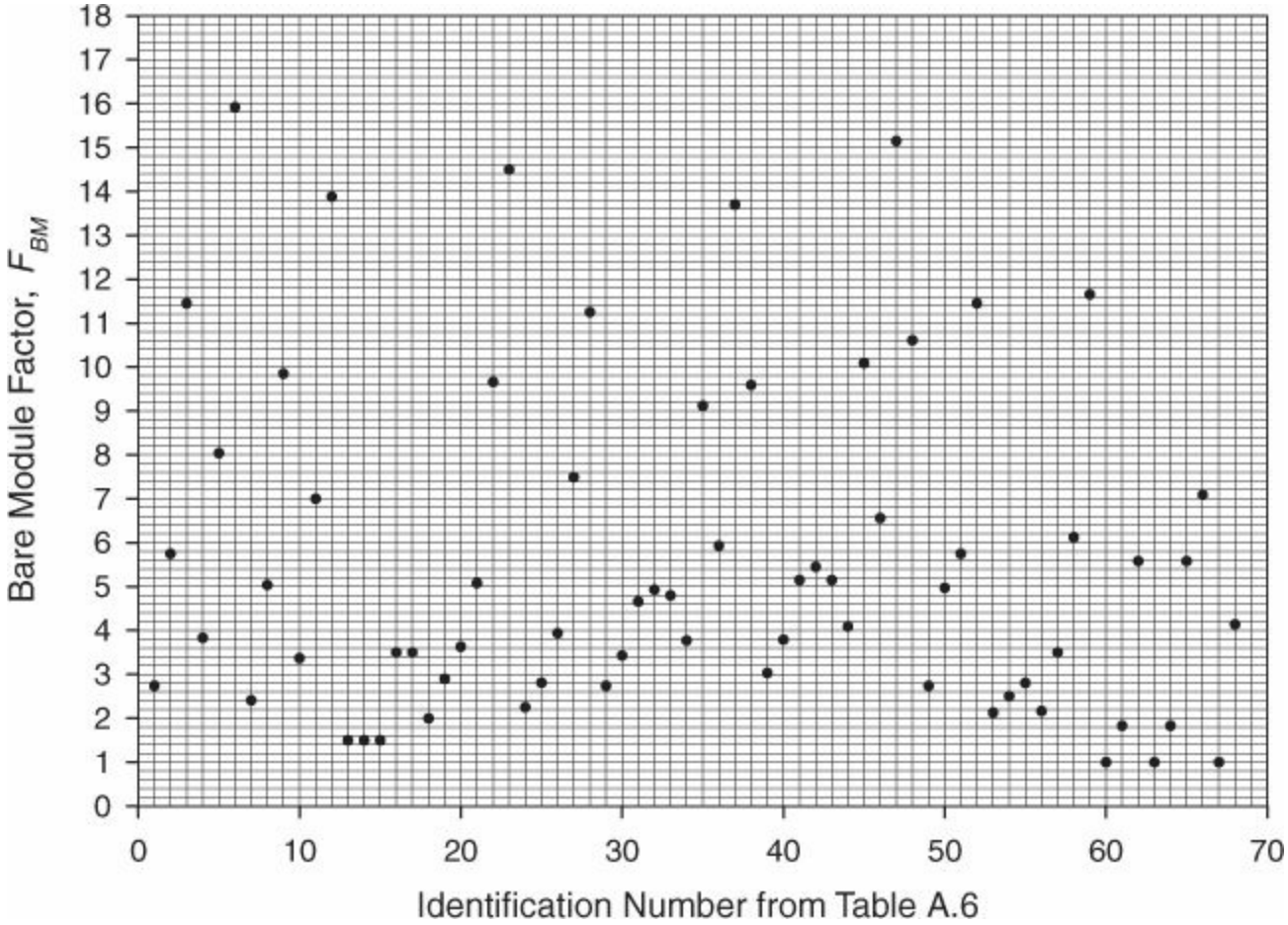


Figure A.19. Bare Module Factors for Equipment in Table A.6 (Average Data from References [1, 2, 3, 6, 7, and 8])

Table A.7. Bare Module Factors for Conveyors, Crystallizers, Dryers, Dust Collectors, Filters, Mixers, Reactors, and Screens

Equipment Type	Equipment Description	Bare Module Factor, F_{BM}
Blenders	Kneader	1.12*
	Ribbon	1.12*
	Rotary	1.12
Centrifuges	Auto batch separator	1.57*
	Centrifugal separator	1.57
	Oscillating screen	1.57*
	Solid bowl w/o motor	1.27
Conveyors	Apron	1.20
	Belt	1.25
	Pneumatic	1.25*
	Screw	1.10
Crystallizers	Batch	1.60
Dryers	Drum	1.60
	Rotary, gas fired	1.25
	Tray	1.25
Dust Collectors	Baghouse	2.86*
	Cyclone scrubbers	2.86*
	Electrostatic precipitator	2.86*
	Venturi scrubber	2.86*
Filters	Bent	1.65*
	Cartridge	1.65*
	Disc and drum	1.65*
	Gravity	1.65*
	Leaf	1.65
	Pan	1.65*
	Plate and frame	1.80
	Table	1.65*
	Tube	1.65*
Mixers	Impeller	1.38*
	Propeller	1.38
	Turbine	1.38
Reactors	Autoclave	4.0*
	Fermenter	4.0*
	Inoculum tank	4.0*
	Jacketed agitated	4.0*
	Jacketed nonagitated	4.0*
	Mixer/settler	4.0*
Screens	DSM	1.34*
	Rotary	1.34*
	Stationary	1.34*
	Vibrating	1.34

When possible, bare module factors are taken to be equal to the Field Installation Factors from Guthrie [2]. Items marked * are estimates.

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Chapter 0. Outcomes Assessment

If you are reading this chapter, you are either a student about to begin the design class that culminates your chemical engineering training or you are a professor planning to teach that same class. The design class is often called the *capstone* class, because not only is it the ultimate class in the chemical engineering curriculum, but also it is where students are expected to apply knowledge gained earlier in the curriculum to the solution of a comprehensive chemical engineering design problem.

Outcomes assessment is the process of determining whether students have learned what the faculty expects them to have learned. The term *learned* is used in this context to include both subject matter (math, chemistry, fluid mechanics, etc.) and skills (report writing, oral presentations, teamwork). Outcomes assessment can be understood by analogy to process control. In process control, a process has a set point—temperature, for example. If the exit temperature is measured and it is not at the desired value, there may be a feedback loop that alters, for example, the flowrate of a cooling water stream in a heat exchanger to bring the temperature to the desired value, i.e., the set point. In outcomes assessment, the faculty determines the knowledge and skills (learning outcomes) it expects graduates to have mastered. This is the set point. Then the faculty measures the level of mastery of the desired knowledge and skills, and, if the measurement is not at the set point, there should be feedback to students to ensure that the deficiencies are corrected for the current students. In addition, there should be changes made to the curriculum to ensure that future students are closer to the desired set point. This process is analogous to feedback control and is illustrated in Figure 0.1. Several nested feedback loops are illustrated, because assessment results can be obtained from alumni, from seniors about to graduate, and at any point in the curriculum. Before the advent of outcomes assessment, the traditional model for higher education was more analogous to feed-forward control, as illustrated in Figure 0.2. In this model, the outcomes are assumed based on the content of the curriculum. The weakness of feed-forward control is that the output is assumed based on a model of the process (curriculum, in this example), but prediction of the correct output is completely dependent on the validity of the model.

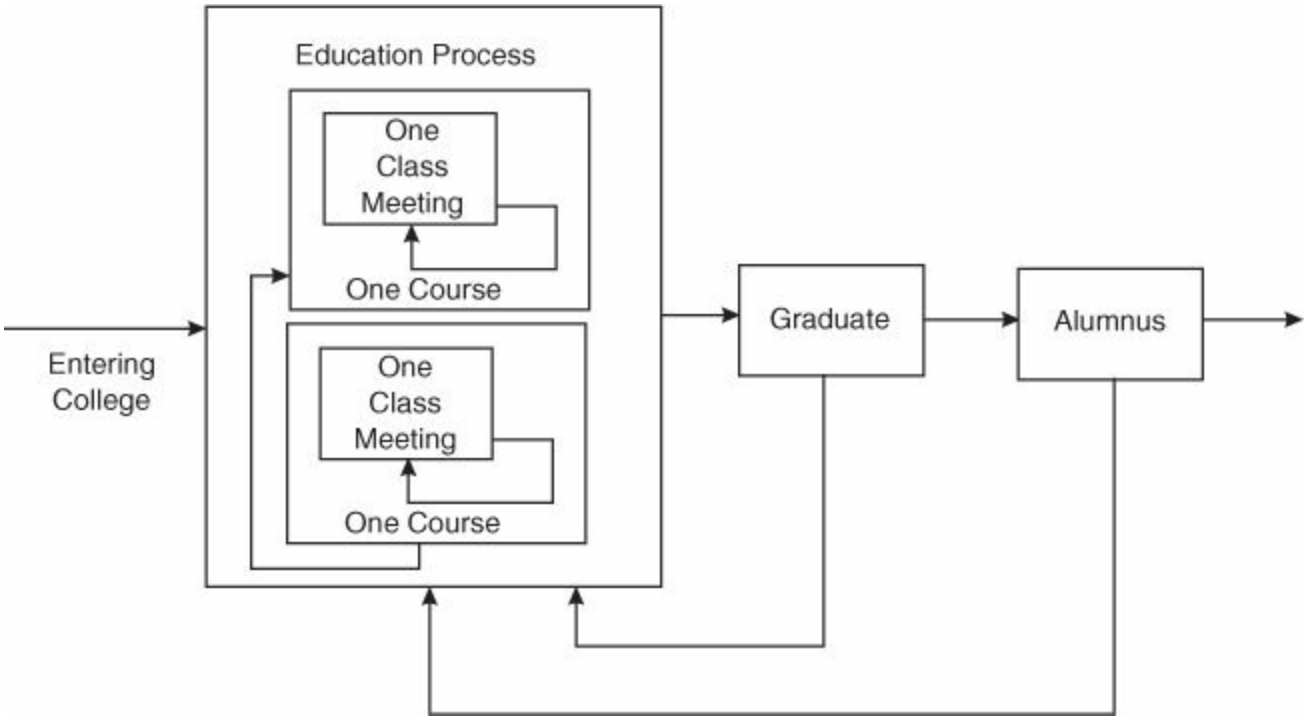


Figure 0.1. Feedback Model for Higher Education

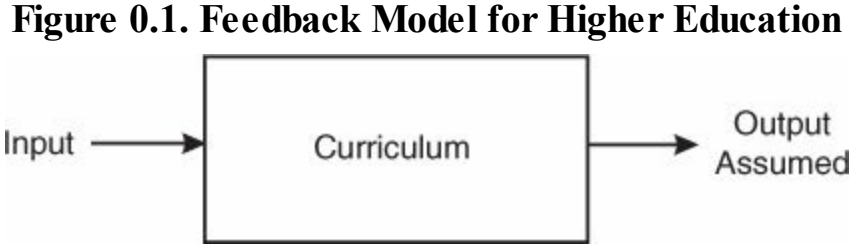


Figure 0.2. Feed-Forward Model of Higher Education

So what is done with outcomes assessment results? As discussed above, one possibility is feedback to improve student learning. This is termed *formative assessment*. Another possibility is to use the results to prove that students have achieved the desired outcomes. This is termed *summative assessment*. Both forms of assessment are necessary. Summative assessment is necessary to satisfy current accreditation requirements and, particularly at state-supported institutions, to satisfy the requirements of governing bodies (e.g., boards of trustees). Formative assessment is necessary to improve student learning to ensure that the desired learning outcomes are achieved.

So why include this topic in a process design textbook? There are two reasons. One is that accreditation of all engineering programs by ABET is now based on outcomes assessment [1]. The second reason is that it is believed that the capstone design class is one of the most logical places in the curriculum for outcomes assessment. Both the faculty and students can perform assessment in the capstone design class. Because this is the class that culminates a student's undergraduate experience and it is the class in which students are expected to apply what they have learned earlier in the curriculum, there is no better opportunity to assess learning outcomes before students graduate. By performing this assessment before graduation, there is opportunity for feedback to students, possibly in the form of remedial instruction, in case any of the desired outcomes are not met.

In what follows, students will first be shown how to assess themselves, followed by methods that instructors can use to assess student outcomes in the design class.

0.1. Student Self-Assessment

There are two ways to describe what you should have learned before receiving your chemical engineering degree. One is to list all of the skills and subject matter you should have learned. This is curriculum dependent, so the list in one department may differ from the list in another department, although the lists between departments will probably have at least 75% common material. However, accreditation requirements state that a department's objectives and outcomes must be published, so your department's expectations for you are probably easy to find either on the Web or in your catalog (or both). You can compare your current level of achievement to your department's expectations. As you proceed through the design class, if you encounter something you do not fully understand, you should take this opportunity to learn it. In many cases, it will be something that your instructor believes you already know, so, by taking the time to catch up, you will be moving closer to the desired outcomes of your department. If it is something that was never covered in an earlier class, you should still take the time to learn it. After you graduate, you will encounter many aspects of chemical engineering that were not part of the undergraduate curriculum, and you will have to learn them on your own. It is better to practice this skill while in school. If you believe that you should be taught all aspects of chemical engineering in school, then you are either being unrealistic or you want a ten-year undergraduate degree! As are all professions, chemical engineering is ever changing. As professionals, chemical engineers are expected to continue to learn throughout their careers. Besides,

one of your department's outcomes is undoubtedly that you should have the ability to educate yourself. Therefore, the capstone class often requires you to teach yourself new material—on purpose.

A second, more general method for describing what you have learned is known as Bloom's Taxonomy of educational objectives [2]. This is known as the **cognitive domain**, and it includes knowledge, thinking, and the application of knowledge, certainly the issues most applicable to chemical engineering education. (The other domain is known as the **affective domain**, and it includes attitudes and values. This domain will not be discussed here.)

Bloom's Taxonomy has six levels:

1. **Knowledge:** In this context, knowledge means facts, definitions, technical jargon, and so on. Knowledge is most often tested using multiple-choice questions. The primary skill necessary to be successful at this level is memorization, which, by now, you know is not sufficient to be successful as a chemical engineer. If you know that mass and energy are always conserved, or if you know that the ideal gas law is $PV = nRT$, you have demonstrated this level of cognitive achievement.
2. **Comprehension:** Comprehension means that you understand what something means. The simplest way to demonstrate comprehension is to explain something in your own words. For example, if you can explain the meaning of each term in the Navier-Stokes equations, you have reached this level of cognitive achievement. For the ideal gas law, if you can explain its meaning in your own words, including the assumptions of non-interacting molecules and molecules that have no volume, you are at the comprehension level of cognitive achievement. Comprehension is most often tested with short answer and essay questions.
3. **Application:** Application means that you can apply the knowledge mastered at levels 1 and 2 to solve problems. If you have reached the capstone design class, then you most certainly have achieved this level of cognitive achievement. Achievement of application is the minimum standard to pass lower-level engineering classes. Problems must be solved, and the problems you have been solving at the end of textbook chapters for the past few years demonstrate application. If you can solve a problem that requires use of the ideal gas law (without specifically being told to use it), then you have reached this level of cognitive achievement. Most of the problems in this book in Section 2 (engineering economics) are at this level.
4. **Analysis:** Analysis is generally described as the ability to break a complex problem down into its component parts. The more difficult end-of-chapter problems you have been assigned are often at this level. For example, a problem that requires use of both material and energy balances, and requires you to determine when to use each one, is an analysis problem. The problems in this book in Section 1, Chapters 5–6, and in Section 4, particularly those in Chapters 22 and 24, are at this level, because these problems require you to break down a process flowsheet into its component parts.
5. **Synthesis:** Synthesis is putting pieces of a problem together to make a whole. It is possible that you have not yet been given this challenge. In Section 3, Chapters 12–13, where a chemical process is constructed (synthesized) from its component parts, you will meet this challenge. In completing a process design, the concept of a base case will be introduced. A base case is a reasonable first estimate of a process design that has not yet been optimized. Construction of a base case involves synthesis.
6. **Evaluation:** Evaluation is the use of judgment when obtaining a problem solution. It is the use

of judgment in choosing among alternatives. A simple example of evaluation might be checking someone else's work for errors. In the context of design, optimization, which is discussed in Chapter 14, is a very common mechanism of evaluation. In optimization, the "best" solution is sought using constraints and judgment. If you take the base-case design discussed above and improve it based on your engineering judgment, which may be based on optimization, experience, or heuristics, you are performing evaluation.

As a student, you can reflect on your undergraduate education using Bloom's Taxonomy and determine what level you believe that you have achieved to date, and you can trace your progress through level 6 before you graduate. By that time, you should have had experiences through level 6. It is levels 4–6 that are required for success with a company or in graduate school.

0.2. Assessment by Faculty

The capstone class is one of the most logical opportunities for program assessment, because it is where students are expected to apply previously learned knowledge. Another advantage is that the capstone design experience is something that is already being done; therefore, outcomes assessment can be performed with only an incremental effort. The question is how to measure learning outcomes. Several methods are suggested below, many of which the authors have used successfully.

One measure that the authors use every year is a classroom assessment technique related to the memory matrix or categorizing grid [3]. On the first day of the design class, students are told that this is the class where they apply what they have learned thus far, and they are asked to enumerate the concepts they believe they have learned prior to the design class. Quite often, the initial response is to list the names of all classes taken in the chemical engineering curriculum. At that point, those classes are listed on the board and students are asked to fill in what they learned in each class. The resulting list provides a good idea of what students believe they have learned. There are always topics that are omitted. If you believe a key topic has been omitted, ask the class about it. If they all agree that it was their omission, that is a good sign. If they all disclaim any knowledge of the topic, or even its definition, that is a sign that you may want to include this topic somewhere in the design class, especially if you think it is important. This provides feedback to students. If you think this topic was omitted from the syllabus or not learned by students in an earlier class, then you should consider finding a method to ensure that it is learned in the future. This is a delicate matter, of course, but it is made somewhat easier by the accreditation requirement that course objectives be included in the syllabus. One result of this requirement is that many faculties now discuss course content more than they did in the past. The authors can send interested instructors results of this exercise from our classes.

Another method for obtaining assessment results from capstone experiences is to develop a rubric containing attributes expected from a design project and evaluate the finished product within its context. In this situation, the term *rubric* means a procedure. The advantage of a well-defined rubric is that it makes it easier to obtain consistency in evaluation between multiple evaluators. A portion of a rubric that can be used for evaluating the technical content of design reports is shown in Figure 0.3. A composite score, which must be an integer, is entered only for the attribute in bold. It is an average of the characteristics under each attribute. If the average of all scores is significantly less than 3, it is believed that feedback is required, both to current students in the form of remedial work and into the curriculum to improve the performance of students when they are assigned a similar design project. This complete rubric, as well as others currently used by the authors for oral presentations, written

reports, and laboratory reports, is available at http://www.che.cemr.wvu.edu/ugrad/outcomes/. By using a rubric for assessment purposes, it is possible to determine the success in student achievement of each attribute considered to be an important component of the whole. By merely assigning a grade, only a composite evaluation is obtained. This method reveals the details and can also be used to make subjective evaluation of design projects more objective.

Attribute	1–Not Acceptable	2–Below Expectations	3–Meets Expectations	4–Exceeds Expectations	Score
Design of equipment, analysis of performance of existing equipment, understand interrelationship between equipment in process					
Design of individual equipment	Major errors in individual equipment design	Some errors in equipment design	Equipment designed correctly	Unique aspects of equipment design enhance result	
Understand interrelationship between equipment on flowsheet	No understanding of equipment interrelationship	Minimum understanding of equipment interrelationship	Clear understanding of equipment interrelationship	Exploitation of equipment interrelationship to enhance result	
Constraints/limitations of individual equipment and flowsheet understood	Constraints/ limitations not understood	Not all constraints/ limitations understood	Constraints/ limitations clearly understood	Exploitation of constraints/ limitations to enhance result	
Response to questions indicates understanding of chemical engineering principles	Response to questions demonstrates lack of understanding	Response to questions shows gaps in understanding	Response to questions shows clear understanding	Response to questions shows superior understanding	
Significance of conclusions understood	Lack of understanding	Gaps in understanding	Clear understanding	Superior understanding	

Figure 0.3. Portion of a Rubric for Evaluating Design Projects

One of the authors' favorite methods for obtaining assessment results is from the questions and follow-up questions after oral design report presentations [4]. Students' responses to questions and follow-up questions can reveal their true understanding of what they did and the principles they applied to arrive at the solution to the problem. In many ways, this is similar to a Ph.D. dissertation defense. The authors use a series of projects over the senior year for assessment purposes. From these, feedback can be provided several times over the senior year. For a program that has only one project, another way to get similar information is from interim presentations or interim review meetings in which students are asked to explain their thought patterns. Students will always make errors; after all, they are still students. However, if a significant number of students make the same error or have the same misconception, that is a significant result and should be noted. Documentation of questions asked (to the instructor or to a TA) can reveal the same type of information.

An important assessment principle is that skills should be developed over time, so students may demonstrate improvement after receiving feedback. Design is one such skill, as are oral presentations, written reports, teamwork, and so on. The capstone design class usually requires all of these experiences. It is difficult to argue that students have developed any of these skills if they have only one such experience while an undergraduate. Therefore, it is recommended that students receive multiple experiences to develop these skills, with feedback after each experience. One way to do this is by integrating these experiences throughout the curriculum. If this is not possible, then it is suggested that there be multiple experiences with feedback in the capstone experience.

0.3. Summary

The capstone design class, the class for which this book is written, is a logical place for outcomes assessment, because it is where students apply knowledge learned earlier in the curriculum and because, given that the capstone experience already exists, only incremental effort is required. Students can assess their own progress using Bloom's Taxonomy or by comparing their progress to the educational objectives and/or learning outcomes published by their department. Several methods have been described here that the faculty can use to obtain program assessment results.

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Other References

A more comprehensive list of references on curriculum outcomes assessment can be found at http://www.che.cemr.wvu.edu/ugrad/outcomes/.

Chapter 29. Written and Oral Communication

What You Will Learn

- High-quality written and oral communication is essential in all fields of endeavor, including the chemical process industry.

Throughout your career as an engineer, chances are that you will draw on your skills in oral and written communication far more often than you ever imagined. Engineers report that they spend most of their time using some combination of the four communication skills: writing, speaking, reading, and listening [1]. The situation is the same for most engineering students, although their education is apt to have given them far more opportunity to read and to listen than to write and to speak.

Technical writing and oral presentation skills are particularly important to the design engineer. After all, the final product of a design project is generally an oral or written report (and sometimes both). Furthermore, throughout the design process, engineers use feasibility studies, environmental impact reports, meeting minutes, progress reports, status reports, appropriation requests, design notebooks, equipment specification sheets, and personnel evaluations, as well as various letters and memos, to document their work and to communicate their findings to colleagues, company management, clients or potential clients, and possibly the general public.

Any evaluation of your success as an engineer, then, will be based in whole or in large part on the quality of your written and oral communication.

In this chapter, instruction in basic writing skills is not attempted. There are many good texts on technical communication [2–4]. However, guidance in adapting this skill to the area of engineering communication that focuses on process design is provided. The formats and guidelines for written and oral design reports are explained, and strategies for improving one's communication are given. Other types of written reports common in engineering, such as laboratory reports and technical journal articles, are not covered. Many of the same strategies, however, apply to these genres, even though the specific guidelines may not.

A sample student design report and the visuals from the oral presentation of the project are given in Chapter 30 of this book. Also included is a critique of these reports. Examples of the problems described in this chapter are given in the sample report.

29.1. Audience Analysis

In all engineering communication, a crucial step is **audience analysis**. Written or oral reporting is, by definition, a transfer of information. One's success at this transfer hinges on presenting the type, detail, and scope of information that the audience expects with a clarity that avoids misunderstandings. It is important that you do the following:

1. **Identify Your Intended Audience:** Will your report or oral presentation be for fellow chemical engineers, other engineers, managers, executives, clients, or the general public? Both the appropriate level of detail and the focus will vary with the background of the audience. Senior executives, even if they were trained years ago as chemical engineers, may not quickly

understand the mathematical details of your design. More important, they will not be very interested. Rather, they need more of a big-picture focus. How might what you have done impact the bottom line? The public's perception of the company? The long-term viability of your company's technical advantage over its competitors? There may be a broad range of audience backgrounds, especially if the primary recipients of your report forward it to others.

2. **Determine What Response You Want from Your Audience:** Do you want them to approve the project? Do you want them to abandon the project? Do you want them to leave the presentation or finish reading the report confident that you have presented the best alternatives in a way that will help them make the decision? Do you want them to order the correct equipment and materials? Do you want them to be confident that you have studied the most important environmental impacts of the project? Do you want to be certain that your safety recommendations are immediately accepted and implemented?
3. **Imagine Yourself to Be One of Your Audience:** After writing the first draft, read the report as if you were one of the people identified in Step 1, with the indicated background and areas of concern. Read the report or hear the oral presentation as this person would, and imagine what response you would have. What would you do after reading or hearing the report?
4. **Iterate:** Multiple drafts are essential. As is the case when solving any complex problem, one must attempt a solution, evaluate it, and then improve upon it. In succeeding drafts, reconsider your likely audience response. If it is not what you want, you must continue to revise.

29.2. Written Communication

Some of the purposes of putting ideas into writing are

1. To provide a permanent record
2. To get someone to do something (action writing)
3. To instruct someone (informative writing)

Often in engineering writing, all three purposes apply. What you write is a permanent record of your analysis, your conclusions, and your recommendations. Unlike oral communication, written documents must stand on their own, because the author is generally not present to answer questions about the content. Also, these documents will be referred to more than once, often much later than when they were written. Precise wording is crucial, because decisions will often be made by the reader without any further consultation with the writer. Ambiguous words or phrases, gaps in logical developments, and undocumented assumptions can lead the reader to make a wrong decision.

To help both the writer and the reader, various formats are used in written engineering communications. They serve both as a guide for the information flow of the document and as a rough checklist to be sure that important content is not omitted. The reader anticipates the location of specific content within the document; thus, the format helps the reader to understand the document, as well as to skip to those sections of most importance when pressed for time. In the following sections, several formats common to chemical process design are described. The detailed guidelines for each format vary from organization to organization, and a sample format for design reports used at West Virginia University is given in section 29.2.8.

Although a typical set of guidelines is given, it is by no means the only (or necessarily the best) such set for design reports. In fact, the best guidelines in a particular organization are the ones agreed to by that organization. They are, in the best of circumstances, an agreement between both parties, whose

purpose is to make the communication between the writer and the reader more complete, reliable, and efficient. The first step, then, is to determine what your organization's guidelines are.

29.2.1. Design Reports

In general, a **design report** presents the results of a design effort to those who will either implement the design or decide whether the design will be implemented. As with the design process itself (described in Chapter 2), design reports are of varying scope, detail, and complexity. Early on, the order-of-magnitude estimate leads to a relatively short report whose purpose is to persuade the reader either to commit to go forward to the study-estimate stage or to abandon the project in favor of other opportunities. The audience for such a report is typically upper management.

The goal of these early reports is to present the data required for decisions that are quite difficult to make. When the final project may require a capital expenditure of millions or even hundreds of millions of dollars, the stakes are high, and the audience needs enough information to be reasonably confident that the decision is the right one. The audience requires the following:

- A careful analysis of a base case with sufficient detail to provide a context
- Evidence that the most reasonable options have been considered
- A careful analysis of these options
- A statement of and justification for any significant assumptions made
- A finite number of options, with a clear analysis of the advantages and disadvantages
- An estimate of the accuracy of the analysis

The audience for such a report is likely to be less interested in the details of proven technology than in the details and risks of new processes, catalysts, or equipment. The financial, environmental, health, and public perception aspects are likely to be of high concern.

Later design reports (based on preliminary design, definitive, and detailed estimates) are apt to have more technical audiences of process engineers, engineering managers, project engineers, purchasing agents, and so on. They will be more interested in the details that allow the design to proceed to a final, constructed, and operating plant. One outcome of any successful design report, however, is the informed decision of the readers to do something—to commit the company to more detailed design (or not), to order equipment, to start up a plant, to go after new markets, or to modify a process to increase yield or reduce environmental impact.

29.2.2. Transmittal Letters or Memos

The report stands on its own, but it is usually sent to the readers with a cover sheet giving a broad overview of the document. This is a memo if the recipient is a fellow employee of your organization; it is a letter if the recipient is a client or an employee of a different organization. Some engineers may mistakenly treat this transmittal memo or letter as merely a tag formally indicating who is doing the transmitting, when, and to whom. However, the real purpose and distinct value of this sheet is to convince the potential reader to become a bona fide reader. To do this, the transmittal memo must contain a very brief statement of the scope and of the most important conclusion or recommendation of the report. It must catch the attention of the recipient. The reward of a good transmittal memo is that your report is read (at least in part).

29.2.3. Executive Summaries and Abstracts

Design reports can be long, and they often must contain very detailed information that will be of interest to only a small fraction of the readers of the document. All readers, however, benefit from a broad overview of the project being reported, with key assumptions, results, conclusions, and recommendations given. This overview is called an **executive summary**. Its length is governed by the guidelines of the organization. Some companies impose a one- or two-page maximum, whereas some organizations (especially government agencies) encourage longer executive summaries that are, in effect, short reports. Some guidelines suggest that the executive summary should be no more than 5% or 10% of the length of the report. The key is to remember that a well-written executive summary will be short enough that busy executives will read it all but will communicate enough information to satisfy these executives, who are unlikely to read the rest of the report.

Some guidelines fail to make the distinction between an executive summary and an abstract. Others define the executive summary as longer than an abstract or more focused on conclusions and recommendations than is the abstract, which may also summarize the procedures used in the analysis. In any case, the executive summary must be focused on the needs of executives whose job is to make the proper decision based on the work you have done, without reading the details contained in the full report. On the other hand, an **abstract** is a very boiled-down version of the complete report and should have the same focus as does the full report. The abstract provides enough information for the reader to decide whether to read the report, and it provides an overview that will help the reader to assimilate the information while reading the report. Even though an abstract or executive summary appears at the beginning of the report, it should be written last. Care should be taken when writing the executive summary and/or abstract that all important results and conclusions are included, because these are often the only sections of the report that are read in their entirety.

An executive summary (or abstract) should be a synopsis of the project being reported, not a description of the report itself. The former is called an **informative executive summary** and may include statements such as, “The total capital investment is $100 million.” The latter would be a **descriptive executive summary** and would include less helpful statements such as, “The total capital investment is given in Section 4 of the report.” If the goal of the summary is to get information to a reader whose time is too valuable to read the report (but who must make an important decision), it is poor strategy to write an executive summary (descriptive) to convince readers that they must then read the report to get any useful information. Rather, the executive summary (informative) should contain all the information necessary for the executive reader to make the decision, and the body of the report should contain the details that will be required by others to implement the decision.

29.2.4. Other Types of Written Communication

Progress reports are often required for long projects. The goals of these (usually short) reports are

1. To indicate the progress made to date
2. To present a schedule for the remainder of the project
3. To explain any unanticipated problems or opportunities encountered
4. To propose or to report on changes in direction from those originally projected
5. To give a synopsis of the important findings of the project

Performance evaluations are periodic (often annual or semiannual) reports of the quality of an employee’s work. They generally include

1. A synopsis of the completed work

2. An evaluation of the quality of that work
3. A list or narrative of the observed strengths and weaknesses
4. Recommendations for improvement
5. Qualitative or quantitative rankings on specific work attributes

Minutes are often taken during design meetings, especially when important decisions are made or when the meetings involve clients. The minutes include a list of important topics discussed, important decisions made, and crucial information communicated to the parties present, as well as the list of attendees and the time and place of the meeting. Without minutes, different attendees will have memories (or even will have notes) of the decisions made that are in conflict. Minutes create the permanent record of the meeting that allows everyone involved to know where things are headed. To be effective, they must be signed by the minutes author and by representatives of each of the groups at the meeting. This typically involves a total of three signatures (client, manager, and author).

Increasingly, **e-mail** within an organization and across the Internet is the medium of choice for rapid communication. Unfortunately, some engineers (and others) fail to apply the same criteria for precision, clarity, and accuracy to e-mail messages that they do to other written communication. These messages can be extremely important, and, although they can be less formal, they must convey the message accurately. Also, some e-mail users forget that their messages are at least as permanent as a paper document. In fact, many more copies may stay around for much longer. In some organizations now, there is a rule that one should not put anything in an e-mail message that one would not want circulated in hard copy throughout the organization (or even outside). Also, any document put on the Internet is potentially available to anyone in the world.

29.2.5. Exhibits (Figures and Tables)

Many of your important results will be presented in figures and tables. When the numerical values are important to the audience, a table is more appropriate. When the trend of the data or the difference between sets of data is important, a graph is better. Figures (graphs and pictures) are numbered sequentially in the order that they are cited in the report. If they are not cited, they are not included. Similarly, tables are numbered sequentially in the order that they are cited. In most reports, these exhibits appear close to the point where they are cited, but care should be taken not to interrupt the flow of the text too much.

The typical kind of graph that engineers use (with two linear scales) is sometimes called a **scatter plot** or an ***x-y* plot**. Care should be taken to choose properly the dependent and independent variables, and the axes must be labeled with the variable name. Usually, an axis is not labeled with the symbol for the variable (because these are not standardized), and it is never labeled with only the units of the variable. The units should be included in the axis label after the variable name. For example, "Manufacturing Cost ($/y)" would be appropriate, but "($/y)" would not. The title of the graph appears at the bottom of the figure, immediately after the figure number. The title should be descriptive and should not merely repeat the axis labels. For example, "Figure 3. Determination of Optimum Pipe Diameter" might be appropriate, whereas "Figure 3. Annualized Cost Versus Pipe Diameter" would not be acceptable.

Other types of figures used in design reports are process (and block) flow diagrams, piping and instrumentation diagrams, pie charts, histograms (bar charts), and scheduling charts. Each is numbered, cited in the text, and titled. Specific format instructions for flow diagrams and P&IDs are

given in Chapter 1. Pie charts and histograms are used to show relative sizes of quantities. For example, the total operating cost has many components, but only the steam cost may be a significant fraction compared with the rest. A pie chart would show this. (Also, the total quantity that the pie represents should always be given.) Relationships between numerical variables, however, are not shown on pie charts or histograms. A scheduling chart is often included in reports of ongoing projects, and these are numbered, titled, and located in the same way as other figures.

Tables contain a number and descriptive title at the top, and each column (except the first in some cases) has a label with appropriate units. Appropriate numbers of significant digits should be shown, and the columns of numbers should line up by their decimal points.

29.2.6. References

When one uses the ideas or words of another author, proper attribution is made in the report. A mark (superscript number, number in brackets, or author name and date in parentheses) is shown in the text at the point where the work is used. The complete citation is given either in a footnote at the bottom of the page or at the end of the body of the report in a separate section. The format for the text mark and for the citation are set in the guidelines of the organization and must be followed.

There are two main reasons for citations of other work. The citation acknowledges the ideas as someone else's, not yours. Such acknowledgment is essential; its absence is plagiarism. (Note that citation is required even when there is no direct quotation of another author.) Also, the citations give the reader guidance to other written sources whose level of detail or focus are different from your report.

With the Internet, it is easy to download text into a file on your computer. To cite this material properly in your report, you must be sure to keep enough authorship data in the file to be able to write the citation. At a minimum, you should include the Internet address (URL) so that you can go back and obtain the author, date, and other information.

29.2.7. Strategies for Writing

The writing process is different for each writer. Some people write best long-hand, others at a computer. Isolation is better for some, but being in the middle of the activity is better for others. Some prefer to spend more time per draft on fewer drafts, whereas others need to get something down on paper (screen), even if it will be modified drastically before the final draft. Here is a strategy that can be quite effective:

1. Define your audience and your purpose.
2. Outline what you want in the report. This may be formal or only a list of topics, statements, or visuals that are key to your message.
3. Start writing early. Writing the introduction is a way of exploring what the problem is. Once you have identified the problem, the focus of the rest of the report will be clearer. Think of the writing of the report as you would any problem, and use one of the problem-solving strategies from this book.
4. In the first draft, focus on the facts and on the logic. Save editing for later.
5. Do not turn in a first draft as a final draft.
6. Set aside the writing for a day before you pick up the hard copy to revise it.
7. Revise for organization, logic, technical content, clarity, and so on.

8. Set aside the hard copy for a day.
9. Revise for grammar, spelling, punctuation, conciseness, word choice, and other elements of editing.
10. Have someone read it aloud to you.
11. Do the final revision.
12. Proofread the hard copy.

This strategy is an example of an ideal process. Other models could be found. We must admit that we do not always follow all these steps, but the more closely we follow them, the better our writing is.

An important issue is writer's block, which is a state of such high anxiety about writing that writing becomes impossible. Much like stage fright, writer's block is autocatalytic. The writing paralysis caused by the anxiety creates increased anxiety, which leads to heightened paralysis. Identifying the cause leads naturally to the cure. The three most common causes are as follows:

1. **Not Fully Understanding What You Are Trying to Explain:** If you are confused about the technical content of your work, it is very difficult to put it down in words.
2. **Having No Clear Sense of Audience or Purpose:** If you do not know who will read your report, how can you communicate with them?
3. **Trying to Turn Out a Final Version Painful Word by Painful Word:** If you want to write the perfect report in one draft, that draft will take far longer than writing multiple drafts.

When a group writes a single report, there are three basic strategies:

1. **Assigned Sections:** This is especially helpful for long reports or when different members of the group have different strengths. A drawback is that the logical connections between the sections can be missed, and this must be corrected by having all members of the group critique all sections of the report between drafts. Finally, one person needs to go through and modify the writing of the sections so that they are written in one style.
2. **Writing by Committee:** On shorter reports, the entire group can meet together, talk about what should be in each section, and decide as a group what the wording should be. This is a difficult strategy to implement, and, in fact, confusing, unfocused writing is often characterized derisively as "written by committee."
3. **Assigned Functions:** Members of the group can be assigned tasks such as preparing the outline, writing the drafts, critiquing the drafts for technical errors, critiquing the drafts for expected audience response, checking for consistency and logical connections, and so on. Again, coordination is the key. Everyone reads all drafts.

29.2.8. WVU Guidelines for Written Design Report

The following guidelines were written by the chemical engineering faculty at West Virginia University and are available at http://www.che.cemr.wvu.edu/publications/projects/index.php. They may be reproduced for use in engineering courses with appropriate attribution to the Web site.

The format for presenting a written design report differs from that of a laboratory report. A laboratory report is more of a scholarly endeavor in which a scientific story is told starting with theory, proceeding through results, discussion, and conclusion. It is usually assumed that the reader will read the entire report. In a design report, the most important conclusions should

appear early in the report, with more detail presented for the reader who reads further into the report. Such is the way of business, where you must effectively convey the bottom line to someone who may not have the time to read the entire report.

Grammar, Punctuation and Spelling

It is important to write using correct spelling, grammar, and punctuation. Incorrect spelling, incorrect grammar, incorrect word usage, and incorrect punctuation make a poor impression on the reader. They can deflect attention from quality technical work. There is no reason for incorrectly spelled words in any report. Spell checkers identify incorrectly spelled words for you, and they also identify words that are often confused with each other. You still must proofread carefully, since a spell checker will not identify a correctly spelled incorrect word (*e.g.*, "too" instead of "two").

For those of you who are unsure of the correct use of punctuation, grammar, etc., the Web site http://grammar.ccc.commnet.edu/grammar is a good reference.

In general, first person (pronouns "I," "we," "me") should be avoided. The passive voice should be used. ("It was done" instead of "I/we did it.") The passive voice will be flagged by your grammar checker unless you disable that option. Others may tell you not to use the passive voice; however, we think it is more formal, and therefore "better," than the alternative. Addressing the reader should also be avoided. ("You should do this." "Seek medical attention.")

The report should be written as a recommendation, not as if the process is already built (unless it is already built!). Therefore, avoid stating, "A 10 m^3 reactor was installed." Instead, write, "It is recommended that a 10 m^3 reactor be used."

Avoid using active verbs with inanimate objects. For example, "This report optimizes…" is incorrect, because a report, which is inanimate, cannot optimize. Instead, try "This report contains the optimization of…"

The most common punctuation errors are the omission of commas and the misuse of semicolons.

Commas must be used to separate introductory phrases and subordinate clauses from the subject of the sentence. For example, there must be a comma in the following sentence before optimization: "On the other hand, optimization yielded…" Similarly, conjunctive adverbs (therefore, however, although) at the beginning of sentences must be followed by commas.

Commas precede coordinating conjunctions (and, but, or) if the clause following the conjunction contains a new subject. For example, a comma is needed before "and" in the following sentence: "The reactor was optimized, and the optimum temperature was found to be 100°C." A comma should not be used in the following sentence because what follows the conjunction refers to the original subject of the sentence: "The reactor was optimized and found to require a temperature of 100°C."

When complete sentences are separated by conjunctive adverbs (therefore, however, although), the conjunctive adverb is preceded by a semicolon and followed by a comma (for example, "A three-compressor configuration was investigated; however, the two-compressor configuration was found to be the optimum").

Semicolons are also used to separate two complete sentences that are written as one sentence.

This should be used sparingly, mostly for effect (for example, “A three-compressor configuration was investigated; it was found to be incredibly expensive”).

It should be observed that the compound adjective “three-compressor” is hyphenated. Another example is high-pressure steam. This occurs only when the compound is used as an adjective (for example, “High-pressure steam was used” but “The steam used was of high pressure”).

Group Reports

Group reports must be edited for consistency. Each group member should read every section and provide feedback to the section authors. Simply assembling individually written sections without editing almost always results in a very poor report. One group member should be designated as the editor. This person should make certain that all figures, tables, equations, etc., are numbered consistently, that font types and sizes are consistent, that formatting such as the indentation spacing, paragraph spacing, justification, etc., are all consistent.

Report Format

The suggested report format is as follows.

Letter of Transmittal

This is a memorandum (if internal) or a letter (if external) to the appropriate person identifying the report. The report is actually an enclosure to this letter. Remember to refer to the original memorandum or problem statement. In order to get the reader’s attention, writing several sentences summarizing the bottom line is essential. You should always sign or initial this memo or letter. This letter stands alone. It contains no figures or tables and does not reference any figures or tables contained within the report.

Title Page

This must include the title, names of all contributors to the report, the business name (class number and name will suffice), and the date.

Abstract or Executive Summary

An abstract or executive summary should start on a new page and nothing else should appear on the same page.

An executive summary is essentially a long abstract. Whereas an abstract is usually less than one typed page, an executive summary may be several pages. An executive summary is usually reserved for a very long report, while an abstract is appropriate for shorter reports. Very long reports may have executive summaries approaching ten pages. It is probably best for the executive summary to be less than 10% of the total report length. For most of our reports, an abstract is appropriate; however, the year-long, senior design project and the third major may be extensive enough to require an executive summary. Some multi-volume reports may contain both an abstract for each volume and an overall executive summary.

At times, an entire report may be an executive summary plus appendices, usually if the report is short. This is essentially a short report without an abstract. In this case, the executive summary should have the same organization as a full report, without separate section headings. It should include key figures and tables but need not include as much discussion as a full report. The Results section may be abbreviated, with additional tables and figures well organized in the appendix. A key difference between an abstract and an executive summary is that an abstract

stands alone. It contains no figures or tables, only rarely contains an equation, and does not refer to any figures (such as references to a PFD—stream numbers, equipment numbers) or tables contained within the report.

Either an abstract or an executive summary should convey to the reader, in a rapid and concise manner, what you did, what you conclude, and what you recommend. This is for the reader who may not read any further or for the reader who is deciding whether or not to read any further. Summarize the bottom line; do not discuss computational details unless they are unique and applicable beyond the report at hand. In an executive summary (but not in an abstract), do not be afraid to use a few well-chosen graphs, pie charts, or histograms to emphasize your important points, but choose these wisely in order to keep the length of the executive summary down.

These instructions suggest that the contents of the abstract and letter of transmittal are similar. Since both sections are supposed to provide a summary of important conclusions, there will be significant repetition of content. The abstract usually contains more information than the letter of transmittal.

Remember the bottom line!

Table of Contents

This is necessary only for longer reports. At the top of the page, the proper title is "Contents," not "Table of Contents." Regardless of whether you include a table of contents, all pages of your report should be numbered, preferably at the top right corner or top center (the latter permits easy two-sided copying). Number, indent, or otherwise indicate sections, subsections, etc.

Introduction

This is for the reader who continues past the abstract. The introduction is a one- or two-paragraph summary of what was assigned, what was done, and (very briefly) how it was done. A summary of the constraints on the problem is appropriate, as well as some perspective on the specific problem in the context of the larger business picture. There should be no results or conclusions in the Introduction section.

Results

The Results section states what was found. It is usually presented without detailed explanations, which are in the Discussion section.

The following are essential components of a results section:

1. Labeled and dated process flow diagram (PFD)—CHEMCAD PFDs are unacceptable.
2. Stream flow tables—These must include temperature, pressure, phase, total mass flowrate, total molar flowrate, and component molar flowrates for every numbered stream.
3. Manufacturing cost summary—Yearly revenue and expense (income from product sales, expenses for raw materials, utilities [itemized], equipment costs if calculated as an annual cost, personnel, etc.) must be included.
4. Investment summary—The cost to build and install plant now (if appropriate to goals of problem) is required. This should be itemized by piece of equipment.

5. Equipment summary—A listing of equipment to be purchased and installed, with specifications, is required. This could be combined with item 4 if the list is not too long.

The above should not simply appear without description. This section is held together by prose that provides the reader with a road map through the tables and figures of item 1—item 5 above. Whether you use figures or tables for the above is your choice. Generally, a figure is used when the trends or relative relationships are more important than the actual numbers. You must decide whether a figure or a table conveys your intent more efficiently. It is also important not to be redundant; do not have a figure and a table illustrating the same point. Make a choice!

Mention the process flow diagram early in the prose of this section, and refer to it often.

Discussion

The discussion section contains explanations of the results. It explains how the results were obtained and what they mean. However, a detailed log of how calculations were done should be avoided. This section is for the reader who wants still more information and is willing to read still further. Here you discuss the reasons for making choices and the reasons for discarding alternatives. This is where you discuss any optimization that was done. You might also discuss nonroutine or unique computational aspects.

For our junior designs, a subsection pertinent to each class is also appropriate.

Conclusions

Nothing new is presented in this section. You should reiterate your important conclusions, which may have already been stated in the abstract, the executive summary, and/or the letter of transmittal. Usually these will involve economics and process modifications. Be concise and clear; avoid lengthy paragraphs. Once again, remember the bottom line!

Recommendations

This section includes recommendations for further action and/or further study. If there are few conclusions and recommendations, these two sections can be combined. Avoid recommendations that are "pie in the sky," such as finding a better catalyst. Also, avoid recommendations that will clearly be studied in subsequent semesters, such as to study the separation section.

References

There are two ways this section can be presented. If you put it at this location in the report, it should contain only references cited in the sections of the report preceding this section. References may be listed by number and cited in the text by this number, either as a superscript or as a number in parentheses or in brackets (preferred). Another method is to cite the reference by the author and year. You should consult the end of a chapter or the end of the book in any of your chemical engineering texts for the correct citation format. If you choose this method, then any references to data sources appearing in the appendix should appear on the page on which that calculation is presented.

No references should appear that are not specifically cited in the report. Software should never be referenced unless you use it as a source of data, as might be the case with Chemcad.

The other alternative is to place the reference section at the very end of the report, and cite all

data references in the appendix in the manner described above for the body of the report.

Figures taken from books or the Web must be cited. Failure to do so is considered plagiarism.

Other Sections

Sometimes, especially for longer reports, specialized additional sections are included, such as Safety, Assumptions, Environmental Concerns, Risks, etc. The author should check with the prospective users of the document to determine the appropriate additional sections and what these sections should include.

Appendix

This section contains your detailed calculations, computer programs, etc. A specific Contents page for the appendix is essential so the reader can easily find a particular calculation. Therefore, pages in the appendix must also be numbered. This numbering may be continuous with the main report, or you may start over. You may also choose to start numbering over for each appendix. If you do the latter, be sure to use a letter indicating the appendix in which the page is contained (*e.g.*, page B-5 means page 5 of Appendix B). Calculations may be hand written but should be legible and easy to follow. Include a copy of the full Chemcad report (including the flowsheet) for your final case at the end.

Other Aspects of the Report

Figures and Tables

Whichever you choose, figures and tables have a specific format. They are numbered in the order in which they appear in the report. They should be embedded in the text where they are cited or appear on the pages immediately following where they are first cited in the prose. Figures and tables are cited by their name, not by a location (above, below). If a figure or table is not cited, it should not appear in the report. Tables have a title at the top. Figures have a caption at the bottom, which, if a graph, should not simply repeat the axes (unacceptable: y versus x; good: plot illustrating . . .). Nothing should appear at the top of a figure. The fact that most software puts a figure title at the top is not a reason for you to have a title at the top. If you put a title at the top of a figure for an oral presentation, the title should be removed for the version used in the written report. There are only figures and tables. Nothing is labeled a graph, sketch, etc. When you refer to a figure or table, Figure #, Stream #, or Table # should be considered a proper name and, therefore, capitalized. Finally, use something other than colors in figures and tables to distinguish between items (different shading, different symbols), since colors are not copied well. It is also strongly suggested that the default gray background on Excel plots be changed to white. Also, on Excel plots, what looks good in color in PowerPoint looks terrible when copied in black and white. Lines and symbols should be black monochrome.

Figures can be scatter plots, bar charts, or pie charts. Use scatter plots when the independent variable (x-axis) is quantitative, *e.g.*, temperature. Use bar charts when a nonquantitative independent variable is being plotted, *e.g.*, cost (y-axis) versus case study number or piece of equipment (x-axis). Use pie charts when the relative amounts of quantities are being compared and the quantities form a whole, *e.g.*, distribution of capital costs between individual equipment.

When pie charts are used, the total quantity (corresponding to the whole pie) should be in a

legend or outside the pie. Each slice should contain the percentage of the pie. When graphs are used, do not use "line charts" (where the *x*-axis has tick marks at irregular intervals) when the independent variable is numerical. Instead, use scatter plots. Increasing magnitude should always be to the right (*x*-axis) and up (*y*-axis). If using grid lines in scatter plots, make sure to use both horizontal and vertical lines. Gridlines help the reader identify the value of data points; however, grid lines should be used sparingly.

Avoid using three-dimensional bar charts or scatter plots, especially when only two variables are used, *i.e.*, if there is only one independent variable. Three-dimensional figures are very difficult to read. That your software uses 3-D plots as a default option is not a good reason to use them.

For axes, use ranges in appropriately round numbers, *e.g.*, from 0 to 20, not from 3.47 to 19.993. If possible, include zero in your scale for the proper perspective.

For plot axes and tables of figures, use the appropriate number of significant figures. The numbers appearing on a figure axis should all contain the same number of decimal places.

When columns of figures appear in a table (and these should be used sparingly), each figure in the column must have the same units. If a total is shown, it should be the sum of all numbers above it. Columns should be lined up by the decimal point or by where the decimal point would be.

The following terminology is used to define the orientation of a table or figure on a page. "Portrait" refers to the way typed text appears, with the long dimension of the paper vertical. This page is in portrait. "Landscape" refers to text, figures, or tables appearing with the long dimension of the paper horizontal. Landscape figures and tables should always be bound facing outward, *i.e.*, the top of the figure or table is closer to the binding.

It is expected that numbers, symbols, and unit abbreviations will be used in the written report. Learn to use the symbols and the equation editor in your word processor, and learn to insert symbols, superscripts, and subscripts in plotting software. For example, use 5°C, not five degrees C. Write $25 million/y instead of 25 million dollars per year. Include lead zeroes in all numbers less than 1, *e.g.*, 0.25 instead of .25. Use 10 m^3 instead of 10 m^3 in both the report and on figures. Items like m^3 are considered unacceptable for reports in this Department.

When reporting large costs, millions of dollars, for example, present no more than three or four significant figures. Just because your spreadsheet reports ten or more significant figures is no reason to present all of them. It is ludicrous to present a preliminary design down to the penny. Remember that people do not expect dollar figures to be in scientific notation. One million dollars should appear as $1 million or $1,000,000.

Equations

Equations may be used in different parts of a report, as needed. The proper format for equations is as follows. Equations are usually centered. All equations are numbered serially, with the equation number usually right-justified. Only the number appears, either in parenthesis or in brackets. Just as with figures and tables, equations should be cited by number. Similarly, Equation # is a proper name and should be capitalized. It is not usual to refer to an equation by number before it appears. Correct and incorrect examples are presented below.

Incorrect:

The relationship for the heat capacity difference is given by Equation 1.

$$C_p - C_v = \frac{\alpha^2 VT}{\kappa_T} \qquad \text{(equation 1)}$$

For an ideal gas, this reduces to Equation 2.

$$C_p - C_v = R \qquad \text{(Eq. 2)}$$

Correct:

The relationship for the heat capacity difference is:

$$C_p - C_v = \frac{\alpha^2 VT}{\kappa_T} \qquad (1)$$

For an ideal gas, Equation 1 reduces to:

$$C_p - C_v = R \qquad (2)$$

It is also considered improper format to include *, ×, or · to indicate multiplication in an equation or anywhere else in a report, except as noted below for exponents. Therefore, $PV = nRT$ is correct. The following are incorrect: $P \times V = n \times R \times T$, $P \cdot V = n \cdot R \cdot T$, $P*V = n*R*T$. Similarly, these symbols should be avoided in units.

It is also incorrect to use the symbol ^ for an exponent in equations or anywhere else in a report.

The terms and symbols used in all equations must be defined, either immediately after the equation or in a comprehensive nomenclature section appearing either immediately after the table of contents or at the end of the report, following the reference list.

Finally, when using exponents, it is not correct to use E format. So, 6.02E23 is incorrect. 6.02×10^{23} is correct.

How Engineering Reports Are Used

An engineering report is essentially never read in its entirety by a single person. Most of the users of these documents are too busy to sit down and read every word. However, you must assume that each word will be read by someone, sometime, and that you will not be around to explain any ambiguous passages. Your report must be useful to the following types of readers:

1. The person who has only a few minutes to read the report. This is often an intelligent, nontechnical person who controls millions of dollars. You must be sure that this person can pick up your report, immediately find the important answers, *i.e.*, the "bottom line," and make the right decision. If the answer is not prominently presented in the Executive Summary or the Abstract, this type of reader will judge your report to be of little value. You cannot afford that judgment.
2. The technical manager. You may assume that this person is a chemical engineer, but you may not assume any specific technical knowledge about the details of your project. This person is busy but may have enough time to read most of the report (but not the appendices). Few engineers will sit down and read a report from beginning to end! One looks for the answers quickly. As soon as these answers are found, one makes a decision and stops reading. Sections might be read in the following order, for example, until the answers are found: Executive Summary, Recommendations, Conclusions, Results,

Discussion, Introduction. Different readers will read the sections in different orders. You must, therefore, take special care to put the information in the correct sections. This is part of the reason why repeating important conclusions in several places in the report (letter of transmittal, abstract, conclusions) is a good idea.

3. The engineer who must use your design. This chemical engineer needs to find details of how you did your calculations and how you reached decisions. The appendices are of special interest to this reader. However, time is of the essence. This reader wants to be able to go immediately to that page or two in your appendices that deals with a specific detail. Without good organization and a good table of contents for the appendices, this is impossible. If this reader cannot find the right information, your effort has been wasted.
4. Others. Many others will try to read your report: mechanical engineers, chemists, environmental activists. Think about these people, too.

What can you do to see if your report meets the needs of these readers? Ask someone who did not author the report to read it, pretending to be one of these readers. A friend, a roommate, or a fellow student might qualify. If they cannot understand what you are trying to say, you have a problem. Remember, if the reader does not find what he or she is looking for or cannot understand what you are trying to say, it really does not matter whether or not the information is in the report somewhere or whether the results are of high quality. And remember, reports written at the last minute will be obvious to an experienced reader. A report with typographical errors, misspelled words, grammar faults, or confusing phrasing is insulting to the reader. That is not the impression that you want to leave with your clients, supervisors, or fellow engineers.

29.3. Oral Communication

Public speaking can be scary at first, but oral communication is crucial in engineering design activities. When done well, it communicates information faster than can the written word, and it allows for immediate communication from the audience to the speaker and between members of the audience. Thus, oral presentations (with questions) provide for a type of feedback control on the communication process, whereas written communications are closer to feed-forward control.

The key to effective oral communication is, as it is for written communication, audience analysis. Include visuals that focus the audience attention on the areas of the project analysis that both you and the audience feel are important. Be sure that the audience receives the information required for making the right decision, and be sure not to bore the audience. If the readers of your report get bored, they may come back to it later. If the attention of your listeners starts to drift, the information is lost.

Before the actual presentation, practice is essential. (It may surprise you to learn that most faculty do not practice their lectures.) If possible, practice in front of real audience members who have agreed to give you feedback. Otherwise, try taping (audio or video) your presentation and critiquing it yourself. If none of these techniques will work, go to a quiet room and give your presentation out loud to yourself. In any case, it is best if you use the actual equipment (overhead projector, slide projector, and/or computer) that you will use in the actual presentation. If this is impossible, use hard copies of your visuals.

Successful oral presentation requires a degree of self-confidence. To avoid a last-minute problem in this regard, give your practice talk far enough in advance that you can make corrections to your talk

and/or your visuals. If your audience says that you need to make major changes, you need to be able to implement these suggestions.

Even when speakers are well prepared and self-confident, often they are nervous. A variety of techniques can be useful to alleviate tension. Here are a few:

- Prepare notes that you can refer to if you draw a blank on what to say next or to be sure that you talk about the key points. The notes should be on stiff note cards that will be easy to hold still and that will not distract you or the audience.
- Practice the presentation in front of a group. You are likely to be most nervous during the first time that you give a presentation.
- On your note cards, print in bold letters "RELAX" or something else that will be a trigger to help you calm down.
- If you tend to speak too quickly during presentations, print "SLOW DOWN" on a note card.
- Even if you never refer to them, note cards can be a kind of security blanket that could help you relax.
- Look at a point just above the heads of your audience. They will think you are making good eye contact, but you can avoid really seeing them.
- Before the start of the presentation, take a deep breath or two to calm down.
- During the presentation, keep focusing on the remainder of the presentation. If you have made a mistake (by omitting to say something that you wanted to include or by not remembering why you chose the reflux ratio that you did), ignore it until the question-and-answer period at the end. Reminding yourself and your audience that your presentation was less than perfect will make it more so.
- If questions during your talk make you nervous, start your talk by asking that the audience save their questions until the end.
- Before the talk begins, go to the room and check it out. Where will you stand during the talk? Would you feel more comfortable and in control if the projector were moved? (Often it can be.) Do you want the lights high or low? By getting used to the environment and making small changes to it, you begin to feel more in control. In a classroom or conference room, you may be able to move chairs or to keep the front row empty, if that would help.
- Avoid looking at one person in the audience throughout the talk. If that person is interested, he or she will show this by facial expressions, and you will feel good. However, if suddenly that person loses interest, you may be devastated.
- Do not allow yourself to be in a rush immediately before your talk. Sit down, take a short walk, whatever will calm you, but do not get into a serious conversation.
- Do not drink too much coffee or other caffeinated beverages before a talk.
- Be sure the computer is working and can read your PowerPoint file, your transparencies are in order, and the pointer is where you want it before the last minute.

During the question-and-answer period, you relinquish part of your control over the situation. You do not know what will be asked, but you must be prepared to answer. Dealing with this uncertainty requires additional strategies:

- Anticipate what the questions will be. Often, especially if you practice the talk with an audience,

many of the questions become obvious. Prepare answers to each of these.

- Admit when you do not know the answer to the question. However, if you have a partial answer, offer that. You should not leave the questioner with the impression that you know nothing about the topic.
- Thank the audience member for the question, even if you do not know the answer. If it is a question that you, too, would like the answer for, tell the audience so. If you will be investigating the issue further, let them know that.
- Do not try to answer the question until you are sure that you know what is being asked. Ask the questioner for clarification if necessary.
- If you need time to think about your answer, restate the question. This not only gives you a few seconds to think, but it also helps to make sure that you are answering the right question.

29.3.1. Formal Oral Presentations

When you are talking to a group (sometimes a large group), the presentation can be quite formal. You may be introduced, and there may be applause after you are finished. In this type of presentation especially, it is important that you have a strong opening and closing and that you focus on keeping the attention of the audience.

Prepare simple, uncluttered visuals that everyone in the room can see. Be sure to see the room before your talk. If the large crowd is going to make you nervous, plan to use the techniques mentioned earlier to make it feel like a smaller audience.

29.3.2. Briefings

Briefings are a very common form of oral presentation, in which a small group of people (as in a conference room) listen to your talk. The size of the audience will mean that audience members are more likely to try to pay attention to your talk than a very large audience would, but you must directly address their needs for information. Again, computer slides or transparencies are usually used, and you should prepare a hard copy set of these for each audience member. Because people more often take notes at a briefing than at a formal oral presentation, the hard copy will help them to focus on your talk. Also, they may find it more helpful to follow your talk by looking at your hard copies rather than at the screen.

Because the audience tends to have a narrow range of background, the briefing tends to be more detailed, and the question period is usually more extensive.

29.3.3. Visual Aids

Most technical presentations are developed around the visuals. Start with a title slide and then a slide that gives the big picture. As with written reports, it is important to obtain the guidelines for oral presentations from your organization. Some are very prescriptive, others not.

A rough guideline is that each visual will be used for one minute; however, this timing varies greatly. Sketch your visuals crudely as you run through what you would like to say. Imagine that you are a typical audience member. Would you have received the right information? Revise your planned visuals to address the gaps or lack of continuity.

A mixture of text visuals and graphics is usually most effective. Tables rarely make good visuals. As you explain the meaning of a trend on a graphic visual, your audience is absorbing the trend itself.

When you present your conclusion, a text visual will probably be better. The best way to improve your visuals (in fact, your entire presentation) is to reflect on your own response to the visuals and presentations of others. What kept your attention? What was confusing? What communicated the most high-quality information? Again, doing a dry run with a friendly audience is a good way to get constructive criticism and feedback in a comfortable environment.

Be prepared to point at the screen to direct the audience attention. Before the presentation, the pointer should not only be located, but also tested by the presenter. One must avoid moving the pointer either so fast or so erratically that the audience is distracted. If the presenter is too nervous, it will be difficult to use any pointer without erratic movement. If this is the case, both hands should be used to steady the pointer. If all else fails, the presenter should find a way to avoid using the pointer. In any case, avoid moving the pointer except when it is in use. The audience will always try to follow a moving pointer.

Right-handed people should always position themselves so that the screen is to their right as they face the audience. Left-handed people should always position themselves so that the screen is to their left as they face the audience. This orientation makes it more comfortable to maintain eye contact with the audience when pointing to the screen.

Slides, transparencies, computer projections, and videos can be used for the visual aids. Each has its own advantages, and one should consider all options before deciding how best to present the material. However, there are two common traps to avoid. Using more than one of these media in a presentation can be impressive if done well; it is invariably disastrous if done without a great deal of rehearsal. Also, one must be prepared with a strategy for continuing if the equipment malfunctions; this can occur especially frequently with state-of-the-art computer projection hardware and software.

There are many guidelines concerning the size of lettering and the density of information to use on visuals. However, the best strategy is to imagine what the audience response would be.

No visual should ever be used in a presentation unless it has been previewed with similar equipment, in a similar room, from the most remote position that an audience member can be located.

29.3.4. WVU Oral Presentation Guidelines

The following guidelines were written by the chemical engineering faculty at West Virginia University and are available at http://www.che.cemr.wvu.edu/publications/projects/index.php. They may be reproduced for use in engineering courses with appropriate attribution.

When presenting an oral report it is important to realize that the audience cannot digest material in the same way as they can when reading a report. There will be no time for them to reread a sentence or paragraph, or to study a table or figure. Therefore, it is incumbent upon the speaker to emphasize the important points. The recommendations that follow, though written for any type of oral presentation, are written within the context of a design presentation.

All oral presentations are organized as follows:

1. Tell the audience what you are going to tell them.
2. Make your presentation.

3. Remind the audience what you told them.

With this in mind, here is one way to organize an oral presentation.

Title Page

Identify the report and the presenters on a visual aid.

Outline

Tell the audience what you are going to tell them, and use a visual aid for reinforcement. This is usually an outline of the report. It is not sufficient to list the structure of the report, *i.e.*, introduction, results, discussion, conclusion. You should include a few words abstracting the contents of each section. Note: this visual should not be titled "Agenda."

Early in your talk, describe the project, flowsheet, etc., in general, before the details. Also, early in your talk, mention the "bottom-line" conclusion.

Results

This follows the outline of the results section of a written report described in the document titled *Written Design Reports*. However, there are a few important points to remember. First, a detailed stream flow table will not be easily seen or understood by your audience. Second, what is effectively communicated in a table in a written report might be best communicated orally using a graph or pie chart. Avoid using complex tables and figures with small print. These can neither be seen in the back of the room nor digested by anyone.

All of the rules on figures and tables in the document entitled *Written Design Reports* extend to oral presentations.

Discussion

Once again, the content is similar to that described in the written report section. The only difference is how you choose to communicate your information.

Conclusions

Here you remind your audience what you told them, usually as a list or outline. Remember the bottom line!

Recommendations

This is self-explanatory. If this section and the conclusion section are both short, they can be combined.

Other Important Points When Making an Oral Presentation

PowerPoint Slide Show

If you are considering using fancy background templates, animation, and/or special effects, think again. They are distracting. Use them sparingly, and only if they add to the effectiveness of the presentation. A simple, color background template is recommended. The background template should be removed or covered when showing large figures, particularly PFDs; such figures should be presented with a white background. Finally, it is also recommended that the font size be set differently on each slide so that the slide appears full.

Content of Visuals

Do not put too much on a visual. A detailed table may not be readable in the back row. When making a visual, put yourself in the audience and ask yourself whether you could learn anything from it if you saw it only for 30 seconds or a minute. Short, concise statements of a few words on the visual, with the speaker providing a more detailed explanation, are sufficient to convey your points. Use colors effectively, but do not go overboard. Test all of your visual aids in the presentation room or in a room of similar size and shape to be sure that all information on your visuals is clearly readable.

The format and rules for presenting figures, tables (use sparingly if at all in oral presentation), equations, etc., are identical to those in the document *Written Design Reports*.

Colors in visuals can be a useful tool. However, colors should be used wisely and effectively. Typically, this means no more than four, as a general rule. Also, try to be consistent in the use of colors; if you use red for the fixed cost of the heat exchangers and blue for the fixed cost of distillation columns, then use the same colors for operating costs for the same equipment.

Presentation Mechanics

Always face the audience. If you have to look at the screen, take a quick glance and then turn back to the audience. If using overheads, you can look at the transparency on the projector rather than turning toward the screen. Be careful not to block the view of a portion of the audience. If someone else is changing your transparencies, stay back next to the screen. If you are changing your own transparencies, step back away from the projector after making the change.

Avoid the following nervous habits: chewing gum, playing with the pointer or something in your pocket, rocking from side to side, or giggling. Approach the oral report with confidence and a firm belief in your abilities and your work.

Never read text visuals word for word, line by line. Visuals should be brief. Your job as a speaker is to amplify the content of the visuals.

Voice

Speak clearly, enunciate carefully, avoid audible pauses, and project your voice. Speaking softly usually implies to the audience that you are unsure of yourself; probing questions will generally follow.

Be Calm

You are in control, not the audience. Beforehand, arrange the room in whatever pattern makes you feel most comfortable. Do you want to point with your left hand or your right? Do you want the shades open or the lights out? Then, do not make last-minute changes in your presentation. Immediately before your presentation, take a few deep breaths and yawn. (This is easier to do if you are not in the presentation room.) If you do not want to be interrupted with questions during the presentation, tell the audience so. And, if they still interrupt, politely tell them that you will be answering that question later. Assume that everything is going to go well.

Notes

To use or not to use? Do whatever will make you most comfortable and in control. If you read entirely from a script, no one will believe that you know what is going on. But no one can remember every detail without notes. When you practice your presentation, try it with and without hand-held notes, if you are not sure which is better. As a novice, you might find that hand-held notes bolster your confidence; however, with practice, you should wean yourself from using notes. Eventually, you will be able to use the content of the visual as your notes.

Audience Analysis ("Know Your Audience")

Just as with a written report, think about the different backgrounds and needs of your audience. Will they get the right message and make the right decisions?

Question and Answer

Admit it when you do not know the answer. Most people ask a question only because they do not know the answer, either. Try to be responsive, not evasive. And prepare for Q & A by imagining the questions that will be asked.

Postmortem

After the presentation, go with your colleagues to a less-tense room and get feedback immediately. Ask your colleagues what you could have done better. If they tell you that you were perfect, tell them that they are not being very helpful. Demand criticism! This is the best time to find out what you did right and what you did wrong. If you wait more than about an hour, the feedback will not be detailed enough to help you.

29.4. Software and Author Responsibility

Word processing, spreadsheet, and graphics software can help an author produce a better final report, but each software package has limitations. It is the author's responsibility to understand these limitations and to overcome them. Some of these software problems are the results of programming errors, some arise from misunderstandings by the software developers of the rules of writing, and some represent differences between technical writing and other forms of written communication.

