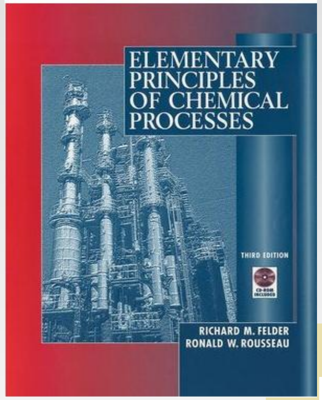
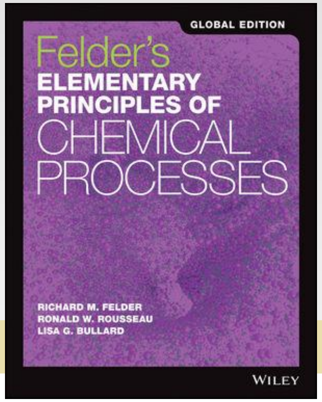




Elementary Principles of Chemical Processes,
3rd or 4th edition,
Wiley & Sons, Inc.
Richard M. Felder, Ronald W. Rousseau, & Lisa G. Bullard.

Student Sample Slides

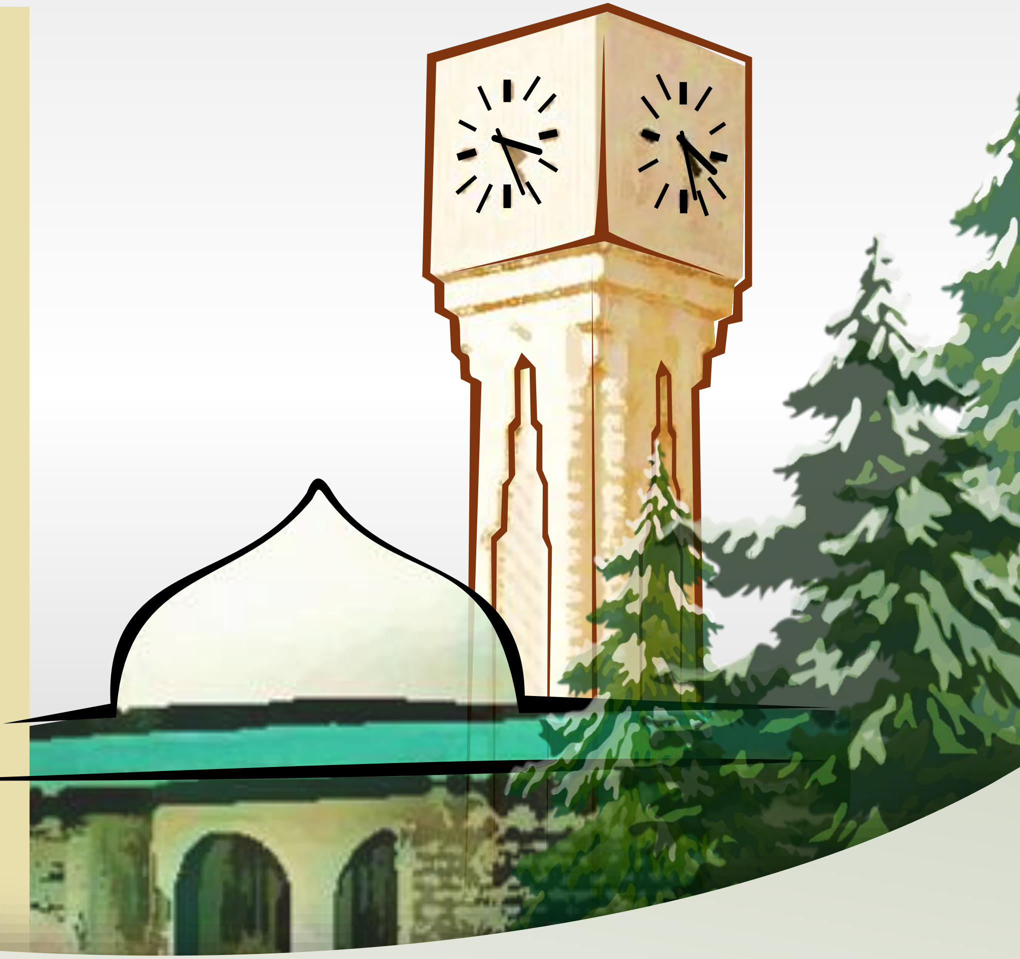
This only a sample of material. Refer to textbook for study of the topics

CHE 0905211

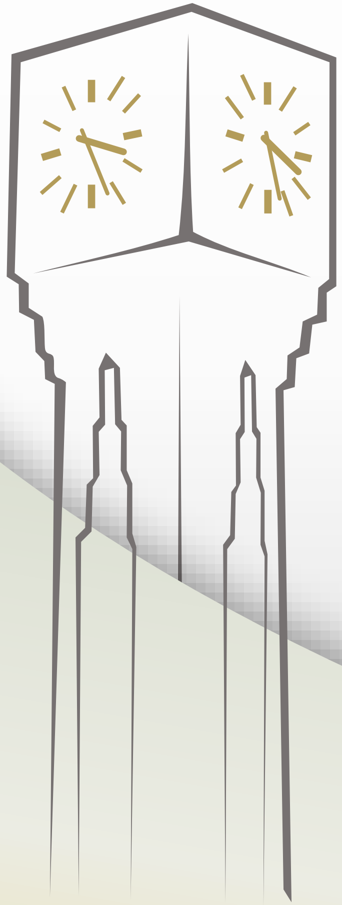
Chemical Engineering Principles 1

Fall 2025

Dr. Hatem Alsyouri	**Chapter 2**



The University of Jordan
Chemical Engineering Department



2.1 Units and Dimensions

Unit and Dimensions

All Measured Quantities Consist of a Number and a Unit.

Dimension
Value
Unit

What's the difference?

Allowed car speed on highway is 120 km/h

Dimension is a property that can be measured (such as *length*, *time*, *mass*) or calculated by multiplying or dividing other dimensions (such as length/time: *velocity*)

Value is the numerical value or worth of the dimension.

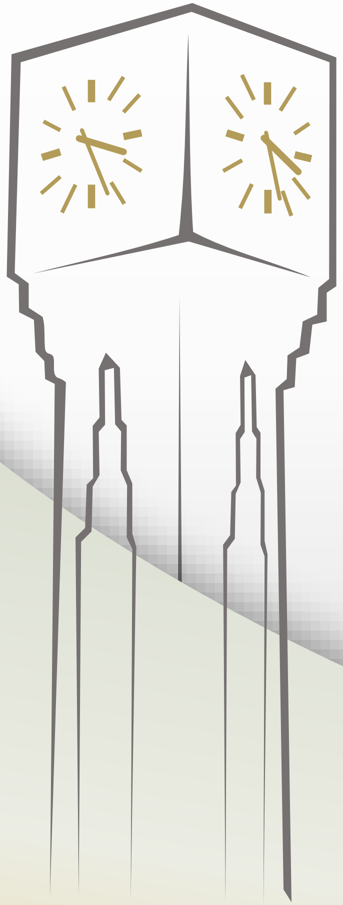
Unit are the means of expressing the dimension such as: *ft* or *cm* for length, and *hour* or *seconds* (for time).

Classification of Dimensions

1. **Basic (or fundamental)** dimension/units are those that can be measured independently and are sufficient to describe essential physical quantities.

2. **Derived** dimension/units are those that can be developed in terms of the basic dimensions/units.

Refer to book to for examples of Basic and Derived units. Memorize some samples



2.2 System of Units

Systems of Units

A system of units has the following components:

1. **Base units** for mass. Length, time, temperature, electrical current, and light intensity.
2. **Multiple units** which are defined as *MULTIPLES* or *FRACTIONS* of base units such as minutes, hours, and milliseconds, all of which are defined in terms of the base unit of a second.
3. **Derived units,** are obtained in one of two ways:
    - a) **Compounds units** obtained By multiplying and dividing base or multiple units (cm^2, $\frac{ft}{min}$, $\frac{kg \cdot m}{s^2}$, etc.).
    - b) **Equivalent units** defined in terms of compound units. Examples:

$$1\ N = 1\ \frac{kg \cdot m}{s^2}$$

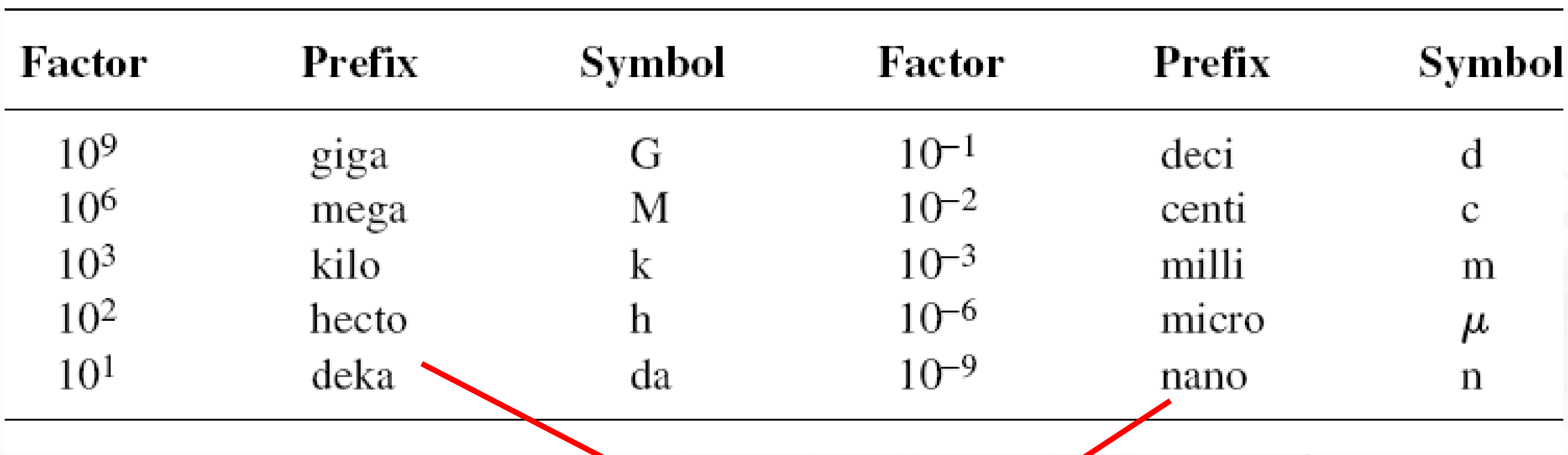
$$1\ dyne = 1\ \frac{g \cdot cm}{s^2}$$

$$1\ lb_f = 32.174\ \frac{lb_m \cdot ft}{s^2}$$

Examples of multiple units

FRACTIONS	**unit**	**MULTIPLES**
	Bite (B)	kB, MB, GB, TB
μm, mm, cm, dm	m	km
μs, ms	s	min, hour, day
mL	L	m^3

Multiple Prefixes



Factor	Prefix	Symbol	Factor	Prefix	Symbol
10^9	giga	G	10^{-1}	deci	d
10^6	mega	M	10^{-2}	centi	c
10^3	kilo	k	10^{-3}	milli	m
10^2	hecto	h	10^{-6}	micro	μ
10^1	deka	da	10^{-9}	nano	n

Remember !

These are multiples not units

Examples

What is the type of the following units?

Class duration is 120 min. *multiple unit (multiple of second)*

Speed of car is 100 km/h. *derived unit (compound)*

Temperature is 40°C. *basic unit*

Weight is 20 $\frac{kg \cdot m}{s^2}$. *derived (compound)*

Pressure is 100 kPa. *derived (equivalent) + multiple*

(1) SI system of units

"*S*ysteme *I*nternationale d'Unites"

(2) The CGS system

(3) American Engineering system

(or English system)

Refer to book to learn the Basic and Derived units in each system

Operations with Units

Addition, Subtraction, Equality

Remember. Numerical values of two quantities may be added, subtracted or equated only if the dimensions and units are the same.

$$\left.\begin{array}{l} 5\ kg + 3\ joules = ? \\ 3\ cm - 1\ s = ? \end{array}\right\}$$

Dimensions are different.
Operation cannot be carried out !

$$3\ x - y = ?$$

$$\left.\begin{array}{l} 3\ cm - 1\ mm = ? \\ 10\ pounds + 5\ grams = ? \end{array}\right\}$$

Dimensions are the same but units are not similar.
Operation cannot be completed until units are the same

$$\left.\begin{array}{l} 3\ cm - 1\ cm = 2\ cm \\ 3\ x - 1\ x = 2\ x \end{array}\right\}$$

Units are the same.
The operation can be completed

Multiplication and Division

Remember. Numerical values and their corresponding units may be always combined by multiplication or division even if units are unlike. However, you cannot cancel units until they are identical.