Above all, though, writers should save their files frequently and make backup copies.

29.4.1. Spell Checkers

Misspellings have always been unacceptable in formal written work. Readers generally have a lower opinion of the ideas expressed when the prose contains misspelled words. With spell checkers being so available, spelling errors have come even more to indicate sloppiness and lack of respect for the audience.

Clearly, one cannot submit a report that has not been subjected to a spell checker. However, no spell checker is perfect. More importantly, they can only check whether the "word" in question is *a* true word, not whether it is *the* word that the author intended. If one writes "to" when "too" is meant (or "preform" instead of "perform"), the spell checker will not correct it.

All spell checkers allow the author to add words to the dictionary. Many technical terms are not in the standard software dictionaries, so it is tempting to put in many words common to the author's subject. However, this is a risky business. If one puts a misspelled word in the user dictionary, nearly all of the author's reports will have that misspelling, without the author having a clue! Also, it is usually far more difficult to remove a user-supplied word from the dictionary than it is to add one.

Most spell checkers automatically suggest another word when they detect a misspelling. If one too quickly accepts the suggestion, rather strange prose can arise. In a technical report, we once somehow accepted the suggestion of "voices" for "VOCs" (volatile organic compounds)!

29.4.2. Thesaurus

In most writing courses, students are warned not to misuse a thesaurus. It is tempting to use a new word, one that sounds more sophisticated. Unfortunately, the probability that the new word can be substituted directly (without a modification of meaning) is nil. The thesaurus is designed to be used to *remind* one of a similar word. If the thesaurus suggests a word that you have no memory of, do not use it. Many satirical papers have been written about the blind use of a thesaurus.

29.4.3. Grammar Checkers

Grammar checkers continue to improve, but most are based on simple rules that apply imperfectly to technical communication. For example, the use of the passive voice is frowned upon in much nontechnical writing, but it can be the more appropriate voice in a technical report. The passive voice places emphasis on the object receiving the action rather than on the subject taking the action. Although the passive voice is often overused in technical writing, it does have its place.

Crude distinctions are often made by spell checkers. For example, some will flag each instance of "affect" and ask if the author meant "effect" (or vice versa). This can be tiresome, but one must be sure to understand the significant difference between these words.

Especially in long sentences, grammar checkers tend to become confused and flag correctly written passive constructions and subject/verb agreement. It is important not to accept the suggested changes too quickly.

Various readability indices are included in grammar checkers. These are crude measures of the ease with which a reader can read and understand a document. Most predate the computer grammar checkers. A document with a good readability index could be totally incomprehensible, and one with a poor index might be quite good. One must not read too much into these indices. However, they do focus on elements of good writing, such as short paragraphs, short sentences, short words, and

straightforward grammatical constructions. Thus, one should watch the readability numbers for sudden shifts to longer words, sentences, and paragraphs. If the same information can be conveyed in a simpler format, it is likely to be more helpful to the reader.

29.4.4. Graphs

For much graphing software, the default graph type is not the common *x*-*y* plot, even though these are by far the most common in technical communication. If the independent variable (on the abscissa or horizontal axis) is numerical and continuous, this type of graph must be used. Bar charts and histograms are used only for nonnumerical or (sometimes) discrete variables. Unfortunately, there is a type of graph that looks vaguely like an *x*-*y* plot but is more like a bar graph. It is called a line chart. The line chart has evenly spaced tick marks on the abscissa, but the numerical values at the ticks are not even intervals! Such a graph is very misleading in technical work and must be avoided.

Most graphing software will automatically choose the scale for both axes. Unfortunately, this is usually not acceptable. For example, it is common practice to use even numbers when both odd and even are not shown and to use numbers ending in 5 or 0 in preference to others. These conventions make it much easier for the reader. Also, there are often constraints (such as 0–100%), and it is sometimes useful to extend axes far beyond the last data point. For example, in a series of graphs, one should use the same scale on each to allow comparisons. Typical graphing software will do almost none of the above automatically. The best strategy is to use user-specified scales on all graphs.

The lettering of the various parts of the graph should be clean and simple, and the more important parts should be in larger font size. This is rarely done automatically. The convention is to put the title of a figure (such as a graph) below the figure, although when the graph is presented by itself (as on a slide), the title may appear at the top. Titles should be properly capitalized: the initial letter of each word (except articles, prepositions, and conjunctions) should be capitalized. All other letters should be lowercase.

Strangely, some graphical software automatically inserts a legend on graphs. Unless there are multiple variables plotted, this should not be done. In any case, a direct label near the curve is more effective. One must avoid default legends such as “Series 1” that are distracting and offer no information.

Default headers and footers on graphs are seldom appropriate. One must override the default to number the pages consecutively in the report and to avoid double titles, multiple pages labeled “Page 1,” and so on.

Most software connects plotted points with line segments (or splines) by default. This is often not appropriate. For example, if the points represent experimental data, only the points should be shown. Also, the joining of points obtained from process simulation on such a graph can obscure the maximum, minimum, and the shifts from one topology to another. More about these details is given in Chapter 14.

29.4.5. Tables

In some word processing and spreadsheet software, the default for numbers in table cells is centered. If this is the case, one must override the default and line up the numbers in a column by their decimal points. Only then can the readers easily compare the numbers or sum them. Also, the default format may be to include many significant digits. One must be careful to include only those digits that are, in fact, significant. Otherwise, either the readers will be misled about the precision of your answers, or

they will discount your answers if they realize that you have exaggerated their precision.

When numbers have four or more digits to the left of the decimal point, they must have commas to help the reader to see quickly the thousands, millions, and so on, places. Only if the numbers are too cumbersome should powers-of-10 notation be used. When it is used, so-called engineering notation is preferred to scientific notation. In **engineering notation**, the power of 10 is always divisible by 3 (analogous to the commas mentioned above). In a column of numbers that all refer to the same kind of property, the format should be the same for each entry.

29.4.6. Colors and Exotic Features

Most software will allow multiple colors, fonts, and other features. Although their use may be tempting, too many changes can be distracting to the readers and cause sensory overload. On slides, use only as many colors as will clarify your results. Most members of your audience will not be able to distinguish between subtle shades in the time available; distinctions should be made with bold contrasts. However, one must not rely on color alone; almost any report will be copied in black-and-white! If your distinctions are not clear when the graphics are reproduced this way, there is a problem.

Reports in which dozens of fonts are used are distracting. Whenever the readers have any trouble focusing on the content, they tend to focus on the variations in font size or type. Thus, one should use a few font changes to focus attention, but the report should not appear to use every available font. Also, the more exotic the font, the less likely it is that the file will be compatible with other word processors.

A very serious problem is the improper use of "3-D" figures. If a graph is a plot of a dependent variable versus one independent variable, the graph is only a two-dimensional representation. Any attempt to make it "faux 3-D" will make it less readable and more confusing. Features such as giving a pie chart a constant thickness or the bars of a bar chart constant depth make the chart less useful in conveying data. Such gimmicks are viewed as such in technical reporting. The same can be said of "shadowing" of two-dimensional figures.

When a graph is truly three-dimensional (two independent variables and one dependent variable), one must be careful to use a perspective that allows the reader to determine easily the height (the dependent axis) at various points. The most useful such perspective is the "isometric" perspective, which involves rotating the straight-on coordinate system by 45° and then tilting it up in back by 30°. In this perspective, the distances perpendicular to the axes are not distorted.

29.4.7. Raw Output from Process Simulators

Process simulation software typically will produce a flowsheet, but this is probably not a true process flow diagram and should not be used as one in a report. There are two reasons for this. First, the simulator-produced flowsheet is unlikely to follow all the conventions of PFDs given in Chapter 1 regarding equipment symbols, line crosses, labels, and so on. Second, the process simulated is not the true process. One "unit" in the process simulator (such as a distillation column) may be several pieces of equipment (tower, condenser, condensate tank, etc.) that need to be shown on a PFD. It is common to simulate a single unit (such as a process-process heat exchanger) as two units to decouple the recycle calculations. Some units, such as a storage tank, require no calculations in the process simulator and thus are not shown on its flowsheet. However, the simulator flowsheet is essential in the appendix of the report if the simulator "report" is included. Care should be taken to use the same

stream numbers in the simulation flowsheet as in the PFD whenever possible.

The report from a process simulator should be included in the appendix, but it serves neither as the main PFD nor as the main flow table. These reports are formatted for use by the user of the software, not by the reader of a report. Therefore, they should be considered as are the calculations in the appendix. They are referred to by the engineers who need to know the details, but they are not of interest to other readers of the report.

29.5. Summary

Effective written and oral communication is crucial to the success of chemical engineering projects and to the success of chemical engineers. The keys to effective technical communication are performing an audience analysis, following the format of the organization, and obtaining and acting on feedback from colleagues.

What You Should Have Learned

- There is no single, correct format for a written report.
- If your company or academic department has a prescribed format, it should be followed.
- Written reports should be written with correct grammar, be correctly punctuated, and be appropriately organized; figures and tables should be neat and legible.
- Oral presentations should be appropriate for the audience, and an oral presentation on the same subject may be presented differently to different audiences.
- Visual aids are meant to enhance the presentation; they are not to be read, word for word, during the presentation.

References

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3. *Effective Communication for Engineers* (New York: McGraw-Hill, 1974).
4. Ulman, J. N., and J. R. Gould, *Technical Reporting*, 3rd ed. (New York: Holt, Rinehart and Winston, 1972).

Problems

1. Obtain the written report guidelines used in your department for laboratory reports. Compare them to those in Section 29.2.8 and explain the differences.
2. Exchange a report you have written for one by a classmate. Spend three minutes skimming the report, and write down answers to the following three questions:
   a. Why was the report written?
   b. What is the author's key conclusion or recommendation?
   c. What would you do, based on the report?

Then discuss your answers to these questions with each other.

3. Obtain the written report guidelines from a firm that employs engineers. Compare them with those in Section 29.2.8 and explain the differences.
4. Ask a chemical engineering student who has not yet taken design to read a report you have written and to point out the difficult passages. Rewrite the report so that it satisfies those concerns.
5. After giving an oral presentation, perform a postmortem analysis with a couple of members of the audience.
6. Write a short (one-paragraph) audience analysis for a design report in your design course.
7. Choose a graphing, drawing, or spreadsheet software package. Investigate the features of the package and make a list of those features that can lead to poor visual aids.
8. Run a grammar checker and spell checker on one of your reports. Accept every change suggested and then reread the report. What do you conclude?

Chapter 30. A Report-Writing Case Study

The purpose of this chapter is to illustrate some of the principles of report writing presented in Chapter 29. In order to accomplish this, we present a written report for a project that a junior engineer might be given in the first several years of employment. This chapter is split into several sections. Each section addresses some of the common errors that are made in report writing. Examples of poor and improved cover memoranda, poor and improved graphics, and poor and improved writing styles are given. A checklist of common errors is also included. Finally, an example is presented of a improved written report that illustrates many of the principles outlined in this chapter and Chapter 29.

It should be noted that the figures and tables concerning the toluene hydrodealkylation problem are presented to illustrate examples of strong and weak graphics and to highlight common mistakes. The absolute values shown for equipment and operating costs are not necessarily accurate.

30.1. The Assignment Memorandum

The assignment memorandum for the project considered in this chapter is shown in Figure 30.1.

This is a good assignment memorandum because it communicates to the junior engineer in a concise manner *what* to do, *why* to do it, *when* to have it completed, and *who* else is involved or interested in the project. Everything is stated clearly; nothing is left for interpretation.

Because the memo indicates *who* is being copied on the memo, the junior engineer knows all of those involved in the loop. The engineer also knows for whom the final report will be prepared. An essential step in preparing a report is knowing the audience.

Because the memo indicates that there are attachments to the memorandum, the recipient of the memo knows whether the document is complete.

The first paragraph provides perspective on the problem (*why* it is assigned). This is essential for the junior engineer to make rational decisions during the assignment.

MEMORANDUM

TO:	Lee Madera, Junior Process Engineer
FROM:	Chris Stafford, Senior Process Engineer
RE:	Benzene Production
DATE:	September 12, 2011
COPIES:	R. T. Hemrick, Principal Process Engineer M. R. Johnson, VP Engineering S. E. Kelley, VP Project Engineering W. C. Lin, VP Sales
ATTACHMENTS:	Preliminary design of benzene process

Currently, the prices of benzene and toluene are such that the production of benzene from toluene via the catalytic hydrodealkylation of toluene is not profitable. However, the price of benzene over the past 15 years has fluctuated wildly (from a low of $0.21/kg to nearly $0.67/kg). Our company is interested in carrying out a feasibility study to determine the minimum price differential between benzene and toluene that will allow the toluene hydrodealkylation process to be profitable. It is recognized that currently the preferred method of producing benzene from toluene is via the disproportionation reaction to yield both benzene and xylenes. However, at present our company has no use for the xylene and would prefer to make just benzene.

With this in mind, your assignment is to determine the process that will minimize the price differential between toluene and benzene required to yield an NPV = 0. This design represents a discounted break-even analysis of the process and will be used as an internal benchmark for comparing competing alternatives to produce benzene. In your analysis, you should use the following economic parameters:

(i) Internal after-tax hurdle rate of 10%, and a taxation rate of 35%
(ii) MACRS depreciation over 6 years for all fixed capital investment
(iii) A project life of 15 years
(iv) A production rate of 68,000 tonne per year of 99.5 wt% pure benzene

The attached preliminary design for a toluene HDA process should be used as a starting point (base case) for your study.

Submit your findings as a short report, not exceeding 8 pages of double-spaced text, plus any tables and figures. Put the details of all your calculations, a PFD, flow table, and so on, in a clearly indexed appendix.

This report is due on September 26, 2011, and will be read by several managers as well as other technical and sales executives. You will also present your major findings in a 15-minute oral presentation on September 27, 2011.

Figure 30.1. Example of a Good Assignment Memorandum

The second and third paragraphs clearly outline *what* is to be done, what the constraints are, and what the deliverables are. If this section were not clear, the junior engineer would either have to guess about the constraints or the specifics of the assignment or have to go back to the senior engineer and ask. If the senior engineer were unavailable to answer questions, this might delay the project. In any case, time would be wasted.

The final paragraph states *when* the assignment is due and when the presentation will be made.

30.2. Response Memorandum

An example of a poor response memorandum is given in Figure 30.2. An example of an improved response memorandum is given in Figure 30.3.

In order to explain the difference between the improved and poor response memos, it is necessary to understand who reads different portions of reports. A secretary reads only the cover memorandum subject in order to determine where to file the report. The senior process engineer, the person who gave you the assignment, may read the entire report. The principal process engineer reads the entire report only if the results are interesting or controversial. The vice presidents will probably not read the entire report. For those who do not read the entire report or who need to decide whether to read the report, the information provided in the cover memorandum is essential.

At any time, there will be many reports circulating within a company. Occasionally, a report may become detached from its cover memorandum. If the attachment is listed as *The Benzene Report*, the cover memorandum may never be matched with the correct report if they become separated. If your company makes benzene, there will probably be many "benzene reports" circulating at one time. Therefore, the complete title should be included on the cover memorandum.

On the "poor" memorandum, report copies are sent to only two individuals. The assignment memorandum was copied to four individuals. Always provide copies of your final product to everyone in the loop based on the original memorandum.

The key problem with the poor memorandum is that it basically states, "Here it is" and nothing else. The poor memorandum provides no information to allow any of the people who receive the report to determine rapidly what the conclusions were or to decide whether they want to read the entire report. Suppose that the conclusion, if the company invested $100,000 in a process modification, the break-even purchase price of toluene would rise to $0.25/kg. It is essential that everyone in the loop know that piece of information immediately. Therefore, a cover memorandum must summarize the key conclusions. What was found, how much it will cost up front (capital cost, if applicable), and what the profitability is (NPV, DCFROR, raw material purchase price) must be stated. In a short report, which is likely to be the rule in industry, the cover memorandum takes the place of an abstract. Therefore, it is imperative to include key results in the cover memorandum.

MEMORANDUM

TO: Chris Stafford, Senior Process Engineer

FROM: Lee Madera, Junior Process Engineer

RE: Benzene Production

DATE: September 26, 2011

COPIES: R. T. Hemrick, Principal Process Engineer
M. R. Johnson, VP Engineering

ATTACHMENTS: The Benzene Report

In response to your memorandum, the attached report details the results of my study on the production of benzene via the catalytic hydrodealkylation of toluene. This process is based on the production of 68,000 tonnes per year of 99.5 wt% benzene. A summary of all the major equipment and operating costs along with other pertinent economic and process information is provided in the report.

Figure 30.2. Example of a Poor Response Memorandum

MEMORANDUM

TO: Chris Stafford, Senior Process Engineer

FROM: Lee Madera, Junior Process Engineer

RE: Benzene Production

DATE: September 26, 2011

COPIES: R. T. Hemrick, Principal Process Engineer
M. R. Johnson, VP Engineering
S. E. Kelly, VP Project Engineering
W. C. Lin, VP Sales

ATTACHMENTS: Report titled: "Evaluation of the Minimum Break-even Price Differential for Benzene and Toluene"

In response to your memorandum of September 12, 2011, regarding the benzene production process, the attached report details the results of my study on the production of 68,000 tonnes/yr of 99.5 wt% benzene via the catalytic hydrodealkylation of toluene. This process yields a discounted break-even cost differential between benzene and toluene of $0.153/kg, $0.034/kg less than for the base case. At the current market price for benzene of $0.27/kg, the price of toluene would have to drop nearly 50% (from the current value of $0.23/kg to $0.117/kg). The fixed capital investment for this project is $5.14 million, and the annual manufacturing costs are $25.42 million/yr. A summary of all the major equipment and operating costs along with other pertinent economic and process information is provided in the report.

If you have any questions regarding this report prior to my presentation on Friday, September 27, 2011, please feel free to contact me at extension 999.

Figure 30.3. Example of an Improved Response Memorandum

30.3. Visual Aids

Figures 30.4 through 30.9 show examples of poor and improved pie charts, tables, and plots. Major points of criticism are shown on the "poor" figures (Figures 30.4, 30.6, and 30.8) in script font, and these errors have been remedied in the corresponding "improved" figures (Figures 30.5, 30.7, and 30.9). Not all the common errors can be shown on these figures, and a comprehensive checklist for figures, tables, and written text is included in Section 30.5.

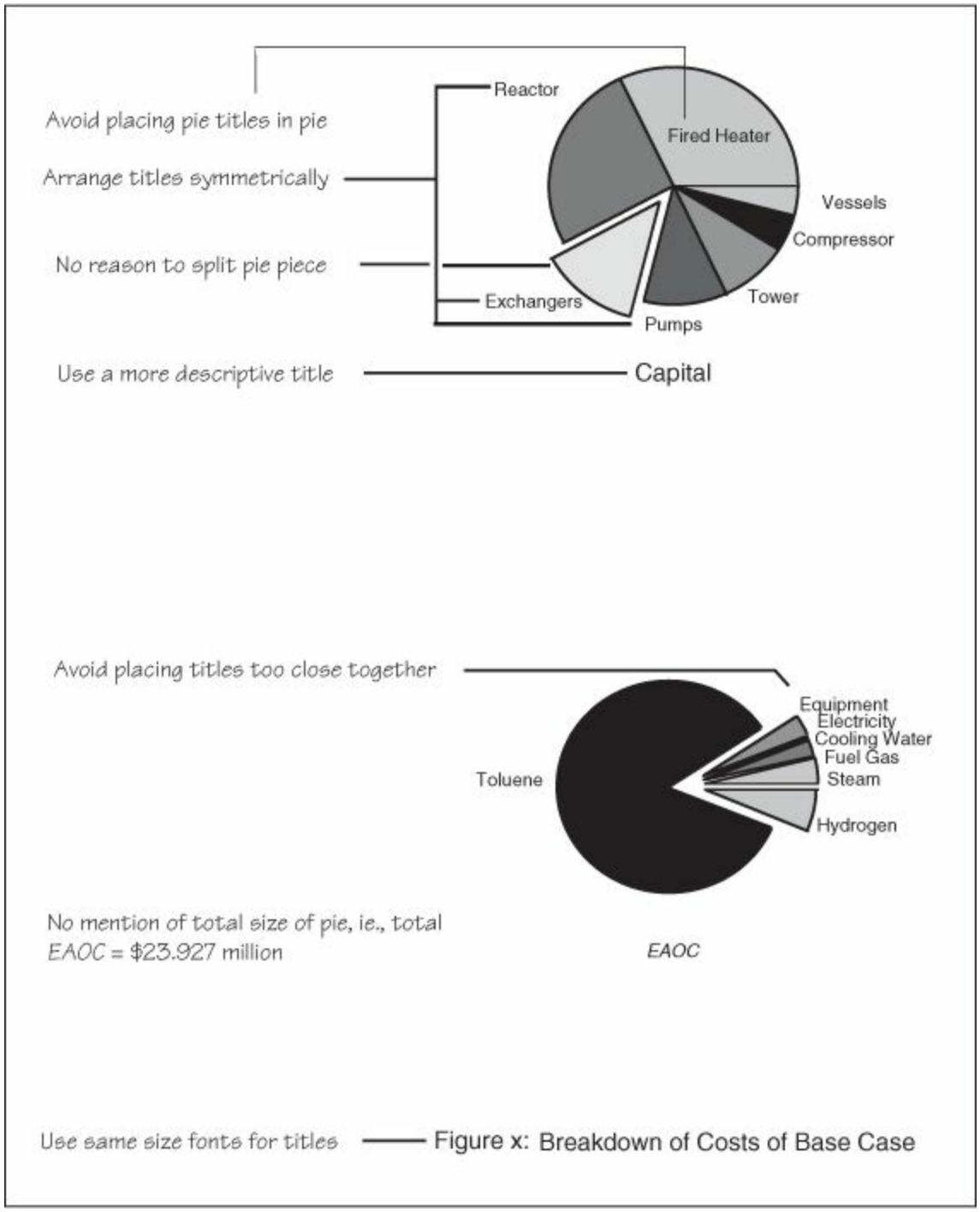


Figure 30.4. Some Common Mistakes Made in Pie Chart Presentation

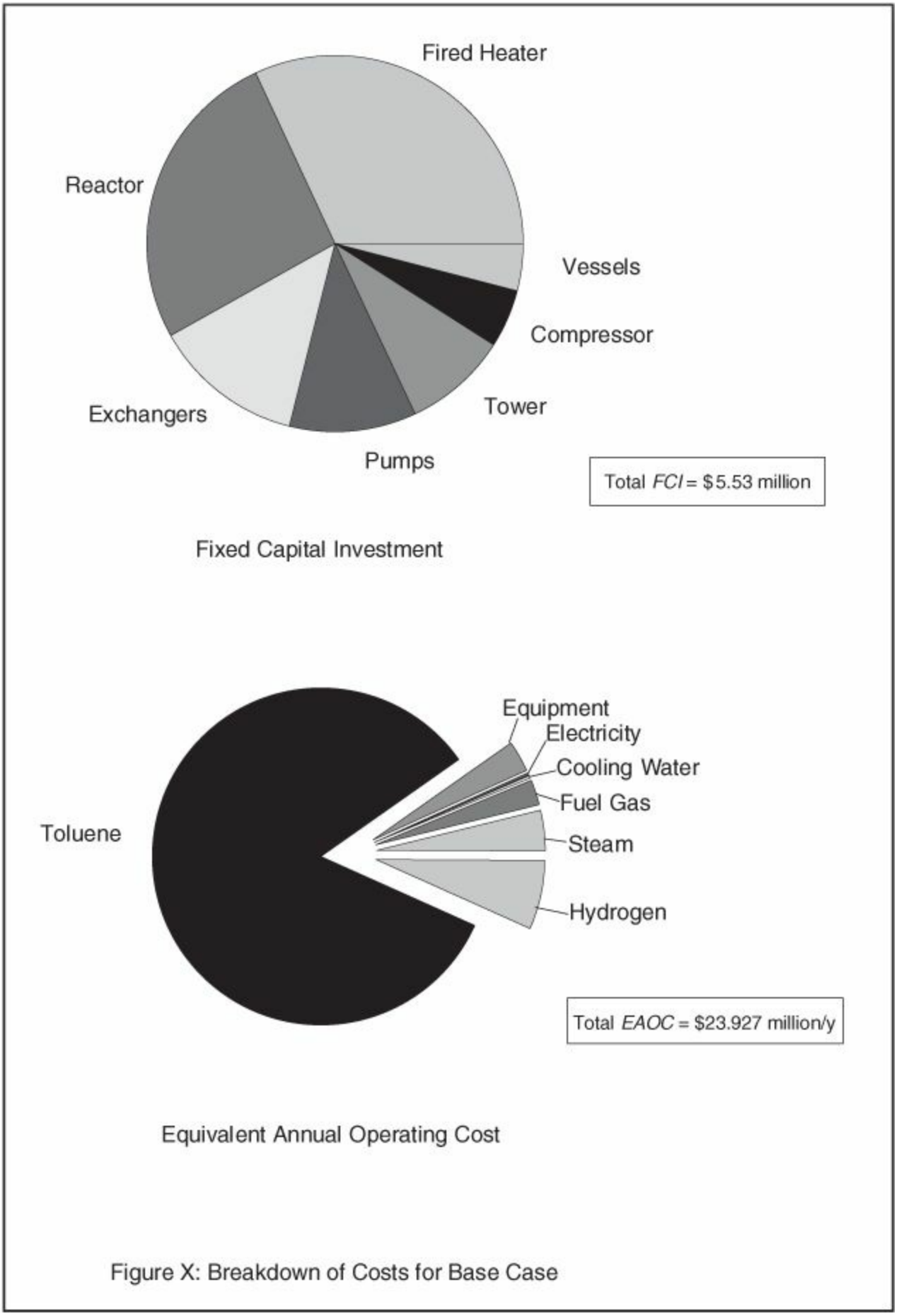


Figure 30.5. Corrected Version of the Pie Chart Shown in Figure 30.4

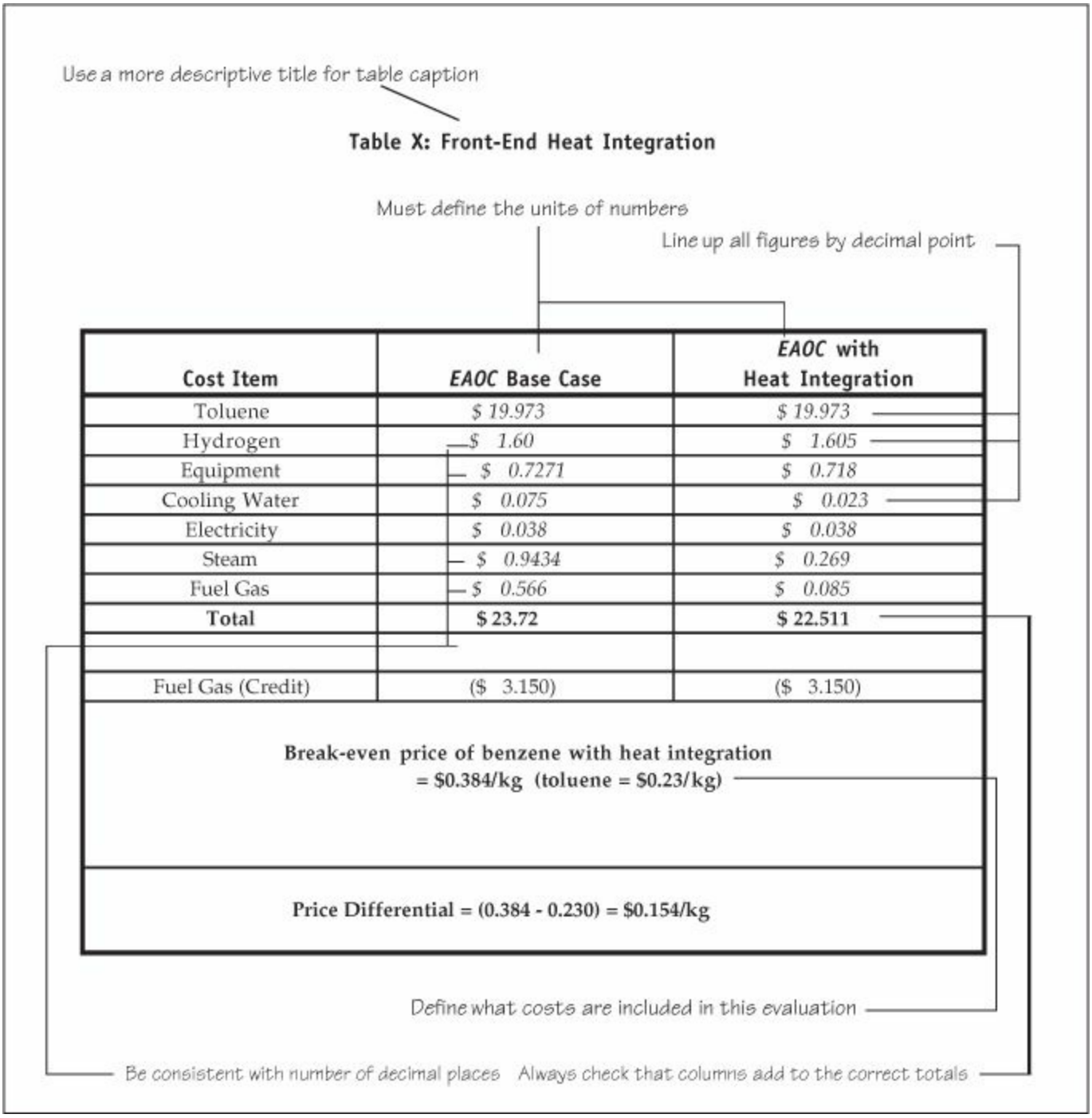


Figure 30.6. Some Common Mistakes Made in Table Presentations

Table X: Economic Impact of Front-End Heat Integration on Process Economics (all *EAOC* cost figures in millions)

Cost Item	*EAOC* Base Case	*EAOC* with Heat Integration
Equipment	$ 0.727	$ 0.718
Steam	$ 0.943	$ 0.269
Fuel gas	$ 0.566	$ 0.085
Cooling water	$ 0.075	$ 0.023
Electricity	$ 0.038	$ 0.038
Toluene	$ 19.973	$ 19.973
Hydrogen	$ 1.605	$ 1.605
Total	**$ 23.927**	**$ 22.711**
Fuel gas (credit)	($ 3.150)	($ 3.150)
Break-even price of benzene with heat integration = $0.384/kg (toluene = $0.23/kg) Break-even costs include utilities, raw materials, maintenance, labor, fixed capital investment, etc.		
Price Differential = (0.384 – 0.230) = $0.154/kg		

Figure 30.7. An Improved Version of the Table Shown in Figure 30.6

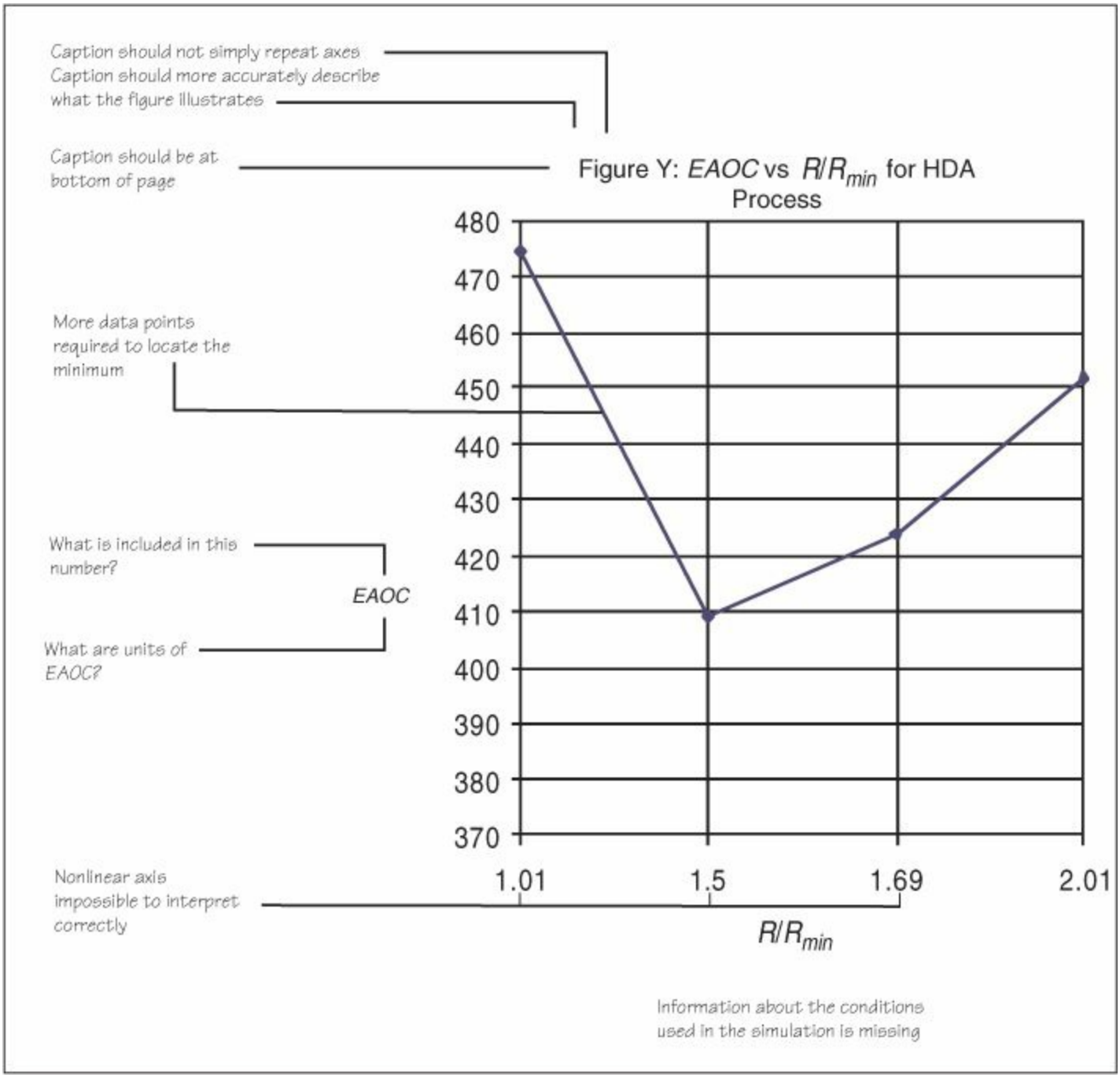


Figure 30.8. Some Common Mistakes Made in Graphical Presentations

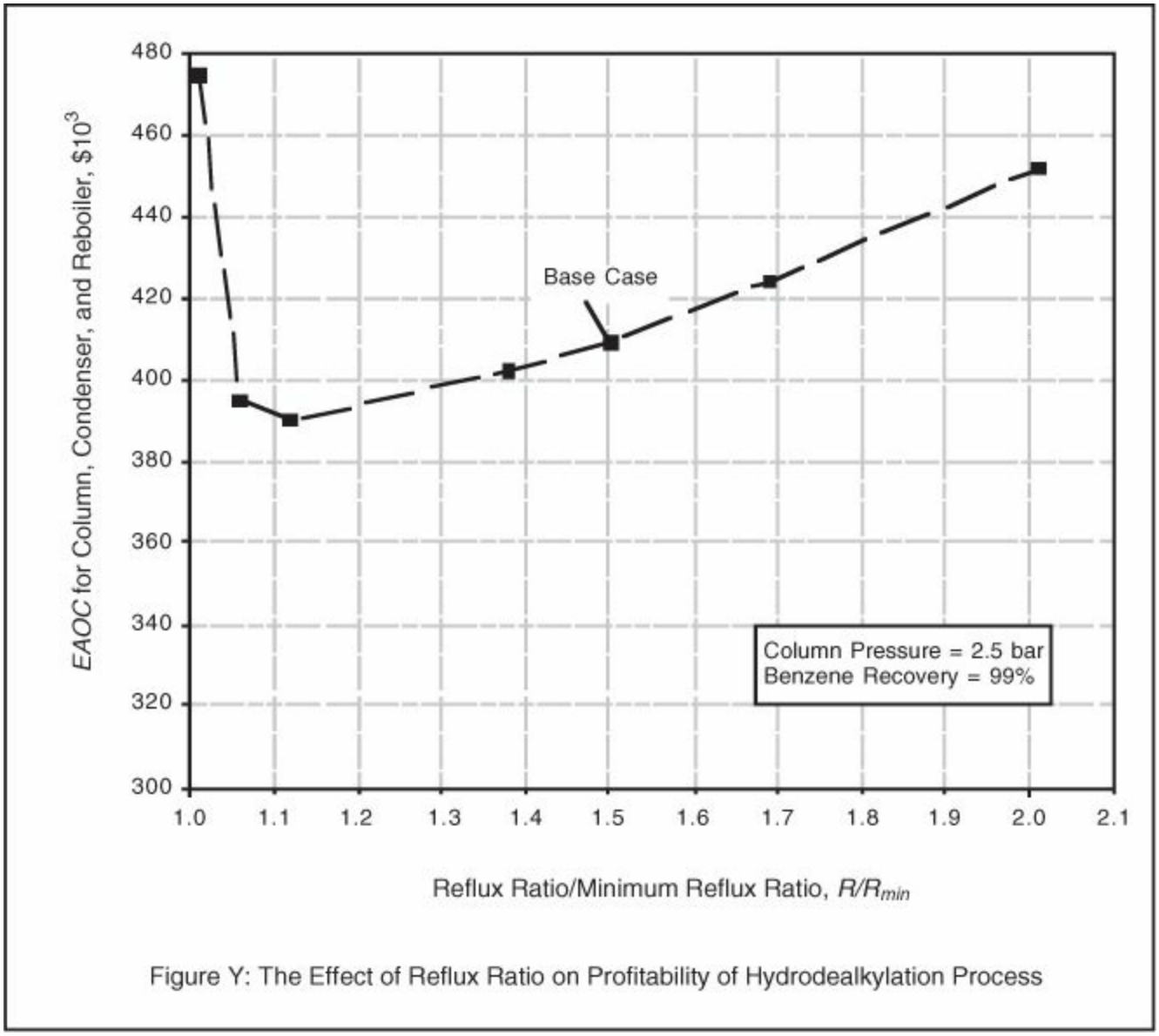


Figure 30.9. Corrected Version of the Graph Shown in Figure 30.8

30.4. Example Reports

Two examples of student reports follow. Section 30.4.1 contains an example of a portion of a student report with suggestions for improvement. Section 30.4.2 contains an example of an improved report.

30.4.1. An Example of a Portion of a Student Written Report

1. Introduction

The purpose of this report is to establish the minimum break-even price differential between benzene and toluene for the production of benzene using the catalytic hydrodealkylation of toluene. In this process, toluene is converted to benzene over a solid catalyst via the following reaction:

$$C_7H_8 + H_2 \rightarrow C_6H_6 + CH_4$$

Use words as well as symbols to identify the major substances in the reaction.

Didn't this info. come from Refs. 1 and 2? If so, you need to include the footnote here.

This reaction is normally carried out at temperatures in the range of 580°C–660°C and at pressures of 35–70 bar. With the development of new catalysts, lower operating pressures, down to 25 bar, may be possible and I assumed this was feasible in this analysis. In the base-case process provided, the reactor consisted of a single-stage adiabatic packed bed of catalyst into which a small stream of recycle gas was fed for temperature control. Over the range of conditions considered here, there are essentially no side reactions.

Reference 3?

Poor wording. Isn't this already the basis of the prelim. design provided with the assignment?

Some readers are very uncomfortable with personal pronouns in technical reports. Are you sure that "I" is appropriate for your audience?

Your readers want to know what process is best and when it should be used; they don't want a step-by-step history of what you did. Remember to focus on their needs.

See your format instructions for ways to improve the organization and usefulness of your report.

2. Base-Case Evaluation

The first step was the analysis of the base case provided. The PFD for this base case is shown in Figure 1. According to the base-case report, the reactor inlet conditions of 600°C and 25 bar have been established to be close to the optimum. As a result, these parameters were not varied in the present study. A summary of the fixed capital investments, operating costs, and the break-even price differential for the base case is given in Table 1 and Figure 1. In order to compare all the costs, I set up an Excel spreadsheet and the data for the base case was input into the program. These numbers are presented as equivalent annual operating costs by amortizing the one-time capital investments over

This is your 2nd Figure 1. Also "EAOC" is used in the figure but hasn't been defined yet.

All the info. in the pie charts (Fig. 1) is given in Table 1. You don't need the figure.

Please use the guidelines. These details are not of interest to the readers.

data were

the life of the project using a 10% discount rate. The break-even price of benzene for this base case is \$0.417/kg ~~compared to the cost of toluene of~~ \$0.23/kg. This yields a break-even cost differential of \$0.187/kg. The details of the break-even analysis are given in the appendix. The cost of manufacturing was estimated from the following equation:

with toluene costing

$$COM_d = 0.180 * FCI + 2.73 \times C_{OL} + 1.23 * (C_{UT} + C_{RM})$$

Don't include both * and × multiplication symbols.

where FCI = fixed capital investment, C_{OL} = cost of operating labor, C_{UT} = cost of utilities, and C_{RM} = cost of raw materials.

Use present tense here.

From Table 1, it is evident that the major costs will be associated with the purchase of toluene and hydrogen. The overall conversion of toluene in the base case will be 99.3%. Potential savings in toluene cost of approximately \$140,000/yr may be realized. This savings would have a minor impact on the differential break-even price of benzene (approx. \$0.003/kg), therefore, the overall conversion of toluene is not considered a variable in the cases studied here. However, the hydrogen cost can be reduced significantly if a suitable separation technique can be found to purify the recycle gas, Streams 5 and 7. Of the remaining costs, the steam, fuel gas, and equipment are the most significant.

;

Wordy. Try "are the keys to the optimization."

The above items provide a focus on where to concentrate the major optimization effort. In this regard, a two level optimization strategy was

Unnecessary and misleading.

two-level

30.4.2. An Example of an Improved Student Written Report

1. Introduction

The purpose of this report is to establish the minimum break-even price differential between benzene and toluene for the production of benzene using the catalytic hydrodealkylation of toluene. In this process, toluene is converted to benzene over a solid catalyst via the following reaction:

$$\underset{toluene}{C_7H_8} + H_2 \rightarrow \underset{benzene}{C_6H_6} + CH_4$$

This reaction is normally carried out at temperatures of 580°C- 660°C and at pressures of 35-70 bar [1, 2]. With the development of new catalysts, operating pressures as low as 25 bar may be possible [3] and are assumed to be feasible in this analysis. In the base-case process provided, the reactor consists of a single-stage adiabatic packed bed of catalyst into which a small stream of recycle gas is fed for temperature control. Over the range of conditions considered here, there are essentially no side reactions.

2. Base-Case Evaluation

The PFD for this base case is shown in Figure 1. The previously reported optimum reactor inlet conditions of 600°C and 25 bar are used. A summary of the fixed capital investments, operating costs, and the break-even price differential for the base case is given in Table 1. They are presented as equivalent annual operating costs by amortizing the one-time capital investments over the life of the project using a 10% discount rate. The break-even sales price of benzene for this base case is \$0.417/kg for a toluene purchase price of \$0.23/kg (a break-even cost differential of \$0.187/kg). The details of the break-even analysis are given in the appendix. The cost of manufacturing is estimated using the following equation:

$$COM_d = 0.180FCI + 2.73C_{OL} + 1.23(C_{UT} + C_{RM}) \quad (1)$$

where FCI = fixed capital investment, C_{OL} = cost of operating labor, C_{UT} = cost of utilities, and C_{RM} = cost of raw materials.

Table 1 shows that the major cost is for toluene. The overall conversion of toluene in the base case is 99.3%, allowing a potential savings in toluene cost of approximately \$140,000/yr. This savings would have only a minor impact (approx. \$0.003/kg) on the differential break-even price of benzene; therefore, the overall conversion of toluene is not considered a variable in the cases studied here. However, the hydrogen cost can be reduced significantly if a suitable separation technique can be found to purify the recycle gas, Streams 5 and 7. Of the remaining costs, the steam, fuel gas, and equipment are the most significant.

TK - 101	P - 101 A/B	E - 101	H - 101	R - 101	C - 101 A/B	E - 102	V - 101	V - 103	E - 103	E - 106	T - 101	E - 104	V - 102	P - 102 A/B	E - 105
Toluene Storage Tank	Toluene Pump	Feed Preheat.	Feed Heater	Reactor	Recycle Gas Compssor	Reactor Effluent Cooler	H.P Phase Separtor	L.P Phase Separtor	Tower Feed Heater	Benz. Reboiler	Benz. Tower	Benz. Conden.	Reflux Drum	Reflux Pumps	Product Cooler

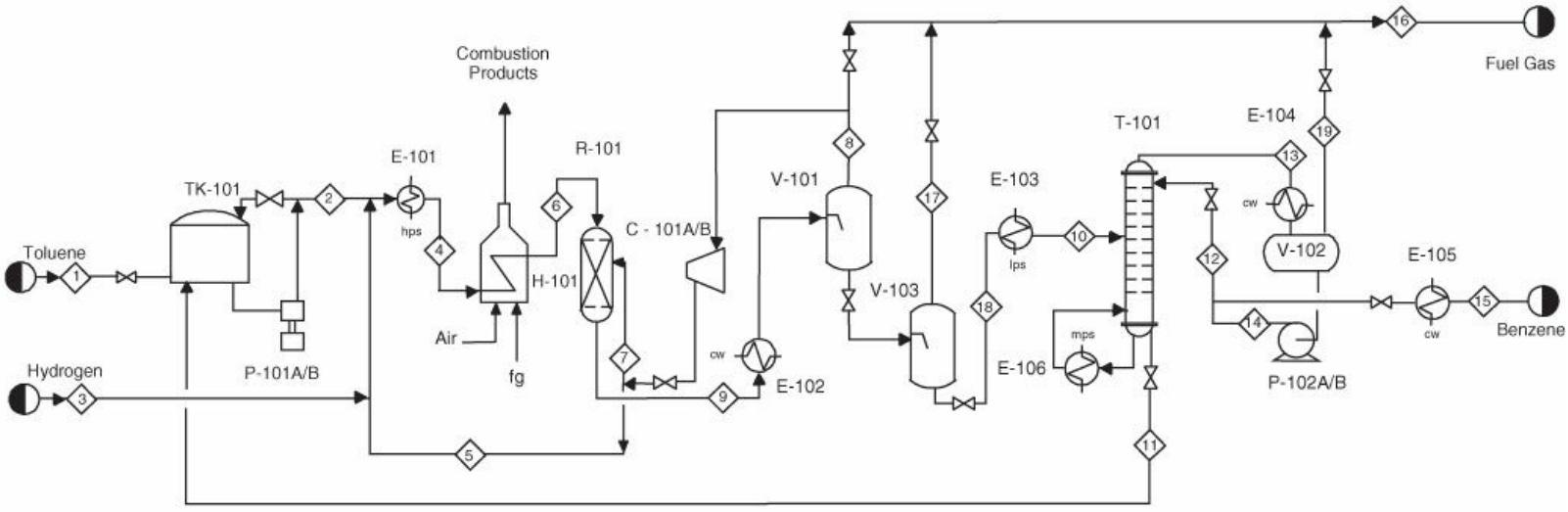


Figure 1 Skeleton Process Flow Diagram (PFD) for the Production of Benzene via the Hydrodealkylation of Toluene

Table 1 Cost Summary for the Base-Case Evaluation of Toluene HDA Process (All fixed capital and *EAOC* cost figures are given in millions.)

Equipment Type	Fixed Capital Investment	% of Total Fixed Costs
Fired heater	$ 1.795	32
Reactor	$ 1.447	26
Exchangers	$ 0.695	13
Pumps	$ 0.579	11
Tower	$ 0.497	9
Compressor	$ 0.289	5
Vessels	$ 0.232	4
Total	**$ 5.534**	**100**

Cost Item	Equivalent Annual Operating Cost (*EAOC*)	% of Total *EAOC*
Equipment	$ 0.727	3.0
Steam	$ 0.943	3.9
Fuel gas	$ 0.566	2.4
Cooling water	$ 0.075	0.3
Electricity	$ 0.038	0.2
Toluene	$19.973	83.5
Hydrogen	$ 1.605	6.7
Total	**$23.927**	**100.0**
Fuel gas (credit)	($ 3.150)	

Break-even price of benzene = $0.417/kg (for toluene at $0.23/kg)

Break-even costs include utilities, raw materials, maintenance, labor, fixed capital investment, and so on.

Price Differential = (0.417 − 0.230) = $0.187/kg

To concentrate the major optimization effort on costs of hydrogen, steam, fuel gas, and equipment, a two-level optimization strategy was employed. The first level focused on topological changes to the process and included the addition of a membrane separation unit to purify the recycle gas (Streams 5 and 7) and the implementation of a heat integration scheme. The second level of optimization focused on changes in operating parameters, particularly the column reflux ratio and the single-pass conversion in the reactor, because significant savings in utilities may be realized by changing these variables. The results of these optimizations are presented in the next sections.

3. Topological Changes to Base-Case PFD

3.1. Membrane Separator

The first topological change attempted was the addition of a membrane separation unit to Stream 8 leaving the high-pressure phase separator. The membrane separation unit separates the recycle gas, sending a hydrogen-rich stream back through the compressor, C-101. This separation reduces the amount of methane in the recycle, and the amount of hydrogen feed required is reduced. Several different cases were screened, and Table 2 shows the results of the best case, where significant reductions in steam, fuel gas, and hydrogen feed costs were obtained. However, these gains were more than offset by the increased cost of electricity (for the compressor), the decrease in fuel gas credit, and the increase in equipment costs due to the larger compressor and the addition of the membrane separation unit. The net result was that the membrane separation unit provided no economic advantage. Consequently, this topological change is not recommended.

Table 2 Economic Impact of Membrane Separation Unit on Process Economics (Permeate available at 10 bar and 85% H_2 purity, all *EAOC* cost figures in millions.)

Cost Item	*EAOC* for Base Case	*EAOC* with Membrane Separator
Equipment	$ 0.727	$ 1.370
Steam	$ 0.943	$ 0.780
Fuel gas	$ 0.566	$ 0.456
Cooling water	$ 0.075	$ 0.065
Electricity	$ 0.038	$ 0.320
Toluene	$19.973	$19.973
Hydrogen	$ 1.605	$ 1.338
Total	**$23.927**	**$24.302**
Fuel Gas (Credit)	($ 3.150)	($ 2.632)
Break-even price of benzene with membrane separator = $0.434/kg (toluene = $0.23/kg)		
Break-even costs include utilities, raw materials, maintenance, labor, fixed capital investment, etc.		
Price Differential = (0.434 − 0.230) = $0.204/kg		

3.2. Heat Integration

The second topological change to the PFD was the addition of heat integration around the reactor, where the benefit would be greatest. Exchanging heat between the reactor effluent, Stream 9, and the high-pressure steam, Stream 4, can significantly reduce cooling water and fuel gas utilities. In addition, the cost of the front-end heat exchange equipment (E-101, E-102, and H-101) might also be reduced. Figure 2(a) shows the base-case configuration, and Figure 2(b) shows the optimized heat exchange configuration around the reactor. Table 3 lists the savings in equipment and utility costs. The use of heat integration eliminates the high-pressure steam usage and reduces significantly the cost and utility demands of the fired heater, yielding a significant economic improvement by reducing the break-even price of benzene to $0.384/kg (break-even price differential of $0.154/kg).

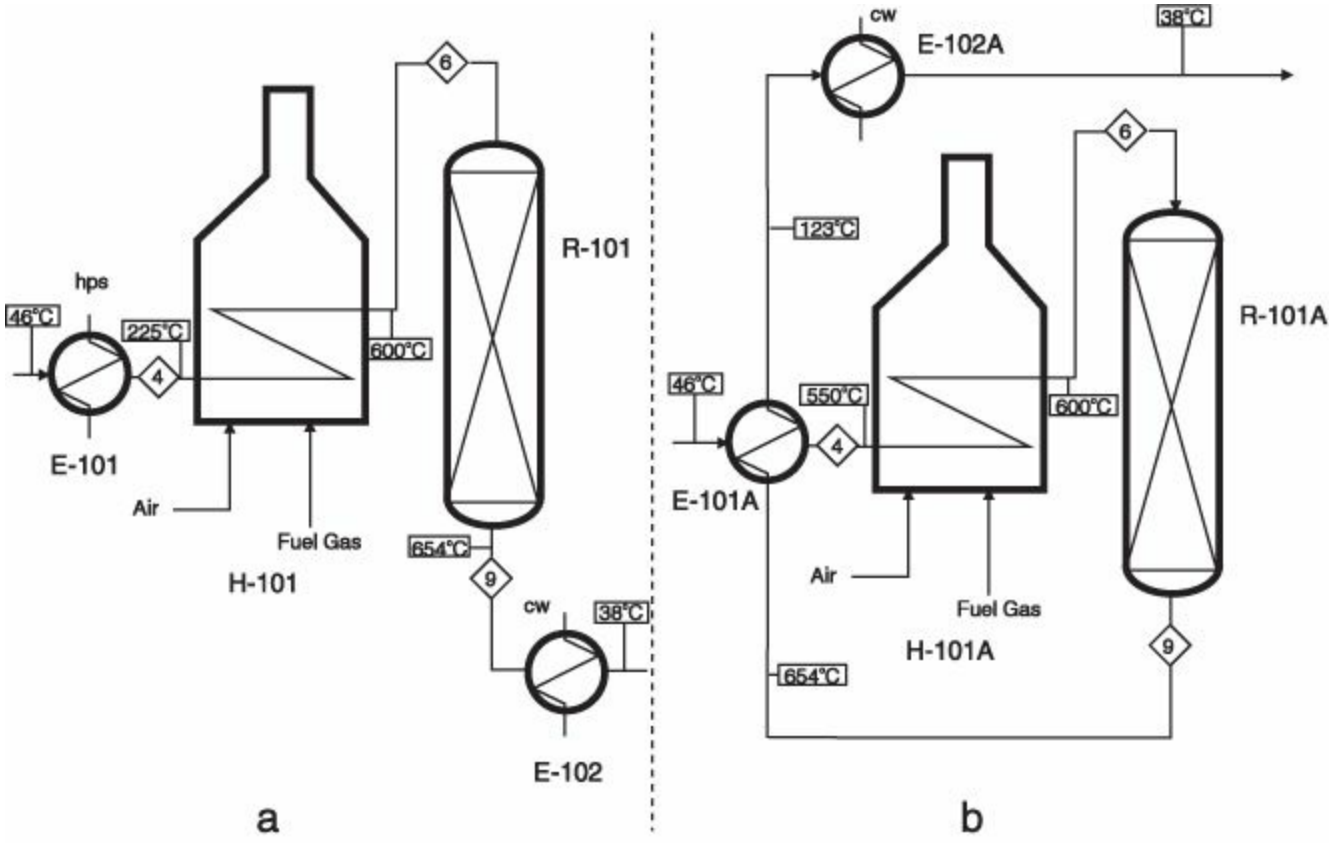


Figure 2 Front End of Toluene HDA Process (a) without Heat Integration and (b) with Heat Integration

Table 3 Economic Impact of Front-End Heat Integration on Process Economics
(All *EAOC* cost figures in millions.)

Cost Item	*EAOC* Base Case	*EAOC* with Heat Integration
Equipment	$ 0.727	$ 0.718
Steam	$ 0.943	$ 0.269
Fuel gas	$ 0.566	$ 0.085
Cooling water	$ 0.075	$ 0.023
Electricity	$ 0.038	$ 0.038
Toluene	$19.973	$19.973
Hydrogen	$ 1.605	$ 1.605
Total	**$23.927**	**$22.711**
Fuel gas (Credit)	($ 3.150)	($ 3.150)
Break-even price of benzene with heat integration = $0.384/kg (toluene = $0.23/kg) Break-even costs include utilities, raw materials, maintenance, labor, fixed capital investment, etc.		
Price Differential = (0.384 − 0.230) = $0.154/kg		

4. Parametric Changes to Base-Case Operation

4.1. Reflux Ratio

Table 1 shows that the two largest utility costs are steam and fuel gas. The heat integration scheme outlined above can reduce these costs significantly. The next largest steam user after E-101 is E-106, the reboiler of T-101. The optimum reflux ratio for column T-101 is 1.12 times the minimum (Figure 3), significantly different from the 1.5 of the base case. For this calculation, it is assumed that costs other than the *EAOC* of the column, reboiler, and condenser are substantially unaffected by changes in column operation. The costs for the optimum reflux are compared to those of the base-case operation (R/R_{min} = 1.5) in Table 4. The overall effect is a small decrease in the break-even price differential of $0.0002/kg.

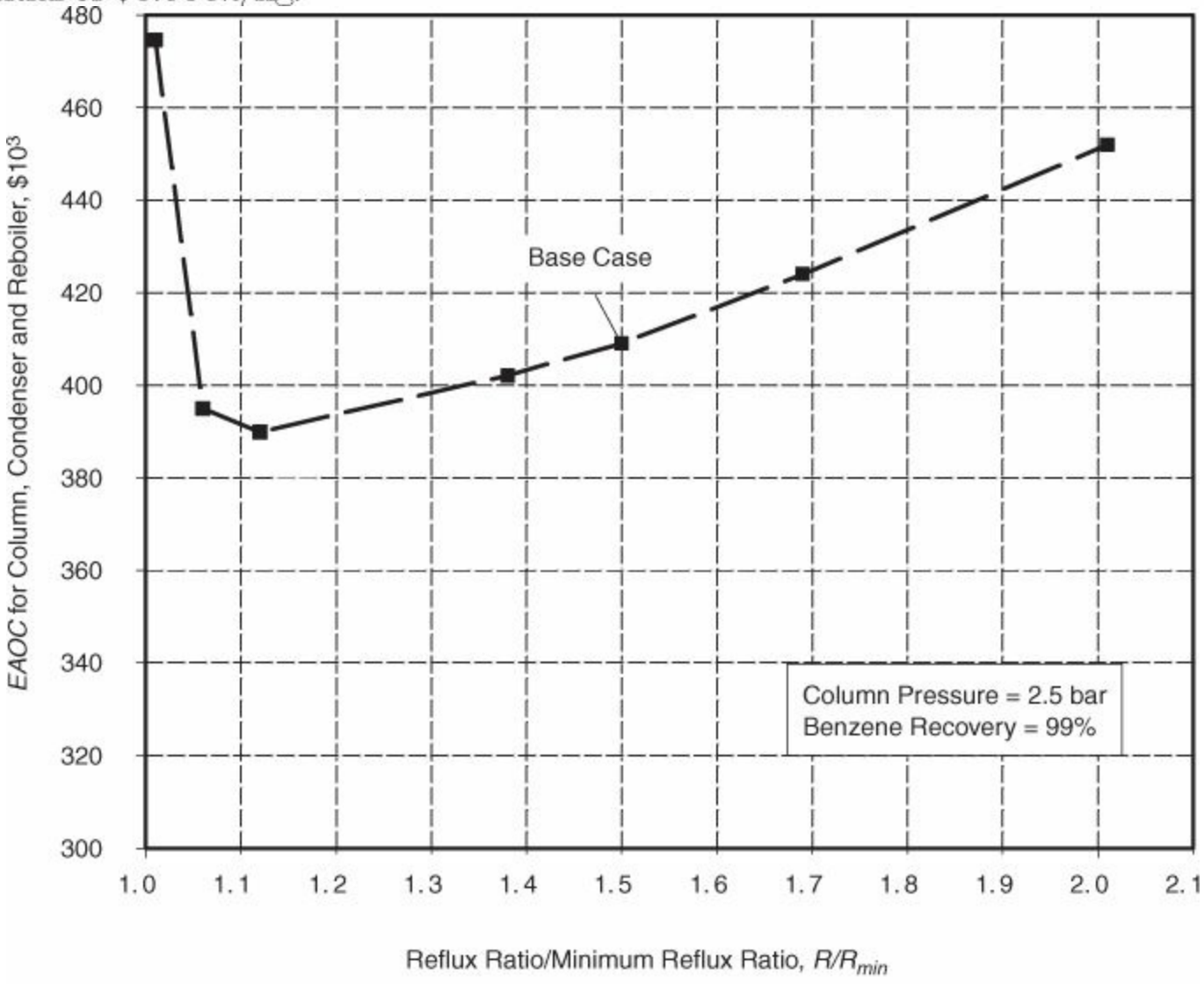


Figure 3 The Effect of Reflux Ratio on Profitability of Hydrodealkylation Process

4.2. Conversion

The final optimization attempted involved the single-pass conversion in the reactor (base-case conditions, T = 600°C, P = 25 bar, conversion = 0.75). The rationale for changing the conversion was that potential savings could be obtained by reducing the amount of toluene recycle; i.e., the size of equipment and utility usage in the recycle loop could be reduced. The results of this optimization are shown in Figure 4, where the break-even price for benzene is plotted as a function of single-pass conversion. The optimum conversion is seen to occur at about 85%, with a break-even price for benzene of $0.383/kg. The results for the optimum conversion are compared to the base case in Table 5. The increase in break-even price for conversions greater than 85% is attributed to an increase in the amount of benzene leaving in the fuel gas. The recovery of this "lost" benzene was not considered in the present analysis but is addressed below in the recommendations section.

Table 4 Economic Impact of Column Optimization on Process Economics (All *EAOC* cost figures in thousands.)

Cost Item	*EAOC* for Base Case R/R_{min} = 1.50	*EAOC* for Optimized Case R/R_{min} = 1.12
Column equipment (T-101, E-102, E-106, V-102, P-102A/B)	$ 132.11	$ 148.03
Cooling water	$ 11.04	$ 9.32
Steam	$ 275.90	$ 239.04
Total	**$ 418.05**	**$ 396.39**
Break-even price of benzene with column optimization = $0.4168/kg (toluene = $0.23/kg) Break-even costs include utilities, raw materials, maintenance, labor, fixed capital investment, etc.		
Price Differential = (0.4168 − 0.230) = $0.1868/kg		

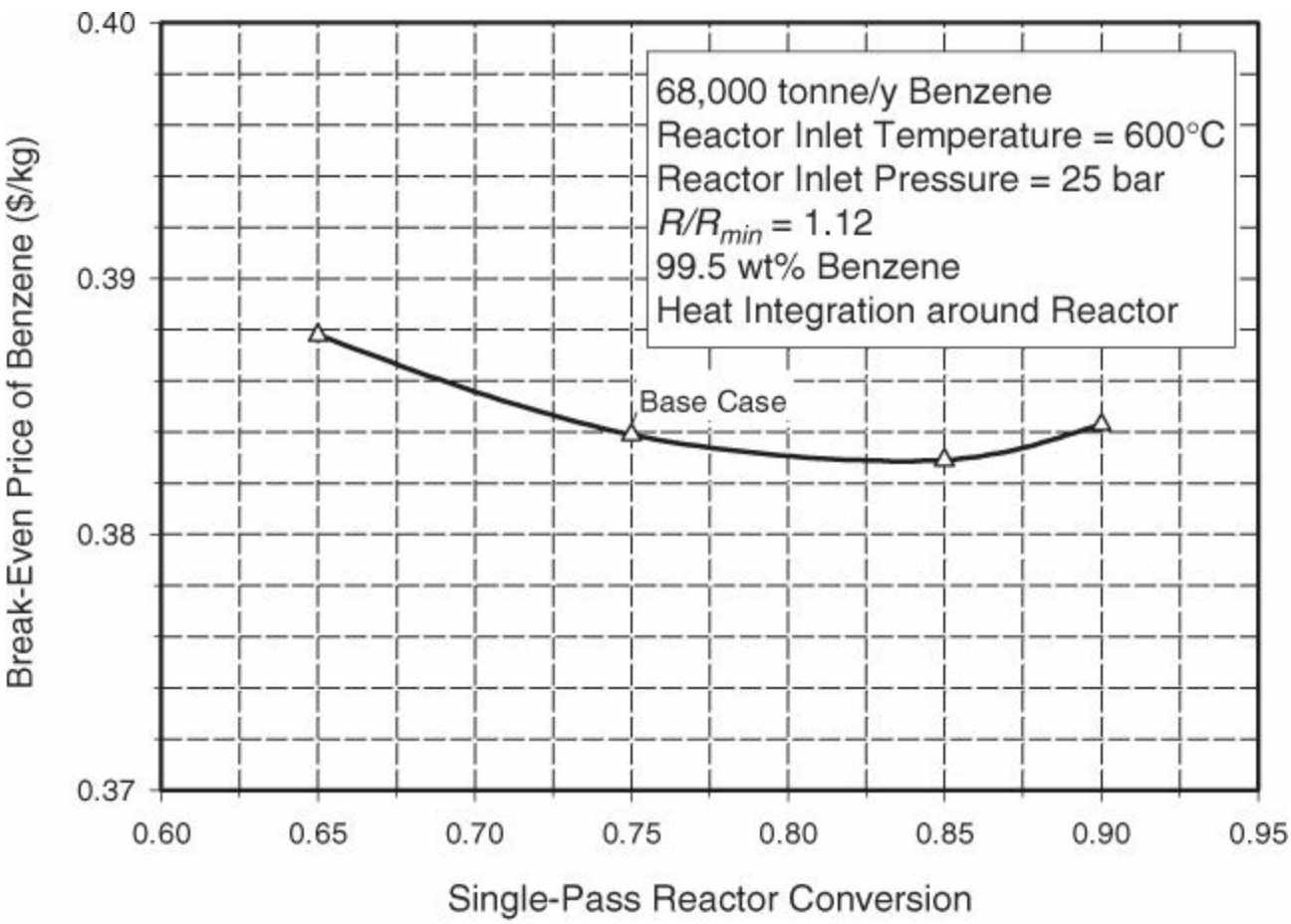


Figure 4 The Effect of Single-Pass Conversion on Break-Even Selling Price of Benzene

Table 5 Economic Impact of Single-Pass Reactor Conversion (Plus Heat Integration) on Process Economics (All *EAOC* cost figures in millions.)

Cost Item	*EAOC* Base Case with Heat Integration Conversion = 0.75	EAOC Optimized Case with Heat Integration Conversion = 0.85
Equipment	$ 0.718	$ 0.675
Steam	$ 0.269	$ 0.243
Fuel gas	$ 0.085	$ 0.068
Cooling water	$ 0.023	$ 0.020
Electricity	$ 0.038	$ 0.035
Toluene	$ 19.973	$ 20.065
Hydrogen	$ 1.605	$ 1.605
Total	**$ 22.711**	**$ 22.711**
Fuel gas (credit)	($ 3.150)	($ 3.161)
Break-even price of benzene with conversion = 0.85 = $0.383/kg (toluene = $0.23/kg)		
Break-even costs include utilities, raw materials, maintenance, labor, fixed capital investment, etc.		
Price Differential = (0.383 − 0.230) = $0.153/kg		

5. Discussion

The results of the present study are summarized in Figure 5, where the results of the different case studies are compared. The minimum break-even price for benzene using the catalytic hydrodealkylation of toluene is $0.383/kg. The recommended process uses significant heat integration around the reactor, with a single-pass conversion in the reactor of 85%. For all cases considered, the ratio of hydrogen to toluene entering the reactor was maintained at 5.1:1 in order to suppress carbon formation. Finally, a reflux ratio of 1.12 times the minimum value was used in the benzene tower, which was determined to be the optimum. The use of a membrane separation unit to purify the recycle hydrogen stream was not found to be economically attractive. The proposed process represents a significant improvement over the base case.

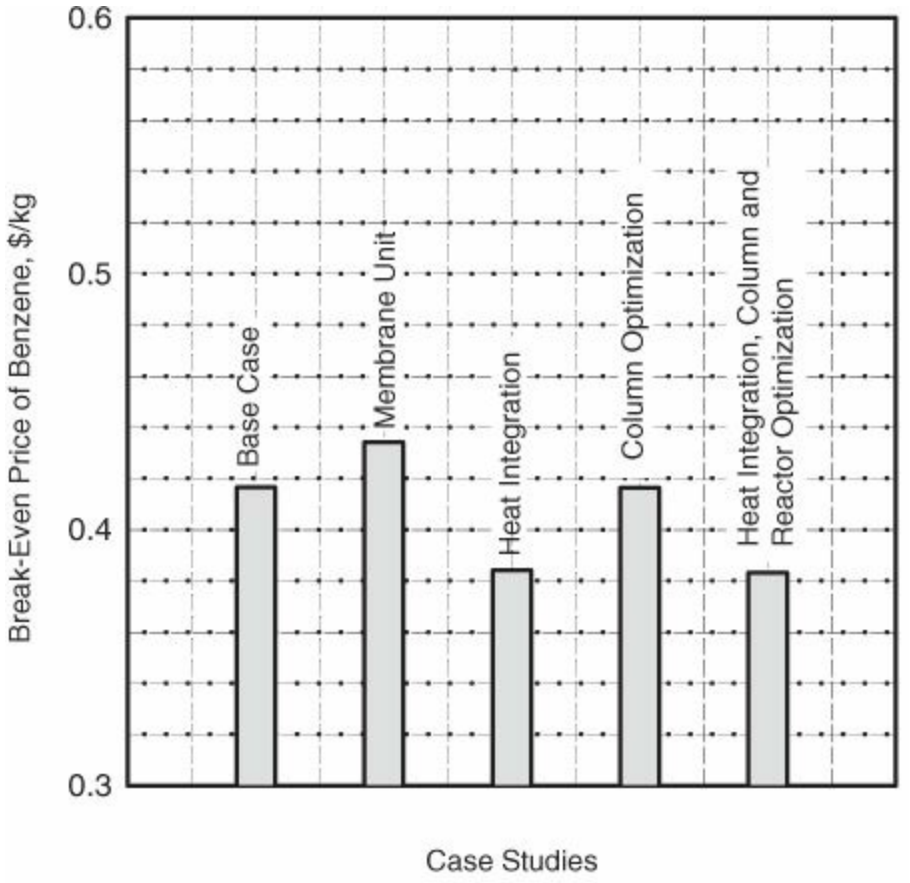


Figure 5 Summary of Results for Process Optimization of Toluene HDA Process

6. Conclusions

The optimum break-even price for benzene using this technology is estimated to be $0.383/kg. With toluene priced at $0.23/kg, this gives a break-even price differential of $0.153/kg. Significant improvements from the base case were made, including heat integration in the front end, column optimization, and increasing the single-pass reactor conversion. The addition of a membrane separation unit to purify the recycle gas stream was found not to be profitable. In summary, the production of benzene from the hydrodealkylation of toluene is not profitable at current market conditions. A significant increase in the price differential between benzene and toluene (>$0.16/kg) must occur before this process becomes economically feasible.