$$3\ \mathrm{N} \times 4\ \mathrm{m} = 12\ \mathrm{N \cdot m}$$

$$\frac{5.0\ \mathrm{km}}{2.0\ \mathrm{h}} = 2.5\ \mathrm{km/h}$$

$$7.0\ \frac{\mathrm{km}}{\cancel{\mathrm{h}}} \times 4\ \cancel{\mathrm{h}} = 28\ \mathrm{km}$$

$$3\ \mathrm{m} \times 4\ \mathrm{m} = 12\ \mathrm{m}^2$$

$$6\ \mathrm{cm} \times 5\ \frac{\mathrm{cm}}{\mathrm{s}} = 30\ \mathrm{cm}^2/\mathrm{s}$$

$$\left(5.0\ \frac{\cancel{\mathrm{kg}}}{\mathrm{s}}\right) \Big/ \left(0.20\ \frac{\cancel{\mathrm{kg}}}{\mathrm{m}^3}\right) = 25\ \mathrm{m}^3/\mathrm{s}$$

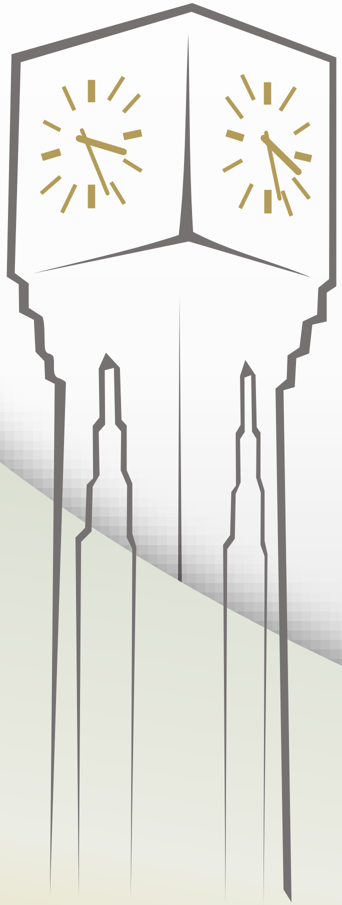
$$\frac{6\ \mathrm{g}}{2\ \mathrm{g}} = 3 \qquad \text{(3 is a \textit{dimensionless} quantity)}$$

Functions

- Trigonometric functions have angular units (radians, degrees).
- All other functions and function arguments, including exponentiation, powers, etc., must be dimensionless.

$$\left.\begin{array}{c} \sin\left(\frac{\pi}{2}\cdots\right) \\ \\ \log(16\cdots) \\ \\ 6^{\,2t\cdots} \end{array}\right\}$$

(….) means unitless



2.3 Conversion of Units

Conversion of Units

$$g \overset{1000}{\longleftrightarrow} kg$$

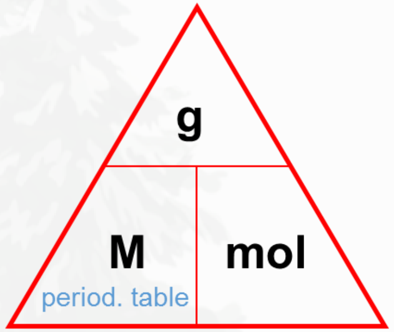
$$mass \overset{M}{\longleftrightarrow} mol$$

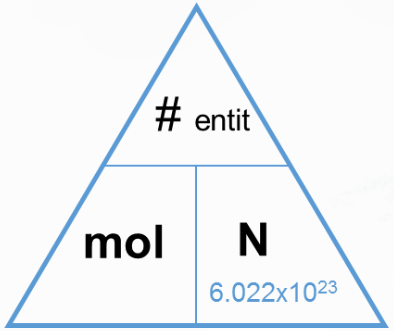
$$mol \overset{N}{\longleftrightarrow} molecules$$

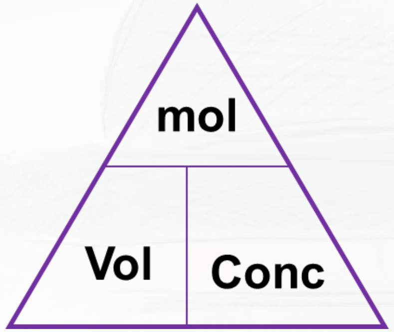
$$mass \overset{D}{\longleftrightarrow} volume$$

Multiply or Divide???


www.faccinefb.com







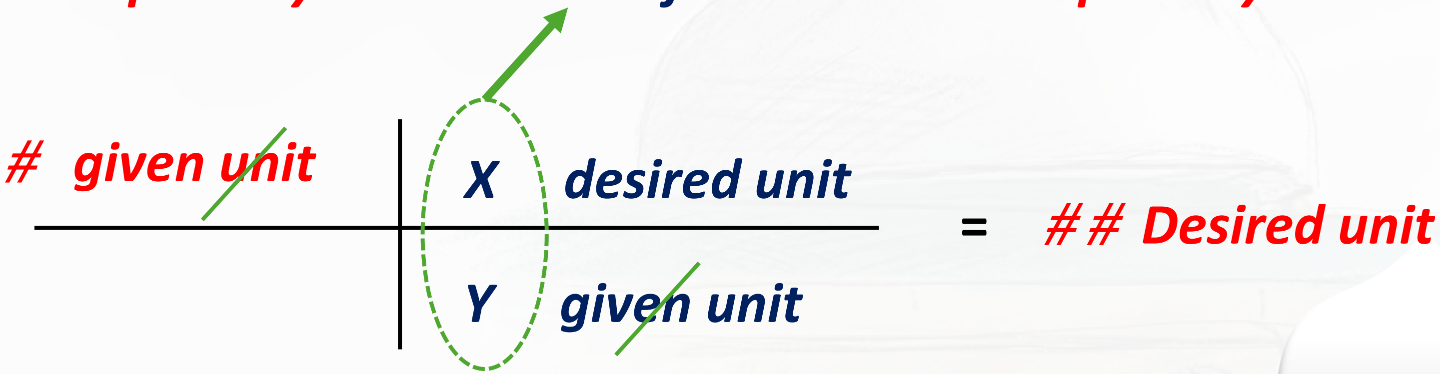
Not needed anymore

Dimensional Analysis for unit conversion

Dimensional analysis:
A method that uses a <u>conversion factor</u> to convert a quantity expressed in one unit to an equivalent quantity in a different unit.

Conversion factor:
States the relationship between two different units.

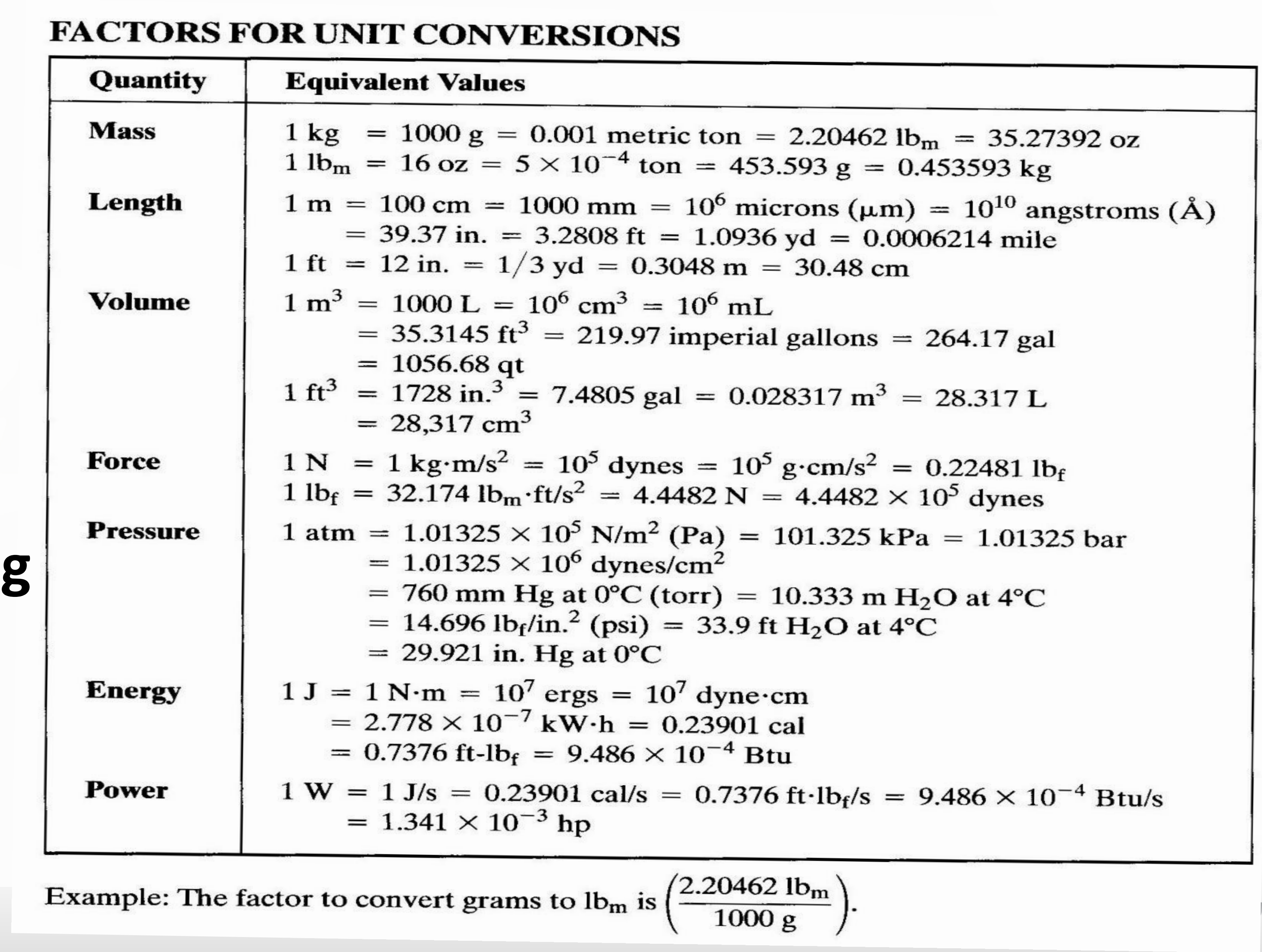
given quantity × conversion factor = Desired quantity



$$\frac{\#\ \cancel{\text{given unit}}}{}\ \left|\ \frac{X\ \text{desired unit}}{Y\ \cancel{\text{given unit}}}\right. = \#\#\ \text{Desired unit}$$

Conversion Table

This table is an important tool. Learn how to use it and always have a hardcopy during lectures



FACTORS FOR UNIT CONVERSIONS

Quantity	Equivalent Values
Mass	$1\ \mathrm{kg} = 1000\ \mathrm{g} = 0.001$ metric ton $= 2.20462\ \mathrm{lb_m} = 35.27392\ \mathrm{oz}$ $1\ \mathrm{lb_m} = 16\ \mathrm{oz} = 5 \times 10^{-4}$ ton $= 453.593\ \mathrm{g} = 0.453593\ \mathrm{kg}$
Length	$1\ \mathrm{m} = 100\ \mathrm{cm} = 1000\ \mathrm{mm} = 10^{6}$ microns (μm) $= 10^{10}$ angstroms (Å) $= 39.37$ in. $= 3.2808$ ft $= 1.0936$ yd $= 0.0006214$ mile 1 ft $= 12$ in. $= 1/3$ yd $= 0.3048\ \mathrm{m} = 30.48\ \mathrm{cm}$
Volume	$1\ \mathrm{m}^3 = 1000\ \mathrm{L} = 10^{6}\ \mathrm{cm}^3 = 10^{6}\ \mathrm{mL}$ $= 35.3145\ \mathrm{ft}^3 = 219.97$ imperial gallons $= 264.17$ gal $= 1056.68$ qt $1\ \mathrm{ft}^3 = 1728\ \mathrm{in.}^3 = 7.4805\ \mathrm{gal} = 0.028317\ \mathrm{m}^3 = 28.317\ \mathrm{L}$ $= 28{,}317\ \mathrm{cm}^3$
Force	$1\ \mathrm{N} = 1\ \mathrm{kg \cdot m/s^2} = 10^{5}$ dynes $= 10^{5}\ \mathrm{g \cdot cm/s^2} = 0.22481\ \mathrm{lb_f}$ $1\ \mathrm{lb_f} = 32.174\ \mathrm{lb_m \cdot ft/s^2} = 4.4482\ \mathrm{N} = 4.4482 \times 10^{5}$ dynes
Pressure	$1\ \mathrm{atm} = 1.01325 \times 10^{5}\ \mathrm{N/m^2}$ (Pa) $= 101.325$ kPa $= 1.01325$ bar $= 1.01325 \times 10^{6}\ \mathrm{dynes/cm^2}$ $= 760$ mm Hg at 0°C (torr) $= 10.333$ m H_2O at 4°C $= 14.696\ \mathrm{lb_f/in.^2}$ (psi) $= 33.9$ ft H_2O at 4°C $= 29.921$ in. Hg at 0°C
Energy	$1\ \mathrm{J} = 1\ \mathrm{N \cdot m} = 10^{7}$ ergs $= 10^{7}$ dyne·cm $= 2.778 \times 10^{-7}\ \mathrm{kW \cdot h} = 0.23901$ cal $= 0.7376\ \mathrm{ft\text{-}lb_f} = 9.486 \times 10^{-4}$ Btu
Power	$1\ \mathrm{W} = 1\ \mathrm{J/s} = 0.23901$ cal/s $= 0.7376\ \mathrm{ft \cdot lb_f/s} = 9.486 \times 10^{-4}$ Btu/s $= 1.341 \times 10^{-3}$ hp