7. Recommendations for Future Work

The loss of benzene to the fuel gas for the improved process presented above represents approximately $640,000/yr in extra raw material (toluene) costs. Although appropriate fuel credit was given in this study, it is recommended that a further study be carried out to investigate methods for recovering this lost benzene. An example of one such method is the use of a pre-fractionator prior to T-101, instead of the two flash separations, to obtain a sharper separation between the noncondensables and benzene and toluene. The maximum potential benefit of this recovery is a reduction in the break-even cost of benzene of $0.012/kg; hence, this option should be considered.

The base-case operating conditions (temperature and pressure) of the reactor were used throughout this study. It is not expected that significant savings can be realized by altering these conditions since the reactor cost has very little impact on the overall break-even price of benzene.

8. References

1. Weiss, A. H., and L. Friedman, "Development of Houdry Detol Process," *Ind. Eng. Chem. Proc. Des. & Dev.* 2 (1963): 163–168.
2. Tarhan, M. O., *Catalytic Reactor Design* (New York: McGraw-Hill, 1983), p. 111.
3. Walas, S. M., *Chemical Process Equipment: Selection and Design* (Stoneham, MA: Butterworth, 1988), p. 29.

9. Appendix

A.1 Calculations for Base-Case Economics
A.1.1 Material and energy balances
A.1.2 Capital cost estimation for equipment and utility cost estimations
A.1.3 Calculation of break-even price of benzene
A.2 Calculations for Membrane Separation Unit
A.2.1 Material and energy balances
A.2.2 Capital cost estimation for equipment and utility cost estimations
A.2.3 Calculation of break-even price of benzene
A.3 Calculations for Column Optimization
A.3.1 Material and energy balances
A.3.2 Capital cost estimation for equipment and utility cost estimations
A.3.3 Calculation of break-even price of benzene
A.4 Calculations for Optimization of Conversion
A.4.1 Material and energy balances
A.4.2 Capital cost estimation for equipment and utility cost estimations
A.4.3 Calculation of break-even price of benzene

30.5. Checklist of Common Mistakes and Errors

The following checklist should be used before finalizing any presentation or report.

30.5.1. Common Mistakes for Visual Aids

1. When including columns of data in tables, the sum of the columns should be included and doubled-checked for correctness.
2. If numbers are included in a table but are not to be added, then care should be taken not to list these numbers in an unbroken vertical column. The natural tendency is for the reader to add the numbers, which may be inappropriate.
3. Either the number of decimal places or the number of significant figures should be the same for all numbers appearing in a table (or report).
4. Place figure numbers and captions below the figure, and table numbers and titles above the table.
5. A note regarding the units of the numbers appearing in a table should be included—for example, "All numbers are in $millions" or similar notation.
6. Pie charts should include the total value of the pie—for example, "The total fixed capital investment is $500,000."
7. Avoid the use of redundant graphics. For example, a pie chart would be redundant if all the same information were included in a table.
8. When presenting comparisons between different cases in the form of multiple tables, make sure that the order of items appearing in these tables is the same for all tables. If the order is changed, then comparisons are made very difficult.
9. When plotting data in the form of a figure, make sure that enough data are plotted. An example of

insufficient data is given in Figure 30.8, where the optimum R/R_{min} value is almost certainly not at 1.50 as shown. Figure 30.9 shows a figure with an appropriate number of data points.

10. All figure and table numbers should be followed by a meaningful caption. Do not simply repeat the axis titles in the caption—for example, "A plot of x vs. y." An additional caption describing the figure, separate from the one with the figure number, should not be included.
11. Never use line graphs. Line graphs are graphs that use an arbitrary x-axis scale having equal spacing between consecutive data points. Figure 30.8 illustrates this type of graph. These graphs are very difficult to interpret and are often misleading.
12. Remember to place all landscape-oriented pages facing outward; rotate 90° counterclockwise.
13. Line up decimal points in columns of tables.
14. The same-size font should be used for axis labels and axis titles. The font size should also be the same for all of the figure and table titles and be the same as that in the main text of the report.
15. If case studies are used in the report, the identification should be consistent throughout the report. For example, in a report with many different case studies, Case 2 should not be referred to as Case B in a table and Case II in a figure.

30.5.2. Common Mistakes for Written Text

It is impossible to list all the errors that might appear in a written report. However, some of the more common mistakes are listed in this section.

Memoranda (Memos)

1. The list of people to copy in a reply memo should be the same as that used in the initiation memo.
2. Be careful to use the correct descriptive titles for attachments and memo subject. For example, for the cover memorandum in Figure 30.3, the subject should read "Evaluation of the Minimum Break-even Price Differential for Benzene and Toluene," and not "Benzene Production" as shown.
3. The significant results of the study or report should be briefly summarized in the memorandum. This enables the person reading it to quickly ascertain the major findings and prioritize the reading of the report (see Section 30.1).

Main Body of Written Report

1. An alternative to using first-person narrative is the passive voice. Some authors claim (insist) that first person (In this report, *I* present *my* findings of a study on . . .) is often clearer and more concise than the passive voice (In this report *the* findings of a study on . . . *are* presented). However, for the novice, a report written in the first person often sounds (reads) unprofessional(ly), and it is safer to stick with the passive voice.
2. When writing chemical reactions, name all ambiguous chemicals in the reactions. For example, the reaction of toluene to yield benzene should be written as

$$\underset{\text{toluene}}{C_7H_8} + H_2 \rightarrow \underset{\text{benzene}}{C_6H_6} + CH_4$$

3. Details of calculation methods and software used should not appear in the main body of the report but rather in the appendix. Software may be cited if specific information is used—for example, if the second virial coefficient for methylene chloride was obtained from the

CHEMCAD databank.

4. Equation numbers should be included in parentheses and be right justified, level with the equation. For example:

$$COM_d = 0.180FCI + 2.73C_{OL} + 1.23(C_{UT} + C_{RM}) \quad (1)$$

In addition, the terms in the equation should always be defined either directly after the equation (which is preferred for written reports) or in a separate notation section at the back of the report (for books and technical papers).

5. The word *data* is plural: The optimization data *are* . . .
6. New results should not be included in the Conclusions section of a report. Such information should have already been included in a separate Discussion section.
7. Try to make specific recommendations that can be quantified. Avoid stating the obvious—for example, "Find cheaper utilities or raw materials." These statements do not improve the report writer's credibility with the reader. Unless one has specific ideas in mind, this type of wishful thinking is detrimental to the credibility of the report.
8. In the References section, only references cited in the report should be included.

Appendix B. Information for the Preliminary Design of Fifteen Chemical Processes

The purpose of the process designs contained in this appendix is to provide the reader with a preliminary description of several common chemical processes. The designs provided are the result of preliminary simulation using the CHEMCAD process simulation software and often contain simplifying assumptions such as ideal column behavior (shortcut method using the Underwood-Gilliland method) and in some cases the use of ideal thermodynamics models (*K*-value = ideal gas, enthalpy = ideal). These designs are used throughout the book in the end-of-chapter problems and provide a starting point for detailed design. The authors recognize that there are additional complicating factors, such as nonideal phase equilibrium behavior (such as azeotrope formation and phase separation), feed stream impurities, different catalyst selectivity, side reaction formation, and so on. The presence of any one of these factors may give rise to significant changes from the preliminary designs shown here. Thus, the student, if asked to perform a detailed process design of these (or other) processes, should take the current designs as only a starting point and should be prepared to do further research into the process to ensure that a more accurate and deeper understanding of the factors involved is obtained.

Following is a list of the sections and projects discussed in this appendix:

B.1 Dimethyl Ether (DME) Production, Unit 200

B.2 Ethylbenzene Production, Unit 300

B.3 Styrene Production, Unit 400

B.4 Drying Oil Production, Unit 500

B.5 Production of Maleic Anhydride from Benzene, Unit 600

B.6 Ethylene Oxide Production, Unit 700

B.7 Formalin Production, Unit 800

B.8 Batch Production of L-Phenylalanine and L-Aspartic Acid, Unit 900

B.9 Acrylic Acid Production via the Catalytic Partial Oxidation of Propylene, Unit 1000

B.10 Production of Acetone via the Dehydrogenation of Isopropyl Alcohol (IPA), Unit 1100

B.11 Production of Heptenes from Propylene and Butenes, Unit 1200

B.12 Design of a Shift Reactor Unit to Convert CO to CO_2, Unit 1300

B.13 Design of a Dual-Stage Selexol Unit to Remove CO_2 and H_2S from Coal-Derived Synthesis Gas, Unit 1400

B.14 Design of a Claus Unit for the Conversion of H_2S to Elemental Sulfur, Unit 1500

B.15 Modeling a Downward-Flow, Oxygen-Blown, Entrained-Flow Gasifier, Unit 1600

B.1. Dimethyl Ether (DME) Production, Unit 200

DME is used primarily as an aerosol propellant. It is miscible with most organic solvents, has a high solubility in water, and is completely miscible in water and 6% ethanol [1]. Recently, the use of DME as a fuel additive for diesel engines has been investigated due to its high volatility (desirable

for cold starting) and high cetane number. The production of DME is via the catalytic dehydration of methanol over an acid zeolite catalyst. The main reaction is

$$\underset{\text{methanol}}{2CH_3OH} \rightarrow \underset{\text{DME}}{(CH_3)_2O} + H_2O \qquad \text{(B.1.1)}$$

In the temperature range of normal operation, there are no significant side reactions.

B.1.1. Process Description

A preliminary process flow diagram for a DME process is shown in Figure B.1.1, in which 50,000 metric tons per year of 99.5 wt% purity DME product is produced. Due to the simplicity of the process, an operating factor greater than 0.95 (8375 h/y) is used.

Fresh methanol, Stream 1, is combined with recycled reactant, Stream 13, and vaporized prior to being sent to a fixed-bed reactor operating between 250°C and 370°C. The single-pass conversion of methanol in the reactor is 80%. The reactor effluent, Stream 7, is then cooled prior to being sent to the first of two distillation columns: T-201 and T-202. DME product is taken overhead from the first column. The second column separates the water from the unused methanol. The methanol is recycled back to the front end of the process, and the water is sent to wastewater treatment to remove trace amounts of organic compounds.

Stream summaries, utility summaries, and equipment summaries are presented in Tables B.1.1–B.1.3.

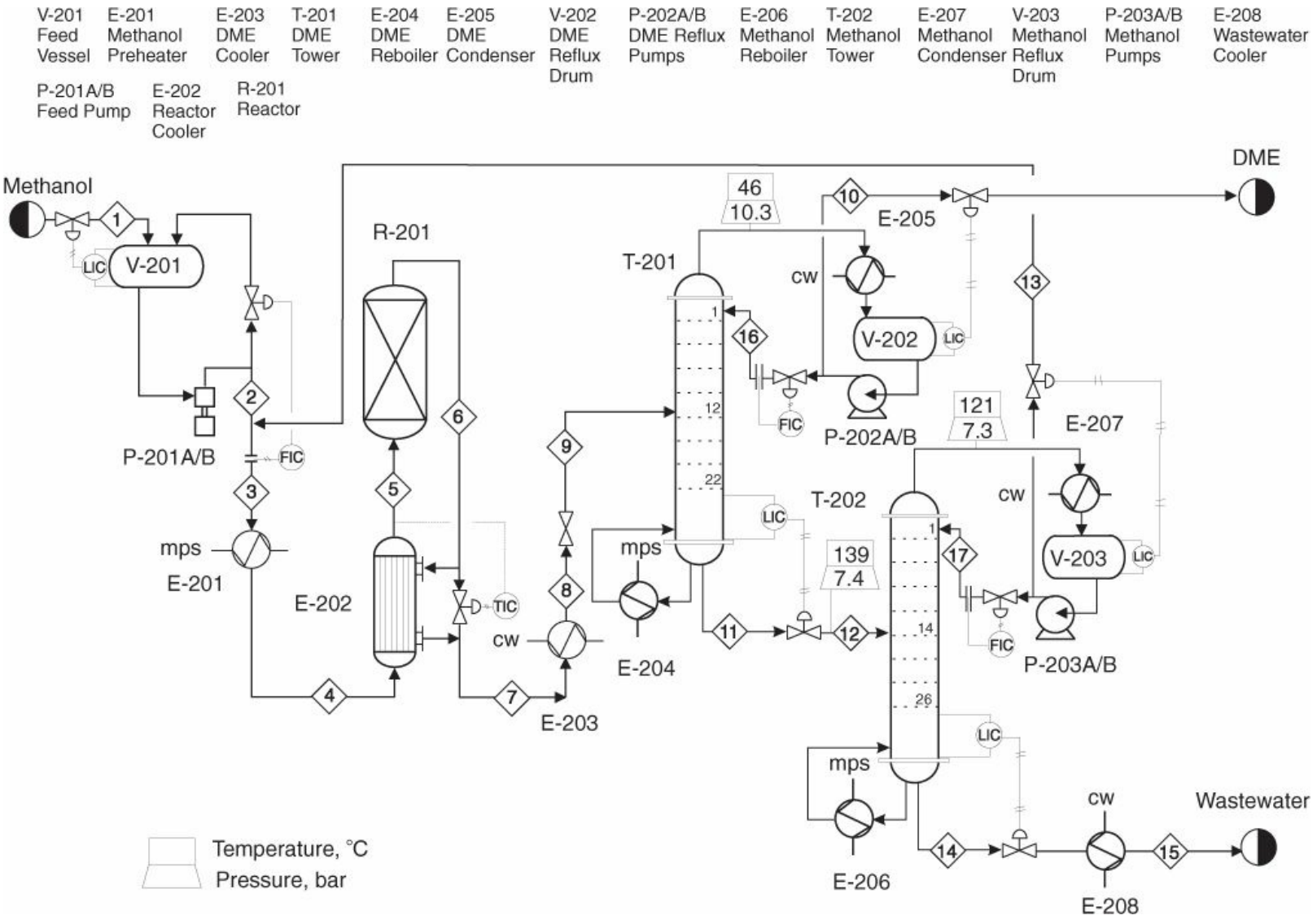


Figure B.1.1. Unit 200: Dimethyl Ether Process Flow Diagram

Table B.1.1. Stream Table for Unit 200

Stream Number	1	2	3	4	5	6	7	8
Temperature (°C)	25	25	45	154	250	364	278	100
Pressure (bar)	1.0	15.5	15.2	15.1	14.7	13.9	13.8	13.4
Vapor fraction	0.0	0.0	0.0	1.0	1.0	1.0	1.0	0.0798
Mass flow (tonne/h)	8.37	8.37	10.49	10.49	10.49	10.49	10.49	10.49
Mole flow (kmol/h)	262.2	262.2	328.3	328.3	328.3	328.3	328.3	328.3
Component flowrates (kmol/h)								
Dimethyl ether	0.0	0.0	1.5	1.5	1.5	130.5	130.5	130.5
Methanol	259.7	259.7	323.0	323.0	323.0	64.9	64.9	64.9
Water	2.5	2.5	3.8	3.8	3.8	132.9	132.9	132.9

Stream Number	9	10	11	12	13	14	15	16	17
Temperature (°C)	89	46	153	139	121	167	50	46	121
Pressure (bar)	10.4	11.4	10.5	7.4	15.5	7.6	1.2	11.4	7.3
Vapor fraction	0.148	0.0	0.0	0.04	0.0	0.0	0.0	0.0	0.0
Mass flow (tonne/h)	10.49	5.97	4.52	4.52	2.13	2.39	2.39	2.17	3.62
Mole flow (kmol/h)	328.3	129.7	198.6	198.6	66.3	132.3	132.3	47.1	113.0
Component flowrates (kmol/h)									
Dimethyl ether	130.5	129.1	1.4	1.4	1.4	0.0	0.0	46.9	2.4
Methanol	64.9	0.6	64.3	64.3	63.6	0.7	0.7	0.2	108.4
Water	132.9	0.0	132.9	132.9	1.3	131.6	131.6	0.0	2.2

Table B.1.2. Utility Summary Table for Unit 200

E-201	E-203	E-204	E-205	E-206	E-207	E-208
mps	cw	mps	cw	mps	cw	cw
7220 kg/h	297,100 kg/h	1250 kg/h	75,120 kg/h	2900 kg/h	142,600 kg/h	28,700 kg/h

Table B.1.3. Major Equipment Summary for Unit 200

Heat Exchangers

E-201
$A = 99.4\ m^2$
Floating head, carbon steel, shell-and-tube design
Process stream in tubes
$Q = 14{,}400$ MJ/h
Maximum pressure rating of 15 bar

E-202
$A = 171.0\ m^2$
Floating head, carbon steel, shell-and-tube design
Process stream in tubes and shell
$Q = 2030$ MJ/h
Maximum pressure rating of 15 bar

E-203
$A = 101.8\ m^2$
Floating head, carbon steel, shell-and-tube design
Process stream in shell
$Q = 12{,}420$ MJ/h
Maximum pressure rating of 14 bar

E-204
$A = 22.0\ m^2$
Floating head, carbon steel, shell-and-tube design
Process stream in shell
$Q = 2490$ MJ/h
Maximum pressure rating of 11 bar

E-205
$A = 100.6\ m^2$
Fixed head, carbon steel, shell-and-tube design
Process stream in shell
$Q = 3140$ MJ/h
Maximum pressure rating of 10 bar

E-206
$A = 83.0\ m^2$
Floating head, carbon steel, shell-and-tube design
Process stream in shell
$Q = 5790$ MJ/h
Maximum pressure rating of 11 bar

E-207
$A = 22.7 m^2$
Floating head, carbon steel, shell-and-tube design
Process stream in shell
$Q = 5960$ MJ/h
Maximum pressure rating of 7 bar

E-208
$A = 22.8\ m^2$
Floating head, carbon steel, shell-and-tube design
Process stream in shell
$Q = 1200$ MJ/h
Maximum pressure rating of 8 bar

Pumps

P-201 A/B
Reciprocating/electric drive
Carbon steel
Power = 7.2 kW (actual)
60% efficient
Pressure out = 15.5 bar

P-202 A/B
Centrifugal/electric drive
Carbon steel
Power = 5.2 kW (actual)
40% efficient
Pressure out = 16 bar

P-202 A/B
Centrifugal/electric drive
Carbon steel
Power = 1.0 kW (actual)
40% efficient
Pressure out = 11.4 bar

Reactor
R-201
Carbon steel
Packed-bed section 7.2 m high filled with catalyst
Diameter = 0.72 m
Height = 10 m
Maximum pressure rating of 14.7 bar

Towers
T-201
Carbon steel
22 SS sieve trays plus reboiler and condenser
24-in tray spacing
Column height = 15.8 m
Diameter = 0.79 m
Maximum pressure rating of 10.6 bar

T-202
Carbon steel
26 SS sieve trays plus reboiler and condenser
18-in tray spacing
Column height = 14.9 m
Diameter = 0.87 m
Maximum pressure rating of 7.3 bar

Vessels
V-201
Horizontal
Carbon steel
Length = 3.42 m
Diameter = 1.14 m
Maximum pressure rating of 1.1 bar

V-202
Horizontal
Carbon steel
Length = 2.89 m
Diameter = 0.98 m
Maximum pressure rating of 10.3 bar

V-203
Horizontal
Carbon steel
Length = 2.53 m
Diameter = 0.85 m
Maximum pressure rating of 7.3 bar

B.1.2. Reaction Kinetics

The reaction taking place is mildly exothermic with a standard heat of reaction, ΔH_{reac} (25°C) = –11,770 kJ/kmol. The equilibrium constant for this reaction at three different temperatures is given below:

T	K_p
473 K (200°C)	92.6
573 K (300°C)	52.0
673 K (400°C)	34.7

The corresponding equilibrium conversions for pure methanol feed over the above temperature range are greater than 99%. Thus this reaction is kinetically controlled at the conditions used in this

process.

The reaction takes place on an amorphous alumina catalyst treated with 10.2% silica. There are no significant side reactions at less than 400°C. At greater than 250°C the rate equation is given by Bondiera and Naccache [2] as:

$$-r_{methanol} = k_0 \exp\left[\frac{-E_0}{RT}\right] p_{methanol} \qquad \text{(B.1.2)}$$

where $k_0 = 1.21 \times 10^6$ kmol/(m^{3}cat.h.kPa), $E_0 = 80.48$ kJ/mol, and $p_{methanol}$ = partial pressure of methanol (kPa).

Significant catalyst deactivation occurs at temperatures greater than 400°C, and the reactor should be designed so that this temperature is not exceeded anywhere in the reactor. The design given in Figure B.1.1 uses a single packed bed of catalyst, which operates adiabatically. The temperature exotherm occurring in the reactor of 118°C is probably on the high side and gives an exit temperature of 368°C. However, the single-pass conversion is quite high (80%), and the low reactant concentration at the exit of the reactor tends to limit the possibility of a runaway.

In practice the catalyst bed might be split into two sections, with an intercooler between the two beds. This has an overall effect of increasing the volume (and cost) of the reactor and should be investigated if catalyst damage is expected at temperatures lower than 400°C. In-reactor cooling (shell-and-tube design) and cold quenching by splitting the feed and feeding at different points in the reactor could also be investigated as viable alternative reactor configurations.

B.1.3. Simulation (CHEMCAD) Hints

The DME-water binary system exhibits two liquid phases when the DME concentration is in the 34% to 93% range [2]. However, upon addition of 7% or more alcohol, the mixture becomes completely miscible over the complete range of DME concentration. In order to ensure that this nonideal behavior is simulated correctly, it is recommended that binary vapor-liquid equilibrium (VLE) data for the three pairs of components be used in order to regress binary interaction parameters (BIPs) for a UNIQUAC/UNIFAC thermodynamics model. If VLE data for the binary pairs are not used, then UNIFAC can be used to estimate BIPs, but these should be used only as preliminary estimates. As with all nonideal systems, there is no substitute for designing separation equipment using data regressed from actual (experimental) VLE.

B.1.4. References

1. "DuPont Talks about Its DME Propellant," *Aerosol Age*, May and June 1982.
2. Bondiera, J., and C. Naccache, "Kinetics of Methanol Dehydration in Dealuminated H-Mordenite: Model with Acid and Basic Active Centres," *Applied Catalysis* 69 (1991): 139–148.

B.2. Ethylbenzene Production, Unit 300

The majority of ethylbenzene (EB) processes produce EB for internal consumption within a coupled process that produces styrene monomer. The facility described here produces 80,000 tonne/y of 99.8 mol% ethylbenzene that is totally consumed by an on-site styrene facility. As with most EB/styrene facilities, there is significant heat integration between the two plants. In order to decouple the operation of the two plants, the energy integration is achieved by the generation and consumption of

steam within the two processes. The EB reaction is exothermic, so steam is produced, and the styrene reaction is endothermic, so energy is transferred in the form of steam.

B.2.1. Process Description [1, 2]

The PFD for the EB process is shown in Figure B.2.1. A refinery cut of benzene is fed from storage to an on-site process vessel (V-301), where it is mixed with the recycled benzene. From V-301, it is pumped to a reaction pressure of approximately 2000 kPa (20 atm) and sent to a fired heater (H-301) to bring it to reaction temperature (approximately 400°C). The preheated benzene is mixed with feed ethylene just prior to entering the first stage of a reactor system consisting of three adiabatic packed-bed reactors (R-301 to R-303), with interstage feed addition and cooling. Reaction occurs in the gas phase and is exothermic. The hot, partially converted reactor effluent leaves the first packed bed, is mixed with more feed ethylene, and is fed to E-301, where the stream is cooled to 380°C prior to passing to the second reactor (R-302), where further reaction takes place. High-pressure steam is produced in E-301, and this steam is subsequently used in the styrene unit. The effluent stream from R-302 is similarly mixed with feed ethylene and is cooled in E-302 (with generation of high-pressure steam) prior to entering the third and final packed-bed reactor, R-303. The effluent stream leaving the reactor contains products, by-products, unreacted benzene, and small amounts of unreacted ethylene and other noncondensable gases. The reactor effluent is cooled in two waste-heat boilers (E-303 and E-304), in which high-pressure and low-pressure steam, respectively, is generated. This steam is also consumed in the styrene unit. The two-phase mixture leaving E-304 is sent to a trim cooler (E-305), where the stream is cooled to 80°C, and then to a two-phase separator (V-302), where the light gases are separated and, because of the high ethylene conversion, are sent overhead as fuel gas to be consumed in the fired heater. The condensed liquid is then sent to the benzene tower, T-301, where the unreacted benzene is separated as the overhead product and returned to the front end of the process. The bottoms product from the first column is sent to T-302, where product EB (at 99.8 mol% and containing less than 2 ppm diethylbenzene [DEB]) is taken as the top product and is sent directly to the styrene unit. The bottoms product from T-302 contains all the DEB and trace amounts of higher ethylbenzenes. This stream is mixed with recycle benzene and passes through the fired heater (H-301) prior to being sent to a fourth packed-bed reactor (R-304), in which the excess benzene is reacted with the DEB to produce EB and unreacted benzene. The effluent from this reactor is mixed with the liquid stream entering the waste-heat boiler (E-303).

Stream summary tables, utility summary tables, and major equipment specifications are shown in Tables B.2.1–B.2.3.

B.2.2. Reaction Kinetics

The production of EB takes place via the direct addition reaction between ethylene and benzene:

$$\underset{\text{benzene}}{C_6H_6} + \underset{\text{ethylene}}{C_2H_4} \rightarrow \underset{\text{ethylbenzene}}{C_6H_5C_2H_5} \qquad \text{(B.2.1)}$$

The reaction between EB and ethylene to produce DEB also takes place:

$$\underset{\text{ethylbenzene}}{C_6H_5C_2H_5} + \underset{\text{ethylene}}{C_2H_4} \rightarrow \underset{\text{diethylbenzene}}{C_6H_4(C_2H_5)_2} \qquad \text{(B.2.2)}$$

Additional reactions between DEB and ethylene yielding triethylbenzene (and higher) are also possible. However, in order to minimize these additional reactions, the molar ratio of benzene to ethylene is kept high, at approximately 8:1. The production of DEB is undesirable, and its value as a

side product is low. In addition, even small amounts of DEB in EB cause significant processing problems in the downstream styrene process. Therefore, the maximum amount of DEB in EB is specified as 2 ppm. In order to maximize the production of the desired EB, the DEB is separated and returned to a separate reactor in which excess benzene is added to produce EB via the following equilibrium reaction:

$$\underset{\text{diethylbenzene}}{C_6H_4(C_2H_5)_2} + \underset{\text{benzene}}{C_6H_6} \leftrightharpoons 2\underset{\text{ethylbenzene}}{C_6H_5C_2H_5} \qquad \text{(B.2.3)}$$

The incoming benzene contains a small amount of toluene impurity. The toluene reacts with ethylene to form ethyl benzene and propylene:

$$\underset{\text{toluene}}{C_6H_5CH_3} + 2C_2H_4 \rightarrow \underset{\text{ethylbenzene}}{C_6H_5C_2H_5} + \underset{\text{propylene}}{C_3H_6} \qquad \text{(B.2.4)}$$

The reaction kinetics derived for a new catalyst are given as

$$-r_i = k_{o,i} e^{-Ei/RT} C^a_{ethylene} C^b_{EB} C^c_{toluene} C^d_{benzene} C^e_{DEB} \qquad \text{(B.2.5)}$$

where i is the reaction number above (B.2.i), and the following relationships pertain:

i	E_i kcal/kmol	$k_{o,i}$	a	b	c	d	e
1	22,500	1.00×10^6	1	0	0	1	0
2	22,500	6.00×10^5	1	1	0	0	0
3	25,000	7.80×10^6	0	0	0	1	1
4	20,000	3.80×10^8	2	0	1	0	0

The units of r_i are kmol/s/m^3-reactor, the units of C_i are kmol/m^3-gas, and the units of $k_{o,i}$ vary depending upon the form of the equation.

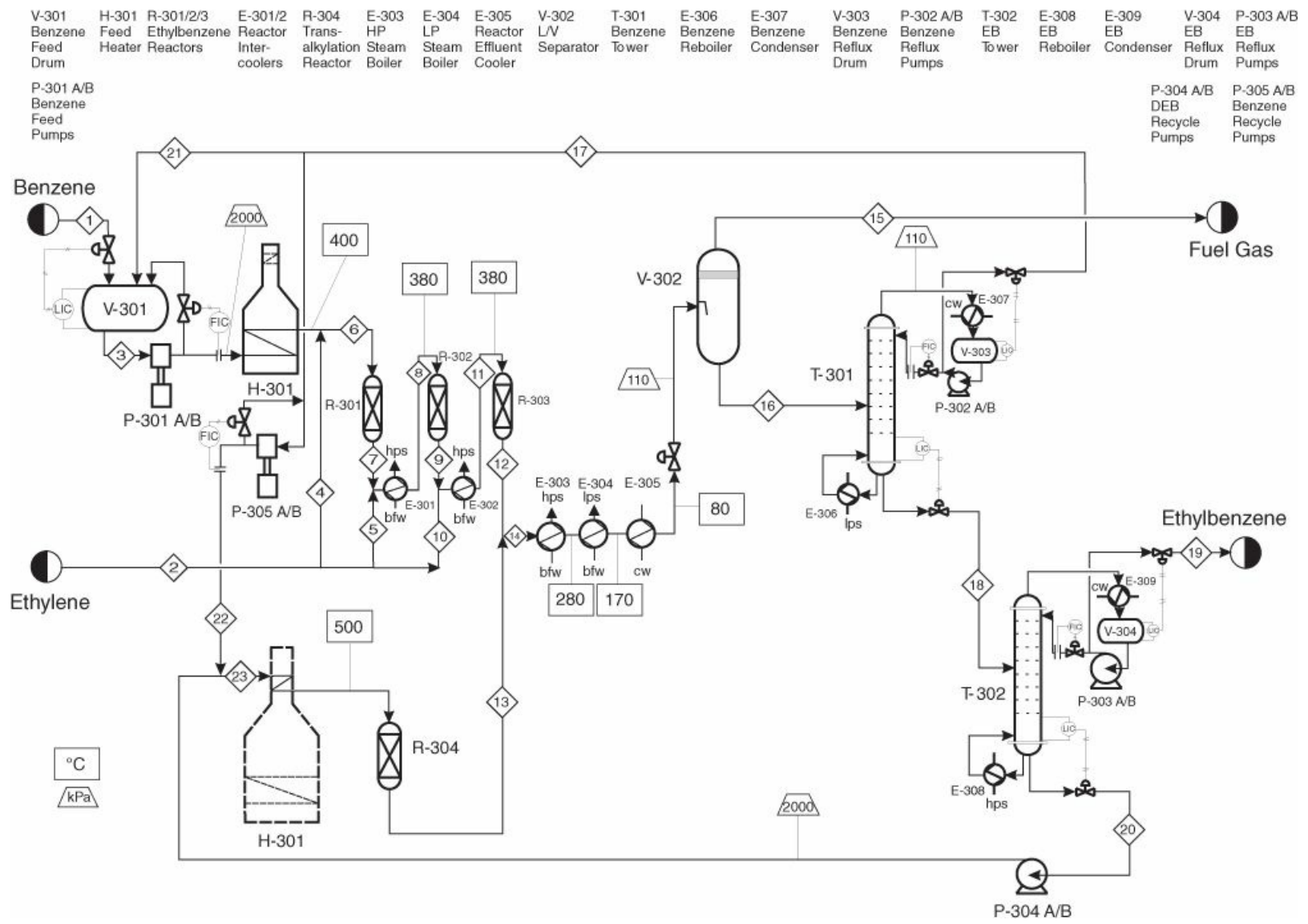


Figure B.2.1. Unit 300: Ethylbenzene Process Flow Diagram

Table B.2.1. Stream Table for Unit 300

Stream Number	1	2	3	4	5	6
Temperature (°C)	25.0	25.0	58.5	25.0	25.0	383.3
Pressure (kPa)	110.0	2000.0	110.0	2000.0	2000.0	1985.0
Vapor mole fraction	0.0	1.0	0.0	1.0	1.0	1.0
Total kg/h	7761.3	2819.5	17,952.2	845.9	986.8	18,797.9
Total kmol/h	99.0	100.0	229.2	30.0	35.0	259.2
Component Flowrates (kmol/h)						
Ethylene	0.00	93.00	0.00	27.90	32.55	27.90
Ethane	0.00	7.00	0.00	2.10	2.45	2.10
Propylene	0.00	0.00	0.00	0.00	0.00	0.00
Benzene	97.00	0.00	226.51	0.00	0.00	226.51
Toluene	2.00	0.00	2.00	0.00	0.00	2.00
Ethylbenzene	0.00	0.00	0.70	0.00	0.00	0.70
1,4-Diethylbenzene	0.00	0.00	0.00	0.00	0.00	0.00

Stream Number	7	8	9	10	11	12
Temperature (°C)	444.1	380.0	453.4	25.0	380.0	449.2
Pressure (kPa)	1970.0	1960.0	1945.0	2000.0	1935.0	1920.0
Vapor mole fraction	1.0	1.0	1.0	1.0	1.0	1.0
Total kg/h	18,797.9	19,784.7	19,784.7	986.8	20,771.5	20,771.5
Total kmol/h	234.0	269.0	236.4	35.0	271.4	238.7
Component Flowrates (kmol/h)						
Ethylene	0.85	33.40	0.62	32.55	33.17	0.54
Ethane	2.10	4.55	4.55	2.45	7.00	7.00
Propylene	1.83	1.81	2.00	0.00	2.00	2.00
Benzene	203.91	203.91	174.96	0.00	174.96	148.34
Toluene	0.19	0.19	0.0026	0.00	0.0026	0.00
Ethylbenzene	24.28	24.28	49.95	0.00	49.95	70.57
1,4-Diethylbenzene	0.87	0.87	4.29	0.00	4.29	10.30

Stream Number	13	14	15	16	17	18
Temperature (°C)	497.9	458.1	73.6	73.6	81.4	145.4
Pressure (kPa)	1988.0	1920.0	110.0	110.0	105.0	120.0
Vapor mole fraction	1.0	1.0	1.0	0.0	0.0	0.0
Total kg/h	4616.5	25,387.9	1042.0	24,345.9	13,321.5	11,024.5
Total kmol/h	51.3	290.0	18.6	271.4	170.2	101.1
Component Flowrates (kmol/h)						
Ethylene	0.00	0.54	0.54	0.00	0.00	0.00
Ethane	0.00	7.00	7.00	0.00	0.00	0.00
Propylene	0.00	2.00	2.00	0.00	0.00	0.00
Benzene	29.50	177.85	8.38	169.46	169.23	0.17
Toluene	0.00	0.00	0.00	0.00	0.00	0.00
Ethylbenzene	21.69	92.25	0.71	91.54	0.92	90.63
1,4-Diethylbenzene	0.071	10.37	0.013	10.35	0.00	10.35

Stream Number	19	20	21	22	23
Temperature (°C)	139.0	191.1	82.6	82.6	121.4
Pressure (kPa)	110.0	140.0	2000.0	2000.0	2000.0
Vapor mole fraction	0.0	0.0	0.0	0.0	0.0
Total kg/h	9538.6	1485.9	10,190.9	3130.6	4616.5
Total kmol/h	89.9	11.3	130.2	40.0	51.3
Component Flowrates (kmol/h)					
Ethylene	0.00	0.00	0.00	0.00	0.00
Ethane	0.00	0.00	0.00	0.00	0.00
Propylene	0.00	0.00	0.00	0.00	0.00
Benzene	0.17	0.00	129.51	39.78	39.78
Toluene	0.00	0.00	0.00	0.00	0.00
Ethylbenzene	89.72	0.91	0.70	0.22	1.12
1,4-Diethylbenzene	0.0001	10.35	0.00	0.00	10.35

Table B.2.2. Utility Summary Table for Unit 300

Stream Name	bfw to E-301	bfw to E-302	bfw to E-303	bfw to E-304	cw to E-305
Flowrate (kg/h)	851	1121	4341	5424	118,300
Stream Name	**lps to E-306**	**cw to tE-307**	**hps to E-308***	**cw to E-309**	
Flowrate (kg/h)	4362	174,100	3124	125,900	

*Throttled and desuperheated at exchanger

Table B.2.3. Major Equipment Summary for Unit 300

Heat Exchangers

E-301
$A = 62.6\ m^2$
1-2 exchanger, floating head, stainless steel
Process stream in tubes
$Q = 1967$ MJ/h
Maximum pressure rating of 2200 kPa

E-302
$A = 80.1\ m^2$
1-2 exchanger, floating head, stainless steel
Process stream in tubes
$Q = 2592$ MJ/h
Maximum pressure rating of 2200 kPa

E-303
$A = 546\ m^2$
1-2 exchanger, floating head, stainless steel
Process stream in tubes
$Q = 10{,}080$ MJ/h
Maximum pressure rating of 2200 kPa

E-304
$A = 1567\ m^2$
1-2 exchanger, fixed head, carbon steel
Process stream in tubes
$Q = 12{,}367$ MJ/h
Maximum pressure rating of 2200 kPa

E-305
$A = 348\ m^2$
1-2 exchanger, floating head, carbon steel
Process stream in shell
$Q = 4943$ MJ/h
Maximum pressure rating of 2200 kPa

E-306
$A = 57.8\ m^2$
1-2 exchanger, fixed head, carbon steel
Process stream in shell
$Q = 9109$ MJ/h
Maximum pressure rating of 200 kPa

E-307
$A = 54.6\ m^2$
1-2 exchanger, floating head, carbon steel
Process stream in shell
$Q = 7276$ MJ/h
Maximum pressure rating of 200 kPa

E-308
$A = 22.6\ m^2$
1-2 exchanger, fixed head, carbon steel
Process stream in shell
$Q = 5281$ MJ/h
Maximum pressure rating of 200 kPa

E-309
$A = 17.5\ m^2$
1-2 exchanger, floating head, carbon steel
Process stream in shell
$Q = 5262$ MJ/h
Maximum pressure rating of 200 kPa

Fired Heater

H-301

Required heat load = 22,376 MJ/h
Design (maximum) heat load = 35,000 MJ/h
Tubes = Stainless steel
75% thermal efficiency
Maximum pressure rating of 2200 kPa

Pumps

P-301 A/B

Positive displacement/electric drive
Carbon steel
Actual power = 15 kW
Efficiency 75%

P-302 A/B

Centrifugal/electric drive
Carbon steel
Actual power = 1 kW
Efficiency 75%

P-303 A/B

Centrifugal/electric drive
Carbon steel
Actual power = 1 kW
Efficiency 75%

P-304 A/B

Centrifugal/electric drive
Carbon steel
Actual power = 1.4 kW
Efficiency 80%

P-305 A/B

Positive displacement/electric drive
Carbon steel
Actual power = 2.7 kW
Efficiency 75%

Reactors

R-301

316 stainless steel packed bed, ZSM-5 molecular sieve catalyst
$V = 20\ m^3$
11 m long, 1.72 m diameter
Maximum pressure rating of 2200 kPa
Maximum allowable catalyst temperature = 500°C

R-303

316 stainless steel packed bed, ZSM-5 molecular sieve catalyst
$V = 30\ m^3$
12 m long, 1.97 m diameter
Maximum pressure rating of 2200 kPa
Maximum allowable catalyst temperature = 500°C

R-302 316 stainless steel packed bed, ZSM-5 molecular sieve catalyst $V = 25\ m^3$ 12 m long, 1.85 m diameter Maximum pressure rating of 2200 kPa Maximum allowable catalyst temperature = 500°C	**R-304** 316 stainless steel packed bed, ZSM-5 molecular sieve catalyst $V = 1.67\ m^3$ 5 m long, 0.95 m diameter Maximum pressure rating of 2200 kPa Maximum allowable catalyst temperature = 525°C
Towers	
T-301 Carbon steel 45 SS sieve trays plus reboiler and total condenser 42% efficient trays Feed on tray 19 Additional feed ports on trays 14 and 24 Reflux ratio = 0.3874 24-in tray spacing Column height = 27.45 m Diameter = 1.7 m Maximum pressure rating of 300 kPa	**T-302** Carbon steel 76 SS sieve trays plus reboiler and total condenser 45% efficient trays Feed on tray 56 Additional feed ports on trays 50 and 62 Reflux ratio = 0.6608 15-in tray spacing Column height = 28.96 m Diameter = 1.5 m Maximum pressure rating of 300 kPa
Vessels	
V-301 Carbon steel Horizontal L/D = 5 $V = 7\ m^3$ Maximum operating pressure = 250 kPa	**V-303** Carbon steel Horizontal L/D = 3 $V = 7.7\ m^3$ Maximum operating pressure = 300 kPa
V-302 Carbon steel with SS demister Vertical L/D = 3 $V = 10\ m^3$ Maximum operating pressure = 250 kPa	**V-304** Carbon steel Horizontal L/D = 3 $V = 6.2\ m^3$ Maximum operating pressure = 300 kPa

B.2.3. Simulation (CHEMCAD) Hints

A CHEMCAD simulation is the basis for the design. The thermodynamics models used were K-val = UNIFAC and Enthalpy = Latent Heat.

It should be noted that in the simulation a component separator was placed after the high-pressure flash drum (V-302) in order to remove noncondensables from Stream 16 prior to entering T-301. This is done in order to avoid problems in simulating this tower. In practice, the noncondensables would be removed from the overhead reflux drum, V-303, after entering T-301.

As a first approach, both towers were simulated as Shortcut columns in the main simulation, but subsequently each was simulated separately using the rigorous TOWER module. Once the rigorous TOWER simulations were completed, they were substituted back into the main flowsheet and the simulation was run again to converge. A similar approach is recommended. The rigorous TOWER module provides accurate design and simulation data and should be used to assess column operation,

but using the shortcut simulations in the initial trials speeds up overall conversion of the flowsheet.

B.2.4. References

1. William J. Cannella, "Xylenes and Ethylbenzene," *Kirk-Othmer Encyclopedia of Chemical Technology*, online version (New York: John Wiley and Sons, 2006).
2. "Ethylbenzene," *Encyclopedia of Chemical Processing and Design*, Vol. 20, ed. J. J. McKetta (New York: Marcel Dekker, 1984), 77–88.

B.3. Styrene Production, Unit 400

Styrene is the monomer used to make polystyrene, which has a multitude of uses, the most common of which are in packaging and insulated Styrofoam beverage cups. Styrene is produced by the dehydrogenation of ethylbenzene. Ethylbenzene is formed by reacting ethylene and benzene. There is very little ethylbenzene sold commercially, because most ethylbenzene manufacturers convert it directly into styrene.

B.3.1 Process Description [1, 2]

The process flow diagram is shown in Figure B.3.1. Ethylbenzene feed is mixed with recycled ethylbenzene, heated, and then mixed with high-temperature, superheated steam. Steam is an inert in the reaction, which drives the equilibrium shown in Equation (B.3.1) to the right by reducing the concentrations of all components. Because styrene formation is highly endothermic, the superheated steam also provides energy to drive the reaction. Decomposition of ethylbenzene to benzene and ethylene, and hydrodealkylation to give methane and toluene, are unwanted side reactions shown in Equations (B.3.2) and (B.3.3). The reactants then enter two adiabatic packed beds with interheating. The products are cooled, producing steam from the high-temperature reactor effluent. The cooled product stream is sent to a three-phase separator, in which light gases (hydrogen, methane, ethylene), organic liquid, and water exit in separate streams. The hydrogen stream is further purified as a source of hydrogen elsewhere in the plant. The benzene/toluene stream is currently returned as a feed stream to the petrochemical facility. The organic stream containing the desired product is distilled once to remove the benzene and toluene and distilled again to separate unreacted ethylbenzene for recycle from the styrene product.

$$\underset{\text{ethylbenzene}}{C_6H_5C_2H_5} \overset{1}{\rightleftharpoons} \underset{\text{styrene}}{C_6H_5C_2H_3} + \underset{\text{hydrogen}}{H_2} \qquad \text{(B.3.1)}$$

$$\underset{\text{ethylbenzene}}{C_6H_5C_2H_5} \overset{3}{\rightarrow} \underset{\text{benzene}}{C_6H_6} + \underset{\text{ethylene}}{C_2H_4} \qquad \text{(B.3.2)}$$

$$\underset{\text{ethylbenzene}}{C_6H_5C_2H_5} + \underset{\text{hydrogen}}{H_2} \overset{4}{\rightarrow} \underset{\text{toluene}}{C_6H_5CH_3} + \underset{\text{methane}}{CH_4} \qquad \text{(B.3.3)}$$

The styrene product can spontaneously polymerize at higher temperatures. Because product styrene is sent directly to the polymerization unit, experience suggests that as long as its temperature is maintained at less than 125°C, there is no spontaneous polymerization problem. Because this is less than styrene's normal boiling point, and because low pressure pushes the equilibrium in Equation (B.3.1) to the right, much of this process is run at vacuum.

Stream tables, utility summaries, and major equipment summaries are given in Tables B.3.1, B.3.2, and B.3.3, respectively.

B.3.2. Reaction Kinetics

The styrene reaction may be equilibrium limited, and the equilibrium constant is given as Equation (B.3.4).

$$K = \left(\frac{y_{sty} y_{hyd} P}{y_{eb}} \right) \qquad \text{(B.3.4)}$$

$$\ln K = 15.5408 - \frac{14{,}852.6}{T}$$

where T is in K and P is in bar.

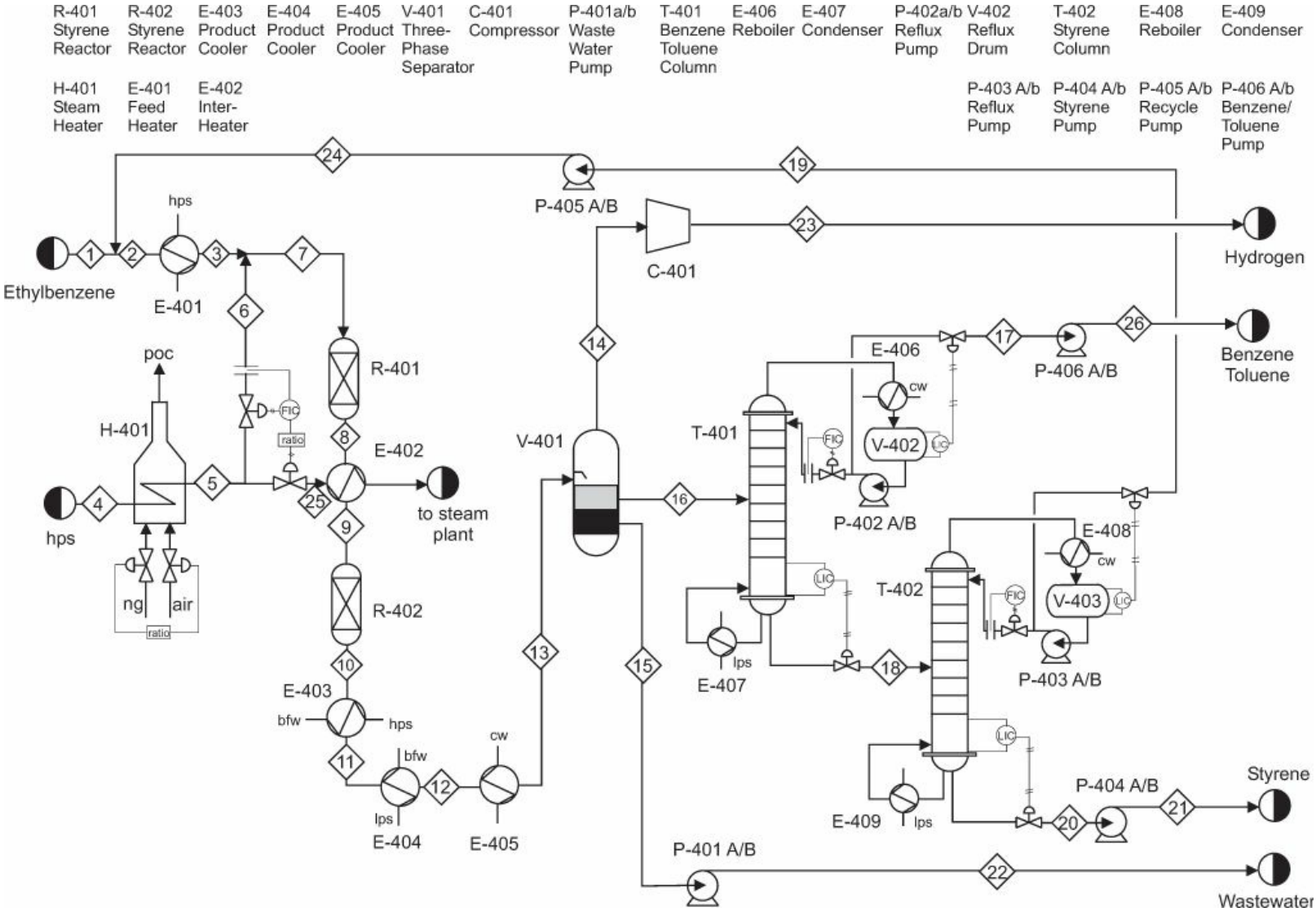


Figure B.3.1. Unit 400: Styrene Process Flow Diagram

Table B.3.1. Stream Tables for Unit 400

Stream Number	1	2	3	4	5
Temperature (°C)	136.0	116.0	240.0	253.7	800.0
Pressure (kPa)	200.0	190.0	170.0	4237.0	4202.0
Vapor mole fraction	0.00	0.00	1.00	1.00	1.00
Total flow (kg/h)	13,052.2	23,965.1	23,965.1	72,353.7	72,353.7
Total flow (kmol/h)	123.42	226.21	226.21	4016.30	4016.30
Component Flowrates (kmol/h)					
Water	0.00	0.00	0.00	4016.30	4016.30
Ethylbenzene	121.00	223.73	223.73	0.00	0.00
Styrene	0.00	0.06	0.06	0.00	0.00
Hydrogen	0.00	0.00	0.00	0.00	0.00
Benzene	1.21	1.21	1.21	0.00	0.00
Toluene	1.21	1.21	1.21	0.00	0.00
Ethylene	0.00	0.00	0.00	0.00	0.00
Methane	0.00	0.00	0.00	0.00	0.00

Stream Number	6	7	8	9	10
Temperature (°C)	722.0	566.6	504.3	550.0	530.1
Pressure (kPa)	170.0	160.0	150.0	135.0	125.0
Vapor mole fraction	1.00	1.00	1.00	1.00	1.00
Total flow (kg/h)	54,045.0	78,010.2	78,010.2	78,010.2	78,010.2
Total flow (kmol/h)	3000.00	3226.21	3317.28	3317.28	3346.41

Component Flowrates (kmol/h)					
Water	3000.00	3000.00	3000.00	3000.00	3000.00
Ethylbenzene	0.00	223.73	132.35	132.35	102.88
Styrene	0.00	0.06	91.06	91.06	120.09
Hydrogen	0.00	0.00	90.69	90.69	119.38
Benzene	0.00	1.21	1.28	1.28	1.37
Toluene	0.00	1.21	1.52	1.52	1.86
Ethylene	0.00	0.00	0.07	0.07	0.16
Methane	0.00	0.00	0.31	0.31	0.65
Stream Number	**11**	**12**	**13**	**14**	**15**
Temperature (°C)	267.0	180.0	65.0	65.0	65.0
Pressure (kPa)	110.0	95.0	80.0	65.0	65.0
Vapor mole fraction	1.00	1.00	0.15	1.00	0.00
Total flow (kg/h)	78,010.2	78,010.2	78,010.2	255.6	54,045.0
Total flow (kmol/h)	3346.41	3346.41	3346.41	120.20	3000.00
Component Flowrates (kmol/h)					
Water	3000.00	3000.00	3000.00	0.00	3000.00
Ethylbenzene	102.88	102.88	102.88	0.00	0.00
Styrene	120.09	120.09	120.09	0.00	0.00
Hydrogen	119.38	119.38	119.38	119.38	0.00
Benzene	1.37	1.37	1.37	0.00	0.00
Toluene	1.86	1.86	1.86	0.00	0.00
Ethylene	0.16	0.16	0.16	0.16	0.00
Methane	0.65	0.65	0.65	0.65	0.00

Stream Number	16	17	18	19	20
Temperature (°C)	65.0	69.9	125.0	90.8	123.7
Pressure (kPa)	65.0	45.0	65.0	25.0	55.0
Vapor mole fraction	0.00	0.00	0.00	0.00	0.00
Total flow (kg/h)	23,709.6	289.5	23,420.0	10,912.9	12,507.1
Total flow (kmol/h)	226.21	3.34	222.88	102.79	120.08
Component Flowrates (kmol/h)					
Water	0.00	0.00	0.00	0.00	0.00
Ethylbenzene	102.88	0.10	102.78	102.73	0.05
Styrene	120.09	0.00	120.09	0.06	120.03
Hydrogen	0.00	0.00	0.00	0.00	0.00
Benzene	1.37	1.37	0.00	0.00	0.00
Toluene	1.86	1.86	0.00	0.00	0.00
Ethylene	0.00	0.00	0.00	0.00	0.00
Methane	0.00	0.00	0.00	0.00	0.00

Stream Number	21	22	23	24	25
Temperature (°C)	123.8	65.0	202.2	91.0	800.0
Pressure (kPa)	200.0	200.0	140.0	200.0	4202.0
Vapor mole fraction	0.00	0.00	1.00	0.00	1.00
Total flow (kg/h)	12,507.1	54,045.0	255.6	10,912.9	18,308.7
Total flow (kmol/h)	120.08	3000.00	120.20	102.79	1016.30

Component Flowrates (kmol/h)					
Water	0.00	3000.00	0.00	0.00	1016.30
Ethylbenzene	0.05	0.00	0.00	102.73	0.00
Styrene	120.03	0.00	0.00	0.06	0.00
Hydrogen	0.00	0.00	119.38	0.00	0.00
Benzene	0.00	0.00	0.00	0.00	0.00
Toluene	0.00	0.00	0.00	0.00	0.00
Ethylene	0.00	0.00	0.16	0.00	0.00
Methane	0.00	0.00	0.65	0.00	0.00

Stream Number	26
Temperature (°C)	70.0
Pressure (kPa)	200.00
Vapor mole fraction	0.00
Total flow (kg/h)	289.5
Total flow (kmol/h)	3.34
Component Flowrates (kmol/h)	
Water	0.00
Ethylbenzene	0.10
Styrene	0.00
Hydrogen	0.00
Benzene	1.37
Toluene	1.86
Ethylene	0.00
Methane	0.00

Table B.3.2. Utility Summary for Unit 400

E-401	E-403	E-404	E-405
hps 7982 kg/h	bfw → hps 18,451 kg/h	bfw → lps 5562 kg/h	cw 3,269,746 kg/h
E-406	**E-407**	**E-408**	**E-409**
cw 309,547 kg/h	lps 7550 kg/h	cw 1,105,980 kg/h	lps 21,811 kg/h

Table B.3.3. Major Equipment Summary for Unit 400

Compressors and Drives

C-401
Carbon steel
$W = 134$ kW
60% adiabatic efficiency

D-401 A/B
Electric/explosion proof
$W = 136.7$ kW
98% efficiency

Heat Exchangers*

E-401
Carbon steel
$A = 260$ m^2
Boiling in shell, condensing in tubes
1 shell—2 tube passes
$Q = 13{,}530$ MJ/h

E-402
316 stainless steel
$A = 226$ m^2
Boiling in shell, process fluid in tubes
1 shell—2 tube passes
$Q = 8322$ MJ/h

E-403
316 stainless steel
$A = 1457$ m^2
Boiling in shell, process fluid in tubes
1 shell—2 tube passes
$Q = 44{,}595$ MJ/h

E-404
Carbon steel
$A = 702$ m^2
Boiling in shell, process fluid in tubes
1 shell—2 tube passes
$Q = 13{,}269$ MJ/h

E-405
316 stainless steel
$A = 1446$ m^2
cw in shell, process fluid in tubes
1 shell—2 tube passes
$Q = 136{,}609$ MJ/h

E-406
Carbon steel
$A = 173$ m^2
Process fluid in shell, cooling water in tubes
1 shell—2 tube passes
$Q = 12{,}951$ MJ/h

E-407
Carbon steel
$A = 64$ m^2
Steam in shell, steam condensing in tubes
Desuperheater—steam saturated at 150°C
1 shell—2 tube passes
$Q = 15{,}742$ MJ/h

E-408
Carbon steel
$A = 385$ m^2
Process fluid in shell, cooling water in tubes
1 shell—2 tube passes
Q = 46,274 MJ/h

E-409
Carbon steel
$A = 176$ m^2
Boiling in shell, steam condensing in tubes
Desuperheater—steam saturated at 150°C
1 shell—2 tube passes
$Q = 45{,}476$ MJ/h

Fired Heater

H-401
Fired heater-refractory-lined, stainless-steel tubes
Design $Q = 23.63$ MW
Maximum $Q = 25.00$ MW

Pumps

P-401 A/B
Centrifugal/electric drive
Stainless steel
$W = 2.59$ kW (actual)
80% efficient

P-402 A/B
Centrifugal/electric drive
Carbon steel
$W = 1.33$ kW (actual)
80% efficient

P-403 A/B
Centrifugal/electric drive
Carbon steel
$W = 0.574$ kW (actual)
80% efficient

P-404 A/B
Centrifugal/electric drive
Carbon steel
$W = 0.775$ kW (actual)
80% efficient

P-405 A/B
Centrifugal/electric drive
Carbon steel
$W = 0.825$ kW (actual)
80% efficient

P-406 A/B
Centrifugal/electric drive
Carbon steel
$W = 0.019$ kW (actual)
80% efficient

Reactors

R-401
316 stainless steel, packed bed
Cylindrical catalyst pellet (1.6 mm × 3.2 mm)
Void fraction = 0.4
$V = 25$ m^3
9.26 m tall, 1.85 m diameter

R-402
316 stainless steel, packed bed
Cylindrical catalyst pellet (1.6 mm × 3.2 mm)
Void fraction = 0.4
$V = 25$ m^3
9.26 m tall, 1.85 m diameter

Towers

T-401
Carbon steel
$D = 3.0$ m
61 sieve trays
54% efficient
Feed on tray 31
12-in tray spacing
1-in weirs
Column height = 61 ft = 18.6 m

T-402
Carbon steel
$D = 6.9$ m
158 bubble cap trays
55% efficient
Feed on tray 78
6-in tray spacing
1-in weirs
Column height = 79 ft = 24.1 m

Vessels

V-401
Carbon steel
$V = 26.8$ m^3

V-402
Horizontal
Carbon steel
$L/D = 3$
$V = 5$ m^3

V-403
Horizontal
Carbon steel
$L/D = 3$
$V = 5$ m^3

* See Figure B.3.1 and Table B.3.1 for shell- and tube-side pressures.

The equilibrium calculation is given as

$$\underset{\substack{1 \\ 1\text{-}x}}{C_6H_5C_2H_5} \rightleftharpoons \frac{1}{2} \underset{\substack{0 \\ x}}{C_6H_5C_2H_3} + \underset{\substack{0 \\ x}}{H_2}$$

total = $N + 1 + x$ includes N moles of inert steam

$$K = \frac{x^2 P}{(1-x)(N+1+x)} \tag{B.3.5}$$

where P is in bar.

Equation (B.3.5) can be used to generate data for equilibrium conversion, x, versus P, T, and N.

The kinetic equations are adapted from Snyder and Subramaniam [3]. Subscripts on r refer to reactions in Equations (B.3.1)–(B.3.3), and the positive activation energy can arise from nonelementary kinetics; it is thought that perhaps these kinetics are an elementary approximation to nonelementary kinetics.

$$r_1 = 10.177 \times 10^{11} \exp\left(-\frac{21{,}708}{RT}\right) p_{eb} \tag{B.3.6}$$

$$r_2 = 20.965 \exp\left(\frac{7804}{RT}\right) p_{sty}\, p_{hyd} \tag{B.3.7}$$

$$r_3 = 7.206 \times 10^{11} \exp\left(-\frac{49675}{RT}\right) p_{eb} \tag{B.3.8}$$

$$r_4 = 1.724 \times 10^{6} \exp\left(-\frac{26857}{RT}\right) p_{eb}\, p_{hyd} \tag{B.3.9}$$

where p is in bar, T is in K, R = 1.987 cal/mol K, and r_i is in mol/m^3-reactor s.

You should assume that the catalyst has a bulk density of 1282 kg/m^3, an effective diameter of 25 mm, and a void fraction = 0.4.

B.3.3 Simulation (CHEMCAD) Hints

Results for the simulation given here were obtained using SRK as the K-value and enthalpy options in the thermodynamics package.

B.3.4 References

1. Shiou-Shan Chen, "Styrene," *Kirk-Othmer Encyclopedia of Chemical Technology*, online version (New York: John Wiley and Sons, 2006).
2. "Styrene," *Encyclopedia of Chemical Processing and Design*, Vol. 55, ed. J. J. McKetta, (New York: Marcel Dekker, 1984), 197–217.
3. Snyder, J. D., and B. Subramaniam, "A Novel Reverse Flow Strategy for Ethylbenzene Dehydrogenation in a Packed-Bed Reactor," *Chem. Engr. Sci.* 49 (1994): 5585–5601.

B.4. Drying Oil Production, Unit 500

Drying oils are used as additives to paints and varnishes to aid in the drying process when these products are applied to surfaces. The facility manufactures drying oil (DO) from acetylated castor oil (ACO). Both of these compounds are mixtures. However, for simulation purposes, acetylated castor oil is modeled as palmitic (hexadecanoic) acid ($C_{15}H_{31}COOH$) and drying oil is modeled as 1-tetradecene ($C_{14}H_{28}$). In an undesired side reaction, a gum can be formed, which is modeled as 1-octacosene ($C_{28}H_{56}$).

B.4.1 Process Description

The process flow diagram is shown in Figure B.4.1. ACO is fed from a holding tank where it is mixed with recycled ACO. The ACO is heated to reaction temperature in H-501. The reaction does not require a catalyst, since it is initiated at high temperatures. The reactor, R-501, is simply a vessel with inert packing to promote radial mixing. The reaction is quenched in E-501. Any gum that has been formed is removed by filtration. There are two holding vessels, V-502 A/B. One of them is used to hold reaction products, while the other one feeds the filter (not shown). This allows a continuous flow of material into Stream 7. In T-501 the ACO is separated and recycled, and in T-502, the DO is purified from the acetic acid. The contents of Streams 11 and 12 are cooled (exchangers not shown) and sent to storage.

Stream summary tables, utility summary tables, and major equipment specifications are shown in Tables B.4.1–B.4.3.

B.4.2 Reaction Kinetics

The reactions and reaction kinetics are adapted from Smith [1] and are as follows:

$$\underset{ACO}{C_{15}H_{31}COOH(l)} \xrightarrow{k_1} \underset{acetic\ acid}{CH_3COOH(g)} + \underset{DO}{C_{14}H_{28}(l)} \qquad \text{(B.4.1)}$$

$$\underset{DO}{2C_{14}H_{28}(l)} \xrightarrow{k_2} \underset{gum}{C_{28}H_{56}(s)} \qquad \text{(B.4.2)}$$

where

$$-r_1 = k_1 C_{ACO} \qquad \text{(B.4.3)}$$

$$-r_2 = k_2 C_{DO}^2 \qquad \text{(B.4.4)}$$

and

$$k_1 = 5.538 \times 10^{13} \exp(-44{,}500/RT) \qquad \text{(B.4.5)}$$

$$k_2 = 1.55 \times 10^{26} \exp(-88{,}000/RT) \qquad \text{(B.4.6)}$$

The units of reaction rate, r_i, are kmol/m^{3}s, and the activation energy is in cal/mol (which is equivalent to kcal/kmol).

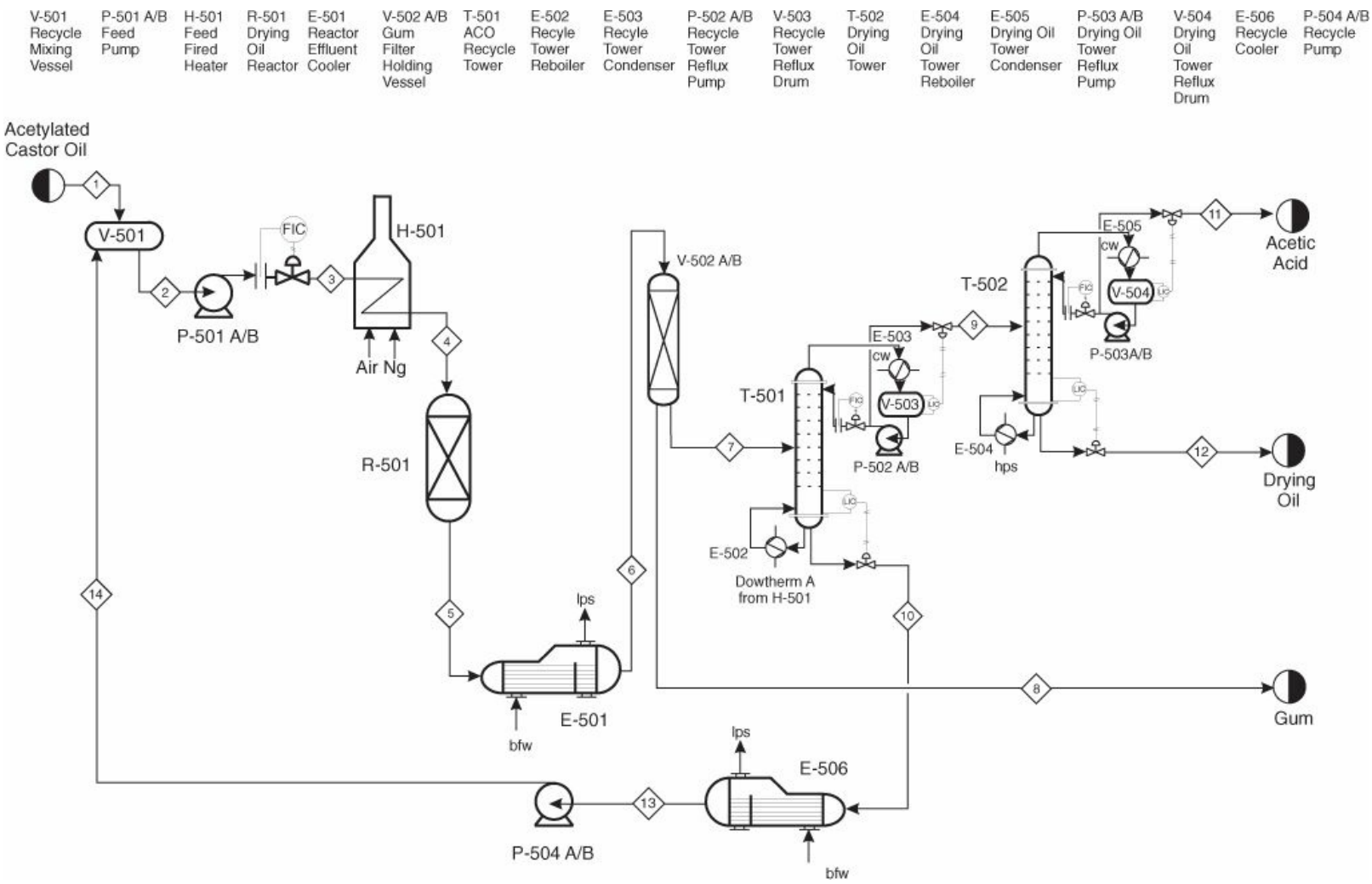


Figure B.4.1. Unit 500: Drying Oil Process Flow Diagram

B.4.3 Simulation (CHEMCAD) Hints

If you want to simulate this process and 1-octacosene is not a compound in your simulator's database, you can add gum as a compound to the simulator databank using the following physical properties:

- Molecular weight = 392
- Boiling point = 431.6°C
- For the group contribution method add the following groups:

  1 – CH_3 group

  25 >CH_2 groups

  1 = CH_2 group

  1 = CH– group

Table B.4.1. Stream Table for Unit 500

Stream Number	1	2	3	4
Temperature (°C)	25.0	151.0	151.1	380.0
Pressure (kPa)	110.0	105.0	230.0	195.0
Vapor mole fraction	0.00	0.00	0.00	0.00
Flowrate (kg/h)	1628.7	10,703.1	10,703.1	10,703.1
Flowrate (kmol/h)	6.35	41.75	41.75	41.75
Component flowrates (kmol/h)				
Acetic acid	0.00	0.00	0.00	0.00
1-Tetradecene (drying oil)	0.00	0.064	0.064	0.064
Hexadecanoic acid (ACO)	6.35	41.69	41.69	41.69
Gum	0.00	0.00	0.00	0.00

Stream Number	5	6	7	8
Temperature (°C)	342.8	175.0	175.0	175.0
Pressure (kPa)	183.0	148.0	136.0	136.0
Vapor mole fraction	0.39	0.00	0.00	0.00
Flowrate (kg/h)	10,703.1	10,703.1	10,703.1	0.02
Flowrate (kmol/h)	48.07	48.07	48.07	4.61×10^{-5}
Component flowrates (kmol/h)				
Acetic acid	6.32	6.32	6.32	0.00
1-Tetradecene (drying oil)	6.38	6.38	6.38	0.00
Hexadecanoic acid (ACO)	35.38	35.38	35.38	0.00
Gum	4.61×10^{-5}	4.61×10^{-5}	0.00000	4.61×10^{-5}

Stream Number	9	10	11	12
Temperature (°C)	108.0	344.8	119.2	252.8
Pressure (kPa)	125.0	90.0	105.0	125.0
Vapor mole fraction	0.00	0.00	0.00	0.00
Flowrate (kg/h)	1628.7	9074.4	378.6	1250.0
Flowrate (kmol/h)	12.67	35.40	6.29	6.38
Component flowrates (kmol/h)				
Acetic acid	6.32	0.00	6.28	0.03
1-Tetradecene (drying oil)	6.32	0.06	0.01	6.31
Hexadecanoic acid (ACO)	0.04	35.34	0.00	0.04
Gum	0.00	0.00	0.00	0.00

Stream Number	13	14
Temperature (°C)	170.0	170.0
Pressure (kPa)	65.0	110.0
Vapor mole fraction	0.00	0.00
Flowrate (kg/h)	9074.4	9074.4
Flowrate (kmol/h)	35.40	35.40
Component flowrates (kmol/h)		
Acetic acid	0.00	0.00
1-Tetradecene (drying oil)	0.06	0.06
Hexadecanoic acid (ACO)	35.34	35.34
Gum	0.00	0.00

Table B.4.2. Utility Summary Table for Unit 500

E-501	E-502	E-503	E-504	E-505	E-506
bfw→lps	Dowtherm A	cw	hps	cw	bfw→lps
2664 kg/h	126,540 kg/h	24,624 kg/h	425 kg/h	5508 kg/h	2088 kg/h

Table B.4.3. Major Equipment Summary for Unit 500

Fired Heater

H-501

Total heat duty required = 13,219 MJ/h = 3672 kW
Design capacity = 4000 kW
Carbon steel tubes
85% thermal efficiency

Heat Exchangers

E-501

$A = 26.2\ m^2$
1-2 exchanger, floating head, stainless steel
Process stream in tubes
$Q = 6329$ MJ/h

E-502

$A = 57.5\ m^2$
1-2 exchanger, floating head, stainless steel
Process stream in shell
$Q = 5569$ MJ/h

E-503

$A = 2.95\ m^2$
1-2 exchanger, floating head, stainless steel
Process stream in shell
$Q = 1029$ MJ/h

E-504

$A = 64.8\ m^2$
1-2 exchanger, floating head, stainless steel
Process stream in shell
$Q = 719$ MJ/h

E-505

$A = 0.58\ m^2$
1-2 exchanger, floating head, stainless steel
Process stream in shell
$Q = 230$ MJ/h

E-506

$A = 919\ m^2$
1-4 exchanger, floating head, stainless steel
Process stream in tubes
$Q = 4962$ MJ/h

Pumps

P-501 A/B

Centrifugal/electric drive
Carbon steel
Power = 0.9 kW (actual)
80% efficient
$NPSH_R$ at design flow = 14 ft of liquid

P-502 A/B

Centrifugal/electric drive
Stainless steel
Power = 1 kW (actual)
80% efficient

P-503 A/B

Centrifugal/electric drive
Stainless steel
Power = 0.8 kW (actual)
80% efficient

P-504 A/B

Stainless steel/electric drive
Power = 0.3 kW (actual)
80% efficient
$NPSH_R$ at design flow = 12 ft of liquid

Reactor

R-501

Stainless steel vessel
$V = 1.15\ m^3$
5.3 m long, 0.53 m diameter

Towers	
T-501 Stainless steel 56 sieve trays plus reboiler and condenser 25% efficient trays Total condenser Feed on tray = 32 Reflux ratio = 0.15 12-in tray spacing, 2.2-in weirs Column height = 17 m Diameter = 2.1 m below feed and 0.65 m above feed	**T-502** Stainless steel 35 sieve trays plus reboiler and condenser 52% efficient trays Total condenser Feed on tray = 23 Reflux ratio = 0.52 12-in tray spacing, 2.8-in weirs Column height = 11 m Diameter = 0.45 m
Vessels	
V-501 Horizontal Carbon steel L/D = 3 $V = 2.3\ m^3$	**V-503** Horizontal Stainless steel L/D = 3 $V = 2.3\ m^3$
V-502 Vertical Stainless steel L/D = 5 $V = 3\ m^3$	**V-504** Horizontal Carbon steel L/D = 3 $V = 0.3\ m^3$

B.4.4 Reference

1. Smith, J. M., *Chemical Engineering Kinetics*, 3rd ed. (New York: John Wiley and Sons, 1981), 224–228.

B.5. Production Of Maleic Anhydride From Benzene, Unit 600

Currently, the preferred route to maleic anhydride in the United States is via isobutene in fluidized-bed reactors. However, an alternative route via benzene may be carried out using a shell-and-tube reactor, with catalyst in the tubes and a cooling medium being circulated through the shell [1, 2].

B.5.1 Process Description

A process flow diagram for the reactor section of the maleic anhydride process is shown in Figure B.5.1. Benzene is vaporized in E-601, mixed with compressed air, and then heated in a fired heater, H-601, prior to being sent to a packed-bed catalytic reactor, R-601, where the following reactions take place:

$$\underset{\text{benzene}}{C_6H_6} + 4.5O_2 \xrightarrow{k_1} \underset{\text{maleic anhydride}}{C_4H_2O_3} + 2CO_2 + 2H_2O \qquad \text{(B.5.1)}$$

$$\underset{\text{benzene}}{C_6H_6} + 7.5O_2 \xrightarrow{k_2} 6CO_2 + 3H_2O \qquad \text{(B.5.2)}$$

$$\underset{\text{maleic anhydride}}{C_4H_2O_3} + 3O_2 \xrightarrow{k_3} 4CO_2 + H_2O \qquad \text{(B.5.3)}$$

$$\underset{\text{benzene}}{C_6H_6} + 1.5O_2 \xrightarrow{k_4} \underset{\text{quinone}}{C_6H_4O_2} + 2H_2O \qquad \text{(B.5.4)}$$

All the reactions are highly exothermic. For this reason, the ratio of air to benzene entering the reactor is kept very high. A typical inlet concentration (Stream 6) of approximately 1.5 vol% of benzene in air is used. Cooling is achieved by circulating molten salt (a mixture of sodium nitrite and sodium nitrate) cocurrently through the shell of the reactor and across the tubes containing the catalyst and reactant gases. This molten salt is cooled in two external exchangers—E-602 and E-607—prior to returning to the reactor.

The reactor effluent, Stream 7—containing small amounts of unreacted benzene, maleic anhydride, quinone, and combustion products—is cooled in E-603 and then sent to an absorber column, T-601, which has both a reboiler and condenser. In T-601, the vapor feed is contacted with recycled heavy organic solvent (dibutyl phthalate), Stream 9. This solvent absorbs the maleic anhydride, quinone, and small amounts of water. Any water in the solvent leaving the bottom of the absorber, T-601, reacts with the maleic anhydride to form maleic acid, which must be removed and purified from the maleic anhydride. The bottoms product from the absorber is sent to a separation tower, T-602, where the dibutyl phthalate is recovered as the bottoms product, Stream 14, and recycled back to the absorber. A small amount of fresh solvent, Stream 10, is added to account for losses. The overhead product from T-602, Stream 13, is sent to the maleic acid column, T-603, where 95 mol% maleic acid is removed as the bottoms product.

The overhead stream is taken to the quinone column, T-604, where 99 mol% quinone is taken as the top product and 99.9 mol% maleic anhydride is removed as the bottoms product. These last two purification columns are not shown in Figure B.5.1 and are not included in the current analysis.

Stream summaries, utility summaries, and equipment summaries are presented in Tables B.5.1–B.5.3.

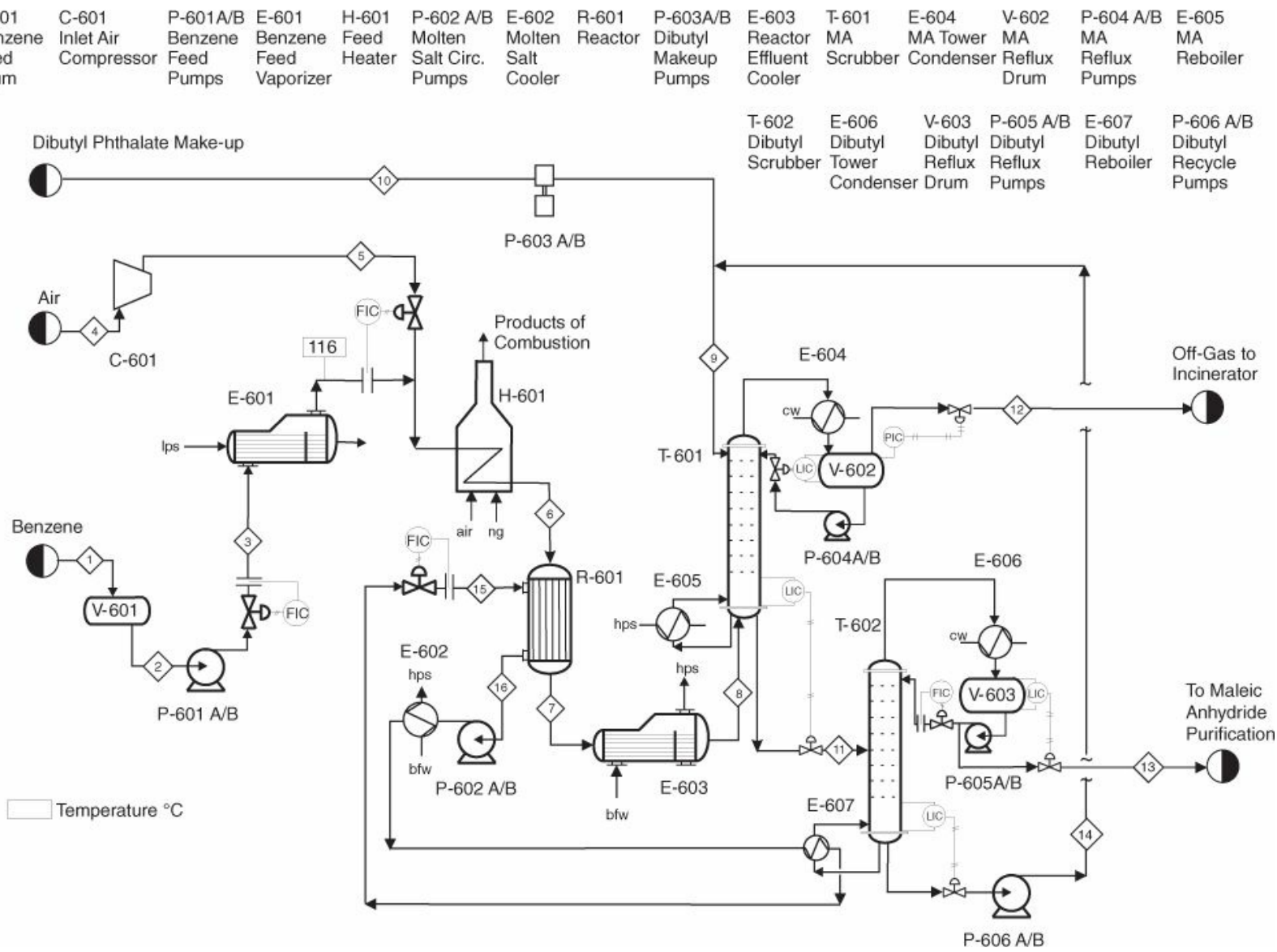


Figure B.5.1. Unit 600: Maleic Anhydride Process Flow Diagram

Table B.5.1. Stream Table for Unit 600

Stream Number	1	2	3	4	5	6	7	8
Temperature (°C)	30	30	30	30	170	460	608	270
Pressure (kPa)	101	101	280	101	250	235	220	215
Total kg/h	3304	3304	3304	80,490	80,490	83,794	83,794	83,794
Total kmol/h	42.3	42.3	42.3	2790.0	2790.0	2832.3	2825.2	2825.2
Component Flowrates (kmol/h)								
Maleic anhydride	0.0	0.0	0.0	0.0	0.0	0.0	26.3	26.3
Dibutyl phthalate	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Nitrogen	0.0	0.0	0.0	2205.0	2205.0	2205.0	2205.0	2205.0
Water	0.0	0.0	0.0	0.0	0.0	0.0	91.5	91.5
Oxygen	0.0	0.0	0.0	585.0	585.0	585.0	370.2	370.2
Benzene	42.3	42.3	42.3	0.0	0.0	42.3	2.6	2.6
Quinone	0.0	0.0	0.0	0.0	0.0	0.0	0.7	0.7
Carbon dioxide	0.0	0.0	0.0	0.0	0.0	0.0	129.0	129.0
Maleic acid	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Sodium nitrite	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Sodium nitrate	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Stream Number	9	10	11	12	13	14	15	16
Temperature (°C)	330	320	194	84	195	330	419	562
Pressure (kPa)	82	100	82	75	80	82	200	200
Total kg/h	139,191.6	30.6	141,866	81,225	2597	139,269	391,925	391,925
Total kmol/h	500.1	0.1	526.2	2797.9	26.2	500.0	5000.0	5000.0
Component Flowrates (kmol/h)								
Maleic anhydride	0.0	0.0	4.8	0.5	24.8	0.0	0.0	0.0
Dibutyl phthalate	500.1	0.1	500.0	0.0	0.0	500.0	0.0	0.0
Nitrogen	0.0	0.0	0.0	2205.0	0.0	0.0	0.0	0.0
Water	0.0	0.0	0.0	91.5	0.0	0.0	0.0	0.0
Oxygen	0.0	0.0	0.0	370.2	0.0	0.0	0.0	0.0
Benzene	0.0	0.0	0.0	2.6	0.0	0.0	0.0	0.0
Quinone	0.0	0.0	0.4	0.4	0.4	0.0	0.0	0.0
Carbon dioxide	0.0	0.0	0.0	129.0	0.0	0.0	0.0	0.0
Maleic acid	0.0	0.0	1.0	0.0	1.0	0.005	0.0	0.0
Sodium nitrite	0.0	0.0	0.0	0.0	0.0	0.0	2065.6	2065.6
Sodium nitrate	0.0	0.0	0.0	0.0	0.0	0.0	2934.4	2934.4

Table B.5.2. Utility Summary Table for Unit 600

E-601	E-602	E-603	E-604	E-605	E-606
lps	bfw → hps	bfw → hps	cw	hps	cw
1750 MJ/h	16,700 MJ/h	31,400 MJ/h	86,900 MJ/h	19,150 MJ/h	3050 MJ/h
841 kg/h	7295 kg/h	13,717 kg/h	2.08×10^6 kg/h	11,280 kg/h	73,000 kg/h

Table B.5.3. Major Equipment Summary for Unit 600

Compressor and Drives

C-601
Centrifugal/electric drive
Carbon steel
Discharge pressure = 250 kPa
Efficiency = 65%
Power (shaft) = 3108 kW
MOC carbon steel

D-601A/B (not shown on PFD)
Electric/explosion proof
W = 3200 kW
98% efficient

Fired Heater

H-601
Total (process) heat duty required = 26,800 MJ/h
Design capacity = 32,000 kW
Carbon steel tubes
85% thermal efficiency
Design pressure = 300 kPa

Heat Exchangers

E-601
A = 14.6 m^2
1-2 exchanger, floating head, stainless steel
Process stream in tubes
Q = 1750 MJ/h
Design pressure = 600 kPa

E-602
A = 61.6 m^2
1-2 exchanger, floating head, stainless steel
Process stream in shell
Q =16,700 MJ/h
Design pressure = 4100 kPa

E-603
A = 1760 m^2
1-2 exchanger, floating head, stainless steel
Process stream in shell
Q = 31,400 MJ/h
Design pressure = 4100 kPa

E-604
A = 1088 m^2
1-2 exchanger, fixed head, stainless steel
Process stream in tubes
Q = 86,900 MJ/h
Design pressure = 300 kPa

E-605
A = 131 m^2
1-2 exchanger, floating head, stainless steel
Process stream in shell
Q = 19,150 MJ/h
Design pressure = 4100 kPa

E-606
A = 11.7 m^2
1-2 exchanger, floating head, stainless steel
Process stream in shell
Q = 3050 MJ/h
Design pressure = 300 kPa

E-607
A = 192 m^2
1-2 exchanger, floating head, stainless steel
Molten salt in tubes
Q = 55,600 MJ/h
Design pressure = 4100 kPa

Pumps

P-601 A/B
Centrifugal/electric drive
Carbon steel
Power = 0.3 kW (actual)
65% efficient
Design pressure = 300 kPa

P-602 A/B
Centrifugal/electric drive
Stainless steel
Power = 3.8 kW (actual)
65% efficient
Design pressure = 300 kPa

P-603 A/B
Reciprocating/electric drive
Stainless steel
Power = 0.1 kW (actual)
65% efficient
Design pressure = 200 kPa

P-604 A/B
Centrifugal/electric drive
Stainless steel
Power = 6.75 kW (actual)
65% efficient
Design pressure = 200 kPa

P-605 A/B
Centrifugal/electric drive
Stainless steel
Power = 0.7 kW (actual)
65% efficient
Design pressure = 400 kPa

P-606 A/B
Centrifugal/electric drive
Stainless steel
Power = 2.4 kW (actual)
65% efficient
Design pressure = 150 kPa

Reactor

R-601
Shell-and-tube vertical design
Stainless steel
L = 7.0 m
D = 3.8 m
12,100 1-in diameter, 6.4 m length catalyst-filled tubes
Design pressure = 300 kPa

Towers

T-601
Stainless steel
14 sieve trays plus reboiler and condenser
50% efficient trays
Partial condenser
Feeds on trays 1 and 14
Reflux ratio = 0.189
24-in tray spacing, 2.2-in weirs
Column height = 10 m
Diameter = 4.2 m
Design pressure = 110 kPa

T-602
Stainless steel
42 sieve trays plus reboiler and condenser
65% efficient trays
Total condenser
Feed on tray 27
Reflux ratio = 1.24
15-in tray spacing, 1.5-in weirs
Column height = 18 m
Diameter = 1.05 m
Design pressure = 110 kPa

Vessels

V-601
Horizontal
Carbon steel
L = 3.50 m
D = 1.17 m
Design pressure = 110 kPa

V-602
Horizontal
Stainless steel
L = 13.2 m
D = 4.4 m
Design pressure = 110 kPa

V-603
Horizontal
Stainless steel
L = 3.90 m
D = 1.30 m
Design pressure = 110 kPa

B.5.2 Reaction Kinetics

The reactions and reaction kinetics [3] given in Equations (B.5.1)–(B.5.4) are given by the expression

$$-r_i = k_i C_{benzene} \text{ or } -r_3 = k_3 C_{maleic\ anhydride} \quad \text{(B.5.5)}$$

where

$$k_1 = 7.7 \times 10^6 \exp(-25{,}143/RT) \quad \text{(B.5.6)}$$
$$k_2 = 6.31 \times 10^7 \exp(-29{,}850/RT) \quad \text{(B.5.7)}$$
$$k_3 = 2.33 \times 10^4 \exp(-21{,}429/RT) \quad \text{(B.5.8)}$$
$$k_4 = 7.20 \times 10^5 \exp(-27{,}149/RT) \quad \text{(B.5.9)}$$

The units of reaction rate, r_i, are kmol/m^3(reactor)s, the activation energy is given in cal/mol (which is equivalent to kcal/kmol), the units of k_i are m^3(gas)/m^3 (reactor)s, and the units of concentration are kmol/m^3(gas).

The catalyst is a mixture of vanadium and molybdenum oxides on an inert support. Typical inlet reaction temperatures are in the range of 350°C to 400°C. The catalyst is placed in 25 mm diameter tubes that are 3.2 m long. The catalyst pellet diameter is 5 mm. The maximum temperature that the catalyst can be exposed to without causing irreversible damage (sintering) is 650°C. The packed-bed reactor should be costed as a shell-and-tube exchanger. The heat transfer area should be calculated based on the total external area of the catalyst-filled tubes required from the simulation. Because of the high temperatures involved, both the shell and the tube material should be stainless steel. An overall heat transfer coefficient for the reactor should be set as 100 W/m^2°C. (This is the value specified in the simulation.)

B.5.3 Simulation (CHEMCAD) Hints

The CHEMCAD simulation used to generate the PFD shown in Figure B.5.1 has several simplifications that are valid for this system. The removal of trace amounts of noncondensables is achieved after the absorber using a component separator, which avoids problems with column convergence downstream. The formation of maleic acid is simulated by using a stoichiometric reactor and setting the conversion of water to 1.

Tower T-601, the maleic anhydride scrubber, is simulated using the rigorous tower simulator. Tower T-602, the dibutyl phthalate tower, is simulated using the Shortcut column module. Currently, there is

no experimental vapor pressure data for the components in this simulation. It appears that the vapor pressures of the components differ widely, and no azeotropes are known at this time. For this reason, the ideal vapor pressure *K*-value option and the latent heat enthalpy option are used.

In order to simulate the temperature spike in the reactor, the reactor is simulated as a cocurrent, packed-bed kinetic reactor, with a molten salt stream as the utility. This configuration provides a greater temperature differential at the front end of the reactor, where the reaction rate is highest. Countercurrent flow could be investigated as an alternative. The kinetics given above are used in the simulation. Dimensions of the reactor tubes are given in Section B.5.2.

B.5.4 References

1. Felthouse, T. R., J. C. Burnett, B. Horrell, M. J. Mummey, and Y-J Kuo, "Maleic Anhydride, Maleic Acid, and Fumaric Acid," *Kirk-Othmer Encyclopedia of Chemical Technology*, online version (New York: John Wiley and Sons, 2001).
2. "Maleic Acid and Anhydride," *Encyclopedia of Chemical Processing and Design*, Vol. 29, ed. J. J. McKetta (New York: Marcel Dekker, 1984), 35–55.
3. Wohlfahrt, Emig G., "Compare Maleic Anhydride Routes," *Hydrocarbon Processing*, June 1980, 83–90.

B.6. Ethylene Oxide Production, Unit 700

Ethylene oxide is a chemical used to make ethylene glycol (the primary ingredient in antifreeze). It is also used to make polyethylene oxide, and both the low-molecular-weight and high-molecular-weight polymers have many applications including as detergent additives. Because ethylene oxide is so reactive, it has many other uses as a reactant. However, because of its reactivity, danger of explosion, and toxicity, it is rarely shipped outside the manufacturing facility but instead is often pumped directly to a nearby consumer.

B.6.1 Process Description [1, 2]

The process flow diagram is shown in Figure B.6.1. Ethylene feed (via pipeline from a neighboring plant) is mixed with recycled ethylene and mixed with compressed and dried air (drying step not shown), heated, and then fed to the first reactor. The reaction is exothermic, and medium-pressure steam is made in the reactor shell. Conversion in the reactor is kept low to enhance selectivity for the desired product. The reactor effluent is cooled, compressed, and sent to a scrubber, where ethylene oxide is absorbed by water. The vapor from the scrubber is heated, throttled, and sent to a second reactor, followed by a second series of cooling, compression, and scrubbing. A fraction of the unreacted vapor stream is purged, with the remainder recycled to recover unreacted ethylene. The combined aqueous product streams are mixed, cooled, throttled, and distilled to produce the desired product. The required purity specification is 99.5 wt% ethylene oxide.

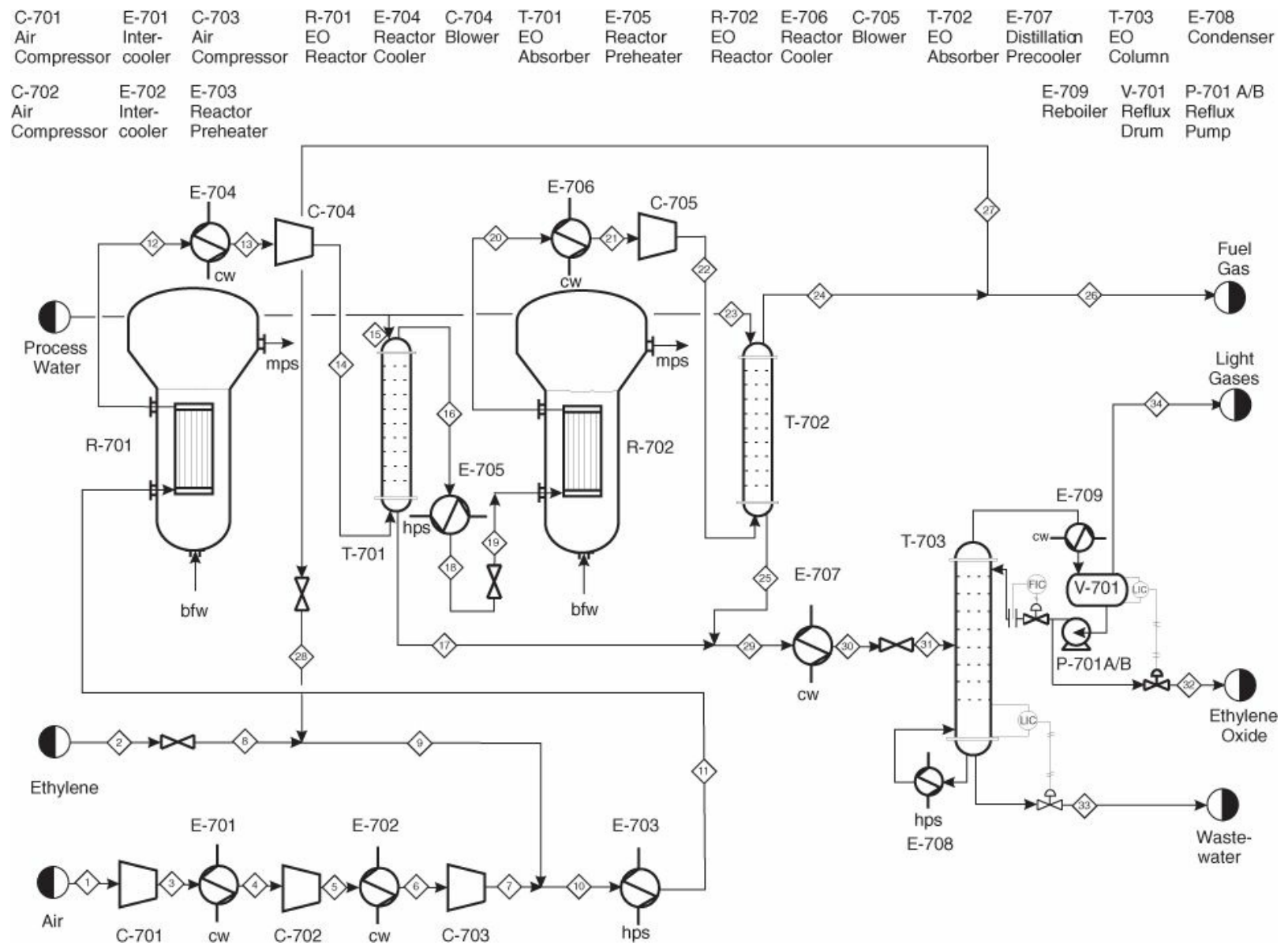


Figure B.6.1. Unit 700: Ethylene Oxide Process Flow Diagram

Table B.6.1. Stream Table for Unit 700

Stream Number	1	2	3	4
Temperature (°C)	25.0	25.0	159.2	45.0
Pressure (bar)	1.0	50.0	3.0	2.7
Vapor mole fraction	1.00	1.00	1.00	1.00
Flowrate (kg/h)	500,000	20,000	500,000	500,000
Flowrate (kmol/h)	17,381.45	712.91	17,381.45	17,381.45
Component flowrates (kmol/h)				
Ethylene	0.0	712.91	0.0	0.0
Ethylene oxide	0.0	0.0	0.0	0.0
Carbon dioxide	0.0	0.0	0.0	0.0
Oxygen	3281.35	0.0	3281.35	3281.35
Nitrogen	14,100.09	0.0	14,100.09	14,100.09
Water	0.0	0.0	0.0	0.0

Stream Number	5	6	7	8
Temperature (°C)	206.1	45.0	195.2	–6.3
Pressure (bar)	9.0	8.7	27.0	27.0
Vapor mole fraction	1.00	1.00	1.00	1.00
Flowrate (kg/h)	500,000	500,000	500,000	20,000
Flowrate (kmol/h)	17,381.45	17,381.45	17,381.45	712.91

Component flowrates (kmol/h)				
Ethylene	0.0	0.0	0.0	712.91
Ethylene oxide	0.0	0.0	0.0	0.0
Carbon dioxide	0.0	0.0	0.0	0.0
Oxygen	3281.35	3281.35	3281.35	0.0
Nitrogen	14,100.09	14,100.09	14,100.09	0.0
Water	0.0	0.0	0.0	0.0
Stream Number	**9**	**10**	**11**	**12**
Temperature (°C)	26.3	106.7	240.0	240.0
Pressure (bar)	27.0	26.8	26.5	25.8
Vapor mole fraction	1.00	1.00	1.00	1.00
Flowrate (kg/h)	524,042	1,023,980	1,023,980	1,023,979
Flowrate (kmol/h)	18,260.29	35,639.59	35,639.59	35,539.42
Component flowrates (kmol/h)				
Ethylene	1047.95	1047.91	1047.91	838.67
Ethylene oxide	6.48	6.47	6.47	206.79
Carbon dioxide	31.71	31.71	31.71	49.56
Oxygen	3050.14	6331.12	6331.12	6204.19
Nitrogen	14,093.02	28,191.39	28,191.39	28,191.39
Water	30.99	30.98	30.98	48.82

Stream Number	13	14	15	16
Temperature (°C)	45.0	63.7	25.0	30.3
Pressure (bar)	25.5	30.2	30.0	30.0
Vapor mole fraction	1.00	1.00	0.00	1.00
Flowrate (kg/h)	1,023,980	1,023,980	360,300	1,015,669
Flowrate (kmol/h)	35,539	35,539	20,000	35,358
Component flowrates (kmol/h)				
Ethylene	838.67	838.67	0.0	837.96
Ethylene oxide	206.79	206.79	0.0	15.45
Carbon dioxide	49.56	49.56	0.0	49.56
Oxygen	6204.19	6204.19	0.0	6202.74
Nitrogen	28,191.39	28,191.39	0.0	28,188.72
Water	48.82	48.82	20,000	63.24

Stream Number	17	18	19	20
Temperature (°C)	51.9	240.0	239.9	240.0
Pressure (bar)	30.0	29.7	26.5	25.8
Vapor mole fraction	0.00	1.00	1.00	1.00
Flowrate (kg/h)	368,611	1,015,669	1,015,669	1,015,669
Flowrate (kmol/h)	20,181.77	35,357.65	35357.66	35,277.47
Component flowrates (kmol/h)				
Ethylene	0.70	837.96	837.96	670.64
Ethylene oxide	191.34	15.45	15.45	175.83
Carbon dioxide	0.01	49.55	49.55	63.44
Oxygen	1.45	6202.74	6202.74	6101.72
Nitrogen	2.68	28,188.72	28,188.72	28,188.72
Water	19,985.58	63.24	63.24	77.13

Stream Number	21	22	23	24
Temperature (°C)	45.0	63.8	25.0	30.1
Pressure (bar)	25.5	30.2	30.0	30.0
Vapor mole fraction	1.00	1.00	0.00	1.00
Total kg/h	1,015,669	1,015,669	60,300	1,008,084
Total kmol/h	35,277.47	35,277.47	20,000	35094.76
Component Flowrates (kmol/h)				
Ethylene	670.64	670.64	0.0	670.08
Ethylene oxide	175.83	175.83	0.0	12.96
Carbon dioxide	63.44	63.44	0.0	63.43
Oxygen	6101.72	6101.72	0.0	6100.28
Nitrogen	28,188.72	28,188.72	0.0	28,186.04
Water	77.13	77.13	20,000	61.96

Stream Number	25	26	27	28
Temperature (°C)	52.3	30.1	30.1	29.5
Pressure (bar)	30.0	30.0	30.0	27.0
Vapor mole fraction	0.00	1.00	1.00	1.00
Flowrate (kg/h)	367,885	504,042	504,042	504,042
Flowrate (kmol/h)	20,182.72	17,547.38	17,547.38	17,547.38
Component flowrates (kmol/h)				
Ethylene	0.57	335.04	335.04	335.04
Ethylene oxide	162.88	6.48	6.48	6.48
Carbon dioxide	0.01	31.71	31.71	31.71
Oxygen	1.43	3050.14	3050.14	3050.14
Nitrogen	2.68	14,093.02	14,093.02	14,093.02
Water	20,015.15	30.99	30.99	30.99

Stream Number	29	30	31	32
Temperature (°C)	52.1	45.0	45.0	86.4
Pressure (bar)	30.0	29.7	10.0	10.0
Vapor mole fraction	0.00	0.00	0.00	0.00
Flowrate (kg/h)	736,497	736,497	736,218	15,514
Flowrate (kmol/h)	40,364.48	40,364.48	40,354.95	352.39
Component flowrates (kmol/h)				
Ethylene	1.27	1.27	1.27	0.0
Ethylene oxide	354.22	354.22	354.22	352.04
Carbon dioxide	0.02	0.02	0.02	0.0
Oxygen	2.89	2.89	2.89	0.0
Nitrogen	5.35	5.35	5.35	0.0
Water	40,000.74	40,000.74	40,000.74	0.35

Stream Number	33	34
Temperature (°C)	182.3	86.4
Pressure (bar)	10.5	10.0
Vapor mole fraction	0.00	1.00
Flowrate (kg/h)	720,703	278.78
Flowrate (kmol/h)	40,002.57	9.53
Component flowrates (kmol/h)		
Ethylene	0.0	1.27
Ethylene oxide	2.18	0.0
Carbon dioxide	0.0	0.02
Oxygen	0.0	2.88
Nitrogen	0.0	5.35
Water	40,000.39	0.0

Table B.6.2 Utility Summary Table for Unit 700

E-701	E-702	E-703	E-704
cw 1,397,870 kg/h	cw 1,988,578 kg/h	hps 87,162 kg/h	cw 5,009,727 kg/h
E-705	**E-706**	**E-707**	**E-708**
hps 135,789 kg/h	cw 4,950,860 kg/h	cw 513,697 kg/h	hps 258,975 kg/h
E-709	**R-701**	**R-702**	
cw 29,609 kg/h	bfw→mps 13,673 kg/h	bfw→mps 10,813 kg/h	

Table B.6.3. Major Equipment Summary for Unit 700

Compressors*

C-701
Carbon steel
Centrifugal
Power = 19 MW
80% adiabatic efficiency

C-702
Carbon steel
Centrifugal
Power = 23 MW
80% adiabatic efficiency

C-703
Carbon steel
Centrifugal
Power = 21.5 MW
80% adiabatic efficiency

C-704
Carbon steel
Centrifugal
Power = 5.5 MW
80% adiabatic efficiency

C-705
Carbon steel
Centrifugal
Power = 5.5 MW
80% adiabatic efficiency

*Note that all compressors have electric-explosion-proof drives with a backup. These units are designated D-701 A/B through D-705 A/B but are not shown on the PFD.

Heat Exchangers

E-701
A = 5553 m^2
1-2 exchanger, floating head, carbon steel
Process stream in tubes
Q = 58,487 MJ/h

E-706
A = 13,945 m^2
1-2 exchanger, floating head, carbon steel
Process stream in tubes
Q = 207,144 MJ/h

E-702
$A = 6255\ m^2$
1-2 exchanger, floating head, carbon steel
Process stream in tubes
$Q = 83{,}202$ MJ/h

E-703
$A = 12{,}062\ m^2$
1-2 exchanger, floating head, carbon steel
Process stream in tubes
$Q = 147{,}566$ MJ/h

E-704
$A = 14{,}110\ m^2$
1-2 exchanger, floating head, carbon steel
Process stream in tubes
$Q = 209{,}607$ MJ/h

E-705
$A = 14{,}052\ m^2$
1-2 exchanger, floating head, carbon steel
Process stream in tubes
$Q = 229{,}890$ MJ/h

E-707
$A = 1478\ m^2$
1-2 exchanger, floating head, carbon steel
Process stream in tubes
$Q = 21{,}493$ MJ/h

E-708
$A = 566\ m^2$
1-2 exchanger, floating head, stainless steel
Process stream condenses in shell
$Q = 43{,}844$ MJ/h

E-709
$A = 154\ m^2$
1-2 exchanger, floating head, stainless steel
Process stream boils in shell
$Q = 14{,}212$ MJ/h

Pump
P-701 A/B
Centrifugal/electric drive
Stainless steel
Power = 4 kW (actual)
75% efficient

Reactors
R-701
Carbon steel, shell-and-tube packed bed
Spherical catalyst pellet, 9 mm diameter
Void fraction = 0.4

R-702
Carbon steel, shell-and-tube packed bed
Spherical catalyst pellet, 9 mm diameter
Void fraction = 0.4

$V = 202\ m^3$ 10 m tall, 7.38 cm diameter tubes 4722 tubes 100% filled with active catalyst $Q = 33{,}101$ MJ/h mps made in shell	$V = 202\ m^3$ 10 m tall, 9.33 cm diameter tubes 2954 tubes 100% filled with active catalyst $Q = 26{,}179$ MJ/h mps made in shell
Towers	
T-701 Carbon steel 20 SS sieve trays 25% efficient trays Feeds on trays 1 and 20 24-in tray spacing, 3-in weirs Column height = 12.2 m Diameter = 5.6 m **T-702** Carbon steel 20 SS sieve trays 25% efficient trays Feeds on trays 1 and 20 24-in tray spacing, 3-in weirs Column height = 12.2 m Diameter = 5.6 m	**T-703** Stainless steel 70 SS sieve trays plus reboiler and condenser 33% efficient trays Total condenser (E-709) Feed on tray 36 Reflux ratio = 0.89 12-in tray spacing, 3-in weirs Column height = 43 m Diameter = 8.0 m
Vessel **V-701** Stainless steel Horizontal L/D = 3.0 $V = 12.7\ m^3$	

Stream summary tables, utility summary tables, and major equipment specifications are shown in Tables B.6.1–B.6.3.

B.6.2 Reaction Kinetics

The pertinent reactions (adapted from Stoukides and Pavlou [3]) are as follows:

$$C_2H_4 + 0.5\,O_2 \rightarrow C_2H_4O \quad \text{(B.6.1)}$$

$$C_2H_4 + 3\,O_2 \rightarrow 2CO_2 + 2H_2O \quad \text{(B.6.2)}$$

$$C_2H_4O + 2.5\,O_2 \rightarrow 2CO_2 + 2H_2O \quad \text{(B.6.3)}$$

The kinetic expressions are, respectively,

$$r_1 = \frac{1.96\exp(-2400/RT)p_{ethylene}}{1 + 0.00098\exp(11{,}200/RT)p_{ethylene}} \quad \text{(B.6.4)}$$

$$r_2 = \frac{0.0936\exp(-6400/RT)p_{ethylene}}{1 + 0.00098\exp(11{,}200/RT)p_{ethylene}} \quad \text{(B.6.5)}$$

$$r_3 = \frac{0.42768\exp(-6200/RT)p^2_{ethylene\ oxide}}{1 + 0.000033\exp(21{,}200/RT)p^2_{ethylene\ oxide}} \quad \text{(B.6.6)}$$

The units for the reaction rates are moles/m^3 s. The pressure unit is bar. The activation energy

numerator is in cal/mol. The catalyst used for this reaction is silver on an inert support. The support consists of 7.5 mm diameter spheres that have a bulk density of 1250 kg/m^3 and a void fraction of 0.4.

B.6.3 Simulation (CHEMCAD) Hints

The following thermodynamics packages are strongly recommended for simulation of this process.

- ***K-values:*** Use a global model of PSRK but use UNIFAC as a local model for T-701 and T-702.
- **Enthalpy:** Use SRK.

B.6.4 References

1. Dever, J. P., K. F. George, W. C. Hoffman, and H. Soo, "Ethylene Oxide," *Kirk-Othmer Encyclopedia of Chemical Technology*, online version (New York: John Wiley and Sons, 2004).
2. "Ethylene Oxide," *Encyclopedia of Chemical Processing and Design*, Vol. 20, ed. J. J. McKetta (New York: Marcel Dekker, 1984), 274 –318.
3. Stoukides, M., and S. Pavlou, "Ethylene Oxidation on Silver Catalysts: Effect of Ethylene Oxide and of External Transfer Limitations," *Chem. Eng. Commun*. 44 (1986): 53–74.

B.7. Formalin Production, Unit 800

Formalin is a 37 wt% solution of formaldehyde in water. Formaldehyde and urea are used to make urea-formaldehyde resins that subsequently are used as adhesives and binders for particle board and plywood.

B.7.1 Process Description [1, 2]

Unit 800 produces formalin (37 wt% formaldehyde in water) from methanol using the silver catalyst process. Figure B.7.1 illustrates the process.

Air is compressed and preheated, fresh and recycled methanol is pumped and preheated, and these two streams are mixed to provide reactor feed. The feed mixture is about 39 mol% methanol in air, which is greater than the upper flammability limit for methanol. (For methanol, UFL = 36 mol%; LFL = 6 mol%.) In the reactor, the following two reactions occur:

$$CH_3OH + \frac{1}{2}O_2 \rightarrow HCHO + H_2O \qquad \Delta H_{rxn} = -37.3 \text{ kcal/mole} \qquad \text{(B.7.1)}$$

methanol — formaldehyde

$$CH_3OH \rightarrow HCHO + H_2 \qquad \Delta H_{rxn} = 20.3 \text{ kcal/mole} \qquad \text{(B.7.2)}$$

methanol — formaldehyde

The reactor is a unique configuration, in which the silver catalyst is in the form of wire gauze, suspended above a heat exchanger tube bank. Because the net reaction is very exothermic, the heat generated in the adiabatic reactor section must be removed quickly, hence the close proximity of the heat-exchanger tubes. The heat exchanger resembles a pool boiler, with a pool of water on the shell side. If the temperature of the effluent is too high, the set point on the steam pressure line is lowered to increase the vaporization of boiler feed water (bfw). In general, the liquid-level controller on the bfw is adjusted to keep the tube bundle fully immersed. The reactor effluent enters an absorber in which most of the methanol and formaldehyde are absorbed into water, with most of the remaining light gases purged into the off-gas stream. The methanol, formaldehyde, and water enter a distillation

column, in which the methanol overhead is recycled; the bottoms product is a formaldehyde/water mixture that contains ≤ 1wt% methanol as an inhibitor. This mixture is cooled and sent to a storage tank, which is sized at four days' capacity. This storage tank is essential, because some of the downstream processes are batch. The composition in the storage tank exceeds 37 wt% formaldehyde, so the appropriate amount of water is added when the downstream process draws from the storage tank. This is not shown in the PFD (Figure B.7.1).

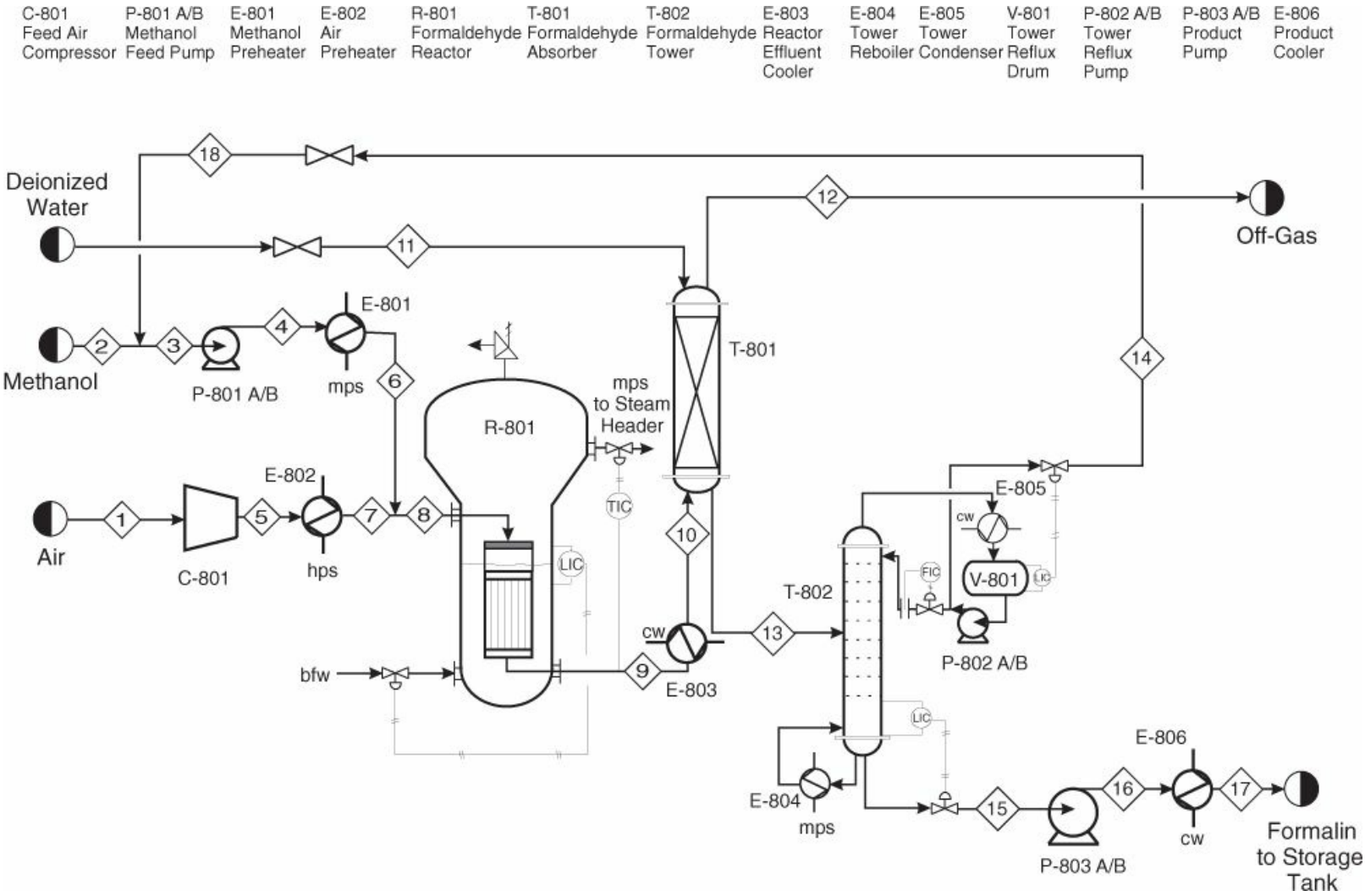


Figure B.7.1. Unit 800: Formalin Process Flow Diagram

Storage of formaldehyde/water mixtures is tricky. At high temperatures, undesirable polymerization of formaldehyde is inhibited, but formic acid formation is favored. At low temperatures, acid formation is inhibited, but polymerization is favored. There are stabilizers that inhibit polymerization, but they are incompatible with resin formation. Methanol, at concentrations between 5 wt% and 15 wt%, can also inhibit polymerizaton, but no separation equipment for methanol currently exists on site, and methanol greater than 1 wt% also causes defective resin production. With ≤1 wt% methanol, the storage tank contents must be maintained between 35°C and 45°C.

Stream summary tables, utility summary tables, and major equipment specifications are shown in Tables B.7.1–B.7.3.

B.7.2 Reaction Kinetics

Due to the very high temperature and large surface area of the wire gauze, the reaction may be considered to be instantaneous.

B.7.3 Simulation (CHEMCAD) Hints

Solutions of formaldehyde and water are very nonideal. Individually, the volatilities are, from most volatile to least volatile, formaldehyde, methanol, and water. However, formaldehyde associates with water so that when this three-component mixture is distilled, methanol is the light key and water is the heavy key. The formaldehyde will "follow" the water. The ESDK *K*-value package in CHEMCAD simulates this appropriately and was used for the simulation presented here. Latent heat should be used for enthalpy calculations. The expert system will recommend these choices. Alternatively, the data provided in Table B.7.4 can be used directly or to fit an appropriate nonideal VLE model.

Table B.7.1. Stream Table for Unit 800

Stream Number	1	2	3	4	5	6
Temperature (°C)	25.0	30.0	40.7	40.8	183.0	150.0
Pressure (kPa)	101.3	120.0	101.3	300.0	300.0	265.0
Vapor fraction	1.0	0.0	0.0	0.00	1.0	1.0
Total kg/h	4210.54	2464.8	3120.3	3120.3	4210.5	3120.3
Total kmol/h	145.94	76.92	99.92	99.92	145.94	99.92
Component flowrates (kmol/h)						
Methanol	0.0	76.92	94.11	94.11	0.0	94.12
Oxygen	30.66	0.0	0.0	0.0	30.66	0.0
Formaldehyde	0.0	0.0	0.0	0.0	0.0	0.0
Water	0.0	0.0	5.81	5.81	0.0	5.81
Hydrogen	0.0	0.0	0.0	0.0	0.0	0.0
Nitrogen	115.28	0.0	0.0	0.0	115.28	0.0
Stream Number	**7**	**8**	**9**	**10**	**11**	**12**
Temperature (°C)	200.0	171.9	200.0	100.0	30.0	84.6
Pressure (kPa)	265.0	255.0	185.0	150.0	150.0	140.0
Vapor fraction	1.0	1.0	1.0	1.0	0.0	1.0
Total kmol/h	4210.5	7330.8	7330.8	7330.8	2576.2	5354.2
Total kg/h	145.94	245.86	278.03	278.03	143.00	224.16
Component flowrates (kmol/h)						
Methanol	0.0	94.12	31.45	31.45	0.0	13.35
Oxygen	30.66	30.66	0.15	0.15	0.0	0.15
Formaldehyde	0.0	0.0	62.67	62.67	0.0	0.04
Water	0.0	5.81	66.82	66.82	143.00	93.68
Hydrogen	0.0	0.0	1.66	1.66	0.0	1.66
Nitrogen	115.28	115.28	115.28	115.28	0.0	115.28

Stream Number	13	14	15	16	17	18
Temperature (°C)	89.9	75.5	106.6	106.7	35.0	73.4
Pressure (kPa)	150.0	130.00	150.00	350.00	315.00	120.00
Vapor mole fraction	0.0	0.0	0.0	0.0	0.0	0.0
Total kg/h	4552.8	655.6	3897.1	3897.1	3897.1	655.6
Total kmol/h	196.87	23.00	173.86	173.86	173.86	23.00
Component flowrates (kmol/h)						
Methanol	18.10	17.19	0.90	0.90	0.90	17.19
Oxygen	0.00	0.00	0.00	0.00	0.00	0.00
Formaldehyde	62.63	0.00	62.63	62.63	62.63	0.00
Water	116.14	5.81	110.33	110.33	110.33	5.81
Hydrogen	0.00	0.00	0.00	0.00	0.00	0.00
Nitrogen	0.00	0.00	0.00	0.00	0.00	0.00

Table B.7.2. Utility Summary Table for Unit 800

E-801	E-802	E-803	E-804
mps 2063 kg/h	hps 45.43 kg/h	cw 23,500 kg/h	mps 18,949 kg/h
E-805	**E-806**	**R-801**	
cw 775,717 kg/h	cw 27,957 kg/h	bfw → mps 3723 kg/h	

Table B.7.3. Major Equipment Summary for Unit 800

Compressor

C-801
Carbon steel
Centrifugal
Power = 183 kW (shaft)
70% efficient

D-801 A/B (not shown on PFD)
Electric/explosion proof
W = 195 kW
95% efficient

Heat Exchangers

E-801
A = 405 m^2
1-2 exchanger, floating head, carbon steel
Process stream in shell
Q = 4111 MJ/h
Maximum pressure rating of 350 kPa

E-802
A = 4.62 m^2
1-2 exchanger, floating head, carbon steel
Process stream in tubes
Q = 76.75 MJ/h
Maximum pressure rating of 350 kPa

E-803
A = 28.16 m^2
1-2 exchanger, floating head, carbon steel
Process stream in shell
Q = 983.23 MJ/h
Maximum pressure rating of 350 kPa

E-804
A = 37.3 m^2
1-2 exchanger, kettle reboiler, stainless steel
Process stream in shell
Q = 37,755 MJ/h
Maximum pressure rating of 250 kPa

E-805
A = 269 m^2
1-2 exchanger, floating head, stainless steel
Process stream in shell
Q = 32,456 MJ/h
Maximum pressure rating of 250 kPa

E-806
A = 41 m^2
1-2 exchanger, floating head, stainless steel
Process stream in tubes
Q = 1169.7 MJ/h
Maximum pressure rating of 400 kPa

Reactors

R-801, Heat-Exchanger Portion
A = 140.44 m^2
Counterflow exchanger, floating head, carbon steel
Process stream in tubes
Q = 8928 MJ/h
Maximum pressure rating of 350 kPa

R-801, Reactor Portion
Thin layers of silver wire gauze suspended above heat exchanger tube bank

Reactors

R-801, Heat-Exchanger Portion
$A = 140.44\ m^2$
Counterflow exchanger, floating head, carbon steel
Process stream in tubes
$Q = 8928$ MJ/h
Maximum pressure rating of 350 kPa

R-801, Reactor Portion
Thin layers of silver wire gauze suspended above heat exchanger tube bank

Pumps

P-801 A/B
Centrifugal/electric drive
Carbon steel
Power = 0.3 kW
80% efficient

P-802 A/B
Centrifugal/electric drive
Carbon steel
Power = 1.7 kW
80% efficient

P-803 A/B
Centrifugal/electric drive
Stainless steel
Power = 0.5 kW
75% efficient

Towers

T-801
Carbon steel
10 m of packing
2-in ceramic Berl Saddles
20 theoretical stages
1.00 kPa/m pressure drop
Diameter = 0.86 m
Packing factor = 45
Maximum pressure rating of 300 kPa

T-802
Stainless steel
31 SS sieve trays plus reboiler and partial condenser
70% efficient trays
Feed on tray 18
Reflux ratio = 37.34
0.6096 m tray spacing, 0.091 m weirs
Column height = 19 m
Diameter = 2.5 m
Maximum pressure rating of 200 kPa

Vessel

V-801
Horizontal
Stainless steel
L/D = 4.0
Volume = $4.2\ m^3$

When simulating an entire process, it is recommended to first use the Shortcut distillation column within the process for the methanol-water/formaldehyde distillation. A rigorous column solver should then be used as a separate item to simulate the column based on the results obtained from the Shortcut column. However, due to the nonideality of the thermodynamics, the actual column simulation using the rigorous column will probably require many more stages than predicted by the shortcut simulation, possibly twice the number. Once the parameters for the rigorous column have been established, the Shortcut column can be replaced by the rigorous column and the simulation rerun to get a converged simulation.

Table B.7.4. *K*-values for Formaldehyde/Water/Methanol System [3]

P(psia) =14.696	Chemical Component		
T (°C)	Formaldehyde	Water	Methanol
0.1	0.123	1.000	0.273
67.1	0.266	0.491	1.094
72.1	0.336	0.394	1.435
74.8	0.374	0.453	1.598
84.6	0.546	0.607	2.559
97.6	0.693	1.105	2.589
99.9	0.730	1.198	2.595
150.1	1.220	2.460	3.004

B.7.4 References

1. Gerberich, H. R., and G. C. Seaman, "Formaldehyde," *Kirk-Othmer Encyclopedia of Chemical Technology*, online version (New York: John Wiley and Sons, 2004).
2. "Formaldehyde," *Encyclopedia of Chemical Processing and Design*, Vol. 23, ed. J. J. McKetta (New York: Marcel Dekker, 1984), 350–371.
3. Gmehling, J., U. Onken, and W. Arlt, *Vapor-Liquid Equilibrium Data Collection*, Chemistry Data Series (Aqueous-Organic Systems, Supplement 1), Vol. 1, Part 1a, DECHEMA, 1981, 474–475.

B.8. Batch Production Of L-Phenylalanine And L-Aspartic Acid, Unit 900

Phenlyalanine and L-aspartic acid are amino acids. When they bond together, the corresponding di-peptide methyl ester is aspartame, known by the brand name NutraSweet or Equal. Production of both amino acids can be accomplished via fermentation of genetically altered bacteria. Production rates of 1000 and 1250 tonnes/y of L-aspartic acid and L-phenylalanine are desired.

B.8.1 Process Description

To accomplish a fermentation process, bacteria must grow in the presence of appropriate nutrients that facilitate the production of the desired product. In a processing context, the fermentation reactor must first be primed with the bacteria and the nutrients. The nutrient feed includes the reactant that the bacteria metabolize to produce the desired amino acid. Air is also sparged into the fermenter as a source of oxygen. All of these feeds are passed through sterilization filters prior to entering the reactor. The bacteria are then allowed to multiply, and the desired product, an amino acid in this case, is produced. In this process, both products are extracellular. After the desired production level of the amino acid is reached, the fermentation broth pH is lowered by addition of sulfuric acid, the bacteria are removed from the fermentation broth by filtration, and the product stream is sent to a holding tank. The addition of acid titrates the amino acid, making it positively charged. The addition of acid is done only for phenylalanine, because L-aspartic acid bypasses the ion exchange column and is crystallized directly via precipitation from solution.

In this process, both amino acids are produced in the same facility. Because fermentation is involved and production levels are low compared with typical commodity chemicals, batch processes are involved. In batch processes, the key variable is the batch time, or the length of time that the unit is

allowed to run. For example, in a batch reactor, the batch time is analogous to the space time in a continuous reactor.

The separation sequence is a continuous process, which is accomplished by a continuous feed from the holding tank. This is not uncommon in batch facilities, because many separation processes are more easily accomplished in the continuous mode. The separation sequence for the two amino acids differs slightly. Phenylalanine is isolated using ion exchange followed by crystallization; in contrast, L-aspartic acid is crystallized directly from the filtered fermentation broth. For phenylalanine, it is adsorbed on the ion exchange resin and subsequently eluted using a basic solution. The addition of base neutralizes the positive charge to promote desorption from the ion exchange resin. For both amino acids, filtration follows crystallization. The product is then sent to storage. The process is shown in Figure B.8.1.

The use of batch processing requires batch scheduling of the type discussed in Chapter 3, which allows use of the same equipment to manufacture both amino acids in the same facility. In this description, only the PFD, reactor calculations, and general descriptions of the separation units are presented. The design of individual equipment, the utility consumption, and the production schedule for the plant are left as exercises for the student. A description of a process to produce four amino acids (including the two amino acids in this process) in the same facility is available at http://www.che.cemr.wvu.edu/publications/projects/large_proj/batch-production_of_amino_acids.pdf. This process description includes possible batch schedules for both the reactors and the separation section.

B.8.2 Reaction Kinetics

L-Aspartic Acid. The reaction of fumaric acid to form L-aspartic acid is an enzymatic conversion carried out using the aspartase activity of bacteria *Escherichia coli (E. coli)* cells according to the following reaction:

$$\underset{\text{fumaric acid}}{C_4H_4O_4} + NH_3 \overset{\text{aspartase}}{\rightleftharpoons} \underset{\text{L-aspartic acid}}{C_4H_7NO_4} \qquad \text{(B.8.1)}$$

The bacteria cells are suspended in a matrix polyacrylamide gel, and the reacting species must diffuse in and out of the matrix. The diffusivities of the substrate (fumaric acid) and product (L-aspartic acid) in the gel decrease as their concentrations increase due to the tendency of the gel to shrink at low pH.

The kinetic model for this reaction follows a Michaelis-Menten form for a reversible reaction, which rearranges to

$$\frac{1}{V_a} = \frac{1}{V_{a,\max}} + \frac{K_{a,M}}{V_{a,\max}\left[C_{FA} - \dfrac{C_{AA}}{KC_{NH_4^+}}\right]} \qquad \text{(B.8.2)}$$

where

C_{FA} is the concentration of fumaric acid (kmol/m^3).

C_{AA} is the concentration of L-aspartic acid (kmol/m^3).

$C_{NH_4^+}$ is the concentration of ammonium ions (kmol/m^3).

K is a reaction equilibrium constant (m^3/kmol).

V_a is the apparent rate of production of L-aspartic acid (kmol/h/kg-gel).

$V_{a,\max}$ is the apparent maximum rate of production of L-aspartic acid (kmol/h/kg-gel).

$K_{a,M}$ is the apparent Michaelis constant for the reaction (kmol/m^3).

Reaction rate parameters have been modified from reference [1] and are used for the current process using a 1.0 M substrate solution at a reaction temperature of 32°C.

$$K_{a,M} = 0.68C_{FA,0}^{1.04}$$

$$V_{a,\max} = \frac{C_{FA,0}^{0.77}}{150}$$

$$K = 88.7 \text{ m}^3/\text{kmol at } 32°\text{C}$$

$$C_{NH_4^+} = 2.04C_{FA}$$

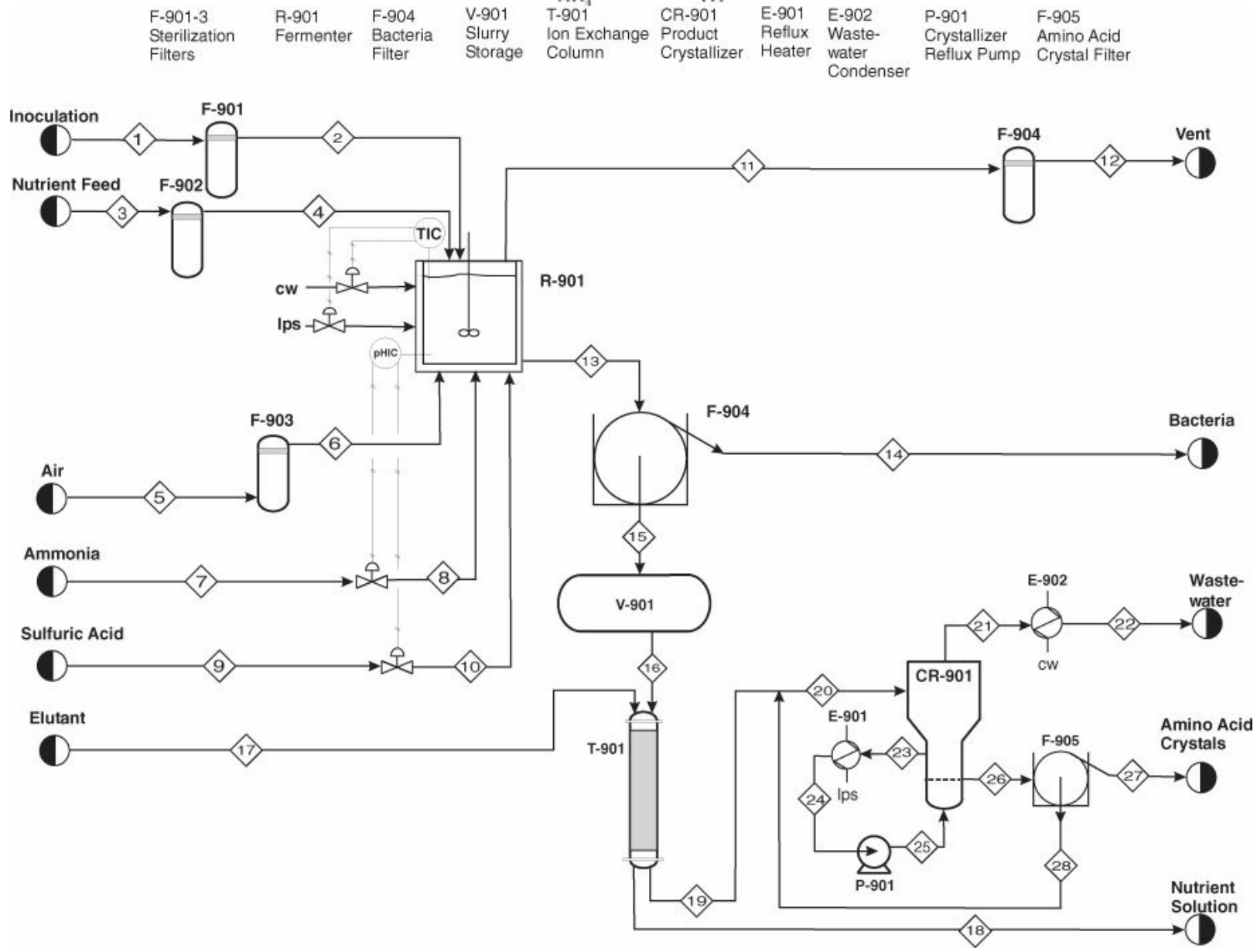


Figure B.8.1. Unit 900: Amino Acid Process Flow Diagram

It should be noted that the relationship $C_{NH_4^+} = 2.04C_{FA}$ can be achieved only in a batch reactor by measuring the concentration of fumaric acid and adjusting the ammonia concentration with time. This approach is assumed here; however, if a fixed amount of ammonia is initially added to the reactor, then the relationship between $C_{NH_4^+}$ and C_{FA} must be found from the material balance and substituted in Equation (B.8.2).

Substituting the above values into Equation (B.8.2) and using the conversion, X, of fumaric acid ($C_{FA} = C_{FA,0}(1 - X)$ and $C_{AA} = C_{FA,0}X$), we get

$$V_a = \frac{VC_{FA,0}}{W}\frac{dX}{dt} = \frac{C_{FA,0}^{0.77}}{150}\left[\frac{(1-2X)}{1-(2+123C_{FA,0}^{1.04})X + 123C_{FA,0}^{1.04}}\right] \qquad \text{(B.8.3)}$$

where

V is the volume of the reacting mass in the reactor (m^3).

W is the weight of the gel (kg) = $V(1-\varepsilon)\rho_{bead}$.

ε is the void fraction of beads in the reacting mass.

ρ_{bead} is the bead density (kg/m^3).

Substituting into Equation (B.8.3), we have

$$\frac{dX}{dt} = \frac{(1-\varepsilon)\rho_{bead}}{C_{FA,0}^{0.23}150}\left[\frac{(1-2X)}{(1+123C_{FA,0}^{1.04}) - (2+123C_{FA,0}^{1.04})X}\right] \qquad \text{(B.8.4)}$$

For the specified initial concentration of fumaric acid of 1.0M = 1 $kmol/m^3$ and with $\rho_{bead} \sim 1000$ kg/m^3 and assuming a voidage of 0.5, Equation (B.8.4) simplifies to

$$\frac{dX}{dt} = 3.33\left[\frac{(1-2X)}{124-125X}\right] \qquad \text{(B.8.5)}$$

Separating variables and integrating Equation (B.8.5) yield the conversion as a function of batch reaction time. This relationship is shown in Figure B.8.2.

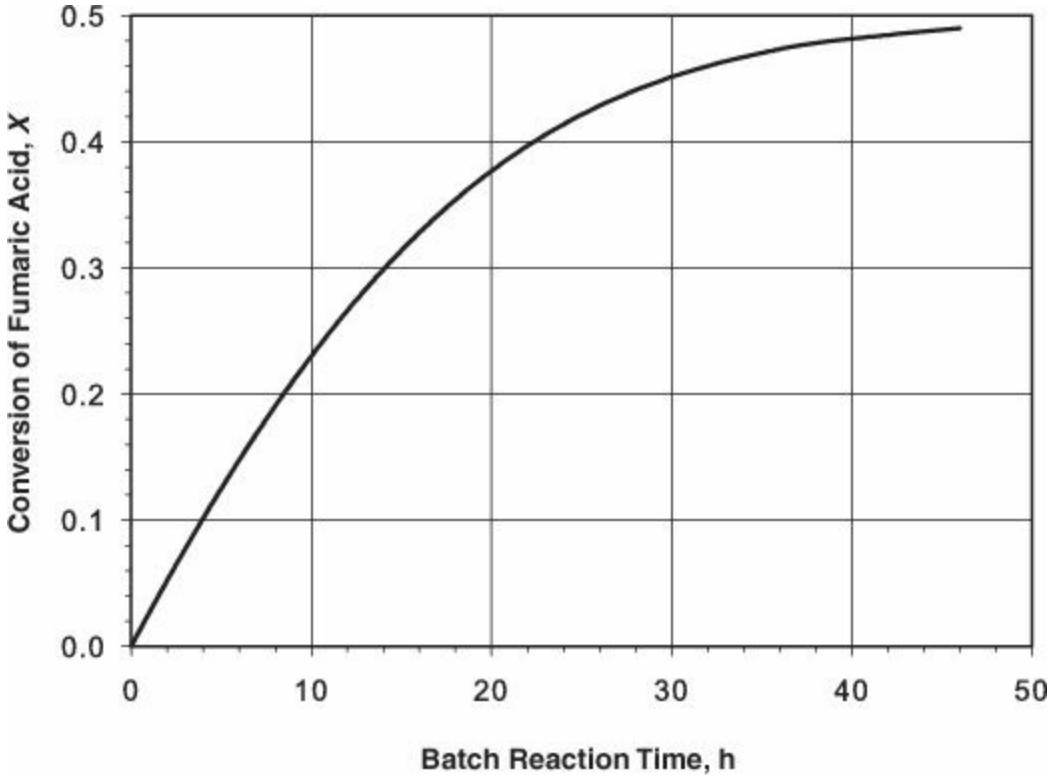


Figure B.8.2. Conversion of Fumaric Acid to L-Aspartic Acid as a Function of Reaction Time

Preliminary Sizing of Reactor R-901. For a conversion of 45% (90% of equilibrium), a reaction time of approximately 30 h is required. Assuming that an additional 5 h is required for filling, cleaning, and heating, the total time for the reaction step is 35 h.