Example: The factor to convert grams to $\mathrm{lb_m}$ is $\left(\dfrac{2.20462\ \mathrm{lb_m}}{1000\ \mathrm{g}}\right)$.

Exercise 1 How many feet is 39.37 inches?

Conversion factor (from table) equality:

1 ft = 12 in

Applicable conversion factors:

$$\frac{1\text{ ft}}{12\text{ in}} \quad \text{or} \quad \frac{12\text{ in}}{1\text{ ft}}$$

$$X\text{ ft} = 39.37\ \cancel{\text{in}}\left(\frac{1\text{ ft}}{12\ \cancel{\text{in}}}\right) \quad \boxed{3.28\text{ ft}}$$

The units must cancel

Exercise 2

How many kilometers is 15,000 decimeters?

$$X\ \text{km} = 15000\ \cancel{\text{dm}} \left(\frac{1\ \cancel{\text{m}}}{10\ \cancel{\text{dm}}}\right)\left(\frac{1\ \text{km}}{1000\ \cancel{\text{m}}}\right) = \boxed{1.5\ \text{km}}$$

Exercise 3

How many seconds is 4.38 days?

$$X\ \mathrm{s} = 4.38\ \cancel{\mathrm{d}}\left(\frac{24\ \cancel{\mathrm{h}}}{1\ \cancel{\mathrm{d}}}\right)\left(\frac{60\ \cancel{\mathrm{min}}}{1\ \cancel{\mathrm{h}}}\right)\left(\frac{60\ \mathrm{s}}{1\ \cancel{\mathrm{min}}}\right)$$

$$= \boxed{378{,}432\ \mathrm{s}}$$

$$= \boxed{3.78 \times 10^{5}\ \mathrm{s}}$$

Exercise 4

From Chemistry class

$$1\ \text{atm} = 760\ \text{mmHg} = 1.013 * 10^5\ \text{Pa} = 1.013\ \text{bar} = \ldots.$$

$$\text{foot (International) ft} = 1/3\ \text{yd} = 0.3048\ \text{m}$$

Convert 800 mmHg (pressure) into bars

$$X\ bar = 800\ \cancel{\text{mmHg}} * \frac{1.013\ \text{bar}}{760\ \cancel{\text{mmHg}}} = 1.066\ \text{bar}$$

Convert 36 mg to g

$$\begin{array}{c|c} 36\ \cancel{\text{mg}} & 1\ \text{g} \\ \hline & 1000\ \cancel{\text{mg}} \end{array} = 0.036\ \text{g}$$

$$(36\ \cancel{\text{mg}}) \times \left(\frac{1\ \text{g}}{1000\ \cancel{\text{mg}}}\right) = 0.036\ \text{g}$$

Exercise 5 - Unsolved

a) Convert 5 kg to g

b) Convert 300 g to kg

c) How many meters is 8.72 cm?

d) Convert 250 kPa into atm

Exercise 6

Convert an acceleration of 1 cm/s² to its equivalent in km/yr²

$$\frac{1\ \text{cm}}{\text{s}^2}\;\Bigg|\;\frac{1\ \text{m}}{100\ \text{cm}}\;\Bigg|\;\frac{1\ \text{km}}{1000\ \text{m}}\;\Bigg|\;\frac{3600^2\ \text{s}^2}{1^2\ \text{h}^2}\;\Bigg|\;\frac{24^2\ \text{h}^2}{1^2\ \text{day}^2}\;\Bigg|\;\frac{365^2\text{day}^2}{1^2\ \text{yr}^2}$$

$$= 9.95\times 10^{9}\ \text{km/yr}^2$$

Exercise 7

Conversion between Systems of Units

Convert 2 km to miles

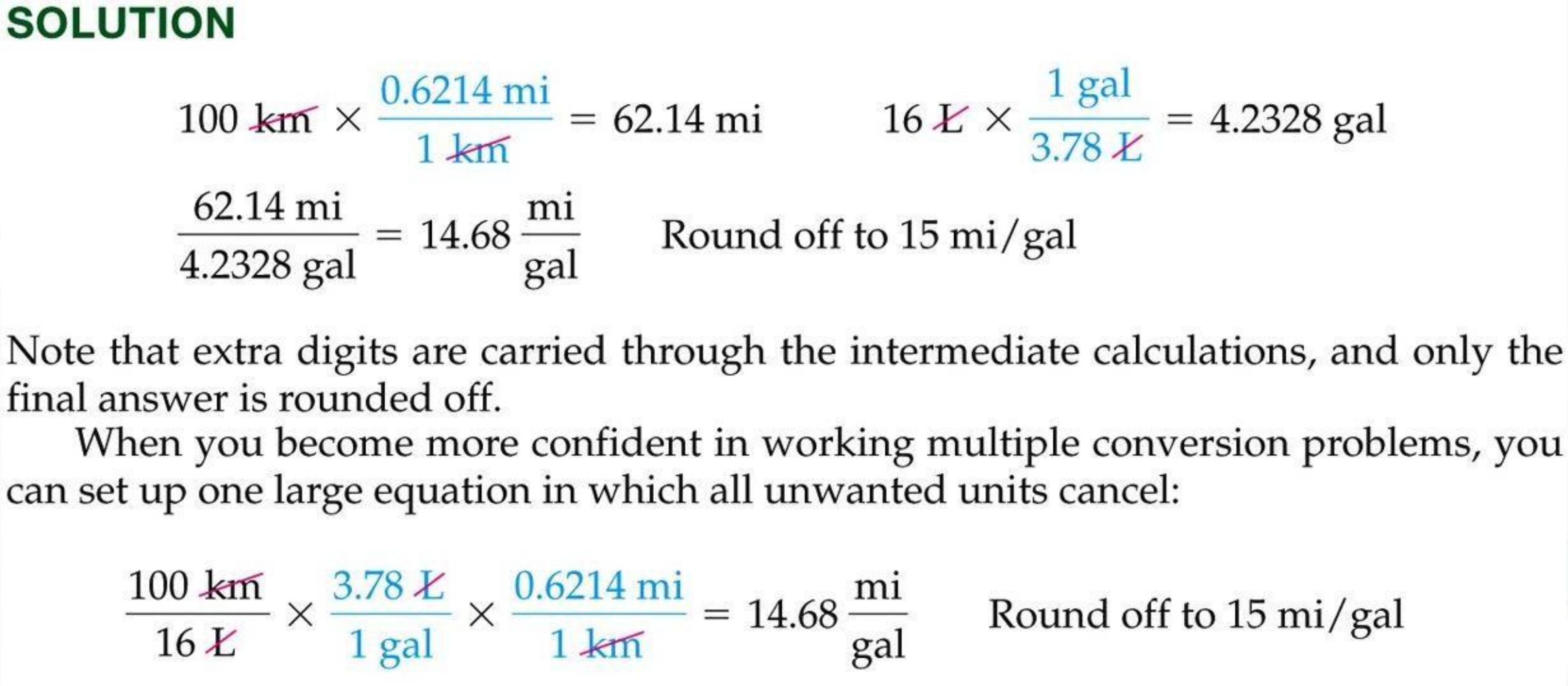
$$\frac{2\ \text{km}}{}\left|\frac{10^5\ \text{cm}}{1\ \text{km}}\right|\frac{1\ \text{in}}{2.54\ \text{cm}}\left|\frac{1\ \text{ft}}{12\ \text{in}}\right|\frac{1\ \text{mile}}{5280\ \text{ft}} = 1.24\ \text{mile}$$

Convert 400 in.^{3}/day to cm^3/min

$$\frac{400\ \cancel{\text{in.}}^3}{\cancel{\text{day}}}\left|\left(\frac{2.54\ \text{cm}}{1\ \cancel{\text{in.}}}\right)^3\right|\frac{1\ \cancel{\text{day}}}{24\ \cancel{\text{hr}}}\left|\frac{1\ \cancel{\text{hr}}}{60\ \text{min}}\right. = 4.55\,\frac{\text{cm}^3}{\text{min}}$$

Exercise 8

A large sport utility vehicle moving at a speed of 125 km/h might use gasoline at a rate of 16 L per 100 km. What does this correspond to in mi/gal?



SOLUTION

$$100\ \cancel{\text{km}} \times \frac{0.6214\ \text{mi}}{1\ \cancel{\text{km}}} = 62.14\ \text{mi} \qquad 16\ \cancel{\text{L}} \times \frac{1\ \text{gal}}{3.78\ \cancel{\text{L}}} = 4.2328\ \text{gal}$$

$$\frac{62.14\ \text{mi}}{4.2328\ \text{gal}} = 14.68\ \frac{\text{mi}}{\text{gal}} \qquad \text{Round off to 15 mi/gal}$$

Note that extra digits are carried through the intermediate calculations, and only the final answer is rounded off.

When you become more confident in working multiple conversion problems, you can set up one large equation in which all unwanted units cancel:

$$\frac{100\ \cancel{\text{km}}}{16\ \cancel{\text{L}}} \times \frac{3.78\ \cancel{\text{L}}}{1\ \text{gal}} \times \frac{0.6214\ \text{mi}}{1\ \cancel{\text{km}}} = 14.68\ \frac{\text{mi}}{\text{gal}} \qquad \text{Round off to 15 mi/gal}$$

2.4 Force and Weight

Force and Weight

Newton's Second Law

$$F = m \cdot a$$ **Force**

$$W = m \cdot g$$ **Weight**

- **Force** is proportional to the product of mass and acceleration (length/time^2) of object.
- **Weight**, is the force exerted on an object by the gravity. It is calculated using the acceleration of gravity at sea level and 45° latitude (g).
- Force and Weight have similar units

Refer to book to learn the units and values of g in different systems of units

(g_c) as a Conversion factor for forces

Refer to book to learn about g_c, its values, and how it is used as a conversion factor from basic to derived units in different systems of unit

Example 1

(a) *SI system.* Calculate the force in Newtons required to accelerate a mass of 4.00 kg at a rate of 9.00 m/s^2.

$$F = ma$$

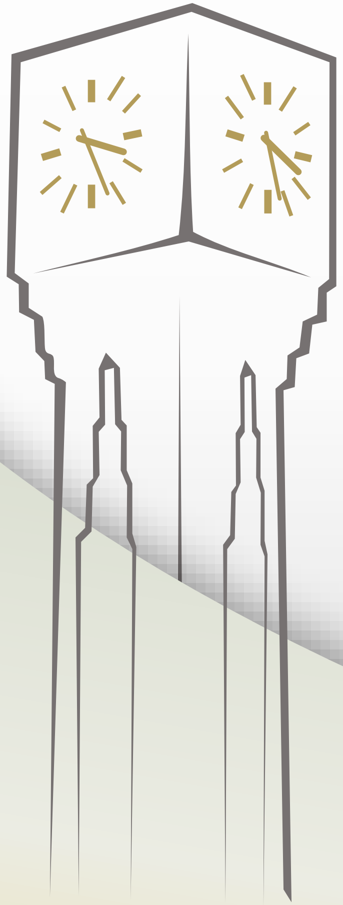
$$F = \begin{array}{c|c|c} 4.00\ \text{kg} & 9.00\ \text{m} & 1\ \text{N} \\ \hline & \text{s}^2 & 1\ \text{kg}\cdot\text{m/s}^2 \end{array} \longrightarrow 1/g_c$$

(b) *American system*. Calculate the force in Ib$_f$ required to accelerate a mass of 4.00 Ib$_m$ at a rate of 9.00 ft/s^2.

$$F = \begin{array}{c|c|c} 4.00\ \text{lb}_\text{m} & 9.00\ \text{ft} & 1\ \text{lb}_\text{f} \\ \hline & \text{s}^2 & 32.174\ \text{lb}_\text{m}\cdot\text{ft/s}^2 \end{array} \longrightarrow 1/g_c$$

$$g_c = \frac{1\ \text{kg}\cdot\text{m/s}^2}{1\ \text{N}} = \frac{32.174\ \text{lb}_\text{m}\cdot\text{ft/s}^2}{1\ \text{lb}_\text{f}}$$

is simply a conversion factor



2.5 Numerical Calculation and Estimation: Scientific Notation

Numerical Calculation - Scientific notations

- A convenient way to represent very large or very small numbers.
- Scientific notation is small number $(0.1 \text{ to } 10) \times 10^{y}$

$$123{,}000{,}000 \;=\; 123{,}0\overleftarrow{00{,}000.} \times 10^{0} \;=\; 1.23 \times 10^{8}$$