Using a reactor size of 37.9 m^3 (10,000 gal) and assuming a 90% fill volume and a voidage of 0.5, the

amount of fumaric acid fed to the batch is (37.9)(0.9)(0.5) = 17.04 m^3, or 17.04 kmol (17.04 × 116 = 1977 kg). The amount of L-aspartic acid produced = (17.04)(0.45) = 7.67 kmol = (7.67)(133) = 1020 kg.

Production rate of L-aspartic acid from a 10,000 gallon reactor is 1020 kg/batch using a batch time of 35 h.

L-Phenylalanine. L-phenylalanine is produced via fermentation using a mutant *Brevibacterium lactofermentum* 2256 (ATCC No. 13869) known as No. 123 [2]. The rate equations for biomass (bacteria, X), substrate (mainly glucose, *S*), and product (L-phenylalanine, *P*) are described by Monod kinetics.

$$\frac{dX}{dt} = \frac{\mu_m S}{K_s + S} X \tag{B.8.6}$$

$$\frac{dS}{dt} = -\frac{1}{Y_{XS}} \frac{\mu_m S}{K_s + S} X \tag{B.8.7}$$

$$\frac{dP}{dt} = \frac{Y_{PS}}{Y_{XS}} \frac{\mu_m S}{K_s + S} X \tag{B.8.8}$$

where

X is the concentration of bacteria (kg/m^3).

S is the concentration of substrate (glucose) (kg/m^3).

P is the concentration of product (L-phenylalanine) (kg/m^3).

μ_m is the maximum specific growth rate (h^{-1}).

K_s is the Monod constant (kg/m^3).

Y_{XS} is biomass yield.

Y_{PS} is product yield.

According to Tsuchida et al. [2], for a culture medium containing 13% glucose, 1% ammonium sulfate, and 1.2% fumaric acid (plus other trace nutrients, etc.) the yield of L-phenylalanine was 21.7 mg/ml after 72 h of cultivation at a temperature of 31.5°C. This represents a yield of approximately 16.7% from glucose by weight. Other amino acids are also produced in small quantities (<5 kg/m^3), with lysine making up approximately 50%.

To obtain a kinetic model of the growth of bacteria and subsequent production of L-phenylalanine and depletion of glucose, the parameters in Equations (B.8.6)–(B.8.8) were back-calculated to give best-fit profiles of *X*, *S*, and *P* compared to published values ([2], Figure 4). The parameter values are shown in Table B.8.1, and the profiles are plotted in Figure B.8.3.

Preliminary Sizing of Reactor R-901. For a reaction time of approximately 60 h, the final concentration of L-phenylalanine is 21.0 kg/m^3. Assuming an additional 5 h for filling, cleaning, and heating gives a total reactor step time of 65 h.

Table B.8.1. Best-Fit Parameters for Monod Kinetics Using *Brevibacterium lactofermentum* 2256 (ATCC No. 13869) Strain No. 123

Parameter	Value
μ_m	0.25 h^{-1}
K_s	105.4 kg/m^3
Y_{XS}	0.07
Y_{PS}	0.167
X_0	0.0114 kg/m^3
S_0	130.0 kg/m^3
P_0	0.0 kg/m^3

Using a 37.9 m^3 (10,000 gal) reactor for the fermentation and assuming that a 90% fill volume is used, the volume of reactants is (37.9)(0.9) = 34.11 m^3.

The amount of L-phenylalanine produced in a 60 h batch reaction is (34.11)(21.0) = 716 kg.

Production rate of L-aspartic acid from a 10,000 gallon reactor is 716 kg/batch, with a reactor step time of 65 h.

Preliminary Information on Other Equipment. As mentioned in the process description, the production of both L-aspartic acid and L-phenylalanine follows similar paths. A brief discussion of the unit operations involved with the separation and purification of the final products is in order, because these operations are not typical of the unit operations covered in this text. Size information is not included for the equipment described next; however, estimates of processing times, where applicable, are given.

Filtration of Bacteria. After reaction, the bacteria must be filtered from the mother liquor prior to storage. The bacteria tend to give rise to slimy filter cakes, and the filtration of such material is best accomplished using a rotary drum filter utilizing a precoat. Typical precoating materials are dolomite, perlite, and cellulose, and these are applied to the drum in a two-stage process prior to filtration. The precoating process involves depositing a layer of the precoat material (5–15 cm thick) on the drum prior to the filtration operation. Once the precoat has been applied, the filtration starts, and the biomass forms a thin layer on the precoat. This layer of biomass is continuously removed, along with a thin layer of the precoat material, using a sharp-edged "Doctor" blade. Additional information is given at http://www.solidliquid-separation.com [3]. Without doing detailed calculations, it is difficult to determine the time required for the precoat stage and filtration stages. For this project you may assume that these steps take 25 h and 5 h, respectively.

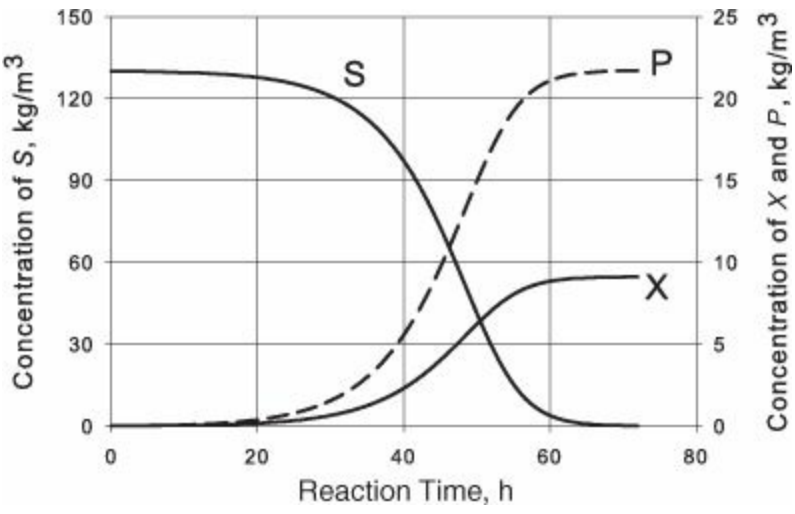


Figure B.8.3. Concentration Profiles as a Function of Reaction Time

Intermediate Storage. The fermentation broth (free of solids, or biomass) leaving the filters is stored in an intermediate storage tank prior to being sent to the ion exchange column (for L-phenylalanine) and on to the crystallizer. The use of an intermediate storage vessel allows the remainder of the process to operate as a continuous process.

Ion Exchange Column. The ion exchange columns operate as semibatch processes. Hydrochloric acid is added to the L-phenylalanine-containing solution and is passed through freshly regenerated ion exchange resin such as Dow's DOWEX MARATHON C [4]. The resin captures the positively charged amino acid. Once the bed is full, it is back-washed with a basic solution of ammonium or sodium hydroxide, which breaks the resin amino acid bond. The resin is subsequently washed free of the hydroxide, and the cycle starts again.

Continuous Crystallizer and Filtration. Draft tube baffle crystallizers can be used for the crystallization of L-aspartic acid and L-phenylalanine. These crystallizers offer the advantages of high circulation rates for efficient mixing. Fines removal is facilitated through the use of baffles, and a certain amount of product classification (crystal size control) is obtained through the elutriating leg. Batch crystallizers could also be used, but product quality and efficiency suffer. The saturated liquid from the crystallizer, containing amino acid crystals, is sent to a filter (such as a rotary drum filter), where the crystals are removed and sent for washing, drying, and packaging. The saturated liquid is returned to the crystallizer for further product recovery, thereby increasing the efficiency of the operation. Both amino acids can be crystallized at temperatures greater than 100°C. Therefore, the crystallization may take place at ambient pressure by removing the excess water through evaporation. The solubilities of L-aspartic acid and L-phenylalanine at 100°C are 67 g/liter and 100 g/liter, respectively.

B.8.3 References

1. Takamatch, T., K. Yamashita, and A. Sumi, "Kinetics of Production of L-Aspartic Acid by Aspartase of Immobilized *E. Coli* Cells," *Japanese Journal of Fermentation Technology* 58, no. 2 (1980): 129–133.
2. Tsuchida, T., K. Kubota, Y. Morinaga, H. Matsui, H. Enei, and F. Yoshinga, "Production of L-Phenylalanine by a Mutant of *Brevibacterium lactofermentum* 2256," *Agric. Bio. Chem.* 51, no. 8 (1987): 2095–2101.
3. http://www.solidliquid-separation.com.
4. DOWEX MARATHON C data sheet, http://www.dow.com/PublishedLiterature/dh_0082/0901b80380082af5.pdf?filepath=liquidseps/pdfs/noreg/17701593.pdf&fromPage=GetDoc.

B.9. Acrylic Acid Production Via The Catalytic Partial Oxidation Of Propylene [1, 2, 3, 4, 5], Unit 1000

Acrylic acid (AA) is used as a precursor for a wide variety of chemicals in the polymer and textile industries. There are several chemical pathways to produce AA, but the most common one is via the partial oxidation of propylene. The usual mechanism for producing AA utilizes a two-step process in which propylene is first oxidized to acrolein and then further oxidized to AA. Each reaction step usually takes place over a separate catalyst and at different operating conditions. The reaction

stoichiometry is given below:

$$C_3H_6 + O_2 \rightarrow C_3H_4O + H_2O$$

acrolein

$$C_3H_4O + \frac{1}{2}O_2 \rightarrow C_3H_4O_2$$

acrylic acid

Several side reactions may occur, most resulting in the oxidation of reactants and products. Some typical side reactions are given below:

$$C_3H_4O + \frac{7}{2}O_2 \rightarrow 3CO_2 + 2H_2O$$

$$C_3H_4O + \frac{3}{2}O_2 \rightarrow C_2H_4O_2 + CO_2$$

acetic acid

$$C_3H_6 + \frac{9}{2}O_2 \rightarrow 3CO_2 + 3H_2O$$

Therefore, the typical process setup consists of a two-reactor system, with each reactor containing a separate catalyst and operating at conditions so as to maximize the production of AA. The first reactor typically operates at a higher temperature than the second.

As with any reaction involving the partial oxidation of a fuel-like feed material (propylene), considerable attention must be paid to the composition of hydrocarbons and oxygen in the feed stream. In the current design, a fluidized-bed reactor is used, which provides essentially isothermal conditions in the reactor and, with the addition of large amounts of steam, allows safe and stable operation. The second safety concern is associated with the highly exothermic polymerization of AA, which occurs in two ways. First, if this material is stored without appropriate additives, then free radical initiation of the polymerization can occur. This potentially disastrous situation is discussed by Kurland and Bryant [1]. Second, AA dimerizes when in high concentrations at temperatures greater than 90°C, and thus much of the separation sequence must be operated under high vacuum in order to keep the bottom temperatures in the columns below this temperature.

B.9.1. Process Description

The process shown in Figure B.9.1 produces 50,000 metric tons per year of 99.9% by mole AA product. The number of operating hours is taken to be 8000/y, and the process is somewhat simplified because there is only one reactor [5]. It is assumed that both reactions take place on a single catalyst to yield AA and by-products. It is imperative to cool the products of reaction quickly to avoid further oxidation reactions, and this is achieved by rapidly quenching the reactor effluent with a cool recycle, Stream 8, of dilute aqueous AA in T-1001. Additional recovery of AA and acetic acid (a by-product) is achieved in the absorber, T-1002. The stream leaving the absorption section is a dilute aqueous acid, Stream 9. This is sent to a liquid-liquid extractor, T-1003, to remove preferentially the acid fraction from the water prior to purification. There are many possible solvents that can be used as the organic phase in the separation; high solubility for AA and low solubility for water are desirable. Some examples include ethyl acrylate, ethyl acetate, xylene, diisobutyl ketone, methyl isobutyl ketone, and diisopropyl ether (DIPE), which is used here. The organic phase from T-1003 is sent to a solvent recovery column, T-1004, where the diisopropyl ether (and some water) is recovered overhead and

returned to the extractor. The bottom stream from this column, Stream 14, contains virtually all the AA and acetic acid in Stream 9. This is sent to the acid purification column, T-1005, where 95% by mole acetic acid by-product is produced overhead, and 99.9% by mole AA is produced as a bottoms product and cooled prior to being sent to storage.

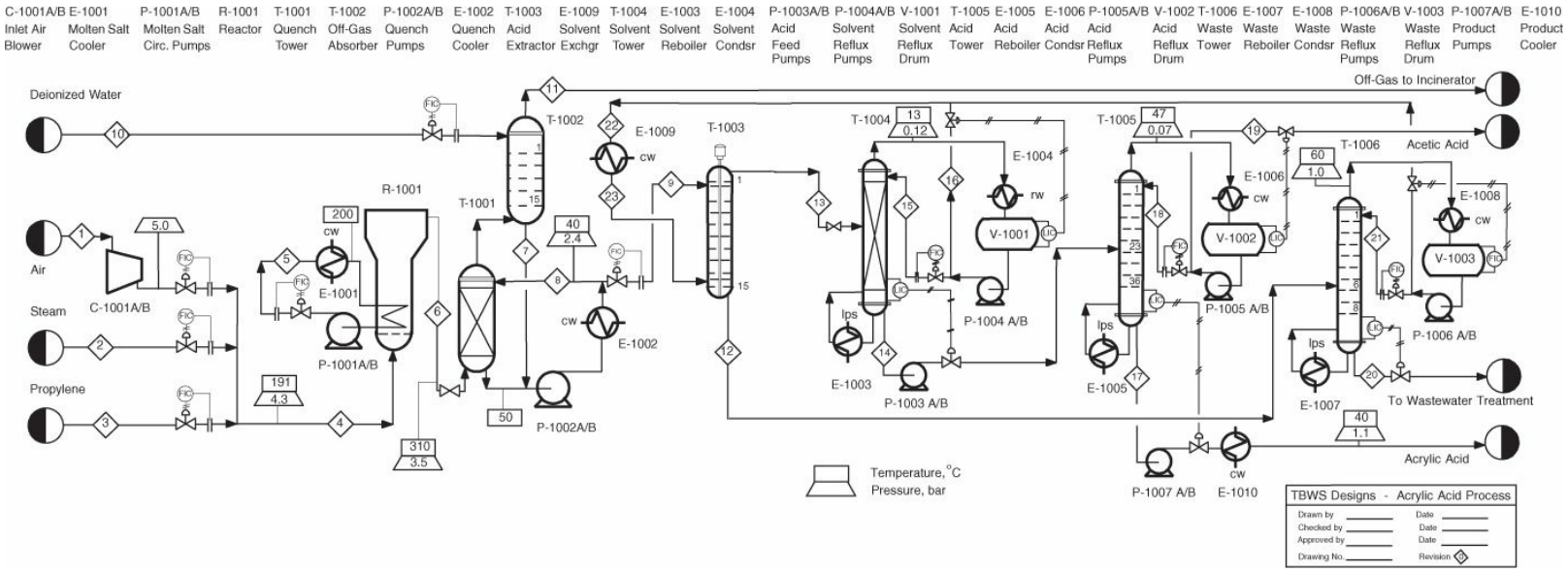


Figure B.9.1. Unit 1000: Production of Acrylic Acid from Propylene PFD (The point where Streams 1 and 2 are mixed with Stream 3 to form Stream 4 actually occurs within Reactor R-1001.)

The aqueous phase from the extractor, Stream 12, is sent to a wastewater column, T-1006, where a small amount of DIPE is recovered overhead and returned to the extractor. The bottoms product, containing water and trace quantities of solvent and acid, is sent to wastewater treatment. Process stream information and preliminary equipment summaries are given in Tables B.9.1 and B.9.2, respectively. A utility summary is also provided in Table B.9.3.

B.9.2. Reaction Kinetics and Reactor Configuration

The reactions taking place are kinetically controlled at the conditions used in the process; that is, equilibrium lies far to the right. The reaction kinetics for the catalyst used in this process are given below:

$$C_3H_6 + \frac{3}{2}O_2 \rightarrow \underset{\textit{acrylic acid}}{C_3H_4O_2} + H_2O \qquad \text{Reaction 1}$$

$$C_3H_6 + \frac{5}{2}O_2 \rightarrow \underset{\textit{acetic acid}}{C_2H_4O_2} + CO_2 + H_2O \qquad \text{Reaction 2}$$

$$C_3H_6 + \frac{9}{2}O_2 \rightarrow 3CO_2 + 3H_2O \qquad \text{Reaction 3}$$

where $-r_i = k_{o,i} \exp\left[-\frac{E_i}{RT}\right] p_{propylene}\, p_{oxygen}$

Table B.9.1. Stream Table for Unit 1000

Stream Number	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23
Temperature (°C)	25	159	25	191	250	310	63	40	40	25	48	40	40	90	13	13	89	47	47	102	60	13	40
Pressure (bar)	1.0	6.0	11.5	4.3	3.0	3.5	1.4	2.4	2.4	5.0	1.0	2.4	2.4	0.19	0.12	3.0	0.16	0.07	1.1	1.1	1.0	3.0	2.8
Vapor fraction	1.0	1.0	1.0	1.0	0.0	1.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Mass flow (tonne/h)	39.05	17.88	5.34	62.27	1075.0	62.27	3.08	1895.	27.46	2.54	37.35	20.87	143.0	6.63	155.3	136.4	6.26	5.28	0.37	20.84	37.37	136.4	136.4
Mole flow (kmol/h)	1362.9	992.3	127.0	2482.2	0.00	2444.0	148.5	85,200.0	1249.6	141.0	1335.4	1156.9	1591.2	93.19	1705.7	1498.0	86.85	90.49	6.34	1156.43	470.2	1498.5	1498.5
Component flowrates (kmol/h)					HiTec Molten Salt																		
Propylene	0.00	0.00	127.0	127.0	0.00	14.7	0.00	0.00	0.00	0.00	14.7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Nitrogen	1056.7	0.00	0.00	1056.7	0.00	1056.7	0.00	0.00	0.00	0.00	1056.7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Oxygen	280.9	0.00	0.00	280.9	0.00	51.9	0.00	0.00	0.00	0.00	51.9	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Carbon dioxide	0.00	0.00	0.00	0.00	0.00	60.5	0.00	0.00	0.00	0.00	60.5	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Water	25.3	992.3	0.00	1017.6	0.00	1165.9	140.9	78,870	1156.7	141.0	150.2	1156.6	198.8	0.30	226.0	198.5	0.00	4.28	0.30	1156.4	126.8	198.7	198.7
Acetic acid	0.00	0.00	0.00	0.00	0.00	6.54	0.65	415	6.08	0.00	0.46	0.03	6.08	6.08	0.00	0.00	0.05	86.07	6.03	0.03	0.00	0.00	0.00
Acrylic acid	0.00	0.00	0.00	0.00	0.00	87.79	6.99	5915	86.81	0.00	0.98	0.00	86.81	86.81	0.00	0.00	86.80	0.14	0.01	0.00	0.00	0.00	0.00
Solvent (diisopropyl ether)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.30	1299.5	0.00	1479.7	1299.5	0.00	0.00	0.00	0.00	343.4	1299.8	1299.8

Table B.9.2. Preliminary Equipment Summary Table for Unit 1000

Equipment	T-1001	T-1002	T-1003	T-1004	T-1005	T-1006	R-1001*
MOC	Stainless steel	Stainless steel	Stainless steel	Stainless steel	Carbon steel	Stainless steel	Carbon steel fluidized bed
Diameter (m)	5.3	3.5	2.2	7.5	2.4	2.3	3.6
Height/length (m)	12	11	9.5	34	25	7.0	10
Orientation	Vertical	Vertical	Vertical	Vertical	Vertical	Vertical	Vertical
Internals	10 m of high-efficiency packing Polyethylene	15 sieve trays + demister Stainless steel	15 perforated plates + mixer Stainless steel	31 m of high-efficiency structured packing Stainless steel	36 sieve plates Stainless steel	8 sieve plates Stainless steel	1451 heat transfer tubes (1420 m^2) filled with molten salt
Pressure (barg)	1.4	1.0	1.4	–1.0	–1.0	0	3.0

*Installed cost of reactor (mid-1996) = $\$2 \times 10^5 [\text{Area } (m^2)]^{0.5}$.

Equipment	P-1001 A/B	P-1002 A/B	P-1003 A/B	P-1004 A/B	P-1005 A/B	P-1006 A/B	P-1007 A/B
MOC	Carbon steel	Stainless steel	Stainless steel	Stainless steel	Carbon steel	Carbon steel	Stainless steel
Power (shaft) (kW)	32.3	106.2	0.9	51.3	1.2	9.0	1.0
Efficiency	75%	75%	40%	75%	40%	60%	40%
Type/drive	Centrifugal/ electric	Centrifugal/ electric	Centrifugal/ electric	Centrifugal/ electric	Centrifugal/ electric	Centrifugal/ electric	Centrifugal/ electric
Temperature (°C)	250	50	90	13	47	60	89
Pressure in (bar)	2.0	1.4	0.19	0.12	0.07	1.0	0.16
Pressure out (bar)	3.6	2.9	2.05	4.62	3.31	4.62	2.46

Equipment	E-1001	E-1002	E-1003	E-1004	E-1005	E-1006	E-1007
Type	Floating-head	Fixed TS	Floating-head reboiler	Floating-head condenser	Floating-head reboiler	Fixed TS condenser	Floating-head reboiler
Duty (MJ/h)	83,400	70,300	101,000	108,300	2230	2280	21,200
Area (m^2)	160	2550	891	7710	19.7	73.3	187
Shell							
Max temp (°C)	40	40	160	10	160	40	160
Pressure (barg)	4.0	4.0	5.0	4.0	5.0	4.0	5.0
Phase	L	L	Cond. steam	L	Cond. steam	L	Cond. steam
MOC	Carbon steel	Carbon steel	Carbon steel	Carbon steel	Carbon steel	Carbon steel	Carbon steel
Tube side							
Max temp (°C)	250	50	90	13	90	47	102
Pressure (barg)	2.0	2.0	–0.81	–0.88	–0.84	–0.93	0.1
MOC	Carbon steel	Stainless steel	Stainless steel	Stainless steel	Carbon steel	Carbon steel	Stainless steel
Phase	L	L	Boiling liq.	Cond. vapor	Boiling liq.	Cond. vapor	Boiling liq.

Equipment	E-1008	E-1009	E-1010
Type	Fixed TS condenser	Floating head	Floating head
Duty (MJ/h)	15,800	8000	698
Area (m^2)	210	19.7	10.3
Shell side			
Max temp (°C)	40	160	40
Pressure (barg)	4.0	5.0	4.0
Phase	L	Cond. steam	L
MOC	Carbon steel	Carbon steel	Carbon steel
Tube side			
Max temp (°C)	60	40	89
Pressure (barg)	0.0	2.0	1.4
MOC	Carbon steel	Carbon steel	Stainless steel
Phase	Cond. vapor	L	L

(*continued*)

Equipment	C-1001 A/B	V-1001	V-1002	V-1003
MOC	Carbon steel	Stainless steel	Carbon steel	Carbon steel
Power (shaft) (kW)	2260	—	—	—
Efficiency	77% Centrifugal	—	—	—
Type/drive	Centrifugal –2 stage/electric	—	—	—
Temperature (°C)	25	—	—	—
Pressure in (bar)	1.0	—	—	—
Pressure out (bar)	5.0	—	—	—
Pressure (barg)	—	–0.88	–0.93	0.0
Diameter (m)	—	2.4	1.0	1.5
Height/length (m)	—	7.2	2.5	4.5
Orientation	—	Horizontal	Horizontal	Horizontal
Internals	—	—	—	—

Table B.9.3. Utility Summary Table for Unit 1000

Utility	cw	cw	lps	rw	lps	cw	lps	cw	lps	cw
Equipment	E-1001	E-1002	E-1003	E-1004	E-1005	E-1006	E-1007	E-1008	E-1009	E-1010
Flow (tonne/h)	1995.0	1682.0	48.5	5182.0	1.07	54.5	10.19	378.0	3.85	16.7

Partial pressures are in kPa, and the activation energies and preexponential terms for re-actions 1–3 are as follows:

i	E_i kcal/kmol	$k_{o,i}$ kmol/m^3 reactor h/(kPa)^2
1	15,000	1.59×10^5
2	20,000	8.83×10^5
3	25,000	1.81×10^8

The reactor configuration used for this process is a fluidized bed, and it is assumed that the bed of catalyst behaves as a well-mixed tank—that is, it is isothermal at the temperature of the reaction (310°C). The gas flow is assumed to be plug flow through the bed, with 10% of the gas bypassing the catalyst. This latter assumption is made in order to simulate the gas channeling that occurs in real fluid-bed reactors.

B.9.3. Simulation (CHEMCAD) Hints

The use of a liquid-liquid extractor requires the use of a thermodynamic package (or physical property data) that reflects the fact that two phases are formed and that significant partitioning of the AA and acetic acid occurs, with the majority going to the organic phase (in this case DIPE). Distribution coefficients for the organic acids in water and DIPE as well as mutual solubility data for water/DIPE are desirable. The process given in Figure B.2 was simulated using a UNIFAC thermodynamics package and the latent heat enthalpy option on CHEMCAD and should give reasonable results for preliminary process design. Much of the process background material and process configuration was taken from the 1986 AIChE student contest problem in reference [5]. The kinetics presented above are fictitious but should give reasonable preliminary estimates of reactor size.

B.9.4 References

1. Kurland, J. J., and D. B. Bryant, "Shipboard Polymerization of Acrylic Acid," *Plant Operations Progress* 6, no. 4 (1987): 203–207.
2. *Kirk-Othmer Encyclopedia of Chemical Technology*, 3rd ed., Vol. 1 (New York: John Wiley and Sons, 1978), 330–354.
3. *Encyclopedia of Chemical Processing and Design*, ed. J. J. McKetta and W. A. Cunningham, Vol. 1 (New York: Marcel Dekker, 1976), 402–428.
4. Sakuyama, S., T. Ohara, N. Shimizu, and K. Kubota, "A New Oxidation Process for Acrylic Acid from Propylene," *Chemical Technology*, June 1973, 350.
5. "1986 Student Contest Problem," *The AIChE Student Annual 1986*, ed. B. Van Wie and R. A. Wills (AIChE, 1986), 52–82.

B.10 Production Of Acetone Via The Dehydrogenation Of Isopropyl Alcohol (IPA) [1, 2, 3, 4], Unit 1100

The prevalent process for the production of acetone is as a by-product of the manufacture of phenol. Benzene is alkylated to cumene, which is further oxidized to cumene hydroperoxide and finally cleaved to yield phenol and acetone. However, the process shown in Figure B.10.1 and discussed here uses isopropyl alcohol (IPA) as the raw material. This is a viable commercial alternative, and a few plants continue to operate using this process. The primary advantage of this process is that the acetone produced is free from trace aromatic compounds, particularly benzene. For this reason, acetone produced from IPA may be favored by the pharmaceutical industry due to the very tight

restrictions placed on solvents by the Food and Drug Administration (FDA). The reaction to produce acetone from IPA is as follows:

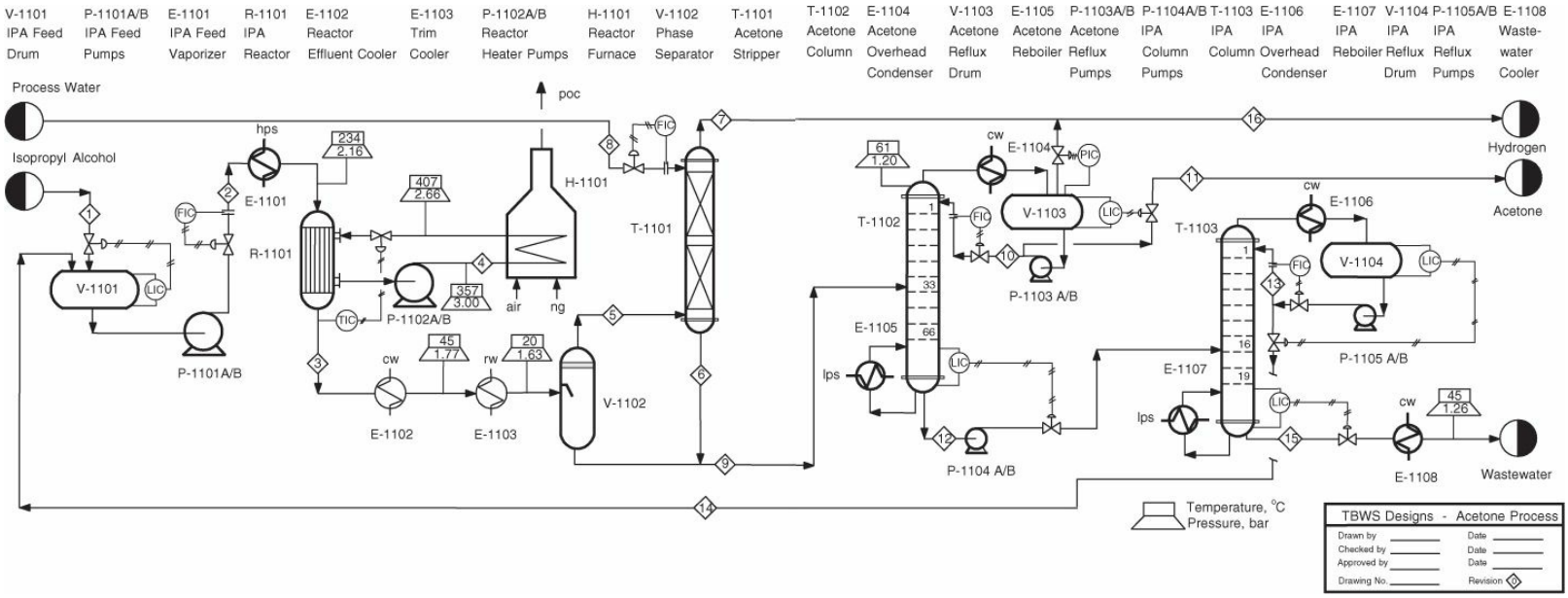


Figure B.10.1. Unit 1100: Production of Acetone from Isopropyl Alcohol PFD

$$(CH_3)_2CHOH \rightarrow (CH_3)_2CO + H_2$$

isopropyl alcohol *acetone*

The reaction conditions are typically 2 bar and 350°C, giving single-pass conversions of 85%–92%.

B.10.1. Process Description

Referring to Figure B.10.1, an azeotropic mixture of isopropyl alcohol and water (88 wt% IPA) is fed into a surge vessel (V-1101), where it is mixed with the recycled unreacted IPA/water mixture, Stream 14. This material is then pumped and vaporized prior to entering the reactor. Heat is provided for the endothermic reaction using a circulating stream of molten salt, Stream 4. The reactor effluent, containing acetone, hydrogen, water, and unreacted IPA, is cooled in two exchangers prior to entering the phase separator (V-1102). The vapor leaving the separator is scrubbed with water to recover additional acetone, and then this liquid is combined with the liquid from the separator and sent to the separations section. Two towers are used to separate the acetone product (99.9 mol%) and to remove the excess water from the unused IPA, which is then recycled back to the front end of the process as an azeotropic mixture. Stream summaries, preliminary equipment, and utility summaries are given in Tables B.10.1, B.10.2, and B.10.3, respectively.

B.10.2. Reaction Kinetics

The reaction to form acetone from isopropyl alcohol (isopropanol) is endothermic, with a standard heat of reaction of 62.9 kJ/mol. The reaction is kinetically controlled and occurs in the vapor phase over a catalyst. The reaction kinetics for this reaction are first order with respect to the concentration of alcohol and can be estimated from the following equation [3, 4]:

$$-r_{IPA} = k_0 \exp\left[-\frac{E_a}{RT}\right] C_{IPA} \quad \frac{\text{kmol}}{\text{m}^3\text{reactor s}}$$

where $E_a = 72.38\text{MJ/kmol}$, $k_0 = 3.51 \times 10^5 \frac{\text{m}^3\text{gas}}{\text{m}^3\text{reactor s}}$, $C_{IPA} = \frac{\text{kmol}}{\text{m}^3\text{gas}}$

In practice, several side reactions can occur to a small extent. Thus, trace quantities of propylene,

diisopropyl ether, acetaldehyde, and other hydrocarbons and oxides of carbon can be formed [1]. The noncondensables are removed with the hydrogen, and the aldehydes and ethers may be removed with acid washing or adsorption. These side reactions are not accounted for in this preliminary design.

For the design presented in Figure B.10.1, the reactor was simulated with catalyst in 2-in (50.4 mm) diameter tubes, each 20 ft (6.096 m) long, and with a cocurrent flow of a heat transfer medium on the shell side of the shell-and-tube reactor. The resulting arrangement gives a 90% conversion of IPA per pass.

B.10.3. Simulation (CHEMCAD) Hints

Isopropyl alcohol and water form a minimum boiling point azeotrope at 88 wt% isopropyl alcohol and 12 wt% water. Vapor-liquid equilibrium (VLE) data are available from several sources and can be used to back-calculate binary interaction parameters or liquid-phase activity coefficients. The process presented in Figure B.3 and Table B.6 was simulated using the UNIQUAC VLE thermodynamics package and the latent heat enthalpy option in the CHEMCAD simulator. This package correctly predicts the formation of the azeotrope at 88 wt% alcohol.

B.10.4 References

1. *Kirk-Othmer Encyclopedia of Chemical Technology*, 3d ed., Vol. 1 (New York: John Wiley and Sons, 1976), 179–191.
2. *Shreve's Chemical Process Industries*, 5th ed., ed. G. T. Austin (New York: McGraw-Hill, 1984), 764.
3. *Encyclopedia of Chemical Processing and Design*, Vol. 1, ed. J. J. McKetta and W. A. Cunningham (New York: Marcel Dekker, 1976), 314–362.
4. Sheely, C. Q., *Kinetics of Catalytic Dehydrogenation of Isopropanol*, Ph.D. Thesis, University of Illinois, 1963.

B.11 Production Of Heptenes From Propylene And Butenes [1], Unit 1200

The background information for this process is taken from Chauvel et al. [1]. This example is an illustration of a preliminary estimate of a process to convert a mixture of C_3 and C_4 unsaturated hydrocarbons to 1-heptene and other unsaturated products. The market for the 1-heptene product would be as a highoctane blending agent for gasoline or in the production of plasticizers. Based on preliminary market estimates, a production capacity of 20,000 metric tons per year of 1-heptene using 8000 operating hours/y was set. This process differs from the other examples in Appendix B in several ways. First, the raw materials to the process contain a wide variety of chemicals. This is typical for oil refinery and some petrochemical operations. Second, no specific kinetic equations are given for the reactions. Instead, the results of laboratory tests using the desired catalyst at different conditions and using different feed materials are used to guide the process engineer to an optimum, or close to an optimum, reactor configuration. The flowsheet in Figure B.11.1 and stream, equipment summary, and utility summary tables, Tables B.11.1–B.11.3, have been developed using such information. It should be noted that a preliminary economic analysis, and hence the feasibility of the process, can be determined without this information, as long as yield and conversion data are available and the reactor configuration can be estimated.

Table B.10.1. Stream Table for Unit 1100

Stream Number	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
Temperature (°C)	25	32	350	357	20	27	33	25	22	61	61	90	83	83	109	33
Pressure (bar)	1.01	2.30	1.91	3.0	1.63	1.63	1.50	2.0	1.63	1.5	1.5	1.4	1.2	1.2	1.4	1.2
Vapor fraction	0.0	0.0	1.0	0.0	1.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0
Mass flow (tonne/h)	2.40	2.67	2.67	35.1	0.34	0.46	0.24	0.36	2.79	4.22	1.88	0.92	8.23	0.27	0.65	0.24
Mole flow (kmol/h)	51.96	57.84	92.62	0.00	39.74	21.14	38.60	20.00	74.02	72.51	32.29	41.73	177.18	5.88	35.85	38.60
Component flowrates (kmol/h)				Molten Salt												
Hydrogen	0.00	0.00	34.78	0.00	34.78	0.00	34.78	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	34.78
Acetone	0.00	0.16	34.94	0.00	4.44	1.93	2.51	0.00	32.43	72.46	32.27	0.16	4.82	0.16	0.00	2.51
Isopropyl alcohol	34.82	38.64	3.86	0.00	0.12	0.10	0.02	0.00	3.84	0.05	0.02	3.82	115.10	3.82	0.00	0.02
Water	17.14	19.04	19.04	0.00	0.40	19.11	1.29	20.00	37.75	0.00	0.00	37.75	57.26	1.90	35.85	1.29

Table B.10.2. Preliminary Equipment Summary Table for Unit 1100

Equipment	P-1101 A/B	P-1102 A/B	P-1103 A/B	P-1104 A/B	P-1105 A/B	V-1101	V-1102
MOC	Carbon steel	Carbon steel	Carbon steel	Carbon steel	Carbon steel	Carbon steel	Carbon steel
Power (shaft) (kW)	0.43	2.53	1.75	0.06	1.45	0.00	0.00
Efficiency	40%	50%	40%	40%	40%	0.00	0.00
Type/drive	Centrifugal/ electric	Centrifugal/ electric	Centrifugal/ electric	Centrifugal/ electric	Centrifugal/ electric	0.00	0.00
Temperature (°C)	25	400	61	90	83	0.00	0.00
Pressure in (bar)	1.13	1.83	1.41	1.93	1.42	0.00	0.00
Pressure out (bar)	3.00	3.00	4.48	2.78	3.25	0.00	0.00
Diameter (m)	0.00	0.00	0.00	0.00	0.00	0.80	0.75
Height/length (m)	0.00	0.00	0.00	0.00	0.00	2.40	2.25
Orientation	0.00	0.00	0.00	0.00	0.00	Horizontal	Vertical
Internals	0.00	0.00	0.00	0.00	0.00	0.00	SS demister
Pressure (barg)	0.00	0.00	0.00	0.00	0.00	0.0	0.63

Equipment	V-1103	V-1104	T-1101	T-1102	T-1103	H-1101	R-1101
MOC	Carbon steel	Carbon steel	Carbon steel	Carbon steel	Carbon steel	Carbon steel	Carbon steel
Diameter (m)	0.83	0.93	0.33	1.25	1.36	0.00	1.85
Height/length (m)	2.50	2.80	3.20	37.0	18.6	0.00	8.0
Orientation	Horizontal	Horizontal	Vertical	Vertical	Vertical	0.00	Vertical
Internals	0.00	0.00	2.5 m of packing 1″ ceramic Raschig rings	66 SS sieve plates @ 18″ spacing	19 SS sieve plates @ 24″ spacing	0.00	448 2″ diameter, 20′ long catalyst filled tubes
Pressure (barg)	0.2	0.2	1.0	0.4	0.4	0.00	2.0
Type	0.00	0.00	0.00	0.00	0.00	Fired heater	0.00
Duty (MJ/h)	0.00	0.00	0.00	0.00	0.00	2730	0.00
Area radiant (m^2)	0.00	0.00	0.00	0.00	0.00	10.1	0.00
Area convective (m^2)	0.00	0.00	0.00	0.00	0.00	30.4	0.00
Tube pressure (barg)	0.00	0.00	0.00	0.00	0.00	2.0	0.00

Equipment	E-1101	E-1102	E-1103	E-1104	E-1105	E-1106	E-1107	E-1108
Type	Float-head vaporizer	Float-head partial cond.	Float-head partial cond.	Fixed TS condenser	Float-head reboiler	Fixed TS condenser	Float-head reboiler	Double pipe
Duty (MJ/h)	3550	3260	563	3095	3500	7340	7390	174
Area (m^2)	70.3	77.6	8.5	39.1	30.9	50.2	65.1	1.6
Shell side								
Max. temp (°C)	234	350	45	61	90	83	109	109
Pressure (barg)	1.0	1.0	1.0	0.2	0.4	0.2	0.4	0.4
Phase	Boiling liq.	Cond. vapor	Cond. vapor	Cond. vapor	Boiling liq.	Cond. vapor	Boiling liq.	L
MOC	Carbon steel	Carbon steel	Carbon steel	Carbon steel	Carbon steel	Carbon steel	Carbon steel	Carbon steel
Tube side								
Max. temp (°C)	254	40	15	40	160	40	160	40
Pressure (barg)	41.0	3.0	3.0	3.0	5.0	3.0	5.0	3.0
Phase	Cond. steam	L	L	L	Cond. steam	L	Cond. steam	L
MOC	Carbon steel	Carbon steel	Carbon steel	Carbon steel	Carbon steel	Carbon steel	Carbon steel	Carbon steel

Table B.10.3. Utility Summary Table for Unit 1100

Utility	hps	cw	rw	cw	lps	cw	lps	cw
Equipment	E-1101	E-1102	E-1103	E-1104	E-1105	E-1106	E-1107	E-1108
Flow (tonne/h)	2.09	77.90	13.50	74.00	1.68	176.00	3.55	4.16

B.11.1. Process Description

Two liquid feed streams containing propylene and butene and a stream of catalyst slurried with 1-hexene are mixed at a pressure of approximately 8 bar prior to being sent to the reactor. The reactor consists of five essentially well-mixed sections, with similar concentrations in each section. Heat removal is achieved by using pump-arounds from each stage through external heat exchangers. The reactor effluent is partially vaporized before being fed to the first of three distillation columns. The first column (T-1201) removes the unreacted C_3 and C_4 components, which are used subsequently as fuel (Stream 7) or sent to LPG storage (Stream 6). The next column (T-1202) separates the 1-hexene product overhead (Stream 10) and sends the bottoms stream to the final column (T-1203). In T-1203, the main 1-heptene product (Stream 13) is taken overhead, and the C_8 and heavier compounds are taken as the bottoms product (Stream 14). The bottoms product is processed off-site to remove the heavy material and to recover spent catalyst.

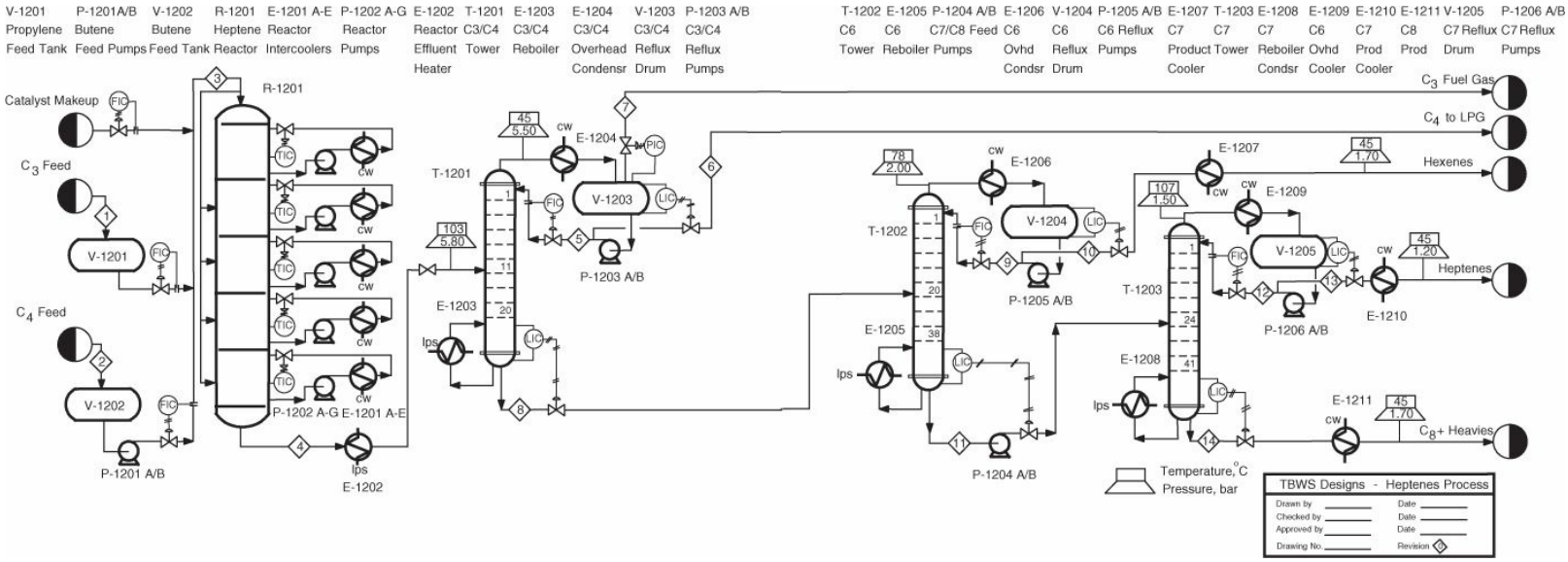


Figure B.11.1. Unit 1200: Production of Heptenes from Propylene and Butenes PFD

B.11.2. Reaction Kinetics

The process given in Figure B.11.1 is based on the liquid-phase catalytic co-dimerization of C_3 and C_4 olefins using an organometallic catalyst. This catalyst is slurried with a small volume of the hexenes product and fed to the reactor with the feed streams. The volume of the catalyst stream is small compared with the other streams and is not included in the material balance given in Table B.11.1. In 1976 (CEPCI = 183), consumption of catalyst amounted to \$9.5/1000 kg of 1-heptene product [1].

The primary reactions that take place are as follows:

$$C_3H_6 + C_3H_6 \rightarrow C_6H_{12}$$

1-*hexene*

$$C_3H_6 + C_4H_8 \rightarrow C_7H_{14}$$

1-*heptene*

$$C_4H_8 + C_4H_8 \rightarrow C_8H_{16}$$

1-*octene*

$$C_3H_6 + 2C_4H_8 \rightarrow C_{11}H_{22}$$

1-*undecene*

Table B.11.1. Stream Table for Unit 1200

Stream Number	1	2	3	4	5	6	7
Temperature (°C)	25	25	26	45	45	45	45
Pressure (bar)	11.6	3.0	8.0	7.7	7.5	6.5	5.0
Vapor fraction	0.0	0.0	0.0	0.0	0.0	0.0	1.0
Mass flow (tonne/h)	3.15	9.29	12.44	12.44	3.68	6.66	0.13
Mole flow (kmol/h)	74.57	163.21	237.78	178.10	64.41	116.45	3.00
Component flowrates (kmol/h)							
Propane	3.56	0.00	3.56	3.56	0.31	0.56	3.00
Propylene	71.06	0.00	71.06	0.00	0.00	0.00	0.00
i-Butane	0.00	29.44	29.44	29.44	16.19	29.28	0.00
n-Butane	0.00	34.41	34.41	34.41	18.65	33.72	0.00
i-Butene	0.00	8.27	8.27	8.27	4.53	8.19	0.00
1-Butene	0.00	90.95	90.95	44.94	24.61	44.49	0.00
1-Hexene	0.00	0.14	0.14	21.21	0.12	0.21	0.00
1-Heptene	0.00	0.00	0.00	26.53	0.00	0.00	0.00
1-Octene	0.00	0.00	0.00	7.41	0.00	0.00	0.00
1-Undecene	0.00	0.00	0.00	2.34	0.00	0.00	0.00

Stream Number	8	9	10	11	12	13	14
Temperature (°C)	151	78	78	135	107	107	154
Pressure (bar)	5.8	4.5	4.5	2.5	4.0	4.0	2.0
Vapor fraction	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Mass flow (tonne/h)	5.64	5.79	1.86	3.79	4.30	2.53	1.26
Mole flow (kmol/h)	58.65	69.84	22.44	36.22	43.78	25.76	10.46
Component flowrates (kmol/h)							
Propane	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Propylene	0.00	0.00	0.00	0.00	0.00	0.00	0.00
i-Butane	0.16	0.50	0.16	0.00	0.00	0.00	0.00
n-Butane	0.69	2.15	0.69	0.00	0.00	0.00	0.00
i-Butene	0.08	0.25	0.08	0.00	0.00	0.00	0.00
1-Butene	0.45	1.40	0.45	0.00	0.00	0.00	0.00
1-Hexene	21.00	64.70	20.79	0.21	0.36	0.21	0.00
1-Heptene	26.52	0.84	0.27	26.26	43.28	25.47	0.79
1-Octene	7.41	0.00	0.00	7.41	0.14	0.08	7.33
1-Undecene	2.34	0.00	0.00	2.34	0.00	0.00	2.34

Table B.11.2. Preliminary Equipment Summary Table for Unit 1200

Equipment	P-1201 A/B	P-1202 A-G*	P-1203 A/B	P-1204 A/B	P-1205 A/B	P-1206 A/B
MOC	Carbon steel	Carbon steel	Carbon steel	Carbon steel	Carbon steel	Carbon steel
Power (shaft) (kW)	6.75	5.13	2.75	0.66	2.15	1.93
Efficiency	40%	70%	40%	40%	40%	40%
Type/drive	Centrifugal/ electric	Centrifugal/ electric	Centrifugal/ electric	Centrifugal/ electric	Centrifugal/ electric	Centrifugal/ electric
Temperature (°C)	25	45	45	151	78	107
Pressure in (bar)	2.97	8.00	5.50	2.50	2.00	1.50
Pressure out (bar)	9.00	9.00	7.55	4.00	4.47	4.00

*Seven identical pumps: five operating + two spares.

Equipment	V-1201	V-1202	V-1203	V-1204	V-1205
MOC	Carbon steel	Carbon steel	Carbon steel	Carbon steel	Carbon steel
Diameter (m)	1.40	1.90	1.10	0.95	0.92
Height/length (m)	4.20	5.7	3.30	2.85	2.75
Orientation	Horizontal	Horizontal	Horizontal	Horizontal	Horizontal
Internals	—	—	—	—	—
Pressure (barg)	20.0	5.0	4.5	1.0	0.5

Equipment	R-1201	T-1201	T-1202	T-1203
MOC	Carbon steel	Carbon steel	Carbon steel	Carbon steel
Diameter (m)	3.00	1.05	1.10	0.90
Height/length (m)	13.0	20.7	26.0	27.3
Orientation	Vertical	Vertical	Vertical	Vertical
Internals	Reactor split into 5 equal sections	20 SS sieve plates @ 24″ spacing	38 SS sieve plates @ 18″ spacing	41 SS sieve plates @ 18″ spacing
Pressure (barg)	7.0	5.0	1.5	1.0

Equipment	E-1201 A-E*	E-1202	E-1203	E-1204	E-1205	E-1206
Type	Fixed TS	Float-head partial vap.	Float-head reboiler	Fixed TS condenser	Float-head reboiler	Fixed TS condenser
Duty (MJ/h)	846	3827	1251	3577	2184	2630
Area (m^2)	61.4	33.8	32.1	128.5	21.1	20.0
Shell side						
Max. temp (°C)	45	160	160	45	160	78
Pressure (barg)	8.0	5.0	5.0	4.0	5.0	1.0
Phase	L	Cond. steam	Cond. steam	Cond. vapor	Cond. steam	Cond. vapor
MOC	Carbon steel	Carbon steel	Carbon steel	Carbon steel	Carbon steel	Carbon steel
Tube side						
Max. temp (°C)	40	103	151	40	135	40
Pressure (barg)	3.0	6.7	4.8	3.0	1.5	3.0
Phase	L	L+V	Boiling liq.	L	Boiling liq.	L
MOC	Carbon steel	Carbon steel	Carbon steel	Carbon steel	Carbon steel	Carbon steel

*Area and duty given for one exchanger; five identical exchangers are needed.

Equipment	E-1207	E-1208	E-1209	E-1210	E-1211
Type	Double pipe	Float-head reboiler	Fixed TS condenser	Double pipe	Double pipe
Duty (MJ/h)	146	2026	2146	372	330
Area (m^2)	2.1	75.3	9.7	3.9	2.4
Shell side					
Max. temp (°C)	78	160	107	107	154
Pressure (barg)	1.0	5.0	0.5	0.3	0.7
Phase	L	Cond. steam	Cond. vapor	L	L
MOC	Carbon steel	Carbon steel	Carbon steel	Carbon steel	Carbon steel
Tube side					
Max. temp (°C)	40	154	40	40	40
Pressure (barg)	3.0	1.0	3.0	3.0	3.0
Phase	L	Boiling liq.	L	L	L
MOC	Carbon steel	Carbon steel	Carbon steel	Carbon steel	Carbon steel

Table B.11.3. Utility Summary Table for Unit 1200

Utility	cw	lps	lps	cw	lps	cw	cw	lps	cw	cw	cw
Equipment	E-1201 A-E	E-1202	E-1203	E-1204	E-1205	E-1206	E-1207	E-1208	E-1209	E-1210	E-1211
Temperature in (°C)	30	160	160	30	160	30	30	160	30	30	30
Temperature out (°C)	40	160	160	40	160	40	40	160	40	40	40
Flow (tonne/h)	20.20*	1.84	0.60	85.50	1.05	62.90	3.49	0.97	51.30	8.90	7.89

*Flow of cooling water shown for one exchanger only.

In order to maximize the selectivity of the heptene reaction, several reactor configurations were considered [1]. The reactor configuration that maximized the heptene production, in a minimum volume, was found to be a plug flow reactor in which the butene feed was introduced at one end and the propylene stream was injected along the side of the reactor. However, due to other considerations such as reactor complexity, it was finally decided to use a reactor with five equal stages in which the concentration in each stage is maintained approximately the same. Heat removal and mixing in each stage are accomplished by withdrawing a stream of material and pumping it through an external heat exchanger and back into the same stage of the reactor. The liquid cascades downward from stage to stage by means of liquid downcomers. The inside of the reactor can thus be considered similar to a five-plate distillation column (without vapor flow). The distribution of the feeds into the different stages is not shown in Figure B.11.1, and the dimensions of the reactor are taken directly from Chauvel et al. [1].

B.11.3. Simulation (CHEMCAD) Hints

All the hydrocarbon components used in the simulation can be considered to be well behaved, that is no azeotrope formation. The simulations were carried out using the SRK VLE and enthalpy packages using the CHEMCAD simulator.

B.11.4. Reference

1. Chauvel, A., P. Leprince, Y. Barthel, C. Raimbault, and J-P Arlie, *Manual of Economic Analysis of Chemical Processes*, trans. R. Miller and E. B. Miller (New York: McGraw-Hill, 1976), 207–228.

B.12. Design of a Shift Reactor Unit to Convert Co To Co_2, Unit 1300

The water-gas shift (WGS) reaction has been traditionally used to produce hydrogen from syngas, which comprises CO and H_2. This process can also be used for producing combustion gas with lower levels of carbon from a carbon-rich syngas. The shift reaction is mildly exothermic and equilibrium limited. Therefore, the extent of reaction becomes limited as the temperature increases along the length of the reactor. A two-stage process with interstage cooling is used to achieve the desired extent of conversion. A higher temperature results in a higher reaction rate, and a chromia-promoted iron oxide catalyst is used in the first stage. The second stage operates at a comparatively lower temperature, where a copper-zinc catalyst is used. The main reaction is

$$CO + H_2O \Leftrightarrow CO_2 + H_2 \qquad \text{(B.12.1)}$$

B.12.1. Process Description

A process flow diagram for a water-gas shift (WGS) reaction system is shown in Figure B.12.1. The

objective of the process is to achieve an overall 90% conversion of CO in the process. Syngas, Stream 1, is first heated in H-1301 before being mixed with steam. The effluent from the first-stage reactor, R-1301, is cooled in E-1301 before being sent to the second reactor stage, R-1302. The residual heat in the effluent from the second-stage reactor is utilized by raising low-pressure steam in E-1302. The reactor effluent is further cooled using cooling water in E-1303 before being sent to the flash separator, V-1301. The off-gas from V-1301 is usually sent to a hydrogen-recovery process or to a combustion system. The bottom product from V-1301 is sent to the wastewater treatment unit.

B.12.2. Reaction Kinetics

The rate equation representing midlife activity of a typical WGS reactor catalyst is given by Rase [1] as

$$-r_{co} = k_0 \exp\left[\frac{-E_0}{RT}\right]\left(y_{co}y_{H_2O} - \frac{y_{co_2}y_{H_2}}{K_{eq}}\right) \qquad \text{(B.12.2)}$$

where

$$k_0 = 0.2986 \text{ kmol/(kg cat. s) for iron catalyst}$$
$$= 0.0090 \text{ kmol/(kg cat. s) for copper-zinc catalyst}$$

$$E_0 = 40{,}739 \text{ kJ/kmol for iron catalyst}$$
$$= 15{,}427 \text{ kJ/kmol for copper-zinc catalyst}$$

$$K_{eq} = \exp\left[-4.33 + \frac{4577.9}{T}\right] \text{ for } 589 \text{ K} < T < 756 \text{ K}$$
$$= \exp\left[-4.72 + \frac{4800}{T}\right] \text{ for } 422 \text{ K} < T < 589 \text{ K}$$

Particle density = 2018 kg/m^3 for iron catalyst
= 2483 kg/m^3 for copper-zinc catalyst

Bulk density = 1121 kg/m^3 for the first bed with iron catalyst
= 1442 kg/m^3 for copper-zinc catalyst

Particle diameter = 1.0 mm for both catalysts

In this process, the steam/CO ratio can be manipulated to affect the CO conversion. The optimum values can be determined by an economic analysis. A higher steam/CO ratio may result in a shorter overall reactor length and less residual CO, but it adds to the cost due to the use of steam and a larger diameter of the reactor(s) to accommodate the larger flowrate. Table B.12.1 shows stream data for a process using a steam/CO ratio of 3 (molar basis).

B.12.3. Simulation (Aspen Plus) Hints

An Aspen Plus simulation is the basis for the design. The Peng-Robinson equation of state is used for the process side. The Ergun equation is used for calculating the pressure drop in the reactors. It should be noted that the steam/CO ratio affects not only the extent of CO conversion but also the temperature in the reactors. The maximum allowable temperature for the catalysts indicated in Table B.12.3 should not be violated.

H-1301 Syngas Heater

R-1301 First-Stage WGS Reactor

E-1301 Interstage Cooler

R-1302 Second-Stage WGS Reactor

E-1302 Low-Pressure Steam Generator

E-1303 Reactor Effluent Cooler

V-1301 Shifted Syngas Separator

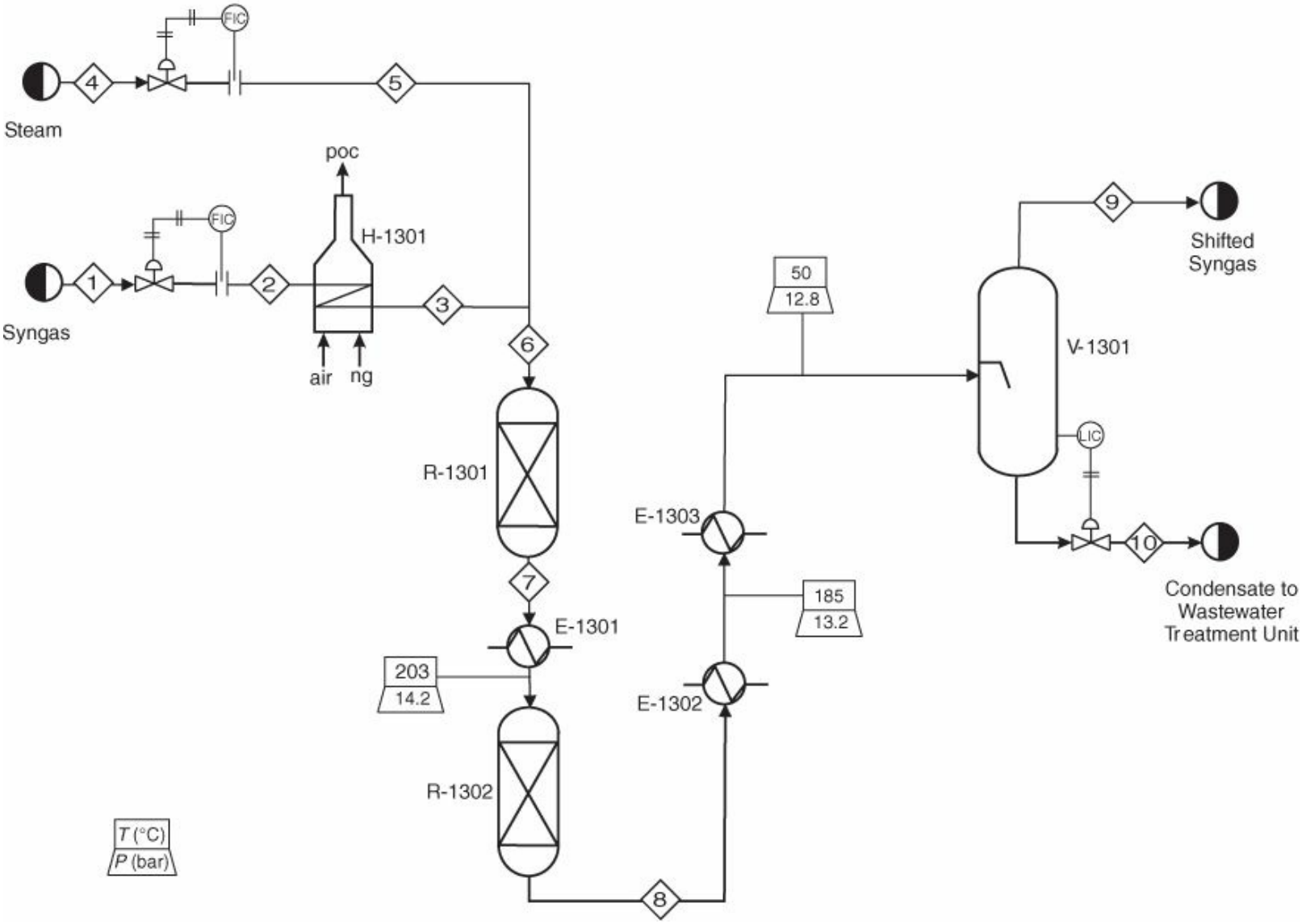


Figure B.12.1. Unit 1300: Shift Reactor Unit Flow Diagram

Table B.12.1. Stream Table for Unit 1300

Stream Number	1	3	4	6
Temperature (°C)	115	320	325	319.7
Pressure (bar)	16.7	15.2	16.2	15.2
Vapor fraction	1.0	1.0	1.0	1.0
Mass flow (kg/h)	2191.2	2191.2	1678.3	3869.5
Mole flow (kmol/h)	100.0	100.0	93.2	193.2
Component flowrates (kmol/h)				
CO	31.3	31.3	0.0	31.3
CO_2	27.7	27.7	0.0	27.7
H_2	40.2	40.2	0.0	40.2
H_2O	0.8	0.8	93.2	94.0
Stream Number	**7**	**8**	**9**	**10**
Temperature (°C)	425.1	250.1	50	50
Pressure (bar)	14.7	13.8	12.7	11.7
Vapor fraction	1.0	1.0	1.0	0.0
Mass flow (kg/h)	3869.5	3869.5	2705.0	1164.5
Mole flow (kmol/h)	193.2	193.2	128.6	64.6
Component flowrates (kmol/h)				
CO	11.6	3.1	3.1	0.0
CO_2	47.4	55.9	55.9	0.0
H_2	59.9	68.4	68.4	0.0
H_2O	74.3	65.8	1.2	64.6

Table B.12.2. Utility Summary Table for Unit 1300

E-1301	E-1302	E-1303
bfw	bfw	cw
688 kg/h	201 kg/h	90,365 kg/h

Table B.12.3. Major Equipment Summary for Unit 1300

Heat Exchangers	
E-1301 $A = 67.2\ m^2$ Floating head, carbon steel, shell-and-tube design Process stream in tubes $Q = 1580$ MJ/h Maximum pressure rating of 19 bar	**E-1302** $A = 31.7\ m^2$ Floating head, carbon steel, shell-and-tube design Process stream in tubes $Q = 455$ MJ/h Maximum pressure rating of 19 bar
E-1303 $A = 62.2\ m^2$ Floating head, carbon steel, shell-and-tube design Process stream in shell $Q = 3764$ MJ/h Maximum pressure rating of 19 bar	
Reactors	
R-1301 Carbon steel, chromia-promoted iron oxide catalyst Catalyst bed height = 2.8 m Diameter = 0.75 m Maximum pressure rating of 19 bar Maximum allowable catalyst temperature = 477°C	**R-1302** Carbon steel, copper-zinc oxide catalyst Catalyst bed height = 1.9 m Diameter = 0.75 m Maximum pressure rating of 19 bar Maximum allowable catalyst temperature = 288°C
Vessel **V-1301** Vertical Carbon steel Length = 1.83 m Diameter = 0.61 m Maximum pressure rating of 19 bar	
Fired Heater **H-1301** Vertical Required heat load = 696 MJ/h Design (maximum) heat load = 800 MJ/h 75% thermal efficiency Maximum pressure rating of 19 bar	

B.12.4. Reference

1. Rase, H. F., *Chemical Reactor Design for Process Plants, Vol. 2: Case Studies and Design Data* (New York: John Wiley and Sons, 1977).

B.13 Design of a Dual-Stage Selexol Unit to Remove CO_2 And H_2S From Coal-Derived Synthesis Gas, Unit 1400

CO_2 capture and sequestration from coal-derived syngas is being strongly considered to reduce environmental pollution. Because of a number of advantages, such as lower solvent loss, higher selectivity toward H_2S, better thermal stability, better water solubility, and lower circulation rate [1],

dimethyl ether of polyethylene glycol (DEPG, Selexol) is very suitable for selective capture of CO_2 and H_2S when the partial pressure of these acid gases is high.

B.13.1. Process Description

A process flow diagram for the dual-stage Selexol unit [1] is shown in Figure B.13.1. The objective of the plant design is to achieve an overall 80% capture of CO_2 in the process and to ensure that the H_2S content of the clean gas is less than 5 ppmv. In addition, the H_2S concentration in Stream 14 should be 45 mol%. In this project, the dual-stage Selexol unit is configured for selective removal of H_2S (first stage) and CO_2 (second stage) from the sour syngas using the Selexol solvent. Most of the H_2S in the syngas is absorbed in the semi-lean solvent as it passes through the H_2S absorber. The off-gas from the top of the H_2S absorber is sent to the CO_2 absorber. A portion of the loaded solvent from the bottom of the CO_2 absorber is cooled in a water cooler, chilled, and then sent to the H_2S absorber. The rich solvent from the bottom of the H_2S absorber is heated by exchanging heat with the lean solvent from the stripper. Then, the syngas goes to a flash vessel (V-1403), called an H_2S concentrator, that helps to decrease the CO_2 content in the rich solvent. The vapor from the flash vessel is recycled back to the H_2S absorber. The bottom stream from the flash vessel goes to the Selexol stripper, which uses a combination of stripping steam and a reboiler for regenerating the solvent. The stripper off-gas, Stream 14, goes to the Claus unit, where the H_2S concentration must be maintained at a desired value for maintaining the Claus furnace temperature. Along with the stripper, the H_2S concentrator plays a key role in generating the desired H_2S concentration in the feed to the Claus unit. Makeup solvent is mixed with the stripped solvent and sent to the top tray of the CO_2 absorber. The remaining portion of the loaded solvent from the bottom of the CO_2 absorber is heated and sent through a series of two flash vessels, called medium-pressure (MP) and low-pressure (LP) flash vessels, respectively, to recover CO_2 for compression in preparation for storage. The semi-lean solvent leaving the LP flash vessel is pumped by P-1402 and then chilled before returning to the fourth tray of the CO_2 absorber. An NH_3 vapor-compression cycle is usually considered for refrigeration. For simplicity, it can be assumed that a refrigerant is available at –20°C.

B.13.2. Simulation (Aspen Plus) Hints

In this study, the solvent, Selexol, is represented by an Aspen Plus databank component with an average molecular weight of 280. The perturbed chain SAFT (PC-SAFT) EOS based on the statistical associating fluid theory (SAFT) is used to represent the thermophysical and transport property of the Selexol system accurately [2]. The DEPG vapor pressure, liquid density, heat capacity, viscosity, and thermal conductivity of the solvent have been regressed in Aspen Plus using published data [3]. Available data in the open literature on vapor-liquid equilibrium between the DEPG solvent and the selected species have been used to adjust the binary interaction parameters [4]. As mentioned before, the plant should be designed for 80% CO_2 capture, for capturing H_2S such that the H_2S concentration in Stream 14 is about 45 mol%. Because of a very high selectivity of H_2S in Selexol (H_2S solubility is about nine times that of CO_2 in the Selexol solvent), the H_2S content of the clean gas becomes much less than 5 ppmv when 80% CO_2 is captured. Consequently, two design

blocks (or controllers) are used. One design block maintains 80% CO_2 capture by manipulating the flowrate of Stream 10. The other design block maintains the H_2S concentration in Stream 14 by manipulating the operating pressure of V-1403. This flowsheet contains a number of recycle streams along with the design blocks. In addition, considerable mass and heat integration exists. Therefore, an appropriate solution strategy must be considered to avoid convergence failure. In Section 16.3 a number of approaches to solve such problems were outlined. The equation-oriented (EO) method is suggested for this problem where a few iterations can be performed using the sequential modular approach to generate a reasonable initial guess.