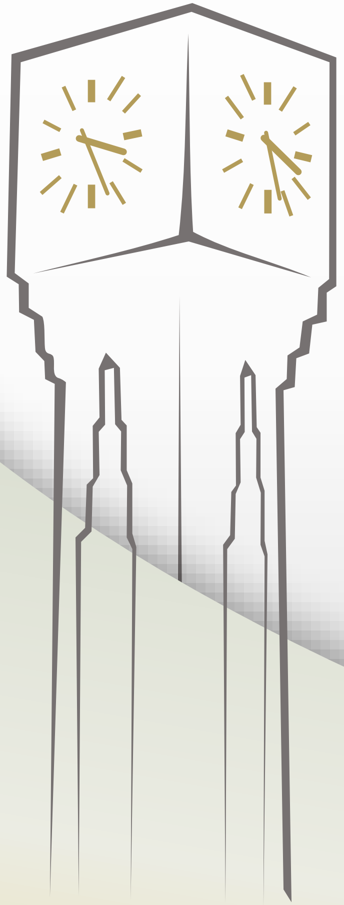
- The value of power = number of moved stages.
- If decimal moves to left (power increases ↑),
- While, if decimal moves to right (the power decreases ↓).

$$0.00025 \;=\; 0\overrightarrow{.00025} \times 10^{0} \;=\; 2.5 \times 10^{-4} \quad \text{or} \quad 25 \times 10^{-5}$$

23,040

0.00304

Section 2.6 contains additional data analysis tools that are not required in this course but are very useful for future reference.



2.6 Dimensional Homogeneity

Dimensional Homogeneity and Dimensionless quantities

- Dimensional homogeneity (or unit consistency) means that all additive terms on both sides of a ***valid equation*** must have the same dimensions (or units).

- Dimensional homogeneity can be used to identify the dimensions and units of terms of quantities in an equation.

$$u(\mathrm{m/s}) = u_0(\mathrm{m/s}) + g(\mathrm{m/s^2})t(\mathrm{s})$$

This equation is dimensionally homogenous, why?

The terms *u*, *uo*, and *g.t* has the same dimension (length/time); or same unit (m/s)

- If an equation is dimensionally homogeneous but its additive terms have inconsistent units, the terms may be made consistent simply by applying the appropriate conversion factors.

Example 2.6-1 Dimensional Homogeneity

Consider the equation $D(\text{ft}) = 3t(\text{s}) - 4$

1. If the equation is valid, what are the dimensions of the constants 3 and 4?

For the equation to be valid, dimensionally homogeneous, each term must have the dimension of length.

$$D(\text{ft}) = 3t(\text{s}) - 4$$

The constant 3	The constant 4
$\boxed{\text{length/time}}$	$\boxed{\text{length}}$

2. If the equation is consistent in its units, what are the units of 3 and 4?

For consistency, the constants must be $\boxed{3\ \text{ft/s}}$ and $\boxed{4\ \text{ft}}$.

3. Derive an equation for distance in meters in terms of time in minutes.

★ Needs attention

Define new variables $D'(\mathrm{m})$ and $t'(\mathrm{min})$.

$$D(\mathrm{ft}) = 3t(\mathrm{s}) - 4$$

$$D(\mathrm{ft}) = \begin{array}{c|c} D'(\mathrm{m}) & 3.2808\ \mathrm{ft} \\ \hline & 1\ \mathrm{m} \end{array} = 3.28D'$$

$$t(s) = \begin{array}{c|c} t'(\mathrm{min}) & 60\ \mathrm{s} \\ \hline & 1\ \mathrm{min} \end{array} = 60t'$$

Substitute these expressions in the given equation

$$3.28D' = (3)(60t') + 4$$

$$D'(\mathrm{m}) = 55t'(\mathrm{min}) + 1.22$$

What are the units of 55 and 1.22?

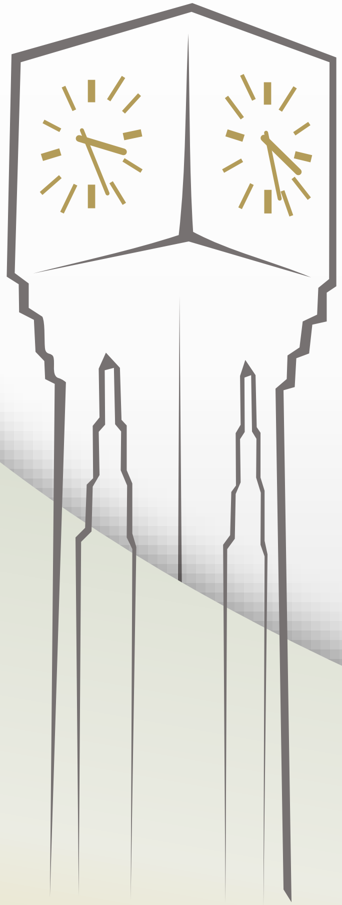
General procedure for rewriting an equation in terms of new variables having the same dimensions but different units:

1. Define new variables that have the desired units.
2. Write expressions for each old variable in terms of the corresponding new variable.
3. Substitute these expressions in the original equation and simplify.