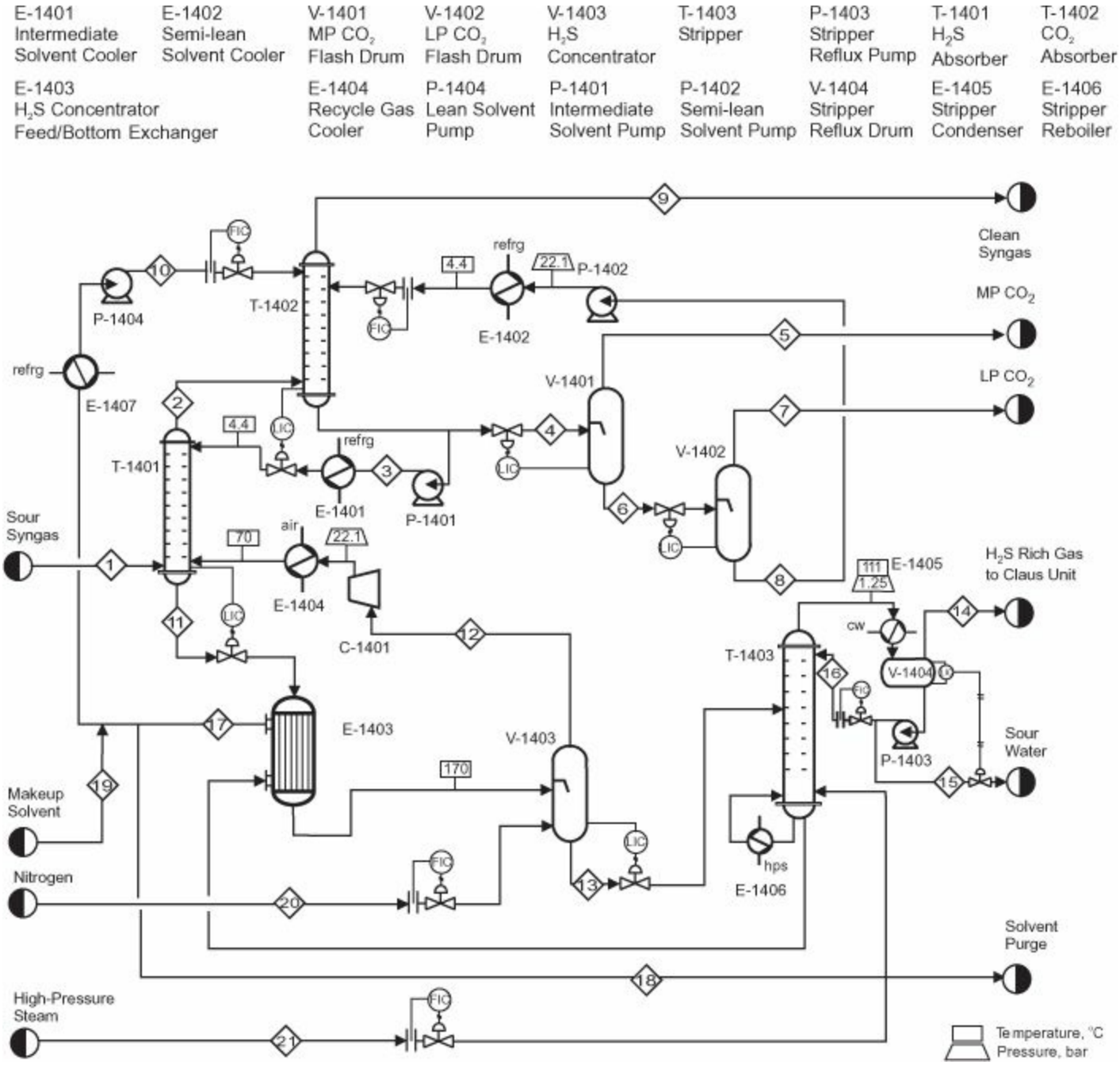


Figure B.13.1. Unit 1400: Selexol Unit Flow Diagram

In Table B.13.3, it can be noted that the duty of heat exchanger E-1403 is very high. Consequently, a large heat-exchange area is calculated. Usually, a proprietary, plate-type heat exchanger is used for this service, which can provide a very high heat-exchange area and achieve a temperature approach as low as 5°C. This can significantly reduce the duties of E-1406 and E-1407.

It should be noted that Stream 5 contains a high amount of H_2. To recover the H_2, the solvent can be

flashed in a vessel that operates at a higher pressure than V-1401, and H_2 can be recycled to T-1402. This introduces another recycle stream. For simplicity, this option is not considered here. Interested students are encouraged to implement this option for H_2 recovery.

Table B.13.1. Stream Table for Unit 1400*

Stream Number	1	2	3	4	5
Temperature (°C)	20.1	7.2	10.8	11.3	9.7
Pressure (bar)	21.4	20.7	23.4	5.1	5.1
Vapor fraction	1.0	1.0	0.0	0.02	1.0
Mass flow (tonne/h)	104.6	123.8	729.1	2209.5	9.62
Mole flow (kmol/h)	5389.0	5888.1	4490.4	13,607.8	270.5
Component flowrates (kmol/h)					
Selexol	0.0	0.0	2430.0	7364.0	0.0
CO	28.8	29.2	0.3	1.0	0.8
CO_2	1114.0	1495.8	446.3	1352.5	187.9
H_2	2468.8	2481.9	13.1	39.8	36.6
H_2O	23.1	4.4	1583.3	4798.1	0.8
N_2	1605.1	1818.3	14.8	44.9	39.4
AR	33.0	34.8	1.3	3.7	2.3
CH_4	48.0	49.2	1.3	3.8	2.7
NH_3	1.1	0.0	0.0	0.0	0.0
		(1.4×10^{-4})	(9.2×10^{-5})	(2.8×10^{-4})	(6.7×10^{-6})
H_2S	67.1	0.0	0.0	0.0	0.0
		(7.9×10^{-4})	(5.5×10^{-4})	(1.7×10^{-3})	(3.2×10^{-5})

*Whenever NH_3 and H_2S flows are low, they are provided inside parentheses for tracking these species through the flowsheet mainly because these species are maintained at a very low level (ppm level) in the clean gas.

Stream Number	6	7	8	9	10
Temperature (°C)	9.7	6.1	6.1	8.2	5.2
Pressure (bar)	5.1	1.5	1.5	20.0	21.7
Vapor fraction	0.0	1.0	0.0	1.0	0.0
Mass flow (tonne/h)	2199.8	28.5	2171.4	66.7	709.04
Mole flow (kmol/h)	13,337.3	655.8	12,681.5	4516.1	4019.2
Component flowrates (kmol/h)					
Selexol	7364.0	0.0	7364.0	0.0	2430.0
CO	0.2	0.2	0.0	27.9	0.0
CO_2	1164.6	638.7	525.9	222.8	0.0
H_2	3.2	3.2	0.0	2429.0	0.0
H_2O	4797.3	6.0	4791.3	3.5	1589.2
N_2	5.5	5.4	0.1	1758.7	0.0
AR	1.4	1.3	0.1	30.0	0.0
CH_4	1.1	1.0	0.1	44.2	0.0
NH_3	0.0	0.0	0.0	0.0	0.0
	(2.7×10^{-4})	(4.2×10^{-5})	(2.29×10^{-4})	(1.4×10^{-6})	(5.0×10^{-11})
H_2S	0.0	0.0	0.0	0.0	0.0
	(1.6×10^{-3})	(2.0×10^{-4})	(1.4×10^{-3})	(5.1×10^{-6})	(2.3×10^{-8})

Stream Number	11	12	13	14	15
Temperature (°C)	12.0	169.3	169.3	50.0	50.0
Pressure (bar)	20.8	10.0	10.0	1.2	5.0
Vapor fraction	0.0	1.0	0.0	1.0	0.0
Mass flow (tonne/h)	738.0	29.2	714.5	5.45	1.54
Mole flow (kmol/h)	4753.8	787.9	4165.9	148.9	85.2
Component flowrates (kmol/h)					
Selexol	2434.2	4.2	2430.0	0.0	0.0
CO	0.3	0.3	0.0	0.0	0.0
CO_2	459.7	395.1	64.6	64.5	0.0
H_2	13.4	13.4	0.0	0.0	0.0
H_2O	1654.5	52.5	1602.0	15.2	85.1
N_2	13.6	212.0	0.9	0.9	0.0
AR	1.3	1.8	0.2	0.2	0.0
CH_4	1.3	1.3	0.0	0.0	0.0
NH_3	3.5	2.4	1.1	1.1	0.0 (0.013)
H_2S	172.0	104.9	67.1	67.0	0.0 (0.081)

Stream Number	16	17	18	19	20	21
Temperature (°C)	50.0	49.0	49.0	30.0	100.0	160.0
Pressure (bar)	1.3	1.2	1.2	1.5	20.0	6.0
Vapor fraction	0.0	0.0	0.0	0.0	1.0	1.0
Mass flow (kg/h)	2.11	709.1	1.5	1.4	5.61	1.63
Mole flow (kmol/h)	117.1	4022.5	8.3	5.0	200.0	90.7
Component flowrates (kmol/h)						
Selexol	0.0	2430.0	5.0	5.0	0.0	0.0
CO	0.0	0.0	0.0	0.0	0.0	0.0
CO_2	0.0	0.0	0.0	0.0	0.0	0.0
H_2	0.0	0.0	0.0	0.0	0.0	0.0
H_2O	116.9	1593.0	3.3	0.0	0.0	90.7
N_2	0.0	0.0	0.0	0.0	199.2	0.0
AR	0.0	0.0	0.0	0.0	0.8	0.0
CH_4	0.0	0.0	0.0	0.0	0.0	0.0
NH_3	0.0 (0.017)	0.0 (5.0×10^{-11})	0.0 (1.0×10^{-13})	0.0	0.0	0.0
H_2S	0.1	0.0 (2.4×10^{-8})	0.0 (4.8×10^{-11})	0.0	0.0	0.0

Table B.13.2. Utility Summary Table for Unit 1400

E-1401	E-1402	E-1405	E-1406	E-1407
refrigerant	refrigerant	cw	hps	refrigerant
5465 kg/h	5798 kg/h	221,400 kg/h	41,400 kg/h	40,032 kg/h

Table B.13.3. Major Equipment Summary for Unit 1400

Heat Exchangers

E-1401
$A = 87.7\ m^2$
Floating head, stainless steel, shell-and-tube design
Process stream in tubes
$Q = 7493$ MJ/h
Maximum pressure rating of 26 bar

E-1402
$A = 100.7\ m^2$
Floating head, stainless steel, shell-and-tube design
Process stream in tubes
Q = 7950 MJ/h
Maximum pressure rating of 25 bar

E-1403
$A = 3344.2\ m^2$
Stainless steel, plate type (usually proprietary)
$Q = 270{,}996$ MJ/h
Maximum pressure rating of 24 bar

E-1404
Carbon steel, finned surface air coolers
$Q = 6720$ MJ/h
Maximum pressure rating of 26 bar

E-1405
$A = 76.5\ m^2$
Floating head, carbon steel, shell-and-tube design
Process stream in shell side
$Q = 9229$ MJ/h
Maximum pressure rating of 8 bar

E-1406
$A = 306.9\ m^2$
Floating head, carbon steel, shell-and-tube design
Process stream in shell side
$Q = 70{,}402$ MJ/h
Maximum pressure rating of 8 bar

E-1407
$A = 436.5\ m^2$
Floating head, stainless steel, shell-and-tube design
Process stream in tubes
$Q = 54{,}893$ MJ/h
Maximum pressure rating of 8 bar

Pumps

P-1401
Centrifugal
Carbon steel
Actual power = 85.2 kW
Efficiency 75%

P-1402
Centrifugal
Carbon steel
Actual power = 1485.1 kW
Efficiency 78%

P-1403
Centrifugal
Carbon steel
Actual power = 0.7 kW
Efficiency 70%

P-1404
Centrifugal
Carbon steel
Actual power = 505.0 kW
Efficiency 75%

Towers	
T-1401 Carbon steel 12 valve trays 24-in tray spacing Column height = 18.0 m Diameter = 3.0 m Maximum pressure rating of 26 bar	**T-1402** Carbon steel 13 valve trays 24-in tray spacing Column height = 25.0 m Diameter = 5.2 m Maximum pressure rating of 25 bar
T-1403 Carbon steel 8 valve trays plus reboiler and condenser 24-in tray spacing Column height = 16.2 m Diameter = 3.6 m Maximum pressure rating of 8 bar	
Vessel	
V-1401 Vertical Carbon steel Length = 15.60 m Diameter = 5.20 m Maximum pressure rating of 25 bar	**V-1402** Vertical Carbon steel Length = 15.45 m Diameter = 5.15 m Maximum pressure rating of 25 bar
V-1403 Vertical Carbon steel Length = 11.20 m Diameter = 3.73 m Maximum pressure rating of 26 bar	**V-1404** Vertical Carbon steel Length = 2.14 m Diameter = 0.71 m Maximum pressure rating of 8 bar
Compressor **C-1401** Carbon steel W = 926,466 kW 75% isentropic efficiency	

B.13.3. References

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B.14. Design of a Claus Unit For the Conversion of H_2S to Elemental Sulfur,

Unit 1500

The Claus process is one of the most common processes for sulfur recovery from acid gases generated in oil and gas refining. The Claus unit is designed to recover sulfur from the acid gas recovered from an acid-gas removal (AGR) unit and the sour gas produced from a sour-water stripper (SWS).

B.14.1. Process Description

The PFD of the Claus process is shown in Figure B.14.1. The Claus unit is designed so that it can process acid and sour-water gases generated in the operation of an integrated gasification combined cycle (IGCC) power plant. Efficient design of a Claus process depends upon high recovery of sulfur and complete destruction of other impurities such as methane and ammonia [1–4]. It should be noted that elemental sulfur, in the operating temperature range of the Claus unit, can exist as S_2 and S_8, among others. For simplicity, only these two sulfur species will be considered.

Acid gas, Stream 2, from an acid-gas removal unit and sour-water gas, Stream 3, from the sour-water stripper are preheated in E-1502 and E-1503, respectively, with high-pressure steam and sent to the reaction furnace, H-1501, for combustion. Preheated, enriched oxygen from an air separation unit (ASU) is used as the oxidant in H-1501. Within the furnace, incomplete combustion of hydrogen sulfide to sulfur dioxide is carried out. Additionally, partial combustion of ammonia can also take place. It is desired that only one-third of the hydrogen sulfide contained in the gases be combusted to form a 2/1 ratio of hydrogen sulfide to sulfur dioxide. This 2/1 ratio of hydrogen sulfide to sulfur dioxide is required to maximize sulfur yield in the downstream reactors. Primary combustion reactions within H-1501 are

$$H_2S + \frac{3}{2}O_2 \xrightarrow{k_1} SO_2 + H_2O \qquad \text{(B.14.1)}$$

$$NH_3 + \frac{3}{4}O_2 \xrightarrow{k_2} \frac{1}{2}N_2 + \frac{3}{2}H_2O \qquad \text{(B.14.2)}$$

These highly exothermic reactions increase the temperature substantially (to about 1450°C) in H-1501. Several side reactions take place. The side reaction shown in Equation (B.14.6) destroys any ammonia not combusted in Reaction (B.14.2).

$$H_2S + SO_2 + H_2 \overset{k_3}{\rightleftharpoons} S_2 + 2H_2O \qquad \text{(B.14.3)}$$

$$H_2S \overset{k_4}{\rightleftharpoons} \frac{1}{2}S_2 + H_2 \qquad \text{(B.14.4)}$$

$$CO_2 + H_2 \overset{k_5}{\rightleftharpoons} CO + H_2O \qquad \text{(B.14.5)}$$

$$NH_3 + \frac{3}{4}SO_2 \xrightarrow{k_6} \frac{1}{2}N_2 + \frac{3}{2}H_2O + \frac{3}{8}S_2 \qquad \text{(B.14.6)}$$

The hot process gas is then cooled in E-1504 to generate high-pressure steam and to quench the reactions taking place. At high operating temperatures, such as those in H-1501, sulfur exists primarily as S_2. As the cooling takes place in E-1504, the equilibrium shifts as shown in Equation B.14.7. Due to the equilibrium shift, the primary sulfur species present at the outlet of E-1504 is S_8.

$$S_2 \overset{k_7}{\rightleftharpoons} \frac{1}{4}S_8 \qquad \text{(B.14.7)}$$

Further cooling is carried out in E-1505 by generating low-pressure steam. This cooled process gas is then sent to V-1501 to separate the liquid sulfur. The process gas is then sent to the first stage of a two-stage process. The process gas is heated in E-1506 with high-pressure steam before being sent to the reactor R-1501, where hydrogen sulfide and sulfur dioxide react in a 2/1 ratio to form elemental sulfur via Equation (B.14.8) (known as the Claus reaction). The reactor effluent is then cooled by generating low-pressure steam in E-1507. The liquid sulfur is then removed in V-1502. The process gas is again preheated in E-1508 with high-pressure steam. The heated gas is sent to the second-stage catalytic reactor R-1502, where the reaction shown in Equation (B.14.8) takes place. The reactor effluent is cooled in E-1509 using cooling water to condense the formed sulfur. The process gas is then sent to a tail-gas treatment unit (not modeled here).

$$H_2S + \frac{1}{2}SO_2 \overset{k_8}{\rightleftharpoons} \frac{3}{16}S_8 + H_2O \qquad \text{(B.14.8)}$$

B.14.2. Reaction Kinetics

Modeling of H-1501 can be simplified by assuming two zones within H-1501: an oxygen-rich zone (known as the flame zone) where faster, exothermic combustion reactions prevail, followed by an oxygen-deficient zone (known as the anoxic zone) where slower, endothermic equilibrium reactions take place.

The combustion reactions will take place homogeneously within the gas phase. The rate equations are of the form [1]

$$-r_i = k_{o,i} \exp\left[\frac{-E_i}{RT}\right] p_{H_2S}^a p_{NH_3}^b p_{O_2}^c \qquad \text{(B.14.9)}$$

where i is the equation number (B.14, i), and

i	E_i kcal/kmol	$k_{o,i}$	a	b	c
1	11,000	1.40×104	1	0	1.5
2	40,000	4.43×106	0	1	0.75

The units of r_i are kmol/s/m^3-reactor, the units of p_i are atm, and the units of $k_{o,i}$ vary depending upon the form of the equation.

The rate equations for the reactions in Equations (B.14.3) through (B.14.6) are [1]

$$-r_3 = 3.58 \times 10^7 \exp\left[\frac{-26.0}{RT}\right]\left(p_{H_2S}p_{SO_2}p_{H_2} - \exp\left[-0.949 - \frac{5840}{T}\right]p_{S_2}p_{H_2O}^2\right) \qquad \text{(B.14.10)}$$

$$-r_4 = 9.17 \times 10^5 \exp\left[\frac{-45.0}{RT}\right]\left(p_{H_2S}p_{S_2}^{0.5} - \exp\left[-5.93 + \frac{10{,}880}{T}\right]p_{S_2}p_{H_2}\right) \qquad \text{(B.14.11)}$$

$$-r_5 = 1.52 \times 10^{12} \exp\left[\frac{-60.3}{RT}\right]\left(C_{CO_2}C_{H_2}^{0.5} - \exp\left[-3.88 + \frac{4166}{T}\right]\frac{C_{CO}C_{H_2O}}{C_{H_2}^{0.5}}\right) \qquad \text{(B.14.12)}$$

$$-r_6 = 2.29 \times 10^4 \exp\left[\frac{-27.5}{RT}\right]C_{NH_3}^{0.25}C_{SO_2}^{0.5} \qquad \text{(B.14.13)}$$

The units of r_i are kmol/s/m^3-reactor, the units of p_i are atm, and the units of C_i are kmol/m^3.

The temperature dependence of the equilibrium between S_2 and S_8 shown in Equation (B.15.7) is given as [1]

$$K_p = \exp\left[-53.67 + \frac{47{,}800}{T[K]}\right] \quad \text{(B.14.14)}$$

The reaction in Equation (B.14.7) is modeled in E-1504.

Equation (B.14.8) is catalyzed in R-1501 and R-1502 by either an alumina or a titanium catalyst. Since Equation (B.14.8) is equilibrium limited and mildly exothermic, the maximum allowable temperature of the catalyst is not a concern. However, significant catalyst deactivation occurs when the temperature is lowered below the dew point of sulfur, since the sulfur will deposit on the catalyst. For this reason, each reactor is operated at a sufficiently high temperature to ensure that no sulfur condenses and deposits on the catalyst. The rate equation for Equation (B.14.8) is [1]

$$-r_8 = 5360 \exp\left[\frac{-7.35}{RT}\right]\left(\frac{p_{H_2S}p_{SO_2}^{0.5} - \exp\left[8.66 - \frac{5550}{T}\right]p_{H_2O}p_{S_8}^{0.1875}}{\left(1 + 1.14\exp\left[\frac{-0.6}{RT}\right]p_{H_2O}\right)^2}\right) \quad \text{(B.14.15)}$$

The units of r_8 are mol/s/kg-cat, and the units of p_i are atm.

B.14.3 Simulation (Aspen Plus) Hints

Due to the low-pressure operation, the ideal gas law was used to model the Claus process. It should be noted that the Aspen Plus model of H-1501 was achieved by dividing it into two zones: H-1501A to model the flame region, and H-1501B to model the anoxic region. Both sections of the furnace are modeled as adiabatic reactors. As substoichiometric oxygen is provided in the furnace to produce an H_2S/SO_2 ratio of 2/1, H-1501A is modeled as a PFR in which the combustion Equations (B.14.1) and (B.14.2) are considered. This is followed by H-1501B, a PFR, in which Equations (B.14.3) through (B.14.6) are considered. Splitting the reaction furnace into two zones is computationally efficient, since the rates of the combustion reactions occurring in the flame region are greatly different from the reactions occurring in the anoxic region. Very fine discretization is required to capture the rapid changes in composition and temperature that occur as a result of the combustion reactions. For the slower equilibrium reactions occurring in the anoxic region, a much coarser discretization can be used. If all reactions are modeled in parallel and the discretization is not fine enough, the model will fail to converge due to the rapid combustion reactions. If, however, the discretization is fine enough to capture the rapid changes due to the combustion reactions, the time for convergence will unnecessarily be increased due to the very fine discretization used for the equilibrium reactions that is not required.

It should be noted that because only combustion reactions are modeled in H-1501A, the actual size of H-1501A is not significant for steady-state simulations as long as oxygen is completely consumed. It should also be noted that in "real" Claus furnaces, a waste heat boiler is an integral part of the furnace and is located at the end of the anoxic zone. For convenience, this exchanger is modeled separately as E-1504.

Physical properties data for S_2 and S_8, if not available in a process simulator databank, can be found in Perry's handbook [5].

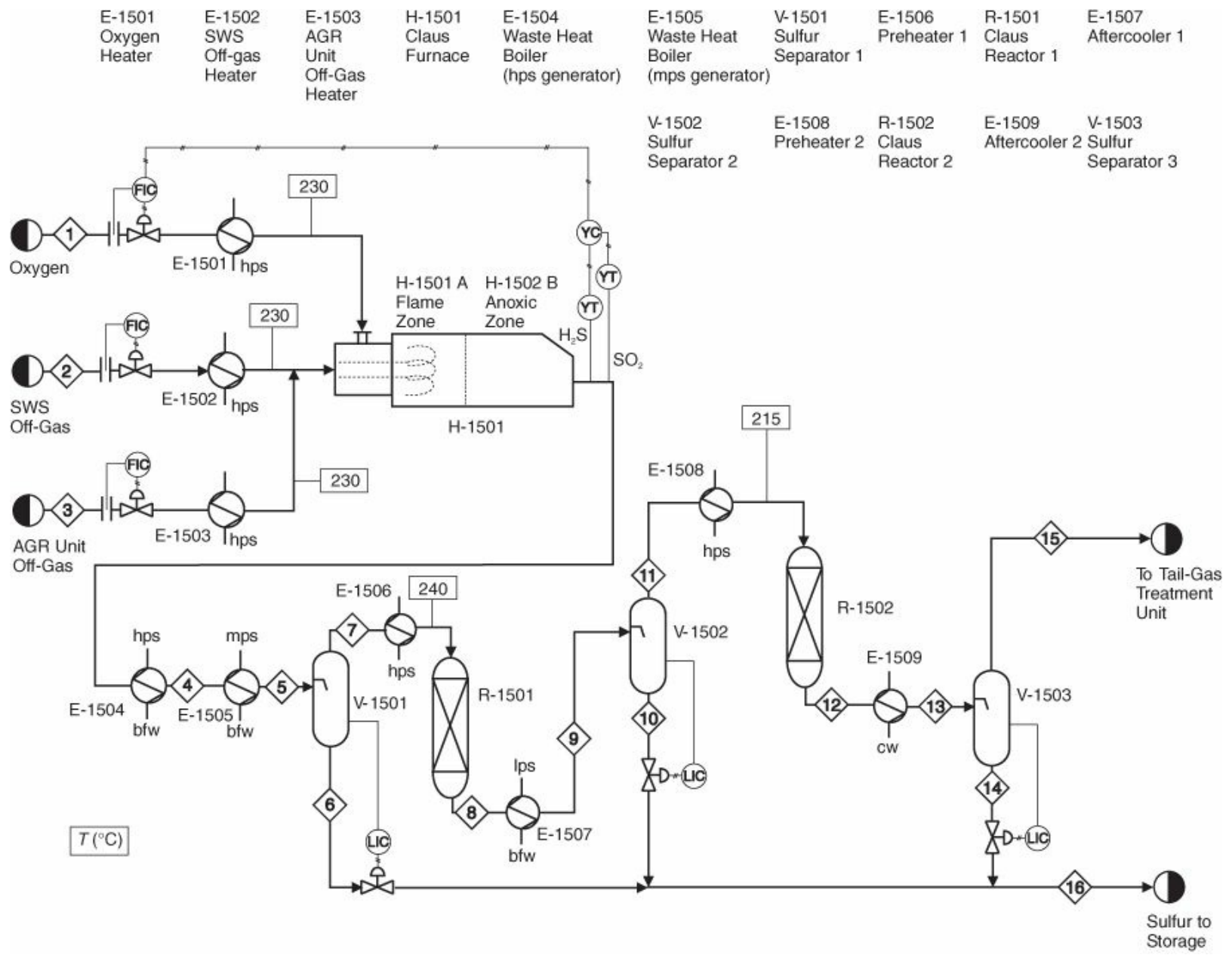


Figure B.14.1. Unit 1500: Claus Unit Process Flow Diagram

Table B.14.1. Stream Table for Unit 1500

Stream Number	1	2	3	4
Temperature (°C)	32	120	50	345
Pressure (bar)	10.0	2.4	2.1	1.7
Vapor fraction	1.0	1.0	1.0	1.0
Mass flow (tonne/h)	3.01	2.2	14.4	19.6
Mole flow (kmol/h)	94.7	85.9	388.1	553.9
Component flowrates (kmol/h)				
Hydrogen sulfide	0.0	23.9	159.1	40.3
Sulfur dioxide	0.0	0.0	0.0	20.1
Water	0.0	0.0	15.6	203.5
Carbon dioxide	0.0	16.9	174.1	142.8
Carbon monoxide	0.0	2.1	0.0	50.3
Oxygen	90.0	0.0	0.0	0.0
Hydrogen	0.0	10.2	0.0	24.2
Nitrogen	4.7	1.3	31.3	57.1
Ammonia	0.0	31.6	7.9	0.0
S_2	0.0	0.0	0.0	0.4
S_8	0.0	0.0	0.0	15.2

Stream Number	5	6	7	8
Temperature (°C)	195	195	195	314
Pressure (bar)	1.6	1.6	1.6	1.3
Vapor fraction	0.97	0.0	1.0	1.0
Mass flow (tonne/h)	19.6	3.72	15.9	15.9
Mole flow (kmol/h)	553.8	15.3	538.5	529.4
Component flowrates (kmol/h)				
Hydrogen sulfide	40.3	0.0	40.3	11.1
Sulfur dioxide	20.1	0.0	20.1	5.5
Water	203.5	0.7	202.8	232.0
Carbon dioxide	142.8	0.0	142.8	142.8
Carbon monoxide	50.3	0.0	50.3	50.3
Oxygen	0.0	0.0	0.0	0.0
Hydrogen	24.2	0.0	24.2	24.2
Nitrogen	57.1	0.0	57.1	57.1
Ammonia	0.0	0.0	0.0	0.0
S_2	0.2	0.2	0.0	0.1
S_8	15.3	14.4	0.9	6.3

Stream Number	9	10	11	12
Temperature (°C)	175	175	175	234
Pressure (bar)	1.2	1.2	1.2	1.0
Vapor fraction	0.99	0.0	1.0	1.0
Mass flow (tonne/h)	15.9	1.51	14.4	14.4
Mole flow (kmol/h)	529.4	6.3	523.1	520.9
Component flowrates (kmol/h)				
Hydrogen sulfide	11.1	0.0	11.1	4.0
Sulfur dioxide	5.5	0.0	5.5	2.0
Water	232.0	0.4	231.6	238.8
Carbon dioxide	142.8	0.0	142.8	142.8
Carbon monoxide	50.3	0.0	50.3	50.3
Oxygen	0.0	0.0	0.0	0.0
Hydrogen	24.2	0.0	24.2	24.2
Nitrogen	57.1	0.0	57.1	57.1
Ammonia	0.0	0.0	0.0	0.0
S_2	0.1	0.1	0.0	0.0
S_8	6.3	5.8	0.5	1.8
Stream Number	**13**	**14**	**15**	**16**
Temperature (°C)	160	160	160	187
Pressure (bar)	0.9	0.9	0.9	0.9
Vapor fraction	1.0	0.0	1.0	0.0
Mass flow (tonne/h)	14.4	0.38	14.0	5.61
Mole flow (kmol/h)	520.9	1.6	519.3	23.15
Component flowrates (kmol/h)				
Hydrogen sulfide	4.0	0.0	4.0	0.0
Sulfur dioxide	2.0	0.0	2.0	0.0
Water	238.8	0.1	238.7	1.2
Carbon dioxide	142.8	0.0	142.8	0.0
Carbon monoxide	50.3	0.0	50.3	0.0
Oxygen	0.0	0.0	0.0	0.0
Hydrogen	24.2	0.0	24.2	0.0
Nitrogen	57.1	0.0	57.1	0.0
Ammonia	0.0	0.0	0.0	0.0
S_2	0.0	0.0	0.0	0.3
S_8	1.8	1.5	0.4	21.7

Table B.14.2. Utility Summary Table for Unit 1500

E-1501	E-1502	E-1503	E-1504
hps	hps	hps	bfw
334.4 kg/h	213.0 kg/h	1574 kg/h	12,382 kg/h

E-1505	E-1506	E-1507	E-1508	E-1509
bfw	hps	bfw	hps	cw
1574 kg/h	531.2 kg/h	1272 kg/h	449.1 kg/h	34,320 kg/h

Table B.14.3. Major Equipment Summary for Unit 1500

Heat Exchangers

E-1501
$A = 84.8\ m^2$
Floating head, carbon steel, shell-and-tube design
Process stream in tubes
$Q = 565$ MJ/h
Maximum pressure rating of 2 bar

E-1502
$A = 54.0\ m^2$
Floating head, carbon steel, shell-and-tube design
Process stream in tubes
$Q = 360$ MJ/h
Maximum pressure rating of 2 bar

E-1503
$A = 114.0\ m^2$
Floating head, carbon steel, shell-and-tube design
Process stream in tubes
$Q = 2659$ MJ/h
Maximum pressure rating of 2 bar

E-1504
$A = 193.7\ m^2$
Floating head, carbon steel, shell-and-tube design
Process stream in tubes
$Q = 28{,}660$ MJ/h
Maximum pressure rating of 2 bar

E-1505
$A = 112.9\ m^2$
Fixed head, carbon steel, shell-and-tube design
Process stream in tubes
$Q = 3619$ MJ/h
Maximum pressure rating of 2 bar

E-1506
$A = 103.3\ m^2$
Floating head, carbon steel, shell-and-tube design
Process stream in tube
$Q = 897$ MJ/h
Maximum pressure rating of 2 bar

E-1507
$A = 105.1\ m^2$
Floating head, carbon steel, shell-and-tube design
Process stream in tube
$Q = 2898$ MJ/h
Maximum pressure rating of 2 bar

E-1508
$A = 48.3\ m^2$
Floating head, carbon steel, shell-and-tube design
Process stream in shell
$Q = 759$ MJ/h
Maximum pressure rating of 2 bar

E-1509
$A = 48.3\ m^2$
Floating head, carbon steel, shell-and-tube design
Process stream in tube
$Q = 1434$ MJ/h
Maximum pressure rating of 2 bar

Reaction Furnace	
R-1501A	**R-1501B**
Furnace (flame zone)	Furnace (anoxic zone)
Refractory lined	Refractory lined
Length = 0.5 m	Length = 4.7 m
Diameter = 2.5 m	Diameter = 2.5 m
Design pressure = 2 bar	Design pressure = 2 bar
Reactors	
R-1501	**R-1502**
Carbon steel	Carbon steel
Packed bed filled with catalyst	Packed bed filled with catalyst
Diameter = 1.22 m	Diameter = 1.22 m
Height = 1.92 m	Height = 1.92 m
Maximum pressure rating of 2 bar	Maximum pressure rating of 2 bar
Vessels	
V-1501	**V-1502**
Horizontal	Horizontal
Carbon steel	Carbon steel
Length = 6.80 m	Length = 5.06 m
Diameter = 2.27 m	Diameter = 1.69 m
Maximum pressure rating of 2 bar	Maximum pressure rating of 2 bar
V-1503	
Horizontal	
Carbon steel	
Length = 5.29 m	
Diameter = 1.76 m	
Maximum pressure rating of 2 bar	

B.14.4. References

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B.15. Modeling a Downward-Flow, Oxygen-Blown, Entrained-Flow Gasifier,

Unit 1600

Gasifiers can be used for generating syngas from coal, petroleum coke (petcoke), biomass, and similar feedstocks. In a gasifier, substoichiometric oxygen is provided to generate syngas with a higher CO/CO_2 ratio. Gasification reactions finally result in substantial conversion of carbon (as high as 98% to 99%). There are various types of gasifiers. In this project, a model of a downward-flow, oxygen-blown, entrained-flow gasifier will be developed.

B.15.1. Process Description

A process flow diagram of the oxygen-blown, entrained-flow gasifier is shown in Figure B.15.1. Illinois no. 6 coal, Stream 1, is mixed with water, Stream 2, to form a slurry. Usually, the slurry is produced in a tank by mixing coal with the appropriate amount of water and then agitating for hours. For simplicity, uniform mixing can be assumed. The slurry along with oxygen (95% pure by weight), Stream 3, is sent to the gasifier. In a typical gasifier operation, the oxygen-to-coal ratio is manipulated to maintain the gasifier exit temperature so that the ash remains molten and it can flow down the gasifier wall. However, it is difficult to measure the gasifier exit temperature reliably and precisely due to the harsh conditions. Therefore, only a ratio controller is shown in Figure B.15.1. The water-to-coal ratio is manipulated to maintain the viscosity of the slurry. A number of reactions take place in a gasifier. For simplicity, only the key reactions will be considered. As the coal enters the gasifier, it gets thermally decomposed, releasing the volatile matter (VM) and tar and leaving behind a high-carbon residue commonly known as char and ash, which contains a number of minerals such as silicon dioxide (SiO_2), aluminum oxide (Al_2O_3), iron oxide (Fe_2O_3), calcium oxide (CaO), and magnesium oxide (MgO). The quantity of the VM can be obtained from the proximate analysis of the coal. The tar produced during the devolatilization reaction cracks further, generating gaseous species and char. For simplicity, char and ash can be assumed to be graphitic carbon and pure silicon dioxide, respectively. The product yield due to devolatilization and tar cracking can be calculated by using the METC Gasifier Advanced Simulation (MGAS) model developed by Syamlal and Bissett [1]. This model is based on analytical data of the coal such as proximate and ultimate assays, tar composition, and so on, from extensive laboratory-scale experiments that characterize the coal. It is assumed that all the sulfur in the coal is converted to H_2S, and all the nitrogen is converted to NH_3. In addition, higher hydrocarbons produced are neglected. As both the devolatilization and tar cracking reactions are usually rapid, they can be combined, and the combined yield of product can be written as

$$Coal \rightarrow \alpha_C C + \alpha_{CO} CO + \alpha_{CO_2} CO_2 + \alpha_{CH_4} CH_4 + \alpha_{H_2} H_2 + \alpha_{H_2O} H_2O + \alpha_{H_2S} H_2S + \alpha_{NH_3} NH_3 + \alpha_{ASH} ASH \quad \text{(B.15.1)}$$

Subsequently, the following reactions take place:

$$CO + 0.5O_2 \xrightarrow{k_1} CO_2 \quad \text{(B.15.2)}$$

$$CH_4 + 2O_2 \xrightarrow{k_2} CO_2 + 2H_2O \quad \text{(B.15.3)}$$

$$H_2 + 0.5O_2 \xrightarrow{k_3} H_2O \quad \text{(B.15.4)}$$

$$C + 0.5O_2 \xrightarrow{k_4} CO \quad \text{(B.15.5)}$$

$$C + CO_2 \xrightarrow{k_5} 2CO \quad \text{(B.15.6)}$$

$$C + H_2O \xrightarrow{k_6} CO + H_2 \quad \text{(B.15.7)}$$

$$CO + H_2O \rightleftharpoons CO_2 + H_2 \quad \text{(B.15.8)}$$

A number of other reactions also take place in the gasifier. For example, hydrogen gasification of char results in methane. Methane participates in methane-steam reforming and methane-CO_2 reforming reactions. There are a number of reactions involving NH_3 that are also not considered here for simplicity. It is very difficult, if not impossible, to calculate precisely the carbon conversion in a gasifier by using the blocks available in commercial process simulators. Complex hydrodynamics, strong interaction between various species, presence of multiple phases, difficulty in characterizing coal, char, tar, and ash are some of the key issues that are difficult to model in a process simulator. For this reason, some deviations from the experimental/literature data will be observed in the Stream 4 results reported in Table B.15.4.

B.15.2. Reaction Kinetics

The product yield (on a mass basis) due to devolatilization and tar cracking (Reaction [B.15.1]) for Illinois no. 6 coal is calculated from Syamlal and Bissett [1] and reported in Table B.15.2.

Table B.15.1. Proximate and Ultimate Analysis of Illinois No. 6 Coal (as Received)

	Proximate				Ultimate				
Coal	Moisture	VM	FC	Ash	C	H	O	N	S
Illinois No. 6	5.86	34.03	50.52	9.59	68.51	4.54	6.98	1.49	3.03

Table B.15.2. Product Yield (Mass Basis) in Reaction (B.15.1) for Illinois No. 6 Coal

Yield Parameter in Reaction (B12.1)	Parameter Value
α_{FC}	0.601
α_{CO}	0.022
α_{CO_2}	0.012
α_{CH_4}	0.096
α_{H_2}	0.010
α_{H_2O}	0.113
α_{H_2S}	0.032
α_{NH_3}	0.018
α_{ASH}	0.096

The reaction kinetics for Reaction (B.15.2) is given by Westbrook and Dryer [2]:

$$-r_{CO} = 8.8 \times 10^{11} \exp\left(-\frac{167{,}504}{RT}\right) C_{O_2}^{0.25} C_{CO} C_{H_2O}^{0.5} \frac{\text{kmol}}{\text{m}^3\text{s}} \quad \text{(B.15.9)}$$

The reaction kinetics for Reaction (B.15.3) is given by Westbrook and Dryer [2]:

$$-r_{CH_4} = 8.47 \times 10^{10} \exp\left(-\frac{202{,}680}{RT}\right) C_{O_2}^{1.3} C_{CH_4}^{0.2} \frac{\text{kmol}}{\text{m}^3\text{s}} \quad \text{(B.15.10)}$$

The reaction kinetics for Reaction (B.15.4) is given by Jones and Lindstedt [3]:

$$-r_{H_2} = 2.72 \times 10^{15} T^{-1} \exp\left(-\frac{167{,}504}{RT}\right) C_{H_2}^{0.25} C_{O_2}^{1.5} \frac{\text{kmol}}{\text{m}^3\text{s}} \quad \text{(B.15.11)}$$

For the char combustion reaction, Equation (B.15.5), the kinetics of the surface reactions available in the open literature for a shrinking-core model [4] is used. For incorporating in a process simulator, the rate expression has been simplified by assuming that the diffusive resistance in the ash layer is the dominating resistance to mass transfer. Further, it is assumed that the char particles have a diameter of 400 μm, and the average operating pressure of the gasifier is 24.5 atm. Subsequently, the reaction kinetics for Equation (B.15.5) can be written as

$$-r_C = 1.63 \times 10^9 \exp\left(-\frac{113{,}070}{RT}\right) y_C^{2/3} y_{O_2} \frac{\text{kmol}}{\text{m}^3\text{s}} \quad \text{(B.15.12)}$$

The kinetics for Equation (B.15.6) is given by Wen et al. [5]:

$$-r_C = 42{,}090 \exp\left(-\frac{175{,}880}{RT}\right) y_C y_{CO_2} \frac{\text{kmol}}{\text{m}^3\text{s}} \quad \text{(B.15.13)}$$

The kinetics for Equation (B.15.7) is given by Wen and Onozaki [5]:

$$-r_C = 42{,}090 \exp\left(-\frac{175{,}880}{RT}\right) y_C y_{H_2O} \frac{\text{kmol}}{\text{m}^3\text{s}} \quad \text{(B.15.14)}$$

The kinetics for Equation (B.15.8) is given by Wen and Onozaki [5]:

$$-r_{CO} = 52.3 \exp\left(-\frac{70{,}071}{RT}\right)\left(y_{CO} y_{H_2O} - \frac{y_{CO_2} y_{H_2}}{K_{eq}}\right) \frac{\text{kmol}}{\text{m}^3\text{s}} \quad \text{(B.15.15)}$$

In Equation (B.15.15),

$$K_{eq} = \exp\left[-3.689 + \frac{4019}{T}\right] \quad \text{(B.15.16)}$$

In the equations provided before, the activation energy is given in kJ/kmol, the units of concentration are kmol/m^3[[FR 3]] (gas), and T is in K whenever a specific unit is needed.

B.15.3. Simulation (Aspen Plus) Hints

In Section 13.7, fundamentals of solids modeling were discussed. Since coal is a heterogeneous mixture of complex materials, it is difficult to calculate its physical properties accurately. Its enthalpy and density can be calculated using appropriate correlations or by using experimental data, if available, at the operating conditions of the gasifier. Coal is declared as type "NC" (nonconventional) in Aspen Plus. The chosen "enthalpy model" is "HCOALGEN," which is a special model for calculating enthalpy of streams comprising coal. A number of empirical correlations are available for calculating heat of combustion, heat of formation, and heat capacity. This enthalpy model can be chosen under Data | Properties | Advanced | NC Props. Selection of correlations can be done by choosing the appropriate "options code" value under "option code" number. The heat of combustion is calculated by the available IGT (Institute of Gas Technology) correlation (option code number 1, value 5), the standard heat of formation is calculated by a heat of combustion-based correlation (option code number 2, value 1), and the heat capacity is calculated by Kirov correlation (option code number 3, value 1). Elements are considered to be in their standard states at 298.15 K and 1 atm (option code number 4, value 1). For calculating the coal density, density model "DCOALIGT" is chosen. This model can be selected under Data|Properties|Advanced|NC Props.

This model uses the IGT correlation for density. For using the models "HCOALGEN" and "DCOALIGT," the proximate, ultimate, and sulfur analyses of coal are needed. The analysis is entered under the tab "Component Attr." of the Stream 1 specification window as per the data provided in Table B.15.1. Sulfur is assumed to be equally distributed in the following "elements": "pyritic," "sulfate," and "organic." In addition, carbon, sulfur, and ash are declared as type "solid," and all other species are declared as "conventional." Stream class "MIXCINC" was chosen so that the substream types "MIXED," "CISOLID," and "NC" are created to support the conventional, solid, and nonconventional species. To promote rapid devolatilization (Equation [B.15.1]) and subsequent combustion of the volatiles (Equations [B.15.2] through [B.15.4]) within a short distance from the entrance of the gasifier, the gasifier burner is designed to promote recirculation of a part of the hot combustion products. The homogeneous and heterogeneous reactions (Equations [B.15.2] through [B.15.8]) continue to take place through the gasifier. To represent these phenomena, a multizonal model can be developed by dividing the gasifier R-1601 into three zones as shown in Figure B.15.2. The first zone is represented by the block R-1601A, where only the reaction in Equation (B.15.1) takes place. R-1601A can be simulated as an "RYield" block. The combustion of the gaseous species (Equations [B.15.2] through [B.15.4]) is considered in the block R-1601B. It is clear from the rate expressions given in Equations (B.15.9) through (B.15.11) that they are very rapid at the gasifier operating temperature (above 1000°C). The oxygen provided is much in excess of the stoichiometric requirement for combustion of the volatiles that get produced in Equation (B.15.1). As a result, reactor R-1601B can be modeled as an "RStoic" reactor in Aspen Plus. The temperature of R-1601A is specified at 500°C, and the required heat is removed from R-1601B. All the homogeneous and heterogeneous reactions (Equations [B.15.2] through [B.15.8]) are considered in R-1601C, which is a PFR. The heat loss to the environment from the gasifier wall is considered by specifying a uniform heat flux from the reactor. Equation (B.15.11) shows that the kinetics of Equation (B.15.4) is very fast. As the gasifier temperature shoots up in the initial region of the gasifier due to the exothermic combustion reactions, reactor R-1601C may fail to converge. The pre-exponential factor in Equation (B.15.11) can be reduced by two to three orders of magnitude to avoid convergence failure. This modification will have negligible effect in the simulation results.

The stream data for the intermediate streams, Stream 51 and Stream 52, are provided in Table B.15.3. Since solids are included in this table and in Table B.15.4, mass flowrates (instead of molar flowrates that are commonly reported in other examples) are given.

Table B.15.3. Stream Table for the Intermediate Streams in Unit 1600

Stream Number	51	52
Temperature (°C)	500	1050
Pressure (bar)	25.3	25.3
Mass flow (tonne/h)	100.0	233.0
Component flowrates (tonne/h)		
Coal	0.0	0.0
C	60.082	60.082
Ash	9.593	9.593
O_2	0.0	40.796
CO	2.157	0.0
H_2	1.027	0.0
CO_2	1.196	30.834
H_2O	11.349	82.018
H_2S	3.221	3.221
N_2	0.0	4.650
CH_4	9.569	0.0
NH_3	1.806	1.806

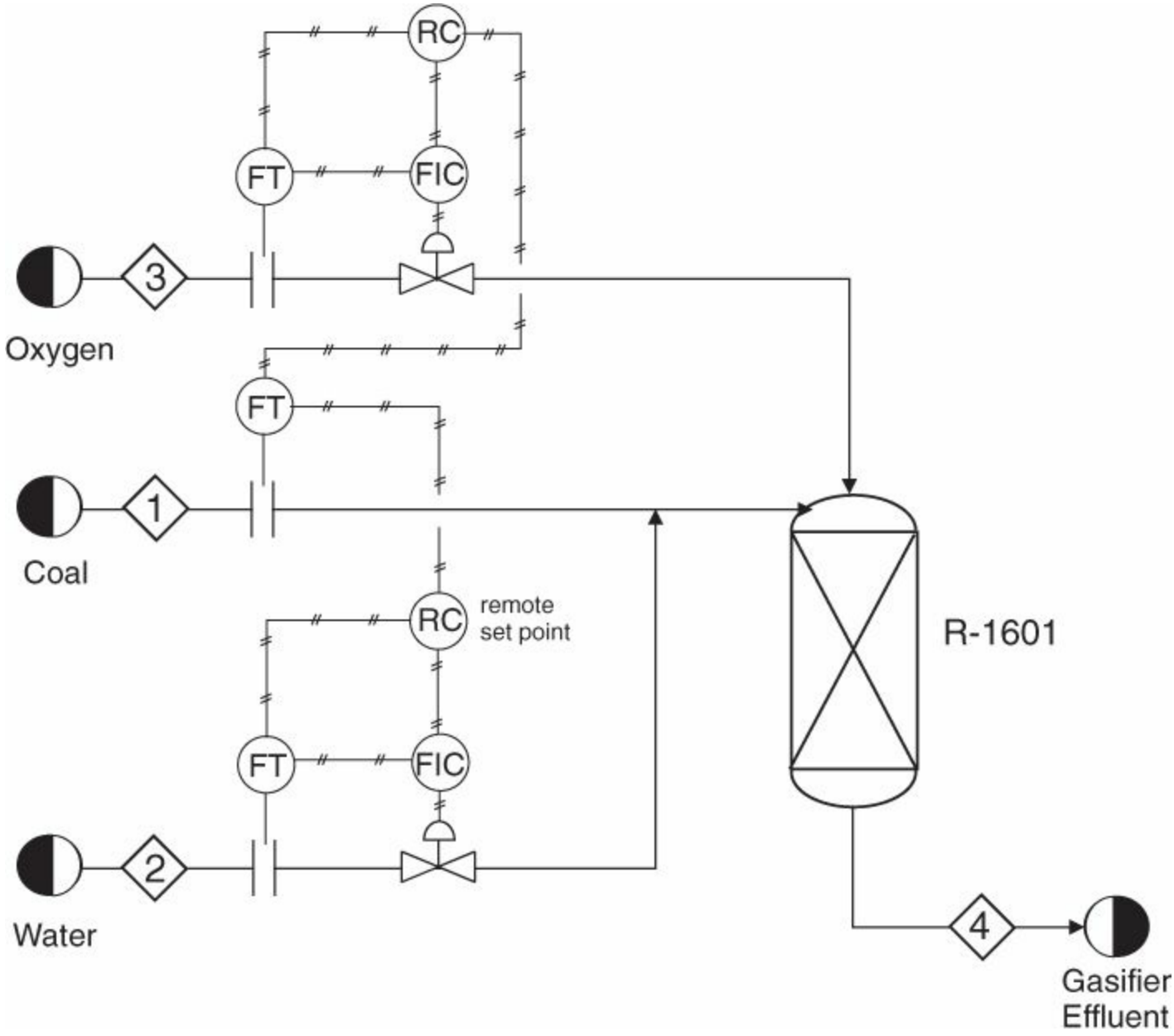


Figure B.15.1. Unit 1600: Flow Diagram of a Downward-Flow, Oxygen-Blown, Entrained-Flow Gasifier

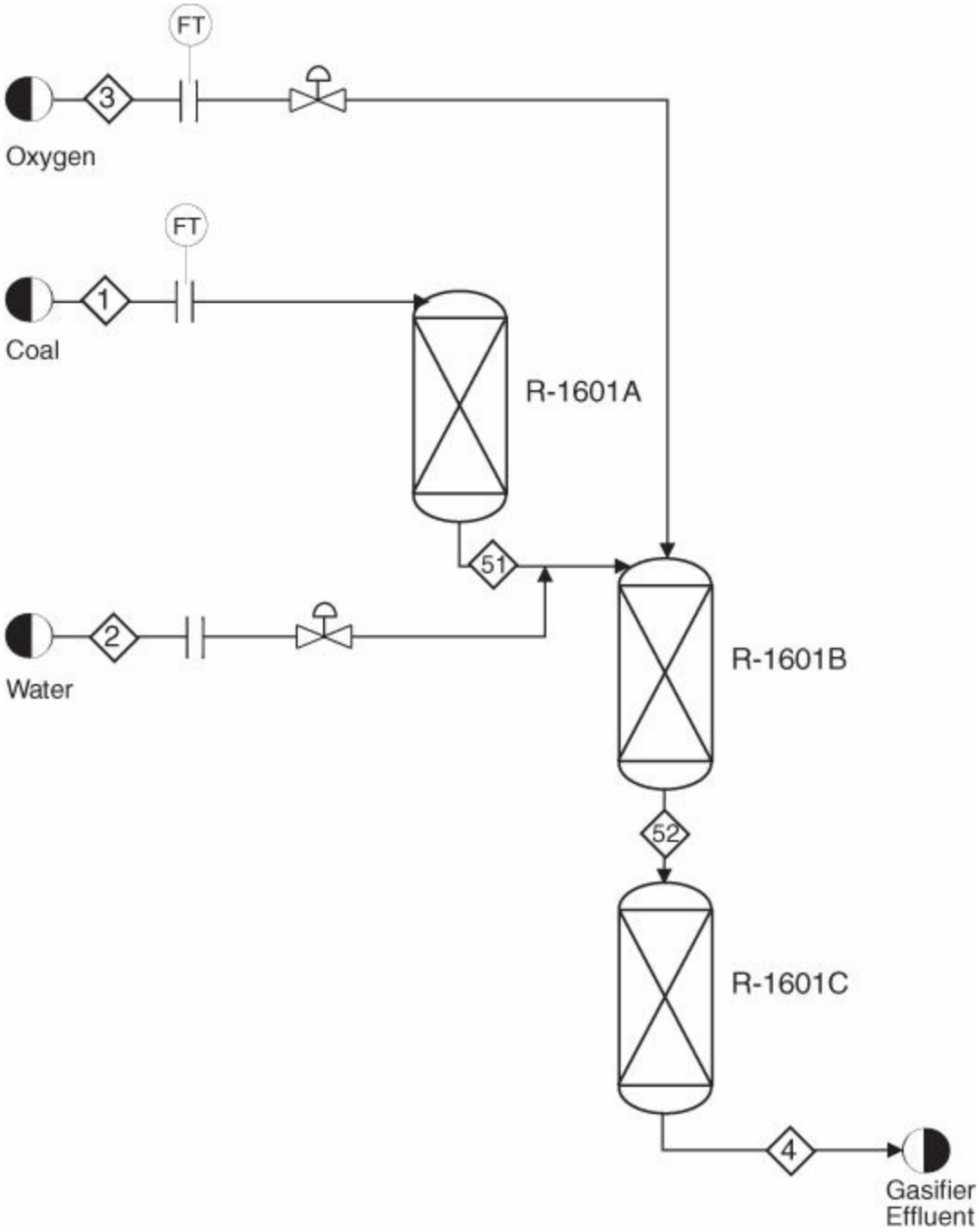


Figure B.15.2. Unit 1600: Multizonal Approach for Modeling a Downward-Flow, Oxygen-Blown, Entrained-Flow Gasifier (Instrumentation Lines Not Shown) (*Note:* This is not a process flow diagram; it is a representation of the simulation strategy.)

Table B.15.4. Stream Table for Unit 1600

Stream No.	1	2	3	4
Temperature (°C)	40	40	50	1143
Pressure (bar)	25.3	26.3	26.3	24.3
Mass flow (tonne/h)	100.0	40.0	93.0	233.0
Component flowrates (tonne/h)				
Coal	100.0	0.0	0.0	0.0
C	0.0	0.0	0.0	3.237
Ash	0.0	0.0	0.0	9.593
O_2	0.0	0.0	88.350	0.0
CO	0.0	0.0	0.0	119.805
H_2	0.0	0.0	0.0	5.319
CO_2	0.0	0.0	0.0	50.884
H_2O	0.0	40.0	0.0	34.485
H_2S	0.0	0.0	0.0	3.221
N_2	0.0	0.0	4.650	4.650
CH_4	0.0	0.0	0.0	0.0
NH_3	0.0	0.0	0.0	1.806

Table B.15.5. Major Equipment Summary for Unit 1600

Reactors **R-1601C** Length = 10 m Diameter = 2 m Maximum pressure rating of 29 bar Maximum allowable temperature = 1900°C Refractory lined Outer wall temperature = 180°C Ambient temperature = 30°C Overall heat transfer coefficient for environmental heat loss calculation = 2 W/m$^{2\circ}$C

B.15.4. References

1. Syamlal, M., and L. A. Bissett, "METC Gasifier Advanced Simulation (MGAS) Model," *Technical Note, NITS Report No. DOE/METC-92/4108*, 1992.
2. Westbrook, C. K., and F. L. Dryer, "Simplified Mechanism for the Oxidation of Hydrocarbon Fuels in Flames," *Combustion Sci. Tech.* 27 (1981): 31–43.
3. Jones, W. P., and R. P. Lindstedt, "Global Reaction Schemes for Hydrocarbon Combustion," *Combustion and Flame* 73 (1988): 233–249.
4. Wen, C. Y., and T. Z. Chaung, "Entrainment Coal Gasification Modeling," *Ind. Eng. Chem Process Des. Dev.* 18 (1979): 684–695.
5. Wen, C. Y., H. Chen, and M. Onozaki, "User's Manual for Computer Simulation and Design of

the Moving Bed Coal Gasifier," *DOE/MC/16474-1390*, 1982.

Appendix C. Design Projects

In this appendix, six design projects are presented. The projects are grouped in pairs, with each pair of projects focused on a given process. The first project in each pair (Projects 1, 3, and 5) deals with an existing facility in which a problem has arisen or in which a change of operating conditions is desired. These types of problems are typically encountered in real operating plants and would be the type of project a young engineer might encounter in his or her first year or two in the plant. These problems often are not completely defined, and not all information is available. In addition, a solution to the problem is required in a fairly short period of time. This situation is not unheard of in the workplace and forces the engineer to make assumptions and analyze situations in which not all the operating variables are known. In analyzing these problems, the information in Section 4, Chapters 19–24, will be very useful. It is not recommended that these problems be given to students without some coverage of the material given in Section 4 of the text.

The second project in each pair (Projects 2, 4, and 6) is more like the typical "design" project that is covered in the senior capstone design course. Here, the student (or group of students) should be familiar with the information given in Sections 1, 2, and 3 and the guidelines for written reports given in Chapter 29 (in this CD).

In the authors' collective experience, the most worthwhile learning experience for the student is obtained during an oral presentation in which the student (or group of students) presents the results to a group of faculty and then defends his or her solutions in a 30–40-minute question-and-answer period. If this method of examination is chosen, the information in Chapter 29 (in this CD) on oral presentations will also be of use.

A note is made to any experienced engineer who may come upon these projects. It is recognized that some of the information given in the flow diagrams reflects poor (and sometimes extremely poor) engineering judgment. In fact, parts of some of the flow diagrams are almost caricatures of how the plant should be designed and operated. This is done intentionally, with the hope that the student will be able to find these gross errors and recommend improvements. The bottom line is that if, by doing these projects, the student can find errors and make improvements, then the transition from student to practicing engineer will have started, and we will have fulfilled our objective in writing this text.

Additional design projects for a variety of processes, suitable for sophomore through senior classes, can be found at our Web site:
http://www2.cemr.wvu.edu/~wwwche/publications/projects/index.html.

Finally, background information for this appendix was obtained from the following sources:

1. *Kirk-Othmer Encyclopedia of Chemical Technology,* 3rd ed. (New York: John Wiley and Sons, 1978).
2. McKetta, J. J., and W. A. Cunningham, eds., *Encyclopedia of Chemical Processing and Design* (New York: Marcel Dekker, 1976).
3. Rase, H. F., *Chemical Reactor Design for Process Plants*, Vol. 2 (New York: John Wiley and Sons, 1977).

Project 1. Increasing the Production of 3-Chloro-1-Propene (Allyl Chloride) in Unit 600

C.1.1. Background

You are currently employed by the TBWS Corp. at the Beaumont, Texas, plant, and you have been assigned to the allyl chloride facility. A serious situation has developed at the plant, and you have been assigned to assist with troubleshooting the problems that have arisen.

Recently, our sister plant in Alabama was shut down by the EPA (Environmental Protection Agency) for violations concerning sulfur dioxide emissions from a furnace in the allyl chloride facility. Fortunately, the Beaumont facility had switched to natural gas as a fuel for its process in early 2000 and hence is currently in compliance with the EPA and Texas regulations. However, the loss of the Alabama plant, albeit for a short time only, has put considerable pressure on the Beaumont plant to fulfill contractual obligations to our customers in Alabama for allyl chloride. Thus, part of your assignment is to advise management concerning the increase in production of allyl chloride that can be made at the Beaumont facility.

Another related issue that has been discussed by management is the long-term profitability of both allyl chloride facilities. Allyl chloride is used as a precursor in the production of allyl alcohol, glycerin, and a variety of other products used in the pharmaceutical industry. More efficient plants have been built recently by our competitors, and we are being squeezed slowly out of the market by these rival companies. We still maintain a loyal customer base due to our excellent technical and customer service departments and our aggressive sales staff. However, we have been losing an ever-increasing share of the market since the mid-2000s. At present, the future looks bleak, and if the profitability and efficiency of our facilities do not increase in the near future, we may well be shut down in the next year or two, when some of our long-term contracts come up for renewal. A second part of your assignment is to look into the overall profitability of the Beaumont allyl chloride facility and determine whether any significant improvements in the overall economics can be made.

C.1.2 Process Description of the Beaumont Allyl Chloride Facility

A process flow diagram (PFD) of the allyl chloride facility is provided in Figure C.1. This process (Unit 600) is the one to which you have been assigned.

Allyl chloride is produced by the thermal chlorination of propylene at elevated temperatures and relatively low pressures. Along with the main reaction, several side reactions also take place. These are shown below.

Main Reaction

$$C_3H_6 + Cl_2 \rightarrow \underset{\textit{allyl chloride}}{C_3H_5Cl} + HCl \qquad \Delta H_{reac,298K} = -112\ \text{kJ/mol}$$

Side Reaction

$$C_3H_6 + Cl_2 \rightarrow \underset{\textit{2-chloropropene}}{C_3H_5Cl} + HCl \qquad \Delta H_{reac,298K} = -121\ \text{kJ/mol}$$

Side Reaction

$$C_3H_6 + 2Cl_2 \rightarrow \underset{\textit{dichloropropene}}{C_3H_4Cl_2} + 2HCl \qquad \Delta H_{reac,298K} = -222\ \text{kJ/mol}$$

Side Reaction

$$C_3H_6 + 3Cl_2 \rightarrow 3C + 6HCl \qquad \Delta H_{reac,298K} = -306\ \text{kJ/mol}$$

carbon

H-601	R-601	J-601	E-601	P-601 A/B	E-602	E-603
Reactor Feed Heater	Fluidized-Bed Reactor	Jet Mixer	Dowtherm Cooler	Dowtherm Pumps	Waste-Heat Boiler	CrudeAllyl Chloride Cooler

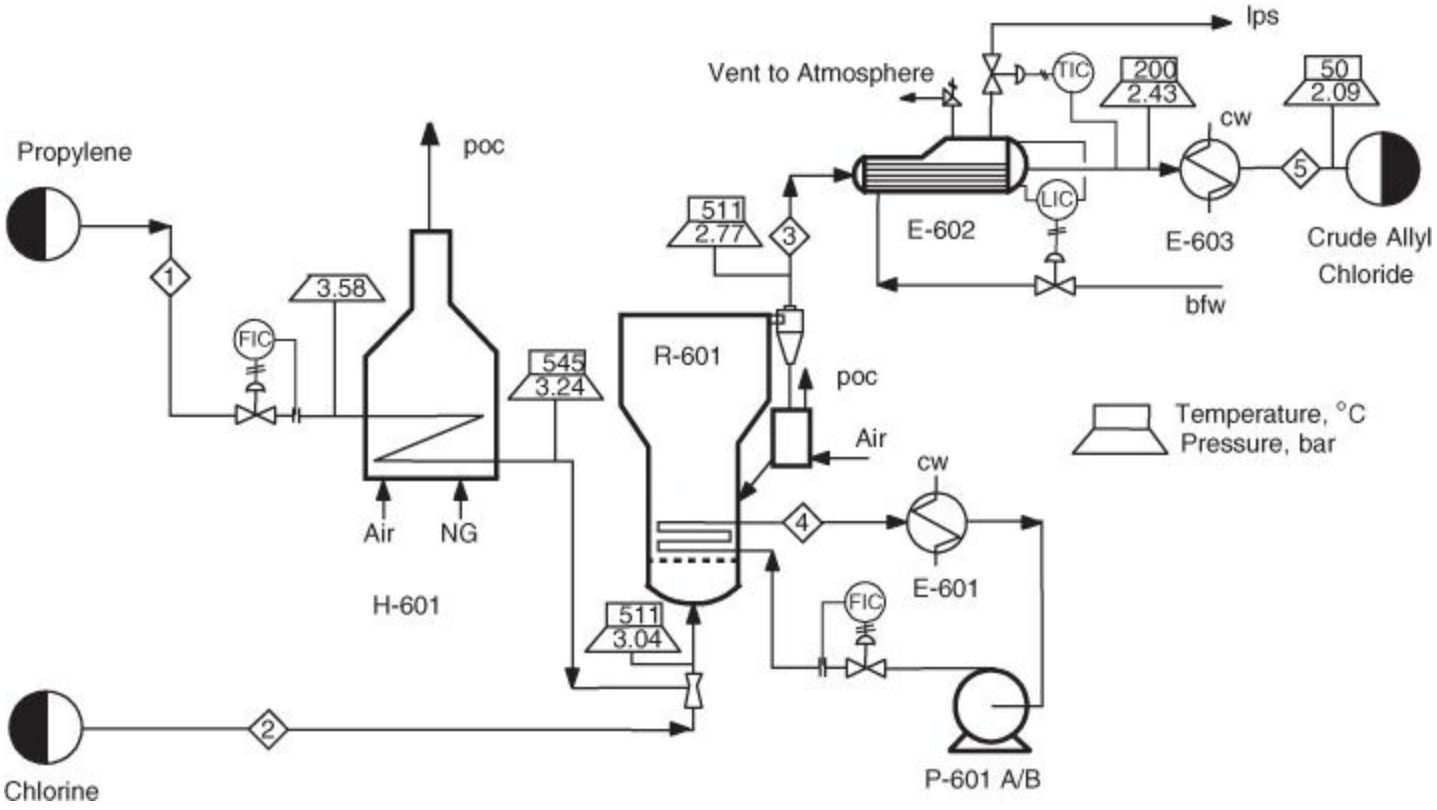


Figure C.1. Process Flow Diagram for the Production of Allyl Chloride (Reaction Section)

The propylene feed is heated in a furnace, fired by natural gas, and brought up to reaction temperature (design conditions are given in Tables C.1 and C.2). The chlorine is mixed with the hot propylene in a mixing nozzle and then fed to the reactor.

During the thermal chlorination process, a significant amount of carbon can be produced, and it has a tendency to deposit on equipment that operates at temperatures greater than 400°C. For this reason, the reactor chosen for this process is a fluidized bed with an inert solid, sand, on the reaction side. The sand provides a large surface area on which the carbon can deposit. It also acts as a scouring agent on the immersed heat transfer tubes in the reactor and prevents the buildup of carbon on the heat transfer surfaces. The carbon, which deposits preferentially on the sand, is removed by combustion in the solids regeneration unit shown in Figure C.1. The regenerated sand is sent back to the reactor, thus maintaining a constant inventory of solids in the reactor. The heat produced in the reactor, by the exothermic chlorination reactions, is removed via the heat transfer tubes through which is circulated a heat transfer medium. The heat transfer fluid is a commercially available coolant called Dowtherm A. Physical properties of this fluid are included in Table C.3 of this assignment.

Table C.1. Flow Summary Table for Unit 600: Crude Allyl Chloride Production Facility

Stream Number	1	2	3	4	5
Temperature (°C)	25	25	511	400	50
Pressure (bar)	11.7	6.44	2.77	11.34	2.09
Vapor fraction	1.0	1.0	1.0	0.0	1.0
Mass flowrate (tonne/h)	3.19	1.40	4.59	16.63	4.59
Molar flowrate (kmol/h)					
Propylene	75.89	—	58.08	—	58.08
Chlorine	—	19.70	—	—	—
Allyl chloride	—	—	15.56	—	15.56
Dichloropropene	—	—	0.46	—	0.46
Dichloropropene	—	—	1.81	—	1.81
Hydrogen chloride	—	—	19.70	—	19.70
Carbon	—	—	*	—	—
Dowtherm A	—	—	—	4.62 kg/s	—
Total mole flow (kmol/h)	75.89	19.70	95.61	4.62 kg/s	95.61

Equipment	Fuel gas (std m^3/h)	Cooling water (kg/s)	bfw (kg/s)	Steam (kg/s)
H-601	131†	—	—	—
E-601	—	14.5 T_{in} = 30°C T_{out} = 40°C	—	—
E-602	—	—	0.333 (90°C)	0.333 (sat. at 6 bar)
E-603	—	6.82 T_{in} = 30°C T_{out} = 40°C	—	—

*Carbon is formed, but at a rate that does not affect the material balance.

†Actual gas flowrate shown; heater efficiency is 90%.

Table C.2. Equipment Design Parameters (Unit 600)

J-601 Jet Mixer

Pressure Drop = 0.20 bar at design conditions
Operating Pressure = 3.24 bar (normal)
= 5.00 bar (maximum)

H-601 Reactor Feed Preheater

Process Side Conditions

Duty = 4000 MJ/h (normal)
5400 MJ/h (maximum)
Operating Pressure = 3.58 bar (normal)
= 4.50 bar (maximum)
Operating Temperature = 545°C (maximum)

R-601 Fluidized-Bed Reactor

Operating Temperature = 511°C (normal)
= 525°C (maximum)
Operating Pressure = 3.04 bar (normal)
= 4.50 bar (maximum)

Dimensions

Square cross section 3.1 × 3.1 m, vessel height = 5 m
Fluidized-bed height = 1.5 m
Heat transfer area = 23.0 m^2
Normal duty = 2188 MJ/h

P-601 A/B Dowtherm A Circulation Pumps

Operating Pressure = 11.0 bar (normal)
= 15.0 bar (maximum)
Operating Temperature = 350°C (normal)
= 400°C (maximum)
ΔP (normal) = 1.55 bar (22.6 psi)
ΔP (maximum) = 2.06 bar (30 psi)
Power (motor) = 2.5 kW
Flowrate = 0.0068 m^3/s (normal)

E-601 Dowtherm A Cooler

Operating Pressure = 11.0 bar (normal)
= 15.3 bar (maximum)
Operating Temperature = 400°C (maximum)
Duty = 2188 MJ/h
Heat Transfer Area = 2.6 m^2
Double-pipe heat exchanger with Dowtherm in inner tube

E-602 Waste-Heat Boiler

Tube Side

Operating Pressure = 2.77 bar (normal)
= 3.50 bar (maximum)

Shell Side

Operating Pressure = 6.0 bar (normal)
= 8.0 bar (maximum)
Duty = 2850 MJ/h
Heat Transfer Area = 57.0 m^2

E-603 Crude Allyl Chloride Cooler

Tube Side

Operating Pressure = 2.43 bar (normal)
= 3.50 bar (maximum)

Shell Side

Operating Pressure = 4.0 bar (normal)
= 5.0 bar (maximum)
Duty = 1025 MJ/h
Heat Transfer Area = 52.0 m^2

The gases leaving the reactor contain unreacted propylene along with the reaction products, as given in the flow table in Table C.1. These hot gases are cooled in a waste-heat boiler and a trim cooler prior to being sent for further processing, including the refining of the allyl chloride and the separation and recycle of unused propylene.

Table C.3. Properties of Dowtherm A: Heat Transfer Fluid

Properties of Dowtherm A:

Temperature Use Range	Liquid	16°C – 400°C
	Gas	257°C – 400°C

Above 400°C Dowtherm A starts to decompose thermally.

Liquid Properties for 350°C–400°C

Thermal Conductivity	0.0943	W/m.K
Specific Heat Capacity	2630	J/kg K
Viscosity	1.4×10^{-4}	kg/m s
Density	680	kg/m^3
Vapor Pressure (400°C)	10.5	bar
Prandtl No. ($C_p\mu/k$)	3.9	

C.1.3. Specific Objectives of Assignment

Your immediate supervisor, Ms. Jane Garcia, has taken you around the allyl chloride facility and told you some of the details of the plant operation. These are summarized in Section C.1.4, Additional Background Information. She has confirmed that the plant is currently operating at close to the design conditions given in Table C.1 and that utility consumption is within a few percent of that shown in Table C.1. In addition, she also provided you with a set of battery limit conditions, Table C.4, for the utilities, feeds, and products, which she has informed you are current and accurate.

Your assignment is to provide a written report to Ms. Garcia by two weeks from now. This report, at a minimum, should contain the following items:

1. A cover letter to your supervisor
2. An executive summary covering the following major points:
   - Findings on how much the throughput of Unit 600 can be increased in the short term (without the purchase of new equipment).
   - Findings of any potential improvements that will increase the profitability of Unit 600. You should provide an estimate of the impact of these changes (assume an internal discount rate for such improvements to be 15% p.a. before tax, and all improvements should be calculated using a five-year project life).
   - The impact that the proposed changes in operations might have on the environment and the health and safety of the plant personnel.
   - Recommendations for immediate changes in plant operations and an estimated time schedule in which these changes might be implemented.
3. A list of assumptions made in carrying out your study
4. An appendix giving details of all important calculations made in your study

The written report should follow the guidelines outlined in Chapter 29 (in this CD).

Table C.4 Battery Limit Conditions for Feeds, Products, and Utilities (Unit 600)

Conditions at which feed and utility streams are available and at which products and utility streams must be returned to the boundary of the process are known as the **battery limit conditions**. For Unit 600 the battery limit conditions that exist are listed below. The limiting conditions are given at the equipment and take into account the pressure loss in the associated supply and return piping.

Utility	**Condition at Equipment**	
Cooling water	5 bar,	30°C
Cooling water return	4 bar,	<45°C
Boiler feed water	6 bar,	90°C
High-pressure steam*	41 bar,	saturated
Medium-pressure steam*	11 bar,	saturated
Low-pressure steam*	6 bar,	saturated
Natural gas	4 bar,	25°C
Feeds and Products	**Condition at Process Boundary**	
Propylene	25°C, saturated vapor	
Chlorine	25°C, saturated vapor	
Crude allyl chloride	50°C, >2.09 bar (Stream 5)	

*Steam pressure at sources, such as waste-heat boilers, may exceed these values in order to overcome pressure losses in header piping.

C.1.4. Additional Background Information

A process flow diagram is provided in Figure C.1, and flow summary and equipment summary tables are given in Tables C.1 and C.2. This information is for the reaction section of Unit 600 only. The separation section is being studied by another group, and you should not consider any changes for this section at this time. The separations section is shown in Figure C.3 and will be considered in Project 2. The data given in the tables and on the PFD reflect the current operating conditions and have been checked recently by your operations department. Some additional information regarding the allyl chloride facility has been provided by Ms. Garcia and is summarized below.

1. The temperature in the reactor should not exceed 525°C, because above this temperature, there is excessive coke production leading to operating problems in the downstream units. It is further recommended that the reactor temperature be maintained at close to 511°C during any changes in process operations.
2. All process exchangers using cooling water are designed to have a 5 psi (0.34 bar) pressure drop on the cooling water side for the design flow rate of cooling water. The velocity of cooling water at design conditions was set at 2 m/s, and long-term operation at velocities above 3.5 m/s is not recommended due to increased erosion.
3. For the fluidized-bed reactor, you may assume that the pressure drop across the bed of sand remains essentially constant regardless of the flowrate.
4. The cyclone and regenerator were designed by the vendor of the equipment to be considerably oversized and are capable of handling any additional loads that might be required during this temporary change in operations.

5. The heat transfer coefficient between the fluidized bed and the immersed heat transfer coils (the outside coefficient) is known not to vary much with fluidizing gas flowrate and may be assumed constant regardless of gas throughput. The heat exchanger in the fluidized bed may be reconfigured so that the three rows of tubes are piped in parallel.
6. Flow of all process and utility streams may be considered to be fully developed turbulent flow. Thus the pressure drop through the equipment will be proportional to the square of the velocity.
7. The conversion of propylene and chlorine in the fluidized bed will be virtually unaffected by changes in gas throughput. This is due to the long gas residence time in the reactor. In fact, the reactor's main purpose is to provide a large surface area for coke deposition and to provide good heat transfer. In addition, small changes in operating pressure of the reactor will not affect the selectivity of the reaction.
8. The crude allyl chloride (Stream 5 in Figure C.1) must be delivered to the separations section at a minimum pressure of 2.9 bar, and a maximum temperature of 50°C.
9. A manufacturer's pump curve for the circulating Dowtherm A pumps is provided for your use and is given in Figure C.2 of this assignment.

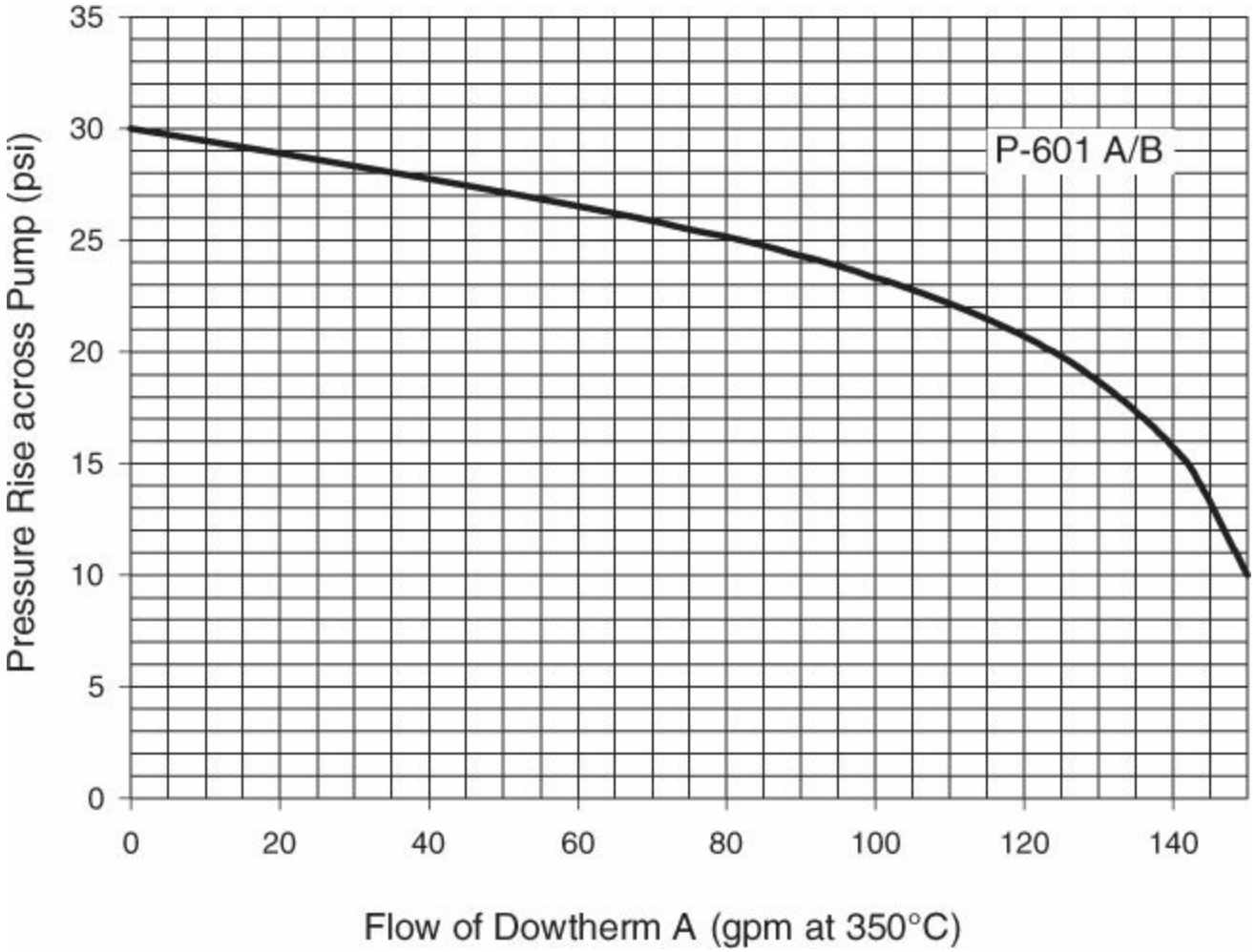


Figure C.2. Pump Curve for P-601 A/B, Dowtherm A Circulation Pumps

10. A set of original design calculations outlining the design of the units is provided for your information. Some units were built slightly differently from these designs.
11. The level of bfw in E-602 is set so that all of the heat transfer tubes are covered.

You have also taken a tour of the plant recently, and in addition to confirming some of the points above with the operators, you make the following observations:

1. The Dowtherm A recirculation pump (P-601 A) is making a high-pitched whining noise.
2. Steam is leaking from the safety relief valve placed on top of E-602.
3. Some of the insulation on the pipe leading from the reactor R-601 to E-602 has come loose and is hanging from the pipe.

C.1.5. Process Design Calculations

Fluidized-Bed Reactor, R-601

Heat generated in reactor = Q_R = 2188 MJ/h

Bed solids are 150 μm sand particles with density (ρ_s) of 2650 kg/m^3

At conditions in the reactor, the process gas has the following properties:

ρ_g = 2.15 kg/m^3 and $\mu_g = 2.25 \times 10^{-5}$ kg/m s

Using the correlation of Wen and Yu [1],

$Re_{p,mf} = [1135.7 - 0.0408\ Ar]^{0.5} - 33.7$

where $$Ar = \frac{d_p^3(\rho_s - \rho_g)\rho_g g}{\mu_g^2} = \frac{(150 \times 10^{-6})^3\,(9.81)(2650 - 2.15)(2.15)}{(2.25 \times 10^{-5})^2} = 372$$

Therefore, $Re_{p,mf} = [1135.7 + 0.0408 \times 372]^{0.5} - 33.7 = 0.2246$

$$Re_{p,mf} = \frac{u_{mf} d_p \rho_g}{\mu_g} \quad \therefore \quad u_{mf} = \frac{(0.2246)\,(2.25 \times 10^{-5})}{(2.15)\,(150 \times 10^{-6})} = 0.0157 \text{ m/s}$$

Total volumetric flow of gas at inlet conditions to the bed = V_{gas} = 0.5674 m^3/s.

Good heat transfer is needed, so the bed will be operated at 5 times u_{mf}, which puts it into the bubbling bed regime.

Free bed area (without heat transfer tubes) = $V_{gas}/5u_{mf}$ = 0.5674/(510.0157) = 7.2 m^2

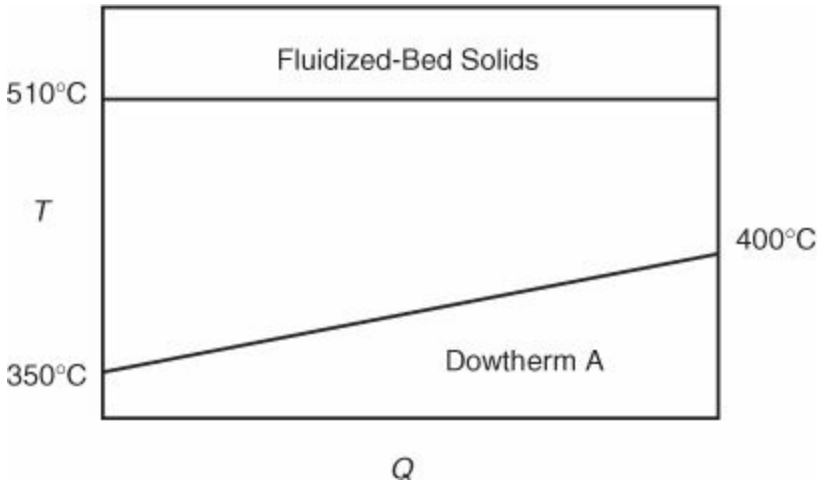
Looking at the heat transfer area for the fluidized bed:

Heat transfer area required in bed = A_0

Overall heat transfer coefficient = U_0

Assume that the fluidized solids are well mixed and isothermal, and assume that the cooling medium enters the bed at 350°C and leaves at 400°C, which is the maximum operating temperature for Dowtherm A.

$$\Delta T_{lm} = \frac{(160 - 110)}{\ln (160/110)} = 133.4°\text{C}$$



Inside film heat transfer coefficient, h_i, is calculated from the Seider-Tate equation:

$Nu = 0.023\ Re^{0.8}\ Pr^{0.33}\ (\mu/\mu_w)^{0.14}$

Assuming a velocity of 1.5 m/s inside a 3-in schedule-40 pipe (ID = 0.0779 m is assumed, OD = 0.0889 m), then

$Re = (0.0779)\ (1.5)\ (680)/(1.4 \times 10^{-4}) = 567 \times 10^3$

$Nu = h_i d/k = 0.023\ (567 \times 10^3)^{0.8}\ (3.9)^{0.33} = 1445$

$h_i = (1445)\ (0.0943)/(0.0779) = 1750\ W/m^2K$

Outside film heat transfer coefficient h_o = 267 W/m^{2}K (from previous plant operating data), and fouling coefficient on inside = 2500 W/m^{2}K.

$d_o / d_i = 0.0889/0.0779 = 1.14$

Ignoring the wall resistance, the overall transfer coefficient U_o is obtained from

$$U_o = \frac{1}{\frac{1}{267} + \frac{1.14}{2500} + \frac{1.14}{1750}} = 206\ \text{W/m}^2\text{K}$$

$$A_0 = \frac{Q_R}{U_o \Delta T_{lm}} = \frac{2188 \times 10^6}{(3600)(206)(133)} = 22.2\ \text{m}^2$$

Now assuming that the tubes are 10 ft long and 3 in in diameter (schedule-40), the heat transfer area per tube is

$\pi d_o L = (3.142)\ (0.0889)\ (10)\ (0.3048) = 0.8513\ \text{m}^2$

$\therefore$ number of tubes required $N_T = 22.2/0.8513 = 27$ tubes.

Using 3 layers of 9 tubes piped in series and placed in horizontal rows in the bed, each row occupies the following csa of bed:

$(9)\ (d_o)\ (L) = (9)\ (0.0889)\ (3.048) = 2.4\ \text{m}^2$

$\therefore$ total csa for bed = 2.4 + 7.2 = 9.6 m^2

Use a square bed with side dimensions = $(9.6)^{0.5}$ = 3.1 m (10.2 ft).

Check Velocity in Tubes

csa for flow of Dowtherm A in tubes = $\pi d_i^2/4 = (3.142)(0.0779)^2/4 = 4.766 \times 10^{-3}$ m^2 flow of Dowtherm A = 6.797×10^{-3} m^3/s

$\therefore$ velocity of Dowtherm A in tubes = $6.797 \times 10^{-3}/4.766 \times 10^{-3} = 1.43$ m/s $\Rightarrow$ assumption is OK

Pressure Drop in Tubes

$Re = 5.41 \times 10^5$ $\therefore$ friction factor $f = 0.0045$ (with $e/d = 0.0006$)

$\Delta P = 2fL_{eq}\rho u^2/\mathrm{d} = (2)\ (0.0045)\ (680)\ (1.43)^2\ L_{eq}/(0.0779) = 161\ L_{eq}$

Now L_{eq} = equivalent length of pipe in three rows of heat transfer pipes in fluidized bed

= (27) (3.048) (1.5) = 123 m (take this as 1.5 times length of pipe to account for fittings)

$\therefore$ $\Delta P = (162)\ (123) = 0.20$ bar

Set bed height (height of sand above distributor plate) = 1.5 m.

This gives a gas residence time in the bed of (7.2) (1.5) (0.45)/0.5674 = 8.6 s. This should be plenty of time because complete reaction should take only about 2–3 s.

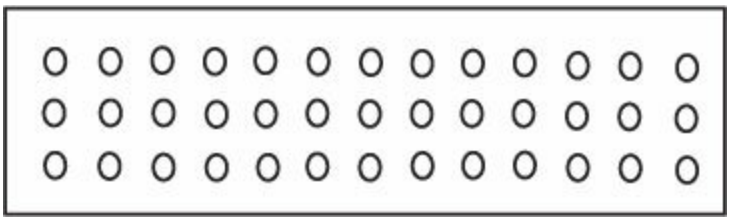
$\Delta P_{bed} = h_{bed}\ \rho_{sand}\ (1 - \varepsilon)g = (1.5)\ (2650)\ (1 - 0.45)\ (9.81) = 0.214$ bar

Assume 0.04 bar for distributor loss and 0.064 bar for cyclones to give the overall equipment pressure drop:

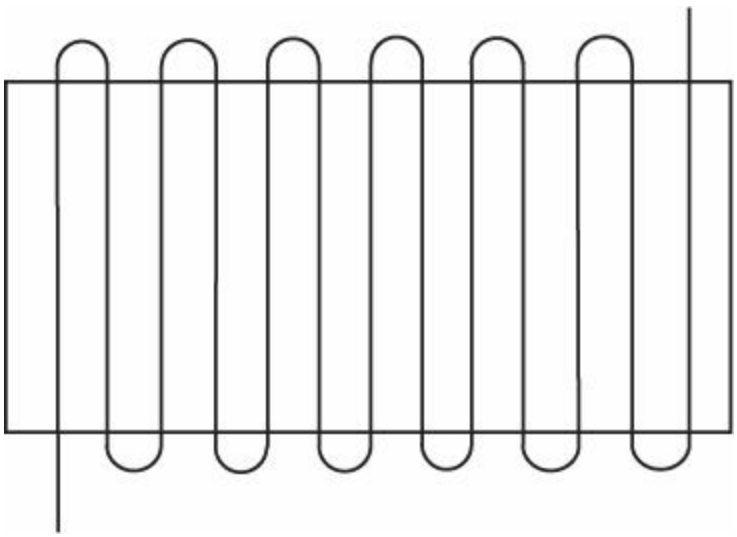
$\Delta P_{reactor} = 0.214 + 0.04 + 0.016 = 0.27$ bar

Design of fluidized bed is given in sketch below:

Side view of bed showing 3 rows of 9 tubes:



Overhead view of bed showing piping arrangement for one row; each row is piped in series with the row below.



For exchanger E-601, $\Delta T_{lm} = (360 - 320)/\ \ln\ (360/320) = 340$°C and $U = 850$ W/m^2 K (approximately equal resistances on both sides and small fouling resistances). Heat transfer area A is

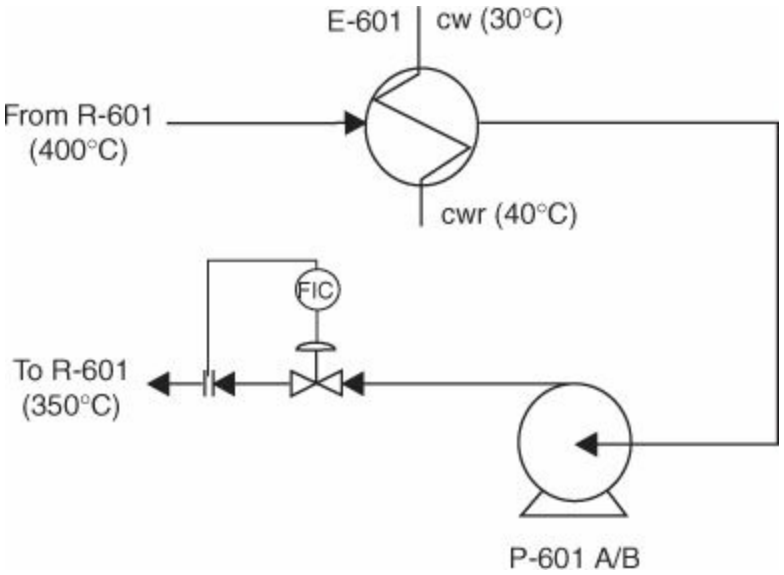
given by

$A = 2188 \times 10^6/(3600)\ (340)\ (850) = 2.1 m^2$

Use a double-pipe heat exchanger because area is small. Considering the Dowtherm A circulation loop shown in the following figure, the following information is given:

Cooling water flowrate = $2188 \times 10^6/(3600)\ (4180)\ (10) = 14.5$ kg/s
Dowtherm flowrate = $2188 \times 10^6/(3600)\ (2630)\ (50) = 4.62$ kg/s
Pressure drop across the exchanger = 0.34 bar for Dowtherm and cooling water
Velocity of cooling water through exchanger set at 2 m/s

Dowtherm A Cooling Loop



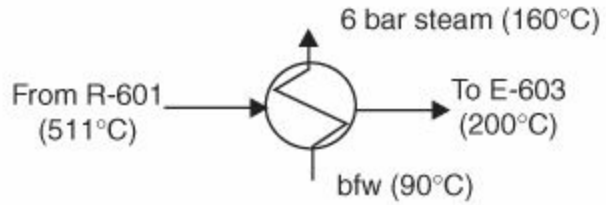
For pumps P-601 A/B, assume

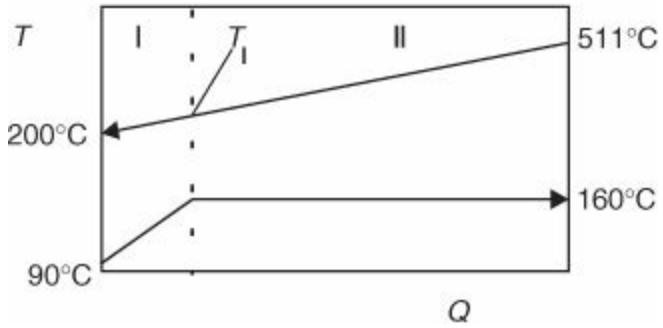
0.34 bar (5 psi) pressure drop across exchanger on Dowtherm side
0.14 bar (2 psi) pressure drop for piping
0.85 bar (12.4 psi) pressure drop across the control valve
0.20 bar (2.9 psi) pressure drop across the reactor exchanger
Total loop pressure drop = 1.53 bar = 22.3 psi
Flow of Dowtherm = $4.62/680 = 6.797 \times 10^{-3}$ m^3/s = 108 gpm
Power required for pumping liquid = $\dot{V}\,\Delta P = (6.797 \times 10^{-3})\ (1.53 \times 10^5) = 1.04$ kW
Assuming an efficiency of 45%, the shaft power = 1.04/0.45 = 2.31 kW.
Use a 2.5 kW pump plus a spare.

Considering the waste heat boiler, E-602, shown in the figure on the following page:

Zone I $U = 90$ W/m^2 K (all resistance on gas side)
Zone II $U = 90$ W/m^2 K (all resistance on gas side)

Waste-Heat Boiler E-602





Heat released as gas cools from 511°C to 200°C is 2850 MJ/h = 792 kW

$$\Delta H_{bfw\text{-}steam} = 2380 \text{ kJ/kg}$$

Steam flowrate = 792/2380 = 0.333 kg/s ($h_L = 376.9$, $h_{L,sat}$ = 675.5, $h_{V,sat}$ = 2756.9 kJ/kg)

$$Q_{90\text{-}160°C,Liq} = (0.333)\,(675.5 - 376.9) = 99 \text{ kW}$$

$$Q_{160°C,\,Liq\text{-}Vap} = (0.333)\,(2756.9 - 675.5) = 693 \text{ kW}$$

For Zone I

$$(T_I - 200)/(510 - 200) = 99/792 \Rightarrow T_I = 238.8°C$$

$$\Delta T_{lm} = \frac{(239 - 160) - (200 - 90)}{\ln \dfrac{(239 - 160)}{(200 - 90)}} = 93.6°C$$

$$A_I Q_I / U_I \Delta T_{lm} F = 99 \times 10^3/(90)(93.6)(1.0) = 11.8 \text{ m}^2$$

For Zone II

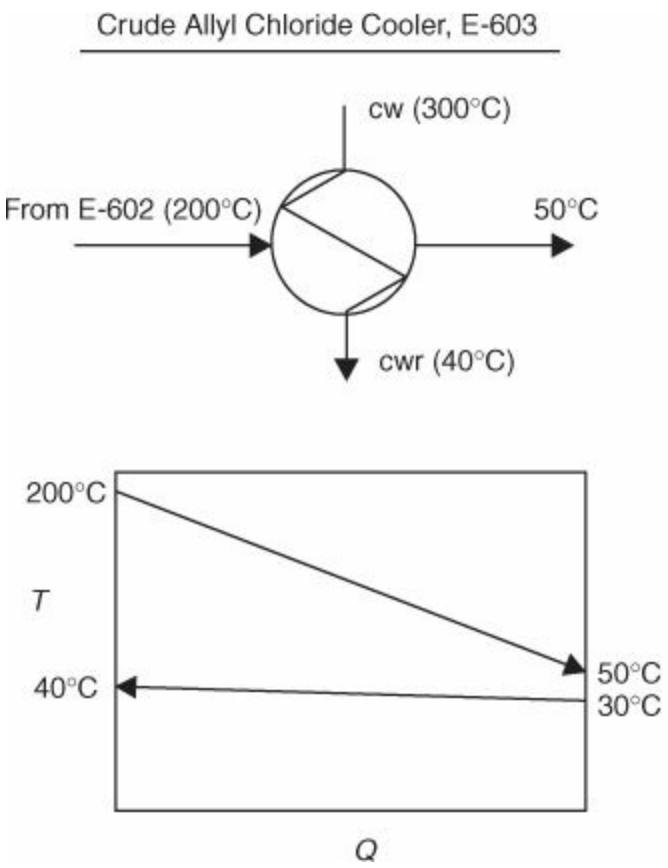
$$\Delta T_{lm} = \frac{(239 - 160) - (511 - 160)}{\ln \dfrac{(239 - 160)}{(511 - 160)}} = 182.4°C$$

$$A_{II} Q_{II} / U_{II} \Delta T_{lm} = 693 \times 10^3/(90)(182.4) = 42.2 \text{ m}^2$$

Total Area $A = A_I + A_{II} = 11.8 + 42.2 = 54 \text{ m}^2$

$$C_{p,gas} = 1490 \text{ J/kg.K}$$

$$Q = m\, C_{p,gas} \Delta T = (4590)\,(1490)\,(200 - 50)/3600 = 0.285 \text{ MW}$$



From the figure above, the following information is calculated:

$$m_{cw} = (0.285 \times 10^6)/(4180)\,(10) = 6.82 \text{ kg/s}$$

$$\Delta T_{lm} = (160 - 20)/\ln(160/20) = 67.3°\text{C}$$

$$U = 90 \text{ W/m}^2\text{ K}$$

$$A = Q/U\Delta T_{lm}F = (0.285 \times 10^6)/(90)\,(67.3)\,(0.95) = 49.5 \text{ m}^2$$

C.1.6. Reference

1. Wen, C. Y., and Y. H. Yu, "A Generalized Method for Predicting Minimum Fluidization Velocity," *AIChE J.* 12, no. 610 (1966).

PROJECT 2. Design and Optimization of a New 20,000-Metric-Tons-per-Year Facility to Produce Allyl Chloride at La Nueva Cantina, Mexico

C.2.1. Background

Recent developments at the Alabama plant have brought into question the stability of our allyl chloride production capacity. It has been noted that the North American market for allyl chloride consumption will probably grow extensively in the next decade and that additional production capacity may be needed. In order to maintain our current market share and to remain competitive in this market, it may become necessary to build a new allyl chloride facility.

With this in mind, a new (grassroots) production facility to produce commercialgrade allyl chloride is being investigated. This facility would most likely be situated in La Nueva Cantina, Mexico, close to our petrochemical facility, which would be able to supply propylene. The supply of chlorine from local manufacturers will also be plentiful. Your group has been given the task of doing a process

estimate for this new facility.

C.2.2. Assignment

Your assignment is to design and optimize a new grassroots 20,000 metric tons per year allyl chloride facility. This facility will produce commercial-grade allyl chloride from the synthesis reaction between propylene and chlorine. The front-end process is to use fluidized-bed technology similar to that currently in use in Unit 600 at Beaumont, Texas (see Project 1). This assignment concerns the design of a new plant, and, except for the fluidized-bed reactor unit, the plant may be reconfigured in any way that you feel is appropriate. For the fluidized-bed reactor, kinetic equations are not available, and therefore your design should be similar to that of the Beaumont unit. With this in mind, the reactor temperature should be close to 511°C, and the ratio of propylene to chlorine into the reactor should remain the same. Although the selectivity of the reaction will change with changes in reactor pressure, you may assume for this preliminary design that the selectivity is unaffected by changes in pressure. Your final design should be the one that maximizes the net present value (NPV) of the project under the following economic constraints:

After-tax internal hurdle rate = 10%
Depreciation = MACRS (6-year schedule; see Chapter 9)
Taxation rate = 15%
Labor costs to be based on U.S. equivalent wage rate
Construction period = 2 years
Project plant life = 15 years after start-up

Additional process information and some hints regarding problem-solving strategy are given below. You should plan to submit your written report in four weeks. The guidelines for written and oral reports given in Chapter 29 (in this CD) should be followed for this assignment.

C.2.3. Problem-Solving Methodology

The optimization of a process as large and complicated as this one is not a trivial matter. To help you in this endeavor the following hints are given. (You may use all or none of them as you see fit.)

1. When initially running case studies using a process simulator, you should use any shortcut methods for simulating distillation columns that are available. Avoid the rigorous methods for this type of preliminary work. You should use the rigorous (tray-to-tray) methods at the end of your work for the optimized case.
2. Establish a base case from the information provided. This should include operating costs and capital investments for the process shown in Figures C.1, C.3, and C.4, using the new production rate of 20,000 metric tons/year. You should make sure that you have included all the equipment and costs.
3. See where the major capital investment and major variable operating costs lie, and use this information to focus on where your optimization should begin.

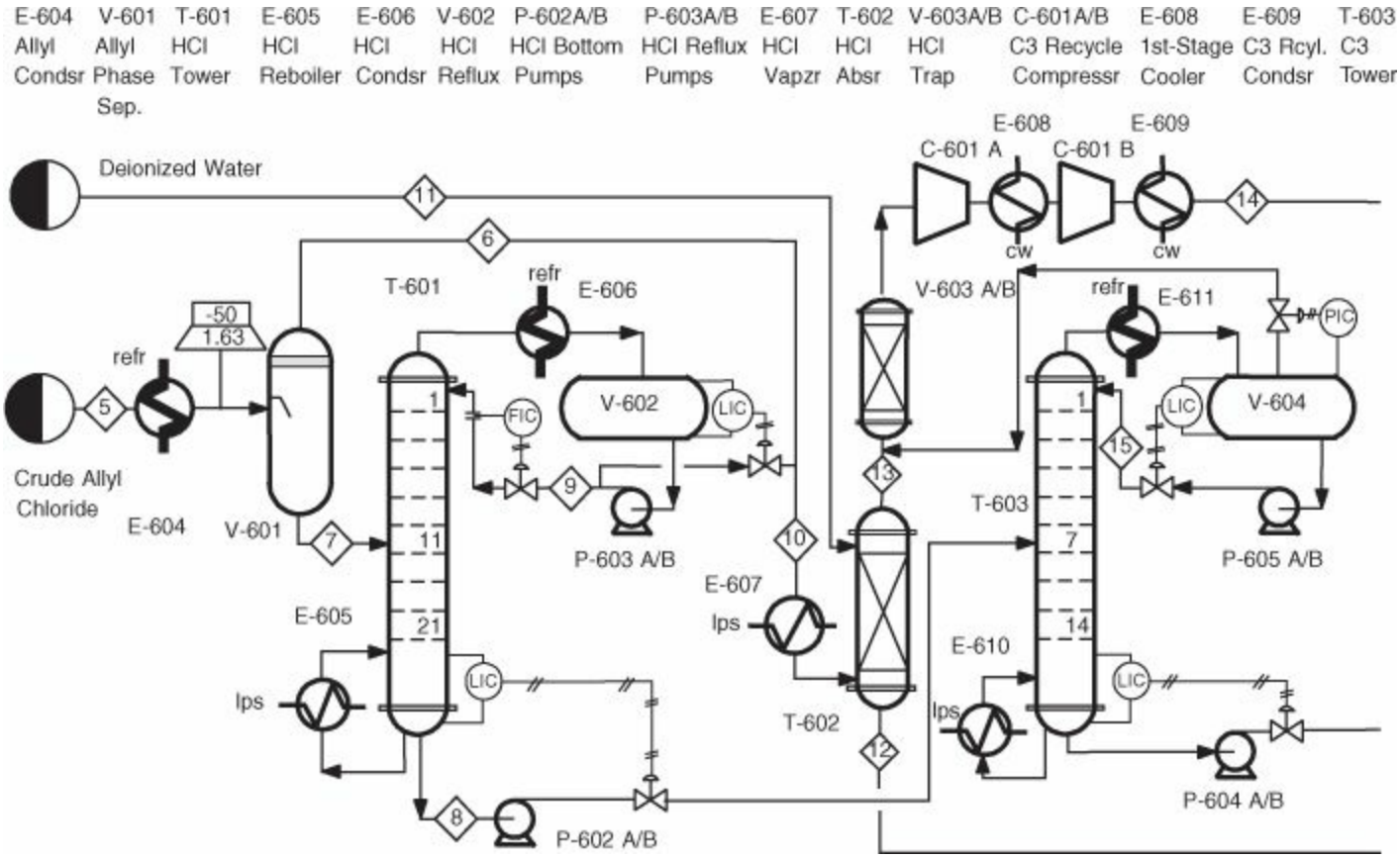
   Note: This is a multivariable optimization, and within the time frame given for solving this problem, you can afford to concentrate on only a few variables. Identify the key decision variables to be manipulated—that is, the variables that have the greatest impact on the NPV.
4. Do not let the computer turn your mind to mush! Think about how changes in operating variables and other things will affect the economics, and try to predict the direction in which the NPV will change as each variable changes. You should be able to rationalize, at least

qualitatively, why a certain change in a variable causes the observed change in the NPV.

C.2.4. Process Information

To help you in this task the following information has been included with this assignment:

1. A flowsheet and a process description for the existing separations section of Unit 600 are included in Figures C.3 and C.4 and Tables C.5 and C.6.



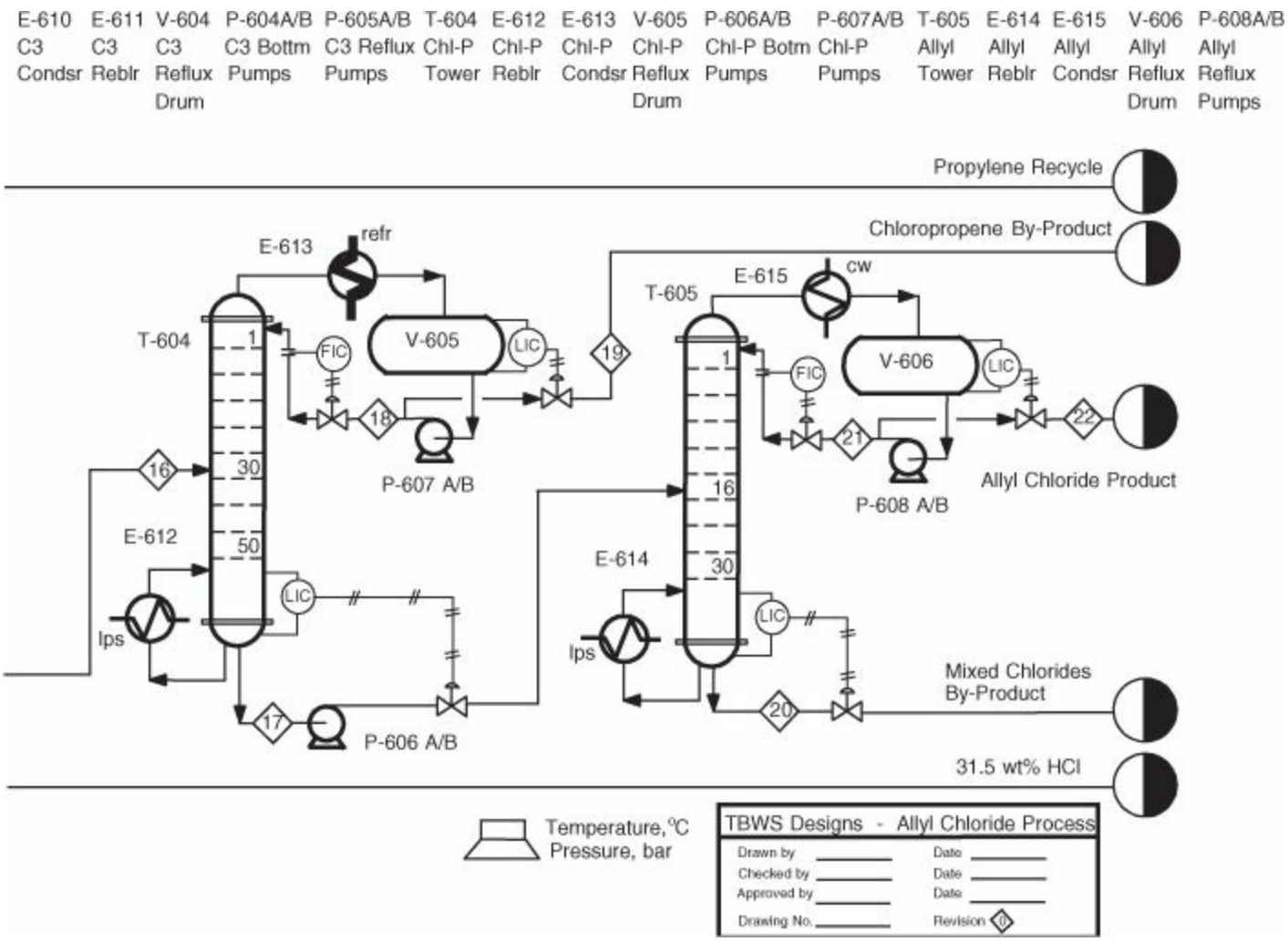


Figure C.3. Separations Section of Allyl Chloride Production Facility (Unit 600)

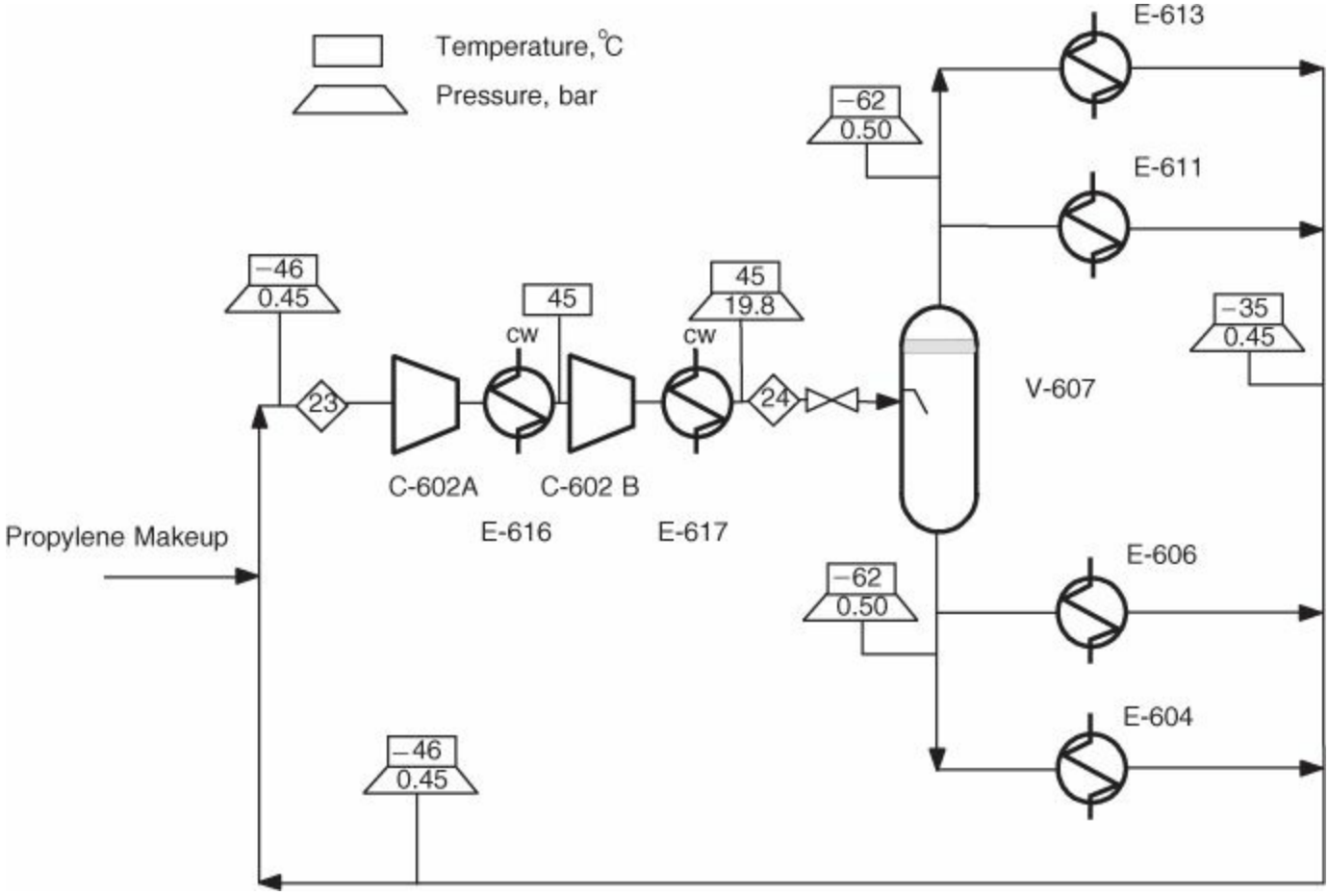


Figure C.4. Propylene Refrigeration Loop for Allyl Chloride Process (Unit 600)

2. Product specifications are included in Table C.7.
3. Note that the current process (Unit 600) is very energy intensive, because very cold temperatures and expensive refrigeration are used throughout the process. Remember that the existing Beaumont plant was designed more than 40 years ago, when electricity and energy were relatively cheap. The optimal process configuration for today's conditions may be significantly different from that of the existing facility!

Table C.5. Flow Summary Table for Allyl Production Process, Figures C.3 and C.4

Stream Number	5	6	7	8	9	10	11	12	13	14
Temperature (°C)	50	–50	–50	46	–57	–56	25	10	10	45
Pressure (bar)	2.09	1.50	1.50	1.50	1.40	1.5	3.0	1.4	1.3	19.9
Vapor fraction	1.0	1.0	0.0	0.0	0.0	0.087	0.0	0.0	1.0	0.0
Mass flowrate (tonne/h)	4.59	0.27	4.32	1.45	0.19	3.14	1.48	2.17	2.44	2.44
Molar flowrate (kmol/h)										
Propylene	58.08	2.72	55.36	0.55	3.65	57.53	0.0	0.0	57.53	58.08
Allyl chloride	15.56	0.01	15.55	15.55	0.0	0.01	0.0	0.01	0.0	0.0
Dichloropropene	0.46	0.0	0.46	0.46	0.0	0.0	0.0	0.0	0.0	0.0
Dichloropropene	1.81	0.0	1.81	1.81	0.0	0.0	0.0	0.0	0.0	0.0
Hydrogen chloride	19.70	4.19	15.51	0.01	1.03	19.69	0.0	19.11	0.58	0.0
Water	0.0	0.0	0.0	0.0	0.0	0.0	82.00	81.88	0.12	0.0
Total molar flowrate (kmol/h)	95.61	6.92	88.69	18.38	4.68	77.23	82.00	101.00	58.23	58.08

Stream Number	15	16	17	18	19	20	21	22	23	24
Temperature (°C)	–40	59	60	30	30	106	55	55	–46	45
Pressure (bar)	1.5	2.0	1.5	1.4	1.4	1.5	1.4	1.4	0.45	19.9
Vapor fraction	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0
Mass flowrate (tonne/h)	0.03	1.42	1.39	1.52	0.04	0.21	0.47	1.18	25.31	25.31
Molar flowrate (kmol/h)										
Propylene	0.81	0.0	0.0	0.0	0.0	0.0	0.0	0.0	602.5	602.5
Allyl chloride	0.0	15.54	15.52	0.84	0.02	0.08	6.13	15.44	0.0	0.0
Dichloropropene	0.0	0.46	0.01	18.99	0.45	0.0	0.0	0.01	0.0	0.0
Dichloropropene	0.0	1.81	1.81	0.0	0.0	1.80	0.0	0.01	0.0	0.0
Hydrogen chloride	0.01	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Water	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Total molar flowrate (kmol/h)	0.82	17.81	17.38	19.83	0.47	1.88	6.13	15.46	602.5	602.5

Table C.6. Process Description of Unit 600

Refer to the process flow diagram for Unit 600, Allyl Chloride Purification Process, Beaumont, Texas (Figure C.3).

Crude allyl chloride, Stream 5, from the reaction section of Unit 600 (Figure C.1) enters the allyl product cooler, E-604, at 50°C and 2.1 bar. This stream is cooled to –50°C using the circulating liquid propylene refrigerant. The two-phase mixture leaving E-604 is fed to V-601, where the liquid stream is taken off and is fed to the HCl column, T-601. The HCl column removes essentially all the HCl and propylene from the cooled crude allyl chloride feed as overhead product at approximately –57°C. This stream is mixed with the vapor coming from V-601 and is fed to E-607, where it is heated with low-pressure steam.

The bottoms product from T-601 contains essentially all the chlorinated hydrocarbon derivatives and a small amount of propylene. This stream is fed to T-603, where the remaining propylene is removed as the overhead product at approximately –40°C. The bottoms product from T-603 is fed to column T-604, where 95 mol% chloropropene is removed overhead at approximately 30°C. The bottom product from T-604 is fed to the allyl tower, T-605, where 99.9% by mole pure allyl chloride is removed as overhead product at 55°C and sent to storage. The bottoms product from T-605 contains 95 mol% 1,2, dichloropropene, and this stream is sent to storage after being cooled in an offsite heat exchanger (not shown on Figure C.3).

The stream leaving E-607 is fed to T-602, where it mixes with water at 20°C. The flow of water is controlled to give an aqueous solution of hydrochloric acid with 31.5 wt% HCl. This concentration of acid is equivalent to a liquid density of 20° Baumé. The use of degrees Baumé is the common method by which hydrochloric acid is specified. The vapor stream leaving T-602 contains all the propylene and small amounts of water and HCl. This stream is sent to one of a pair of acid traps, V-603 A and B, where the water and HCl are removed (by adsorption onto activated carbon). The vapor stream leaving the absorbers is pure propylene. This propylene stream is sent to a two-stage compressor, C-601 A and B, with intercooler E-408 and condenser E-409. The stream leaving the condenser is a liquid at 45°C and is recycled to the propylene storage tank for Unit 600.

Four of the exchangers in Unit 600 (E-604, E-606, E-611, and E-613) require heat to be removed from the process stream at temperatures less than 35°C. In order to do this, a refrigeration system is required. In Unit 600, this is achieved by circulating a stream of cold (–62°C) propylene through these exchangers. The refrigeration loop is shown in the second PFD for Unit 600, Figure C.4. The refrigeration is achieved by taking a high-pressure (20 bar) stream of liquid propylene (45°C) and flashing it down to low pressure (0.5 bar). Cooled liquid and vapor propylene streams (–62°C) are sent to the four process exchangers, where they provide the necessary cooling. The warmed propylene vapor (–46°C) is recycled back to the refrigeration loop compressors C-602 A&B, the intercooler E-616, and the condenser E-617. A makeup propylene stream is provided to account for minor system leaks.

Table C.7. Product Specifications and By-Product Costs (Unit 600)

Product Specifications

Product	Required Purity	Battery Limit Condition
Allyl chloride	> 99.9% by mole allyl chloride	Liq, T < 55°C, P >1.5 bar
By-Product	**Required Purity**	**Battery Limit Condition**
Mixed chlorides	> 95% by mole 1,2-dichloropropene	Liq, T < 50°C, P >1.2 bar
Chloropropene	> 95% by mole chloropropene	Liq, T < 50°C, P >1.2 bar
31.5 wt% hydrochloric acid	31.5 wt% hydrochloric acid ± 0.1 wt %	Liq, T < 45°C, P >1.2 bar

By-product and Waste Stream Selling Prices/Costs

By-Product	Selling Price
Mixed chlorides	$0.10 /kg*
Chloropropene	$0.15 /kg*
31.5 wt% hydrochloric acid (20° Baumé)	From *Chemical Marketing Reporter*

Waste Stream	Cost of Disposal
Waste acid stream (cost of regenerating carbon)	$0.40 /kg of HCl + hydrocarbons collected on carbon

*These are credits that we will receive from our petrochemical complex for supplying these chemicals, which must meet the specifications given above. We may alternatively pay to dispose of these chemicals at a cost of $0.25/kg. For this case, no specifications need to be met (i.e., these streams are now waste streams rather than by-products).

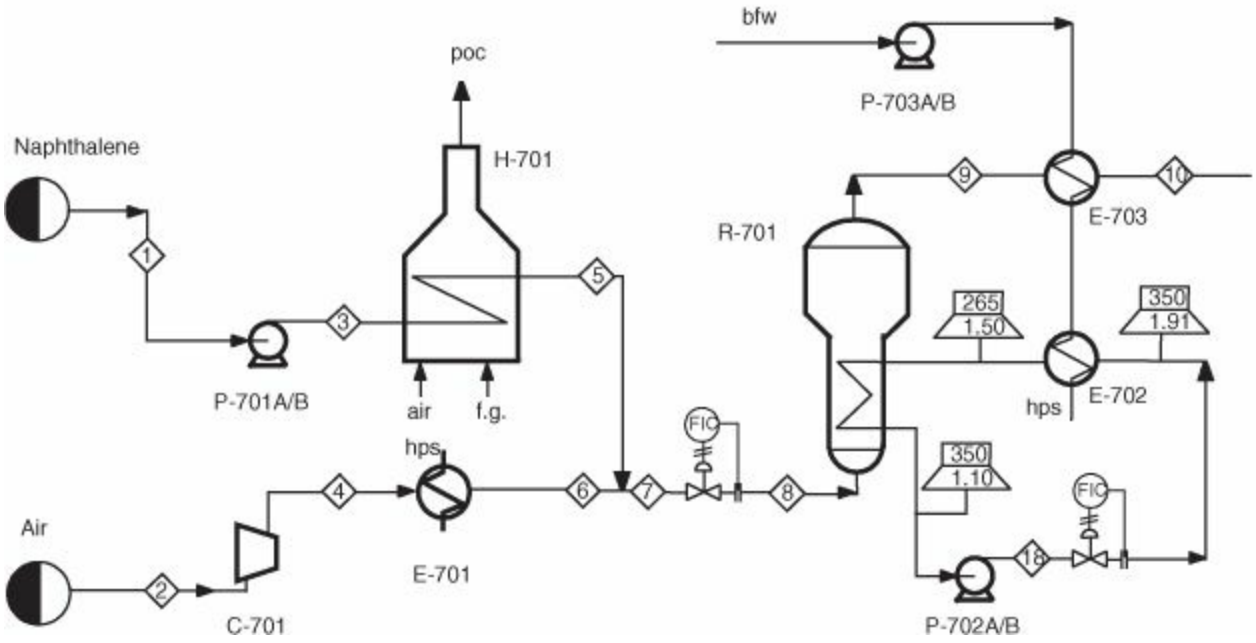
PROJECT 3. Scale-Down of Phthalic Anhydride Production at TBWS Unit 700

C.3.1. Background

You have recently joined the TBWS Chemical Corporation. One of TBWS's major businesses has always been production of phthalic anhydride from naphthalene. Phthalic anhydride production is integrated as part of a large chemical plant, in which naphthalene is produced and in which phthalic anhydride is immediately used to make polyester resins. In recent years, there have been some problems. Some end users have complained about the quality of the resins produced and have taken their business to other companies that produce phthalic anhydride from o-xylene. Therefore, our plant, which had been designed to produce 100,000 metric tons/year of phthalic anhydride from naphthalene, was scaled back to about 80,000 metric tons/year several years ago. We are now forced to scale down production once again due to the loss of another large customer. Marketing informs us that we may lose additional customers. Research is working on development of catalysts for the o-xylene reaction, but their results are not expected for up to a year. There is an immediate need to determine how to scale down operation of our plant to 50% of current capacity (40,000 metric tons/year). We would like to accomplish this without a shutdown, because one is not scheduled for a few months. If 50% scale-down cannot be achieved without a shutdown, we need to know how much scale-down is possible immediately. Specifically, you are to determine the maximum possible scale-

down, up to 50%, under current operating conditions, and you are to define these operating conditions. Furthermore, you are to determine how the plant can be scaled down to 50% of current capacity, what operating conditions are required, and what capital expenditures, if any, are needed. Any suggestions for plant improvements that can be made during shutdown are encouraged. You must clearly define the consequences of any changes that you recommend for this process and the consequences of these changes for other processes that might be affected. It should be noted that one possible scenario is to operate the plant at design capacity for six months of the year and shut down the plant for the remaining six months. Although this solution might work, we are reluctant to lay off our operators for half the year and also to purchase additional storage in order to store enough phthalic anhydride to supply our customers for the six months that the plant is down. You should not consider this option any further.

P-701A/B	C-701	H-701	E-701	R-701	E-702	P-702A/B	E-703	P-703A/B
Naphthalene Feed Pumps	Feed Air Compressor	Air Preheater	Naphthalene Furnace	Fluidized-Bed Reactor	Molten Salt Cooler	Molten Salt Pumps	bfw Preheater	bfw Pumps



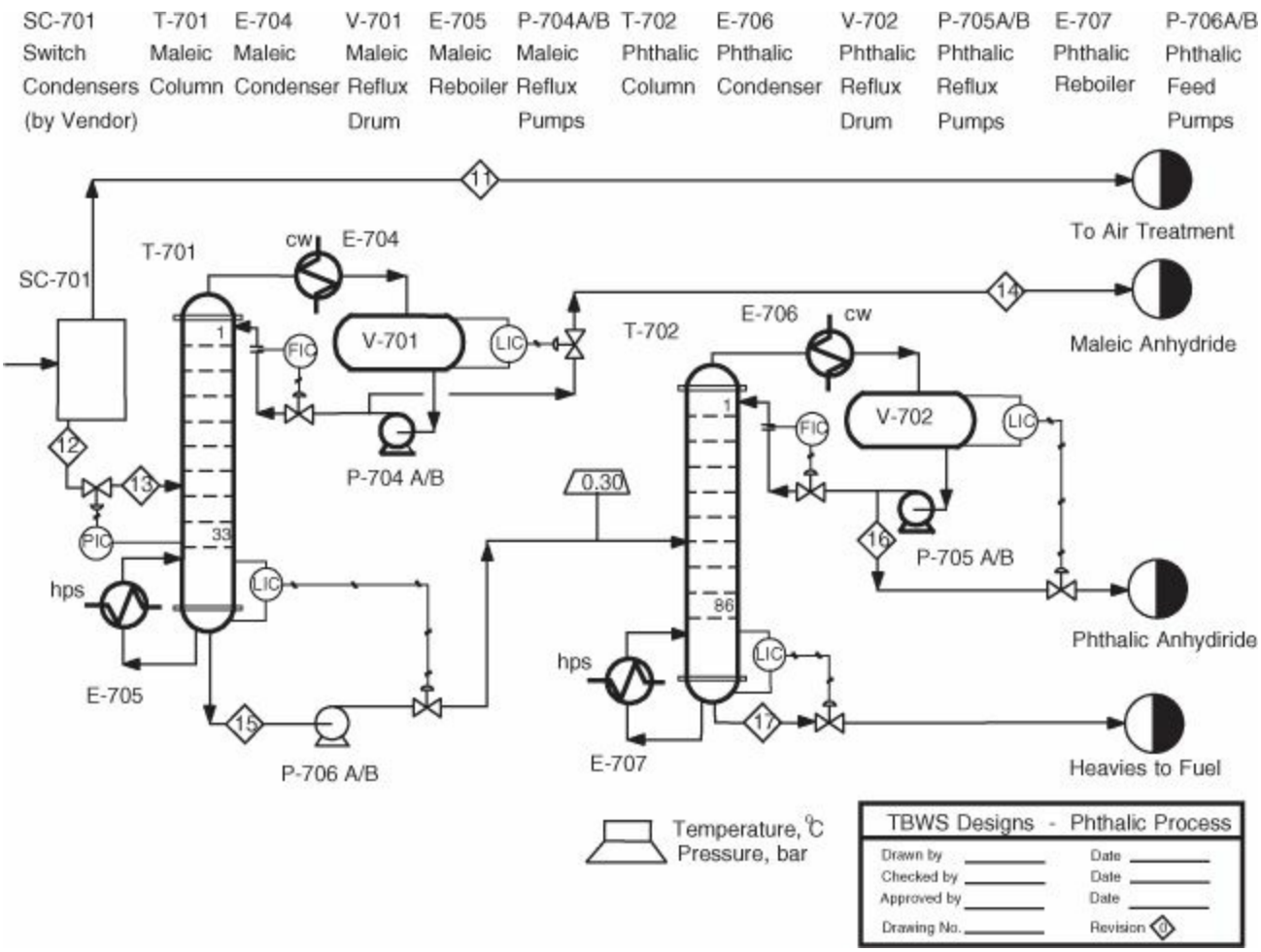


Figure C.5. Process Flow Diagram for the Production of Phthalic Anhydride from Naphthalene (Unit 700)

For your first assignment, you are to address the issues described above for the portion of the process before the switch condensers (see Figure C.5).

C.3.2. Phthalic Anhydride Production

Unit 700 now produces about 80,000 metric tons/y of phthalic anhydride. The feeds are essentially pure naphthalene and excess air. These are pressurized, heated and vaporized (naphthalene), and reacted in a fluidized bed with a vanadium oxide on silica gel catalyst. The reactions are as follows:

$$C_{10}H_8 + \frac{9}{2}O_2 \rightarrow C_8H_4O_3 + 2H_2O + 2CO_2$$

naphthalene *phthalic anhydride*

$$C_{10}H_8 + 6O_2 \rightarrow 2C_4H_2O_3 + 2H_2O + 2CO_2$$

maleic anhydride

$$C_{10}H_8 + \frac{3}{2}O_2 \rightarrow C_{10}H_6O_2 + H_2O$$

naphthoquinone

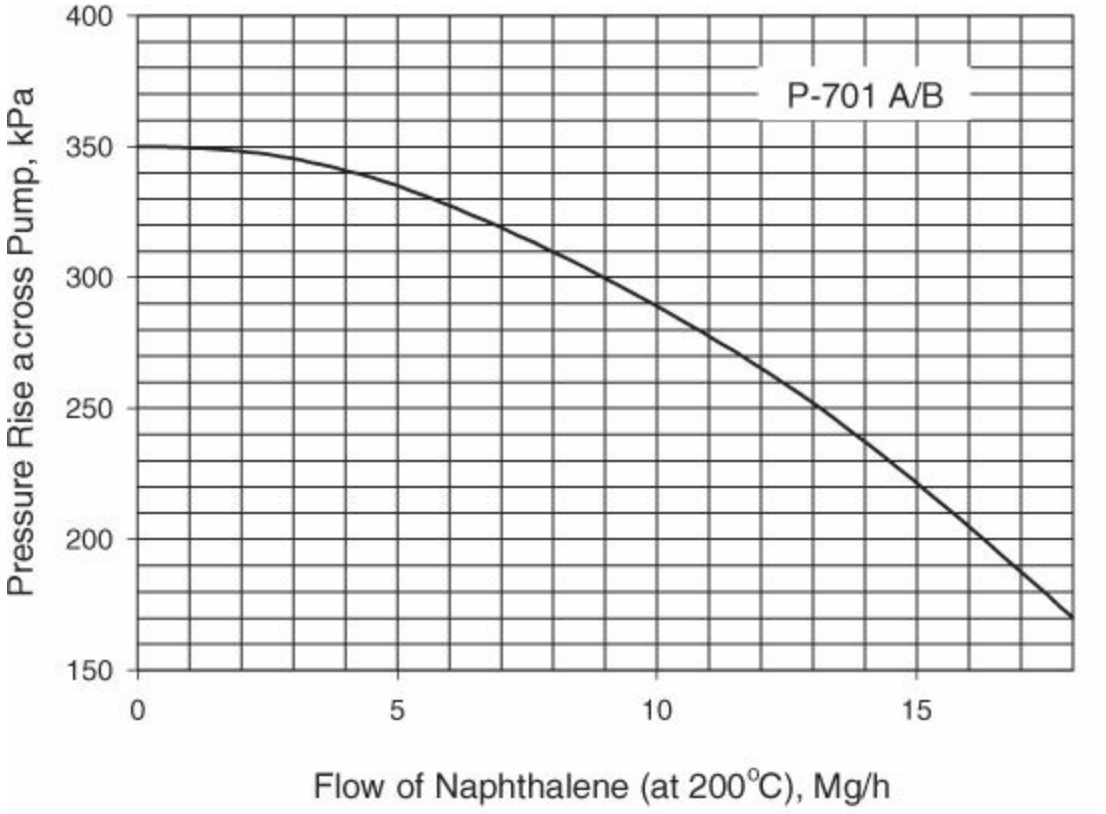
Additionally, the complete and incomplete combustion reactions of naphthalene also occur. The large exothermic heat of reaction is removed by molten salt circulated through coils in the reactor. The molten salt is used to produce high-pressure steam. Total conversion of naphthalene is very close to 100%. The reaction products proceed to a set of devices known as switch condensers. These are described in detail later. Design and operation of these devices are provided under contract by

CONDENSEX. They guarantee us that their condensers can operate at any capacity and provide the same separation as in current operation, as long as the pressure and the composition of the condensable portion of Stream 10 remain constant. The net result of the switch condensers is that essentially all of the light gases and water leave as vapor, with small amounts of maleic and phthalic anhydrides, and that the remaining anhydrides and naphthoquinone leave as liquid. The liquid pressure is then reduced to vacuum for distillation. The first column removes maleic anhydride impurity overhead, and the second column removes the phthalic anhydride product overhead.

Organic waste is burned for its fuel value. The dirty air, Stream 11, must be treated. The anhydrides are scrubbed using water, which is then sent to the on-site wastewater treatment facility.

C.3.3. Other Information

Other pertinent information is appended, including pump and compressor curves, Figure C.6 and Figure C.7; a flow summary table, Table C.8; and an equipment list, Table C.9.



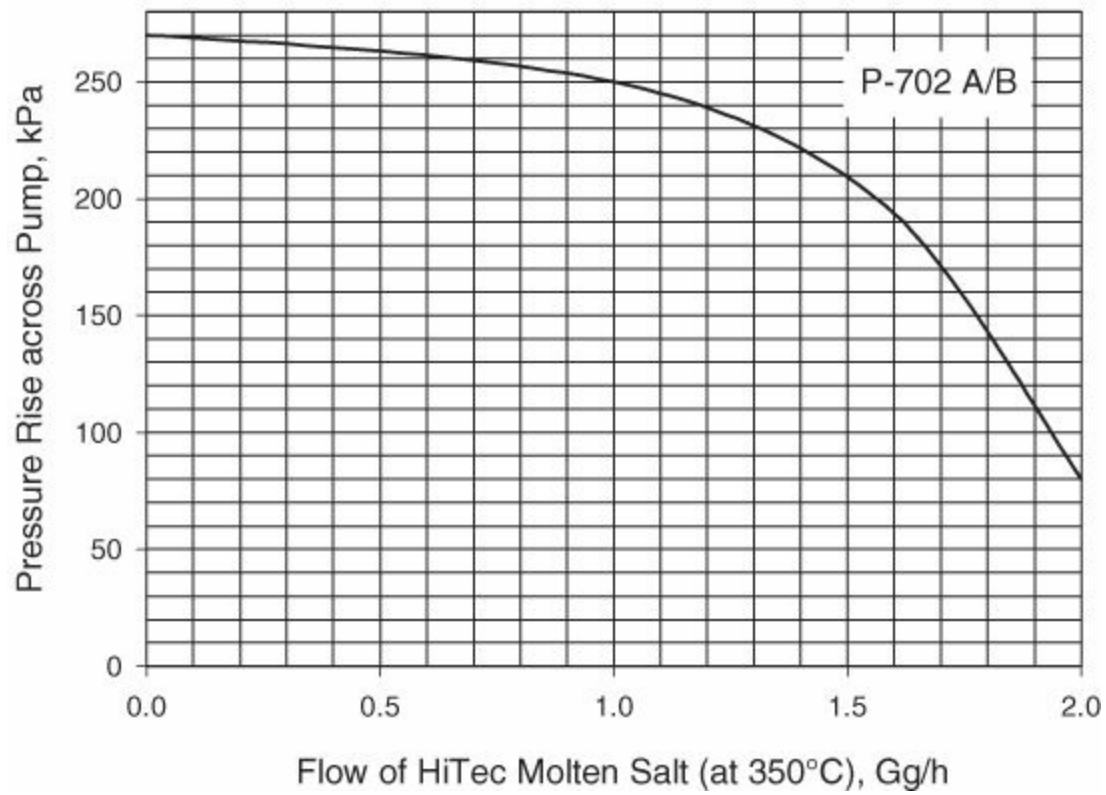
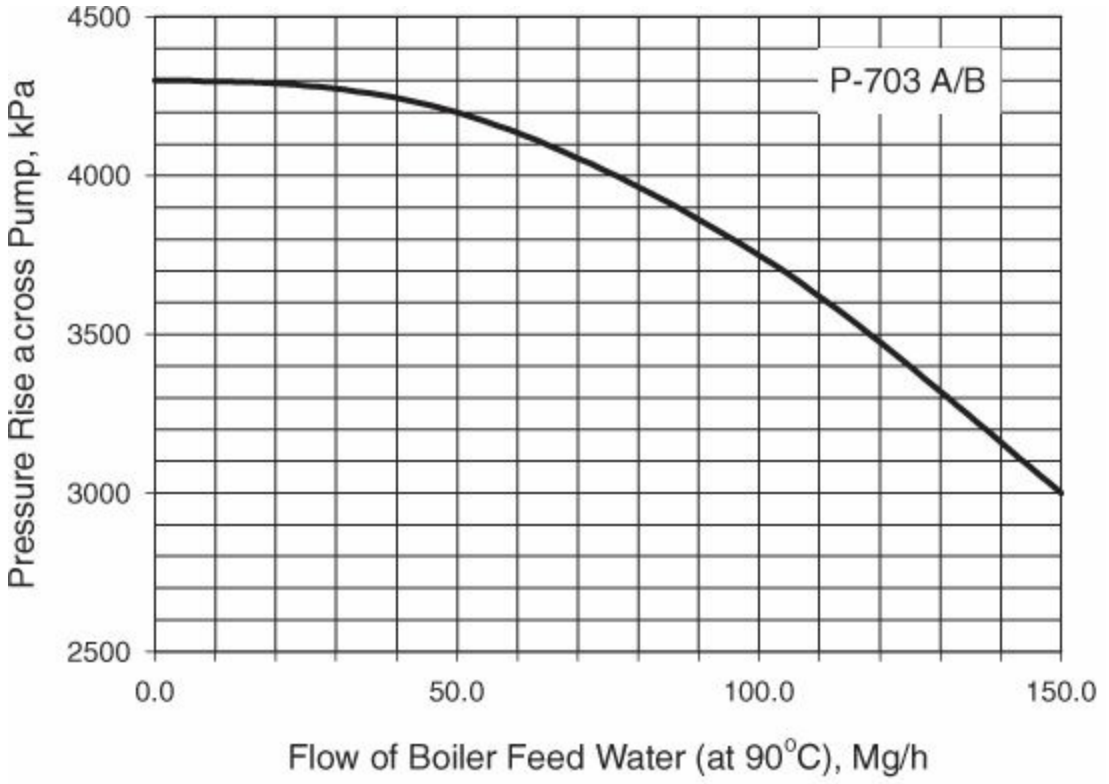


Figure C.6. Pump Curves for P-701 A/B and P-702 A/B



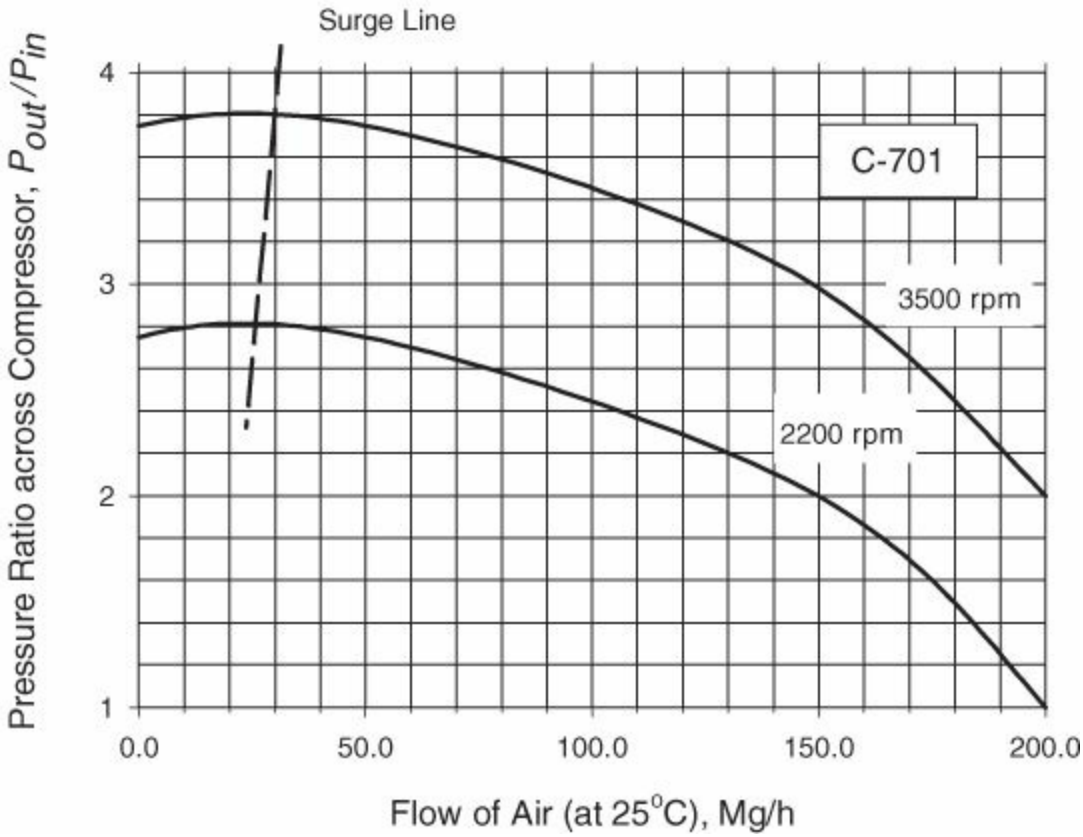


Figure C.7. Pump and Compressor Curves for P-703 A/B and C-701

Table C.8. Flow Summary Table for Current Operation of Phthalic Anhydride Production Facility, Unit 700 (see Figure C.5)

Stream Number	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
Temperature (°C)	200	25	200	164	400	240	263	263	360	160	131	131	131	141	241	190	241	350
Pressure (bar)	0.80	1.01	3.35	3.10	2.85	2.85	2.75	2.25	2.00	1.70	1.40	1.40	0.15	0.11	0.30	0.05	0.20	3.00
Vapor mole fraction	0.0	1.0	0.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Flowrate (tonne/h)	12.82	144.25	12.82	144.25	12.82	144.25	157.07	157.07	157.07	157.07	145.00	12.07	12.07	1.61	10.47	10.06	0.40	1624.72
Flowrate (kmol/h)																		HiTec molten salt
Naphthalene	100.0	0.0	100.0	0.0	100.0	0.0	100.0	100.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Oxygen	0.0	1050.0	0.0	1050.0	0.0	1050.0	1050.0	1050. 0	469.0	469.0	469.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Phthalic anhydride	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	70.0	70.0	0.7	69.0	69.0	0.69	69.0	68.0	0.69	0.0
Maleic anhydride	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0-	16.0	16.0	0.8	15.0	15.0	15.0	0.015	0.015	0.0	0.0
Naphthoquinone	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	2.0	0.0	2.0	2.0	0.08	1.9	0.002	1.91	0.0
Carbon dioxide	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	306.0	306.0	306.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Carbon monoxide	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	50.0	50.0	50.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Nitrogen	0.0	3950.0	0.0	3950.0	0.0	3950.0	3950.0	3950.0	3950.0	3950.0	3950.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Water	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	238.0	238.0	238.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Total (kmol/h)	100.0	5000.0	100.0	5000.0	100.0	5000.0	5100.0	5100.0	5101.0	5101.0	5014.0	86.0	86.0	16.0	71.0	68.0	2.60	17,660

Stream Number	hps to E-701	Conden. from E-701	hps to E-707	Conden. from E-707	hps to E-705	Conden. from E-705	cw to E-706	cwr from E-706	cw to E-704	cwr from E-704	bfw to E-703	bfw to E-702	hps from E-702
Temperature (°C)	254	254	254	254	254	254	30	45	30	45	91	173	254
Pressure (bar)	42.4	42.4	42.4	42.4	42.4	42.4	5.16	4.86	5.16	4.86	42.4	42.4	42.4
Vapor mole fraction	1.0	0.0	1.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0
Total tonnes/h	6.73	6.73	9.36	9.36	1.89	1.89	267.84	267.84	19.62	19.62	104.98	104.98	104.98

Table C.9. Equipment Summaries (Unit 700)

Compressor (assume efficiency independent of flowrate)

C-701 centrifugal, 5670 kW, 80% efficient @ design flowrate and 3500 rpm; can operate at two discrete rpm values, as shown on compressor curve; surge line also shown on compressor curve

Pumps (assume efficiency independent of flowrate)

P-701 A/B centrifugal, 1.3 kW, 50% efficient
P-702 A/B centrifugal, 54 kW, 70% efficient
P-703 A/B centrifugal, 140 kW, 80% efficient
P-704 A/B centrifugal, 0.5 kW, 40% efficient
P-705 A/B centrifugal, 4.4 kW, 50% efficient
P-706 A/B centrifugal, 0.8 kW, 40% efficient

Fired Heater (process fluid flows through a set of tubes with a natural gas or liquid fuel fired flame, providing the radiant and convective heat transfer necessary to heat the fluid to the desired temperature)

H-701 fired heater, $Q = 9{,}350$ MJ/h
Consists of four identical banks of tubes—currently these are all in operation and are operating in parallel—piping and valving exist to run any or all tube banks in any configuration (i.e., series, parallel, etc.)—there is a control system that maintains the temperature of Stream 5 by measuring the temperature of Stream 5 and altering the natural gas and air feed rate.

Heat Exchangers (all one pass on each side, unless otherwise noted; h_i refers to tube side; tube wall resistance negligible, unless otherwise noted)

E-701 Uses high-pressure steam, steam in shell, $Q = 11{,}370$ MJ/h
$A = 695$ m^2, $U = 112$ W/m^2°C, $h_i = 114$ W/m^2°C

E-702 Makes high-pressure steam, steam in shell, $Q = 215{,}407$ MJ/h
$A = 539$ m^2, $U = 2{,}840$ W/m^2°C, $h_i = 3960$ W/m^2°C
hps supplies Unit 700 needs, excess steam used in Unit 300

E-703 Preheats high-pressure bfw, bfw in shell, $Q = 36{,}900$ MJ/h
$A = 1519$ m^2, $U = 57$ W/m^2°C, $h_i = 63$ W/m^2°C

E-704 Total condenser for T-701, condensing fluid in shell
$A = 5.52$ m^2, $U = 600$ W/m^2°C, all resistance on water side

E-705 Reboiler for T-701
$A = 50$ m^2, $U = 1400$ W/m^2°C, approximately equal resistances

E-706 Total condenser for T-702, condensing fluid in shell
$A = 51$ m^2, $U = 600$ W/m^2°C, all resistance on water side

E-707 Reboiler for T-702
$A = 243$ m^2, $U = 1400$ W/m^2°C, approximately equal resistances

Reactor

The reactor is a fluidized bed, which means that the bed temperature is essentially constant and equal to the exit temperature of the gas.

R-701 Fluidized bed with vanadium oxide catalyst coated on silica gel
Molten salt circulated in tubes to remove heat of reaction
Heat-exchange area = 15,850 m^2 (parallel tube banks within reactor)
U = 100 $W/m^{2\circ}C$, all resistance on reactor side
Heat removal required = 2.154×10^5 MJ/h
Reactor pressure drop unaffected by flowrate

Molten Salt Loop

Molten salt is used to remove the heat generated in the reactor. It circulates in a closed loop and is thermally regenerated by making high-pressure steam in E-702. The properties of this molten salt, known as HiTec, may be found in the 6th edition of Perry's, pp. 9–77.

Switch Condenser

SC-701 There are three sets of condensers. Due to the low partial pressure of phthalic anhydride in the stream, it desublimates rather than condenses. Therefore, the process stream is cooled using a low-temperature oil in tubes to promote desublimation. Then after solid is loaded on the heat transfer surface, higher-temperature oil is circulated in the tubes to melt the solid. There are three such devices, one operating in desublimation mode, one operating in melting mode, and one on standby. The net result is a liquid stream containing the condensables, and a vapor stream containing water and the noncondensables. These condensers are designed and maintained under contract by CONDENSEX. They indicate operation at any scale is possible as long as the pressure of Stream 10 remains within 10% of current operating conditions, and as long as the relative composition of the condensables remains approximately constant.

Distillation Columns (For both distillation columns, it may be assumed that weeping begins to occur at 35% of flooding. Both use high-pressure steam and cooling water at the maximum allowable temperature rise.)

T-701 Removes maleic anhydride impurity overhead
Reflux ratio = 0.27
33 trays, 40% efficient, 12-in tray spacing, 2-in weirs
Diameter = 0.84 m, active area = 75% of total area
Q_c = –1230 MJ/h
Q_r = 3220 MJ/h

T-702 Removes phthalic anhydride product overhead
Reflux ratio = 2.43
86 trays, 50% efficient, 18-in tray spacing, 0.75-in weirs
Diameter = 4.2 m, active area = 75% of total area
Q_c = –16,810 MJ/h
Q_r = 15,890 MJ/h

Vessels

V-701 Diameter = 0.50 m, Length = 1.50 m

V-702 Diameter = 1.25 m, Length = 3.75 m

Air Treatment

The organics in Stream 11 are removed in a scrubber, with 10,000 kg of water needed per kg of organic, at the current operating conditions. If the organic content of Stream 11 becomes more concentrated, then the amount of water needed increases by 100 kg per 0.001 mass fraction of organic. The water is sent to the on-site wastewater treatment facility.

C.3.4. Assignment

Your assignment is to provide recommendations as to how much immediate scale-down is possible and what, if any, modifications would be needed to scale down by 50%. For now, you are to consider only the portion of the process prior to the switch condensers. You should also recommend any other changes that you feel should be made to improve performance in Unit 700. Because our plant is due for annual shutdown in a few months, we want specific recommendations as to what should be done at that time and the cost of these alterations and/or modifications.

Specifically, you are to prepare the following by two weeks from now:

1. A written report detailing the maximum scale-down possible, how to achieve 50% scale-down, recommendations, and costs associated with scaling down production in Unit 700.
2. A list of new equipment to be purchased, including size, cost, and materials of construction.
3. An analysis of any change in the annual operating cost created by your recommended modifications.
4. A legible, organized set of calculations justifying your recommendations, including any assumptions made.

C.3.5. Report Format

This report should be brief. Most of the report should be an executive summary, not to exceed five double-spaced, typed pages, that summarizes your diagnosis, recommendations, and rationale. Figures and tables may be included (and do not count against the page limit) in the executive summary. An appendix should be attached that includes items such as the requested calculations. These calculations should be easy to follow. In general, the written report should follow the guidelines given in Chapter 29 (in this CD).

PROJECT 4. The Design of a New 100,000-Metric-Tons-per-Year Phthalic Anhydride Production Facility

C.4.1. Background

The operation of Unit 700, our phthalic anhydride facility, has been successfully scaled down by 50%. Over the long term, we are still considering changing to o-xylene as the raw material. The catalysis and reaction engineering group has finished preliminary research and is very optimistic about its new catalyst. They promise that it will be superior to other versions of o-xylene to phthalic anhydride catalysts in that most side products are minimized. At this point we are uncertain as to whether Unit 700 will be retrofitted to accommodate the new catalyst or whether we will build a new, grassroots facility at another site, nearer to an o-xylene producer.

In order for us to have enough information to make an informed decision, we need a preliminary process design for a grassroots facility to produce phthalic anhydride from what may be assumed to be pure o-xylene. Your job is to prepare a preliminary design for the new 100,000 metric tons/y phthalic anhydride from o-xylene plant, and it must be completed within the next month. You may assume that the o-xylene feed is available at 100°C and 1.1 bar and that the required purity for phthalic and maleic anhydride products is 99.9 wt% and 95.0 wt%, respectively.

C.4.2. Other Information

Concentrated organic waste streams may be burned instead of natural gas only if a fired heater is included in the design. Dilute organic waste streams must be sent to a treatment facility, with the

appropriate operating cost charged. The capital cost of this facility may be assumed to be included in the grassroots cost of the new facility. Other pertinent information is given below and in Tables C.10, C.11, and C.12.

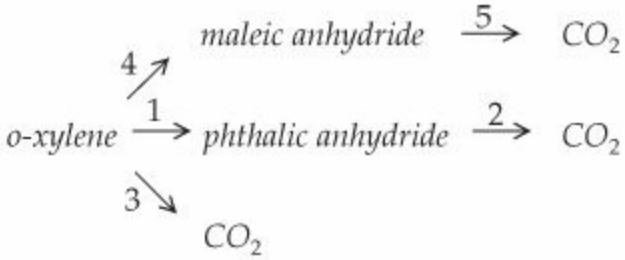
Table C.10. Information on Reaction Kinetics (Unit 700)

The catalysis and reaction engineering group has obtained the following kinetic information regarding the o-xylene to phthalic anhydride reaction. The reactions are

$$\underset{\textit{o-xylene}}{C_8H_{10}} + 3O_2 \rightarrow \underset{\textit{phthalic anhydride}}{C_8H_4O_3} + 3H_2O$$

$$C_8H_{10} + \frac{15}{2}O_2 \rightarrow \underset{\textit{maleic anhydride}}{C_4H_2O_3} + 4H_2O + 4CO_2$$

In addition, the complete combustion reaction for each organic component occurs. The reaction network is given below. As you can see, a major advantage of our catalyst is that CO formation is essentially eliminated and no heavy impurity is made.



The catalyst must operate between 300°C and 400°C, and at pressures between 1 atm and 3 atm. In this range, the kinetics are as follows. (Partial pressures in atmospheres, r_i in kmol h^{-1} (kg catalyst) $^{-1}$, $k_0 = 1$ kmol h^{-1}(kg catalyst)$^{-1}$atm^{-2}, $R = 1.987$ cal/K mole, and T is in K.)

$$r_1 = k_1 p_{xyl} p_{o_2} \qquad \ln\frac{k_1}{k_0} = -\frac{27{,}000}{RT} + 19.837$$

$$r_2 = k_2 p_{pal} p_{o_2} \qquad \ln\frac{k_2}{k_0} = -\frac{31{,}000}{RT} + 20.86$$

$$r_3 = k_3 p_{xyl} p_{o_2} \qquad \ln\frac{k_3}{k_0} = -\frac{28{,}600}{RT} + 18.97$$

$$r_4 = k_4 p_{xyl} p_{o_2} \qquad \ln\frac{k_4}{k_0} = -\frac{27{,}900}{RT} + 19.23$$

$$r_5 = k_5 p_{mal} p_{o_2} \qquad \ln\frac{k_5}{k_0} = -\frac{30{,}400}{RT} + 20.47$$

The lower flammability limit of o-xylene in air is 1 mol%, and the upper flammability limit is 6 mol%. For safety reasons, it is necessary that process conditions not be within these limits. It is also necessary that the o-xylene content of the reactor never exceed 10 mol%, because if that

limit is exceeded, the catalyst no longer operates at the desired selectivity, and the reaction could become oxygen starved, forming significant amounts of CO and other undesired by-products.

At this time, we are unsure as to whether a packed-bed reactor (shell-and-tube type, modeled as a plug flow reactor) or a fluidized-bed reactor (modeled as an isothermal plug flow reactor with 10% feed gas bypass) is the better choice. Please address this in your preliminary design. For the shell-and-tube packed bed, the catalyst would be in the tubes. We do believe, however, that tube diameters exceeding 1 inch in a shell-and-tube configuration would not allow for rapid enough heat removal, causing significant hot spots and subsequent catalyst damage.

For a fluidized bed, the following data may be assumed:

Spherical catalyst particle, diameter range d_p = 300–600μm
Catalyst particle density ρ_{cat} = 1600 kg/m^3
Void fraction at minimum fluidization ε_{mf} = 0.50
Heat transfer coefficient from fluidized bed to tube wall h = 300 W/m^2°C
Reactor should operate between $2u_{mf}$ (bubbling) and $50u_{mf}$ (turbulent)
The reactor has a rectangular cross section (width of sides = w and v)
Range of acceptable side ratios $0.2 < v/w < 5$
Maximum value of v or w = 8 m
Maximum volume of bed displaced by tube banks is 40%
The cost of the fluidized bed should be estimated as 5 times the cost of a vessel of the same volume

For u_{mf}, use the correlation of Wen and Yu:

$$\mathrm{Re}_{mf} = \frac{d_p u_{mf} \rho_g}{\mu} = \left[(33.7)^2 + \frac{0.0408 d_p^3 \rho_g (\rho_s - \rho_g) g}{\mu^2} \right]^{0.5} - 33.7$$

where ρ_g is the density of the gas in the fluidized bed (at average conditions) and ρ_s is the solid catalyst particle density (called ρ_{cat} above).

For a shell-and-tube packed bed, the following data may be assumed:

Catalyst particle diameter d_p = 3 mm
Catalyst particle density ρ_{cat} = 1600 kg/m^3
Void fraction ε = 0.50
Heat transfer coefficient from packed bed to tube wall h = 60 W/m^2°C
Use standard tube sheet layouts as for a heat exchanger
Shell diameter is a function of heat transfer characteristics and frictional losses

It is anticipated that a heat transfer fluid will be used in a closed loop to remove the highly exothermic heat of reaction from either type of reactor. We anticipate that all surplus high-pressure steam made can be sold elsewhere in the plant. Because we have had many years of successful operation using the HiTec molten salt, we anticipate using it again for the new process. However, you should feel free to recommend an alternative if you can justify superior performance at the same cost, or equal performance at a lower cost.

Table C.11. Design of the Switch Condensers and Air Treatment Costs (Unit 700)

These are a complex set of three condensers. Because of the low partial pressure of phthalic anhydride in the stream, it desublimates rather than condenses. Therefore, the process stream is cooled using a low-temperature oil in tubes to promote desublimation. Then, after solid is loaded on the heat transfer surface, gas flow to this condenser is stopped, and higher-temperature oil is circulated in the tubes to melt the solid. There are three such devices, one operating in desublimation mode, one operating in melting mode, and one on standby. The net result is a liquid stream containing the condensables and a vapor stream containing some maleic anhydride, some phthalic anhydride, and all of the noncondensables.

These condensers will once again be designed and maintained under contract by CONDENSEX. They indicate that operation at any scale is possible as long as the pressure of the feed to the condensers is between 1.70 and 2.00 bar. You may assume that all light gases are neither condensed nor dissolved and that 99% of the organics are desublimated and melted. Based on past experience, CONDENSEX suggests that we may estimate the capital cost of these condensers as 15% of all other capital costs for the new process, and that the annual operating cost is 3 times the cost of an equivalent amount of cooling water needed to satisfy the cooling duty from the energy balance on the condenser unit modeled as a component separator.

The following cost of treating the waste (dirty) air stream leaving the switch condensers should be used in your cost estimates:

$$\text{Air Treatment Cost} = \$10^{-4} V_{tot}(0.5 + 1000 x_{or})$$

where V_{tot} = the total volume of "dirty air" to be treated, m^3, and x_{or} = mole fraction of organics in "dirty air" stream.

Table C.12. Simulator Hints (Unit 700)

The following hints were developed for students using the CHEMCAD simulator. These should also provide help to people using other simulator packages.

Use SRK (Soave-Redlich-Kwong) for the VLE and enthalpy options in the thermodynamic package for all the units in this process.

For heat exchangers with multiple zones, it is recommended that you simulate each zone with a separate heat exchanger. For the switch condensers, use a component separator, and then calculate the heat duty from the inlet and outlet streams.

When simulating a process using "fake" streams and equipment, it is imperative that the process flow diagram that you present not include any fake streams and equipment. It must represent the actual process.

C.4.3. Assignment

Your assignment is to provide the following:

1. An optimized preliminary design of a plant to make phthalic anhydride from o-xylene using the new catalyst.
2. An economic evaluation giving the NPV (net present value), after tax, of the new project. For your evaluation you should use the following economic information:
   - After-tax internal hurdle rate = 9%
   - Depreciation = MACRS (6-year schedule given in Chapter 9)
   - Marginal taxation rate of 35%
   - Construction period of 2 years

- Project plant life = 10 years after start-up

Specifically, you are to prepare the following by . . . (four weeks from now):

1. A written report detailing your design and profitability evaluation of the new process
2. A clear, complete, labeled process flow diagram of your optimized process
3. A clear stream flow table giving the *T*, *P*, total flowrate in kg/h and kmol/h, component flowrate in kmol/h, and phase for each important process stream
4. A list of new equipment to be purchased, including size, cost, and materials of construction
5. An evaluation of the after-tax NPV, and the discounted cash flow rate of return on investment (DCFROR) for your recommended (optimized) process
6. A legible, organized set of calculations justifying your recommendations, including any assumptions made

C.4.4. Report Format

This report should be in the standard design report format. It should include an abstract, results, discussion, conclusions, recommendations, and an appendix with calculations. The report format rules given in Chapter 29 (in this CD) should be followed.

PROJECT 5. Problems at the Cumene Production Facility, Unit 800

C.5.1. Background

Cumene (isopropyl benzene) is produced by reacting propylene with benzene. During World War II, cumene was used as an octane enhancer for piston engine aircraft fuel. Presently, most of the worldwide supply of cumene is used as a raw material for phenol production. Typically, cumene is produced at the same facility that manufactures phenol.

The plant at which you are employed currently manufactures cumene in Unit 800 by a vapor-phase alkylation process that uses a phosphoric acid catalyst supported on kieselguhr. Plant capacity is on the order of 90,000 metric tons per year of 99 wt% purity cumene. Benzene and propylene feeds are brought in by tanker trucks and stored in tanks as a liquid.

C.5.2. Cumene Production Reactions

The reactions for cumene production from benzene and propylene are as follows:

$$\underset{\text{propylene}}{C_3H_6} + \underset{\text{benzene}}{C_6H_6} \rightarrow \underset{\text{cumene}}{C_9H_{12}}$$

$$\underset{\text{propylene}}{C_3H_6} + \underset{\text{cumene}}{C_9H_{12}} \rightarrow \underset{\text{p-diisopropyl benzene}}{C_{12}H_{18}}$$

C.5.3. Process Description

The PFD for the cumene production process, Unit 800, is given in Figure C.8. The reactants are fed from their respective storage tanks. After being pumped up to the required pressure (dictated by catalyst operating conditions), the reactants are mixed, vaporized, and heated in the fired heater to the temperature required by the catalyst. The shell-and-tube reactor converts the reactants to desired and undesired products as per the above reactions. The exothermic heat of reaction is removed by producing high-pressure steam from boiler feed water in the reactor. The stream leaving the reactor enters the flash unit, which consists of a heat exchanger and a flash drum. The flash unit is used to

separate the C_3 impurities, which are used as fuel for a furnace in another on-site process. The liquid stream from the flash drum is sent to the first distillation column, which separates benzene for recycle. The second distillation column purifies cumene from the p-diisopropyl benzene (p-DIPB) impurity. Currently, the waste p-DIPB is used as fuel for a furnace. The pressure of both distillation columns is determined by the pressure in the flash drum; that is, there are no pressure-reduction valves downstream of the flash drum.

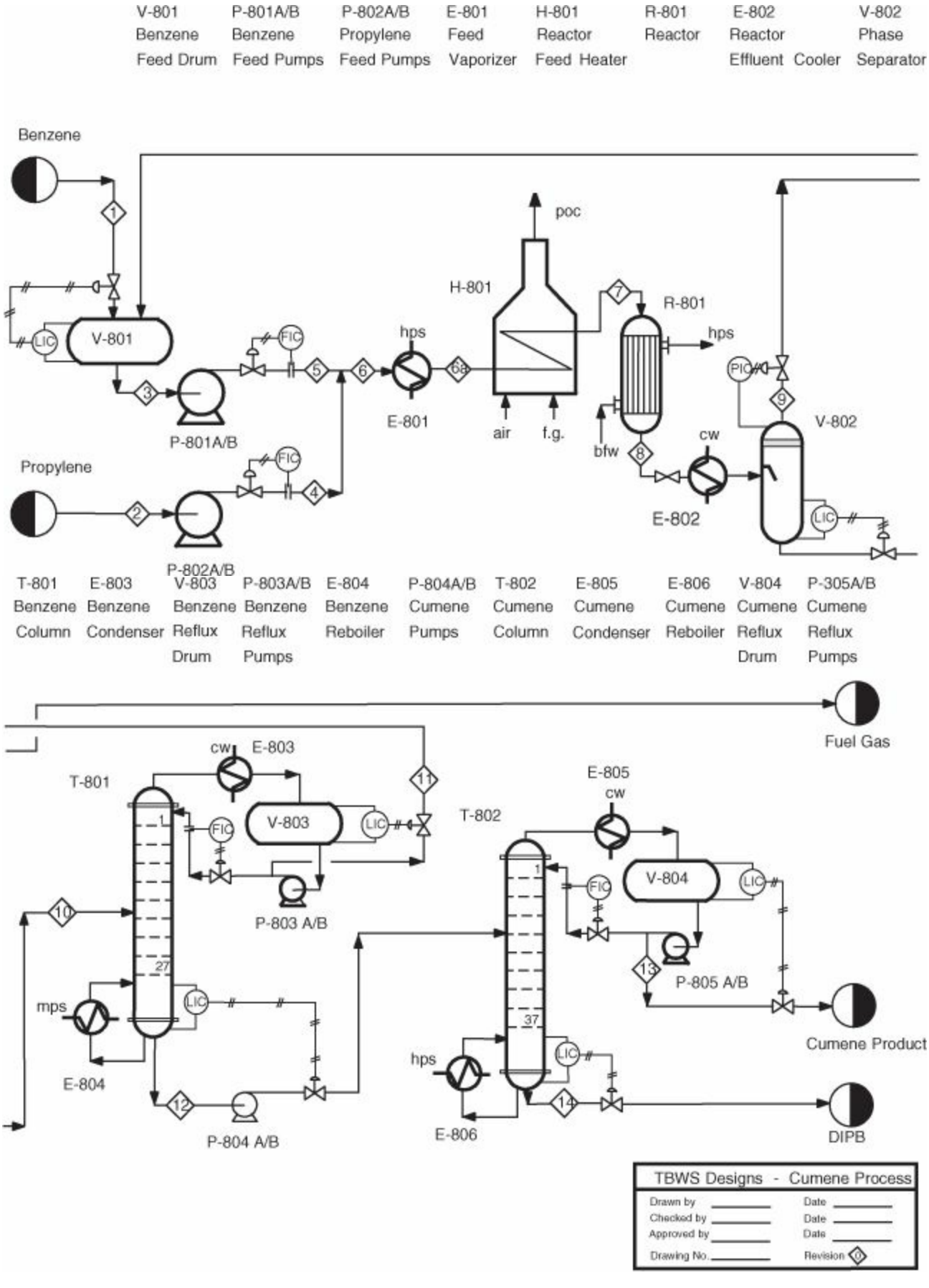


Figure C.8. Process Flow Diagram for the Production of Cumene Process (Unit 800)

C.5.4. Recent Problems in Unit 800

Recently, Unit 800 has not been operating at standard conditions. We have recently switched suppliers of propylene; however, our contract guarantees that the new propylene feed will be within specifications given in Table C.13.

Upon examining present operating conditions, we have made the following observations:

1. Production of cumene has dropped by about 8%, and the reflux in T-801 was increased by approximately 8% in order to maintain 99 wt% purity. The flows of benzene (Stream 5) and propylene (Stream 2) remained the same. Pressure in the storage tanks has not changed appreciably when measured at the same ambient temperature.
2. The amount of fuel gas being produced has increased significantly and is estimated to be 78% greater than before. Additionally, it has been observed that the pressure control valve on the fuel gas line (Stream 9) coming from V-802 is now fully open, although previously it was controlling the flow.
3. The benzene recycle, Stream 11, has increased by about 5%, and the temperature of Stream 3 into P-801 has increased by about 3°C.
4. Production of steam in the reactor has fallen by about 6%.
5. Catalyst in the reactor was changed six months ago, and previous operating history (over last ten years) indicates that no significant drop in catalyst activity should have occurred over this time period.
6. p-DIPB production, Stream 14, has dropped by about 20%.

We are very concerned about this loss in production because we can currently sell all the material we produce.

Another problem that has arisen lately is the malfunction of the feed pumps. This problem arose during a very warm spell when the ambient temperature reached 110°F. A maintenance check showed that P-802 needed a new bearing, and this was taken care of, but P-801 seemed to be OK. The ambient temperature has now returned to a mild 70°F, and both pumps seem to be working fine.

Table C.13. Specifications of Products and Raw Materials

Raw Materials	
Benzene	>99.9 wt% purity
Propylene	≤ 5 wt% propane impurity
Product	
Cumene	>99 wt% purity

Currently, market conditions for cumene are very tight. We are in direct competition with some local companies that have recently built cumene plants. It appears that management is very concerned about our competitiveness because other producers in the area are beginning to undercut our prices. Management wants to find out whether any significant savings in operating costs can be found for Unit 800.

C.5.5. Other Information

Other pertinent information is appended, including a flow table for the process streams at design conditions, that is, prior to the current operating problem, Table C.14; a utility summary table at design conditions, Table C.15; pump curves, Figures C.9 and C.10; a set of design calculations; and an equipment list, Table C.16.

C.5.6. Assignment

Specifically, you are to prepare the following by . . . (two weeks from now):

1. A written report detailing your diagnosis of the operating problems with the plant, along with your recommendations for solving these problems
2. A list of new equipment to be purchased, if any, including size, cost, and materials of construction
3. An analysis of any change in the annual operating cost created by your recommended modifications
4. A legible, organized set of calculations justifying your recommendations, including any assumptions made

C.5.7. Report Format

This report should be brief. Most of the report should be an executive summary, not to exceed five double-spaced, typed pages, which summarizes your diagnosis, recommendations, and rationale. Figures and tables may be included (do not count these against the page limit) in the executive summary. An appendix should be attached that includes items such as the requested calculations. These calculations should be easy to follow. The guidelines given in Chapter 29 (in this CD) should be followed.

Table C.14. Flow Summary Table for Cumene Production at Design Conditions, Unit 800 (Figure C.8)

Stream Number	1	2	3	4	5	6	6a	7	8	9	10	11	12	13	14
Temperature (°C)	25	25	41	28	44	41	214.0	350	350	90	90	57	179	178	222
Pressure (bar)	1.00	11.66	1.01	31.50	31.50	31.25	30.95	30.75	30.25	1.75	1.75	1.75	1.90	1.90	2.10
Vapor mole fraction	0	0	0	0	0.0	0.0	1.0	1.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0
Flowrate (tonne/h)	8.19	4.64	16.37	4.64	16.37	21.01	21.01	21.01	21.01	1.19	19.82	8.18	11.64	11.08	0.56
Flowrates (kmol/h)															
Benzene	105.00	0.0	205.27	0.0	205.27	205.27	205.27	205.27	108.96	7.88	101.08	100.27	0.81	0.81	0.0
Propylene	0.0	105.00	2.89	105.00	2.89	107.89	107.89	107.89	8.86	5.97	2.89	2.89	0.0	0.0	0.0
Propane	0.0	5.27	2.79	5.27	2.79	8.06	8.06	8.06	8.06	5.27	2.79	2.79	0.0	0.0	0.0
Cumene	0.0	0.0	0.94	0.0	0.94	0.94	0.94	0.94	94.39	0.77	93.62	0.94	92.68	91.76	0.92
P-diisopropyl benzene	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.79	0.0	2.79	0.0	2.79	0.03	2.76
Total (kmol/h)	105.00	110.27	211.89	110.27	211.89	322.16	322.16	322.16	223.06	19.89	203.17	106.89	96.28	92.60	3.68

Table C.15. Flow Summary Table for Utility Streams in Unit 800

Stream Name	hps to E-801	Condensate from E-801	mps to E-804	Condensate from E-804	hps to E-806	Condensate from E-806
Temperature (°C)	254	254	185.5	185.5	254	254
Pressure (bar)	42.37	42.37	11.35	11.35	42.37	42.37
Flowrate (tonne/h)	7.60	7.60	3.56	3.56	3.25	3.25

Stream Name	cw to E-802	cw from E-802	cw to E-803	cw from E-803	cw to E-805	cw from E-805
Temperature (°C)	30	45	30	45	30	45
Pressure (bar)	5.16	4.96	5.16	4.96	5.16	4.96
Flowrate (tonne/h)	261.30	261.30	85.88	85.88	87.50	87.50

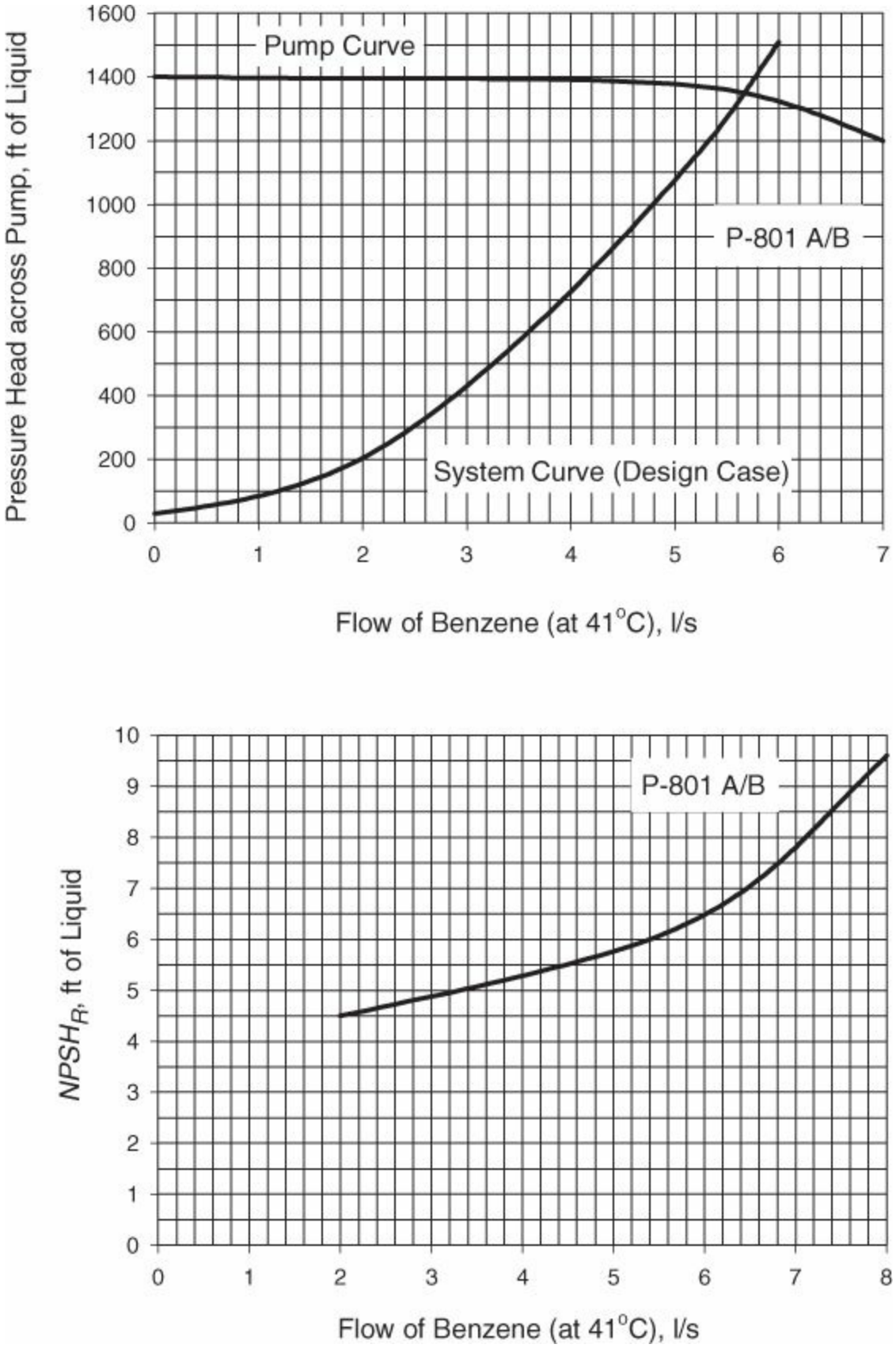
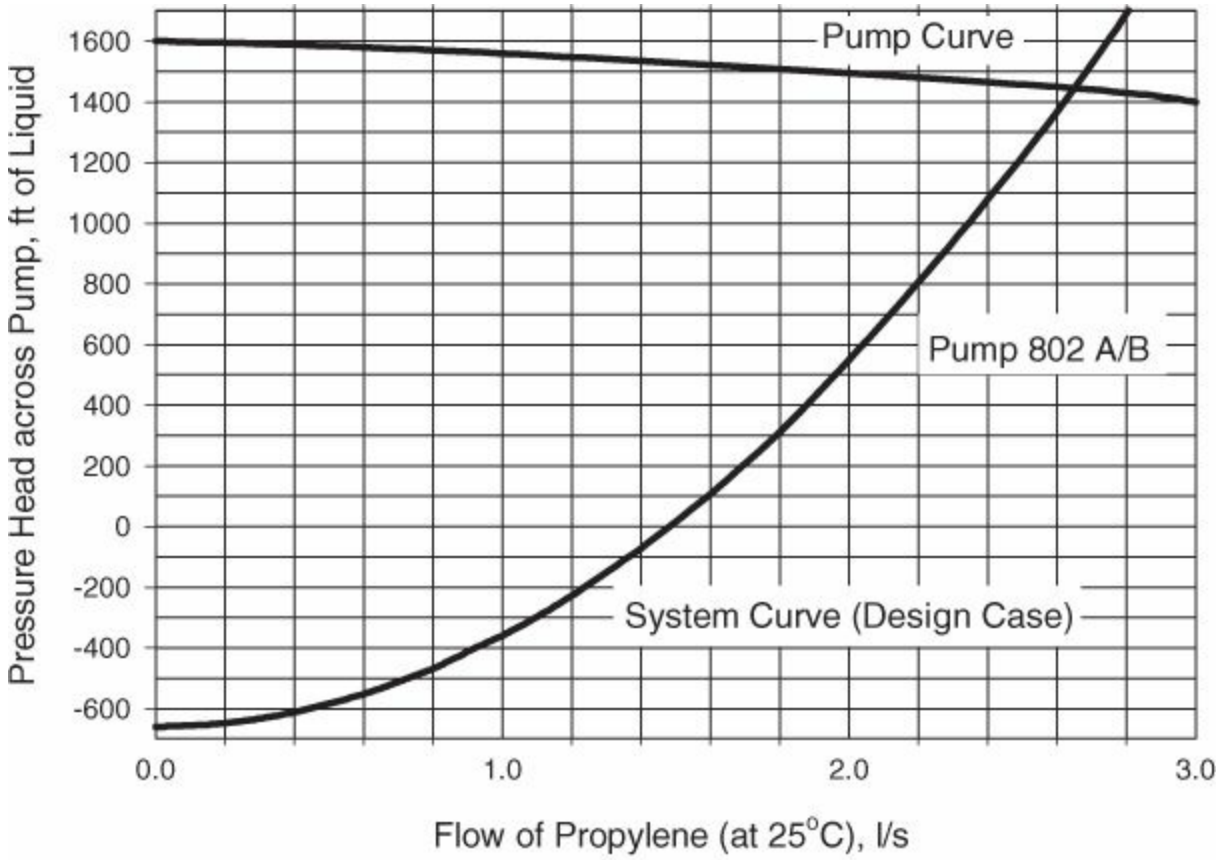


Figure C.9. Pump, System, and NPSH Curves for P-801 A/B



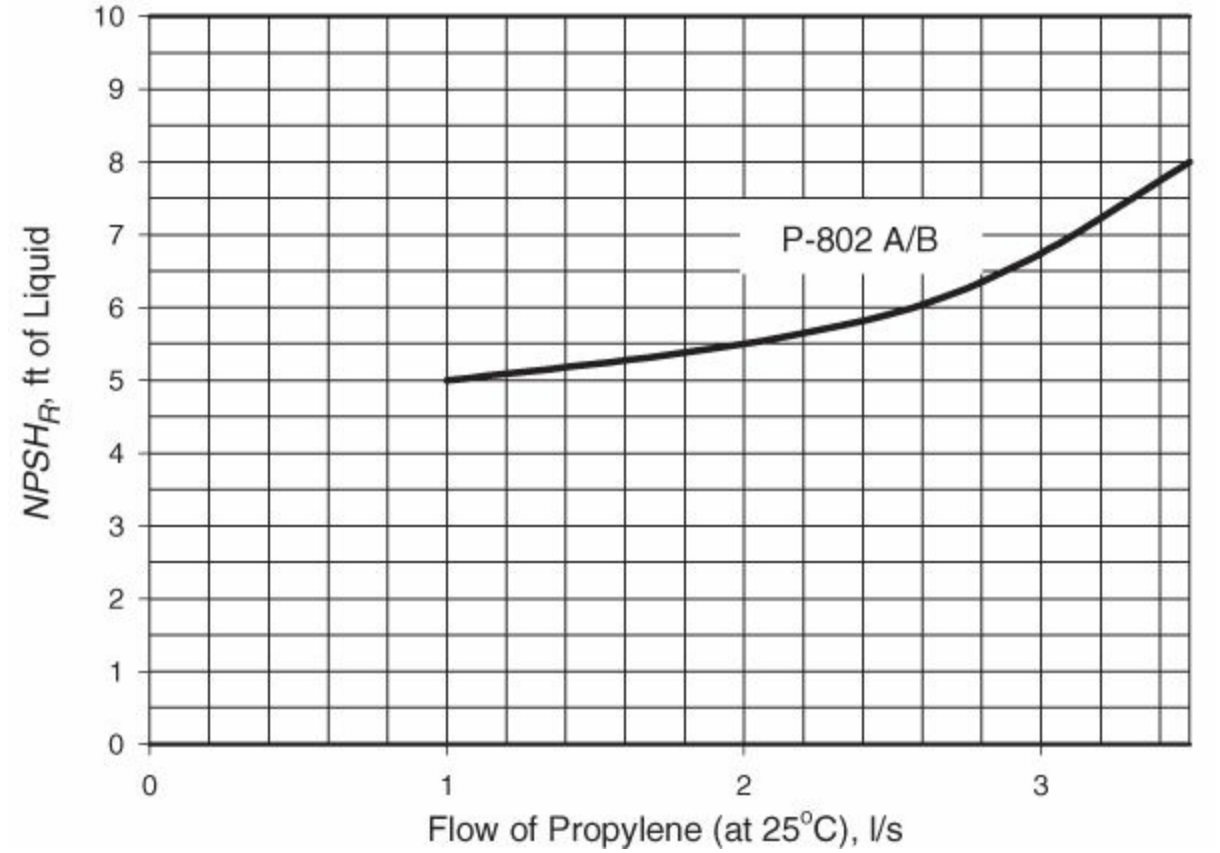


Figure C.10. Pump, System, and NPSH Curves for P-802 A/B

Table C.16. Equipment Summary Table for Unit 800

Tanks (not shown on flowsheet)

TK-801 storage tank for benzene
There are two tanks: one feeding Stream 1 and one in a filling mode.
Each tank is 450 m^3.

TK-802 storage tank for propylene
There are two tanks: one feeding Stream 2 and one in a filling mode.
Each tank is 450 m^3.

Pumps (assume efficiency independent of flowrate)

P-801 centrifugal, 75% efficient, driver rated at 21.9 kW

P-802 centrifugal, 75% efficient, driver rated at 6.8 kW

P-803 centrifugal, 75% efficient, driver rated at 2.4 kW

P-804 centrifugal, 75% efficient, driver rated at 1.0 kW

P-805 centrifugal, 75% efficient, driver rated at 3.3 kW

Heat Exchangers (all one pass on each side, unless otherwise noted; h_i refers to tube side; tube wall resistance negligible, unless otherwise noted)

E-801 uses high-pressure steam, steam in shell, Q = 12,800 MJ/h
A = 20.8 m^2 in two zones
Desubcooling zone: A = 13.5 m^2, U = 600 W/m^2°C, h_i = 667 W/m^2°C
Vaporizing zone: A = 7.3 m^2, U = 1500 W/m^2°C, equal resistances on both sides

E-802 condenser for flash unit, process stream in shell, 1-2 configuration
Q = 16,400 MJ/h, A = 533 m^2

E-803 total condenser for T-801, condensing fluid in shell
A = 151 m^2, U = 450 W/m^2°C, all resistance on water side

E-804 reboiler for T-801
A = 405 m^2, U = 750 W/m^2°C, approximately equal resistances

E-805 total condenser for T-802, condensing fluid in shell
A = 24.0 m^2, U = 450 W/m^2°C, all resistance on water side

E-806 reboiler for T-802
A = 64.0 m^2, U = 750 W/m^2°C, approximately equal resistances

Fired Heater

H-801 Q = 6380 MJ/h (heat actually added to fluid)
Capacity 10,000 MJ/h of heat added to fluid
70% efficiency

Reactor

R-801 shell-and-tube packed bed with phosphoric acid catalyst supported on kieselguhr
Boiler feed water in shell to produce high-pressure steam
Reactor volume = 6.50 m^3, heat exchange area = 342 m^2
234 tubes, 3.0-in (7.62 cm) ID, 6 m long
U = 65 W/m^2°C, all resistance on reactor side
Heat removal required = 9840 MJ/h

Distillation Columns

T-801 removes benzene impurity overhead for recycle
Medium-pressure steam used in reboiler
Cooling water used in condenser, returned at maximum allowable temperature
Reflux ratio = 0.44
27 trays, 50% efficient
24-in tray spacing, 3-in weirs
Diameter = 1.13 m, active area = 75% of total area
Q_c = –5390 MJ/h
Q_r = 7100 MJ/h

T-802 removes cumene product overhead
High-pressure steam used in reboiler
Cooling water used in condenser, returned at maximum allowable temperature
Reflux ratio = 0.63
37 trays, 50% efficient
24-in tray spacing, 3-in weirs
Diameter = 1.26 m, active area = 75% of total area
Q_c = –5490 MJ/h
Q_r = 5520 MJ/h

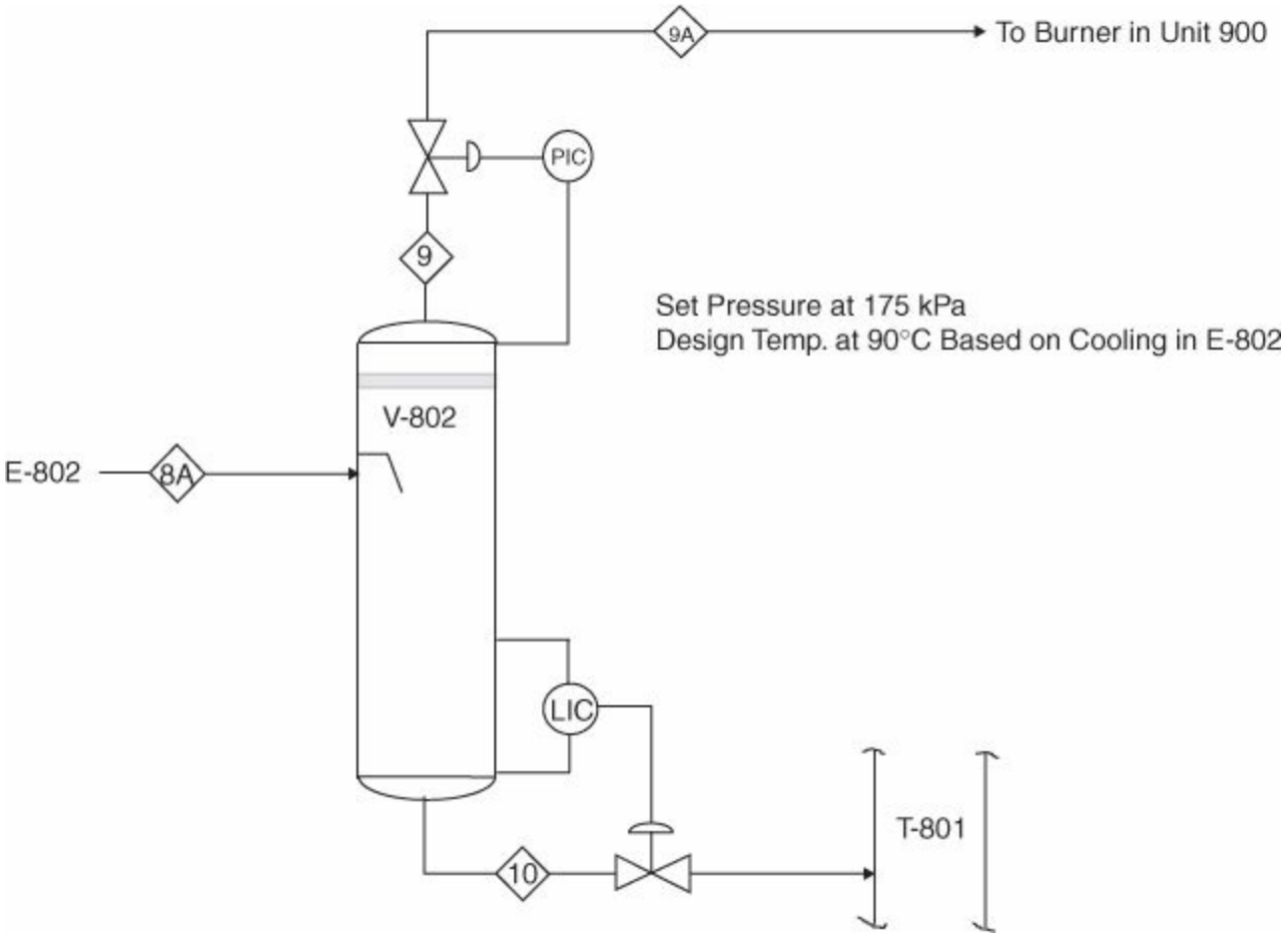
Vessels

V-801	benzene feed drum	4.2 m length, 1.4 m diameter
V-802	flash drum	5.2 m height, 1 m diameter
V-803	T-801 reflux drum	4 m length, 1.6 m diameter
V-804	T-802 reflux drum	6.5 m length, 1.6 m diameter

C.5.8. Process Calculations

Calculations for Fuel Gas Exit Line for V-802

Design flow of fuel gas = 1192 kg/h
Molecular weight of fuel gas = 59.9
Gas viscosity = 9.5×10^{-6} kg/m.s
Gas density = 1.18 (273) P/(293 + 90) (1.01) = 0.00876P kg/m^3 (P in bar)
Destination pressure (in burner in unit 900) = 1.25 bar
$\Delta P_{line} + \Delta P_{valve}$ = 1.75 – 1.25 = 0.50 bar
ΔP_{valve} should be ≅ 0.30 bar and ΔP_{line} = 0.20 bar
Length of line (Stream 9A) ≅ 125 m (equivalent length including fittings)
Average pressure in line, P = (1.45 + 1.25) / 2 = 1.35 bar
Density of gas in line = 0.00876 P = 1.18 kg/m^3
$\Delta P_{line} = 2f \rho u^2 L_e / d_{pipe}$



Look at 3-in, 4-in, and 6-in schedule-40 pipe:

d_{pipe} (nominal)	3 in.	4 in.	6 in.
d_{pipe}(inside) = d_i	0.0779 m	0.1022 m	0.1541 m
$u = 4Q/\pi d_i^2$	58.9 m/s	34.2 m/s	15.0 m/s
$\mathrm{Re} = u\rho d_i/\mu$	5.69×10^5	4.34×10^5	2.88×10^5
e/d_i	0.00059	0.00045	0.0003
f (from friction factor diagram)	0.0046	0.0045	0.0042
$\Delta P_{line} = \frac{2f\rho u^2 L_{eq}}{d_i}$	0.603 bar	0.152 bar	0.018 bar

Choose 4-in schedule-40 pipe.

ΔP_{line} = 0.152 bar and ΔP_{valve} = 0.50 – 0.152 = 0.348 bar

---

Calculations for P-801

Design Conditions (note that 1 kPa = 0.335 ft of water = 0.402 ft of benzene)
LAL (low alarm level) = 5 ft from ground and pump center line is 2 ft from ground
NOL (normal operating level) = 10 ft above ground level

NPSH Calculations (at LAL)
Static head = 5 – 2 = 3 ft of benzene = h_{stat}
P_{supply} = 1.01 bar = 40.7 ft of benzene = h_{supply}

$\Delta P_{friction}$ (in supply line) = 1 psi = 2.8 ft of benzene = $h_{friction}$

Vapor Pressure of Stream 3

$T = 30°C \quad P^* = 54$ kPa
$T = 40°C \quad P^* = 72$ kPa
$T = 50°C \quad P^* = 94$ kPa

Vapor Pressure of Stream 3 = 0.74 bar @ 41°C = 29.7 ft of benzene = h_{vp}

$NPSH_{available} = h_{supply} + h_{static} - h_{friction} - h_{vp} = 40.7 + 3 - 2.8 - 29.7 = 11.2$ ft

$NPSH_{required}$ (from pump curve) = 6.1 ft @ 5.5×10^{-3} m^3/s

$\therefore$ cavitation should not be a problem

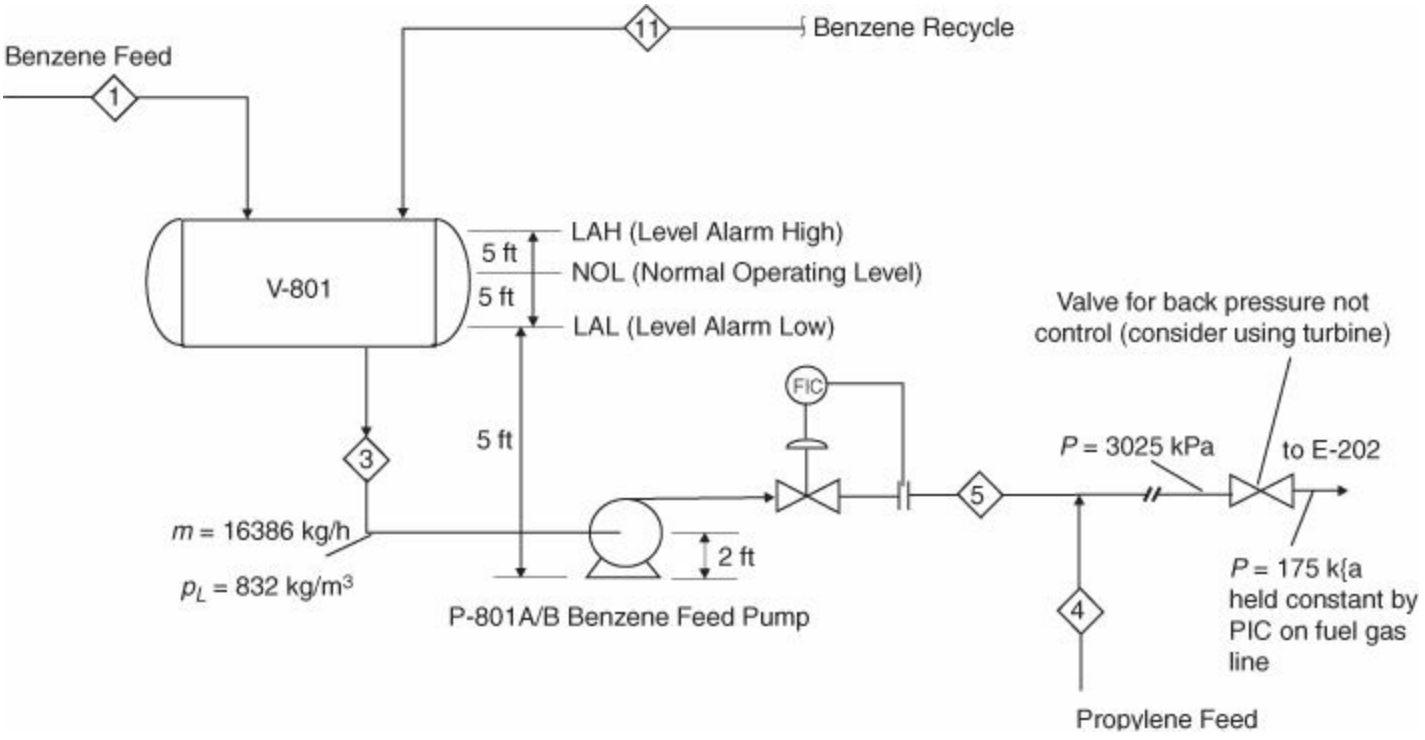
System Curve Calculations

$\Delta P_{friction}$ (discharge) = 31.50 – 1.75 = 29.75 bar = 1196 ft of benzene

$\Delta P_{friction}$ (suction) = 2.8 ft of benzene

$\Delta P_{discharge-tank}$ = 1.75 – 1.01 = 0.74 bar = 30 ft of benzene

ΔP_{static} = 0 (E-801 entrance @ 10 ft above ground level = NOL)



$\therefore$ Required head at design flow = 1199 + 30 + ΔP_{cv} = 1230 ft of benzene + ΔP_{cv}

From pump curve this gives us ΔP_{cv} = 135 ft = 3.36 bar (this is high but OK)

Calculations for P-802

Design Conditions (note that 1 kPa = 0.335 ft of water = 0.666 ft of propylene)
LAL (low alarm level) = 10 ft from ground and pump center line is 2 ft from ground
NOL (normal operating level) = 20 ft from ground

NPSH Calculations (at LAL)

Static head = 10 - 2 = 8 ft of propylene = h_{stat}

$P_{supply} = P_{sat}$ (@25°C) = 11.66 bar = 777 ft of propylene = h_{supply}

$\Delta P_{friction}$ (in supply line) = 0.2 psi = 1 ft of propylene = $h_{friction}$ (3-in schedule 40 pipe

L_e = 20 ft)

Vapor Pressure of Stream 2 = 11.66 bar = 777 ft of propylene = h_{vp}

$NPSH_{available} = h_{supply} + h_{static} - h_{friction} - h_{vp}$ = 777 + 8 – 1 – 777 = 7 ft of propylene
(@ propylene flowrate of 2.57 × 10^{-3} m^3/s)
$NPSH_{required}$ (from pump curve) = 6 ft

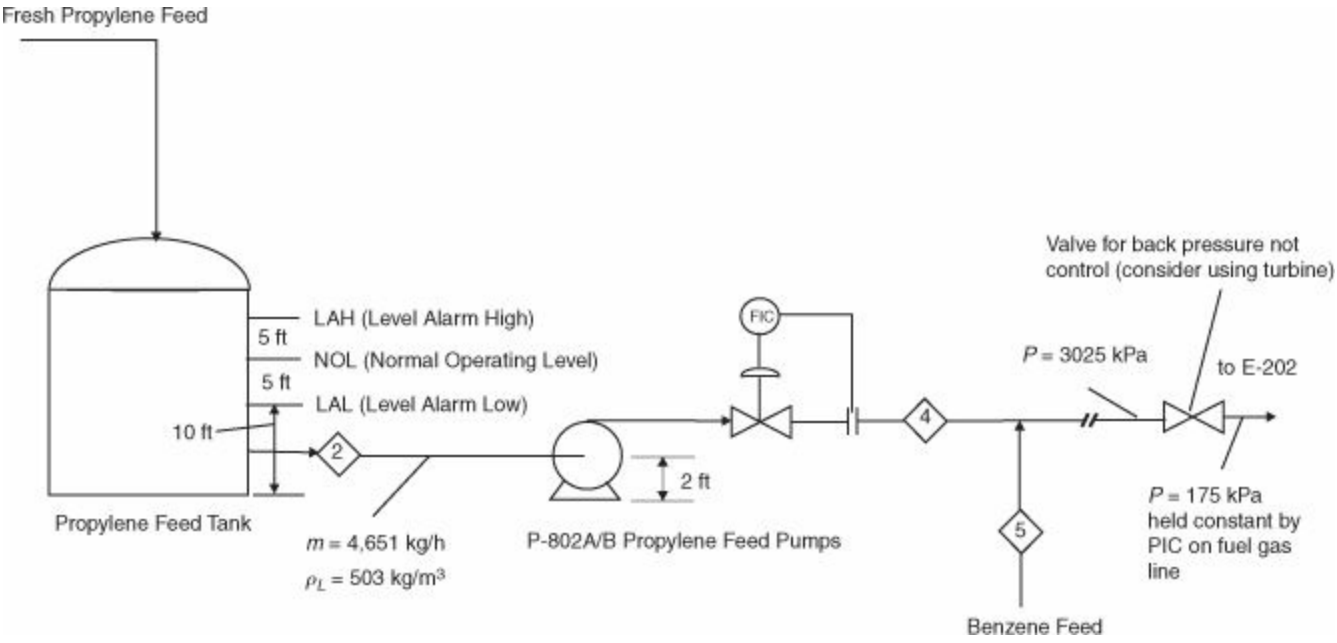
∴ cavitation should not be a problem (put note on P&ID to increase LAL to 12 ft to be safe)

System Curve Calculations

$\Delta P_{friction}$ (discharge) = 31.50 – 1.75 = 29.75 bar = 1981 ft of propylene
$\Delta P_{friction}$ (suction) = 1 ft of propylene
$\Delta P_{discharge\text{-}tank}$ = 1.75 – 11.66 = –9.91 bar = –660 ft of propylene
ΔP_{static} = – 10 ft of propylene

∴ Required head at design flow = 1982 – 660 – 10 + ΔP_{cv} = 1312 ft of propylene + ΔP_{cv}

From pump curve this gives us ΔP_{cv} = 140 ft = 2.10 bar



PROJECT 6. Design of a New, 100,000-Metric-Tons-per-Year Cumene Production Facility

C.6.1. Background

In the opinion of our marketing research department, the demand for phenol-derived plasticizers is on the rise. Therefore, we are investigating the possibility of a new, grass-roots phenol plant to handle the anticipated increase. Because phenol is made from cumene, a grassroots cumene plant would also be necessary. Given your experience in troubleshooting our existing cumene process, we would like you to study the economics of a new cumene plant. Specifically, we would like a complete preliminary design of a grassroots, 100,000 metric ton/y cumene process using benzene and propylene.

We have a new, proprietary catalyst, and the kinetics are included in Table C.17. We would also like you to consider the economics of our continuing to use propylene with 5% propane impurity at

$0.095/lb versus purer propylene feed. In preparing this preliminary design, you should assume that all steam made can be used elsewhere in the plant with the appropriate economic credit, that condensed steam can be returned as boiler feed water for the appropriate credit, and that fuel gas can be burned for credit at its LHV (lower heating value). Additional information is given in Table C.18.

C.6.2. Assignment

Your assignment is to provide the following:

1. An optimized preliminary design of a plant to make cumene from benzene and propylene using the new catalyst
2. An economic evaluation of your optimized process, using the following information:
   - After-tax internal hurdle rate = 9% p.a.
   - Depreciation = MACRS (6-year schedule; see Chapter 9)
   - Marginal taxation rate = 35%

Table C.17 Reaction Kinetics for Cumene Reactions (Unit 800)

The kinetics for the reactions are as follows:

$$\underset{\textit{propylene}}{C_3H_6} + \underset{\textit{benzene}}{C_6H_6} \xrightarrow{k_1} \underset{\textit{cumene}}{C_9H_{12}}$$

$$r_1 = k_1 c_p c_b \quad \text{mole/g cat sec}$$

$$k_1 = 3.5 \times 10^4 \exp\left(\frac{-24.90}{RT}\right)$$

$$\underset{\textit{propylene}}{C_3H_6} + \underset{\textit{cumene}}{C_9H_{12}} \xrightarrow{k_2} \underset{\textit{p-diisopropyl benzene}}{C_{12}H_{18}}$$

$$r_2 = k_2 c_p c_c \quad \text{mole/g cat sec}$$

$$k_2 = 2.9 \times 10^6 \exp\left(\frac{-35.08}{RT}\right)$$

where the units of the activation energy are kcal/mol, the units of concentration are mol/l, and the temperature is in Kelvin.

For a shell-and-tube packed bed, the recommended configuration, the following data may be assumed:

Catalyst particle diameter $d_p = 3$ mm

Catalyst particle density $\rho_{cat} = 1600$ kg/m^3

Void fraction $\varepsilon = 0.50$

Heat transfer coefficient from packed bed to tube wall $h = 60$ W/m^2°C

Use standard tube sheet layouts as for a heat exchanger

If tube diameter is larger than in tube sheet layouts, assume that tube cross-sectional area is 1/3 of shell cross-sectional area

   - Construction period = 2 years
   - Project plant life = 10 years after start-up

Specifically, you are to prepare the following by . . . (four weeks from now):

1. A written report detailing your design and profitability evaluation of the new process
2. A clear, complete, labeled process flow diagram of your optimized process including all equipment and the location of all major control loops
3. A clear stream flow table including T, P, total flowrate in kg/h and kmol/h, component flowrate in kmol/h, and phase for each process stream
4. A list of new equipment to be purchased, including size, cost, and materials of construction
5. An evaluation of the annual operating cost for the plant

Table C.18 Additional Information (Unit 800)

Cost of Manufacture

In order to estimate the cost of manufacture (not including depreciation), COM_d, you should use the following equation:

$$COM_d = 0.180\,FCI + 2.73\,C_{OL} + 1.23\,(C_{UT} + C_{WT} + C_{RM}) \qquad (8.2)$$

The current MACRS method for depreciation should be used in your calculations (see Chapter 9).

Hints for Process Simulator

The CHEMCAD process simulator was used to generate the flow table given in Project 5. The hints given here are specifically directed to CHEMCAD users but should also be applicable for other process simulators.

Use SRK (Soave-Redlich-Kwong) thermodynamics package for VLE and enthalpy calculations for all the equipment in the process.

For heat exchangers with multiple zones, it is recommended that you simulate each zone with a separate heat exchanger. Actual equipment may include several zones, so costing should be based on the actual equipment specifications.

For the reactor, you may use an isothermal reactor to estimate the volume of catalyst and heat-exchange area. For more accurate results, the temperature profile in the reactor should be modeled by completing a differential heat and material balance on the reactor.

For the distillation columns, you should use the Shortcut method (SHOR) to get estimates for the rigorous distillation simulation (TOWR or SCDS). The Shortcut method may be used until an optimum case is near. It is then expected that everyone will obtain a final design using rigorous simulation of the columns.

When simulating a process using "fake" streams and equipment, it is absolutely necessary that the process flow diagram you present not include any "fake" streams and equipment. It must represent the actual process.

6. An analysis of the after-tax NPV (10 years, 9%), and the discounted cash flow rate of return on investment (DCFROR) for your recommended process
7. A legible, organized set of calculations justifying your recommendations, including any assumptions made

C.6.3. Report Format

This report should be in the standard design report format, consistent with the guidelines given in Chapter 29 (in this CD). It should include an abstract, results, discussion, conclusions,

recommendations, and an appendix with calculations.

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