Dimensionless quantities

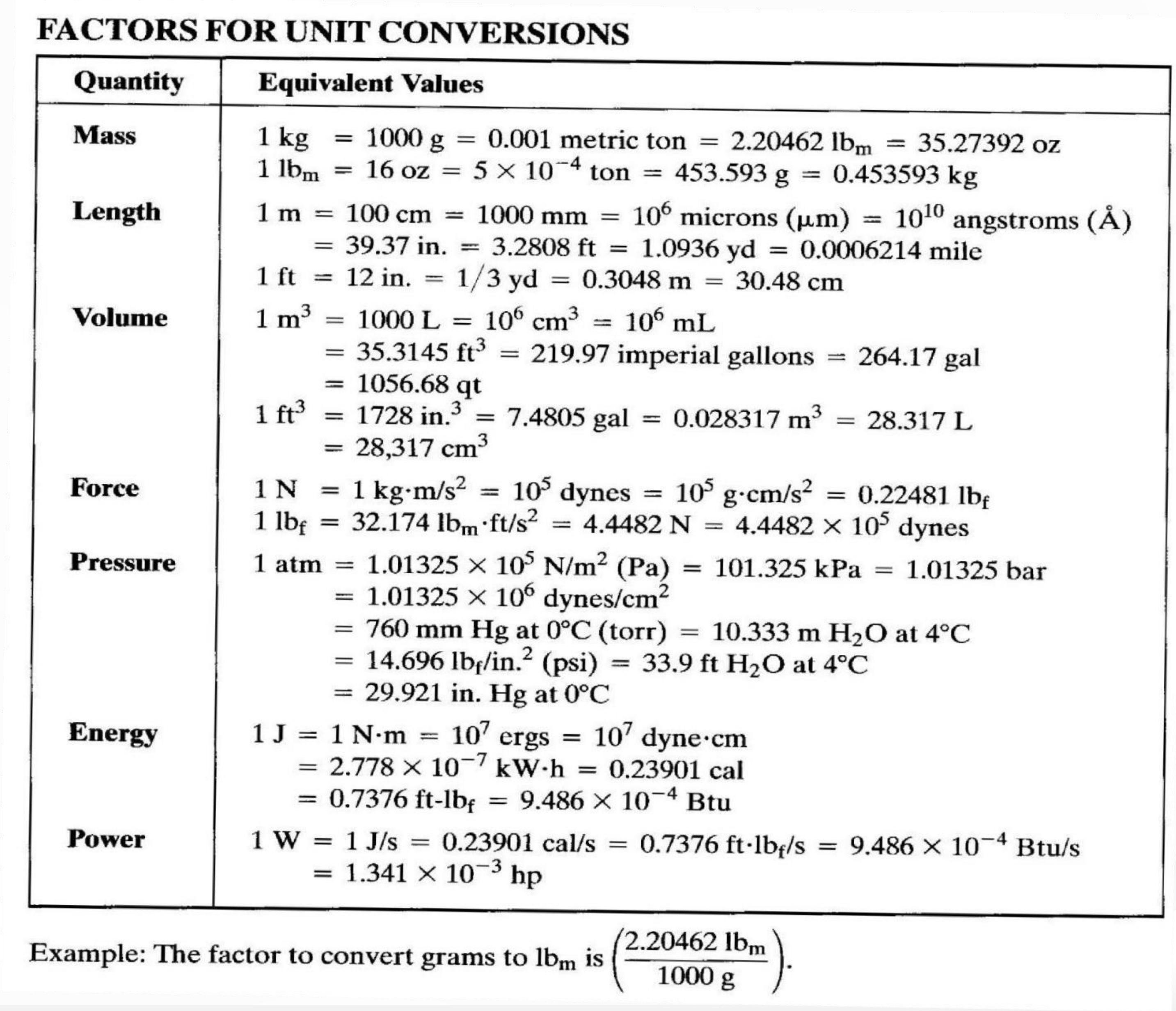
A **dimensionless quantity** can be a pure number or a multiplicative combination of variables with no net dimensions.

Example: $$\left.\frac{M(g)}{M_o(g)} \quad or \quad \frac{D(cm)u(cm/s)\rho(g/cm^3)}{\mu[g/(cm.s)]}\right\}$$ **Dimensionless Group**



Problem Solving

Conversion Table



FACTORS FOR UNIT CONVERSIONS

Quantity	Equivalent Values
Mass	1 kg = 1000 g = 0.001 metric ton = 2.20462 lb_m = 35.27392 oz 1 lb_m = 16 oz = 5×10^{-4} ton = 453.593 g = 0.453593 kg
Length	1 m = 100 cm = 1000 mm = 10^6 microns (μm) = 10^{10} angstroms (Å) = 39.37 in. = 3.2808 ft = 1.0936 yd = 0.0006214 mile 1 ft = 12 in. = 1/3 yd = 0.3048 m = 30.48 cm
Volume	1 m^3 = 1000 L = 10^6 cm^3 = 10^6 mL = 35.3145 ft^3 = 219.97 imperial gallons = 264.17 gal = 1056.68 qt 1 ft^3 = 1728 in.^3 = 7.4805 gal = 0.028317 m^3 = 28.317 L = 28,317 cm^3
Force	1 N = 1 kg·m/s^2 = 10^5 dynes = 10^5 g·cm/s^2 = 0.22481 lb_f 1 lb_f = 32.174 $\text{lb}_m\text{·ft/s}^2$ = 4.4482 N = 4.4482×10^5 dynes
Pressure	1 atm = 1.01325×10^5 N/m^2 (Pa) = 101.325 kPa = 1.01325 bar = 1.01325×10^6 dynes/cm^2 = 760 mm Hg at 0°C (torr) = 10.333 m H_2O at 4°C = 14.696 $\text{lb}_f/\text{in.}^2$ (psi) = 33.9 ft H_2O at 4°C = 29.921 in. Hg at 0°C
Energy	1 J = 1 N·m = 10^7 ergs = 10^7 dyne·cm = 2.778×10^{-7} kW·h = 0.23901 cal = 0.7376 ft-lb_f = 9.486×10^{-4} Btu
Power	1 W = 1 J/s = 0.23901 cal/s = 0.7376 ft·lb_f/s = 9.486×10^{-4} Btu/s = 1.341×10^{-3} hp

Example: The factor to convert grams to lb_m is $\left(\dfrac{2.20462\ \text{lb}_m}{1000\ \text{g}}\right)$.

Exercise 1

1) Convert 23 $lb_m.ft/min^2$ to its equivalent in $kg.cm/s^2$. [answer:

2) Convert 400 $in.^3/day$ to cm^3/min

3) A vehicle consumes gasoline at a rate of 16 L / 100 km. Convert this consumption rate to gal / mile.

Exercise 2

In the equation, $\left(p + \frac{a}{\dot{V}^2}\right) \times (\dot{V} - b) = R \times T$

What are the dimensions of a and b?

Solution

a [=] (pressure)(volume/time)^2
b [=] (volume/time)

Exercise 3

A seed crystal of diameter D (mm) is placed in a solution of dissolved salt and new crystals are observed to nucleate at a constant rate r (crystal/min). Experiments with seed crystals of different sizes show that the rate of nucleation varies with the seed crystal diameter as:

$$r(\text{crystal/min}) = 200D - 10D^2 \quad (\text{D in mm})$$

a) What are the units of constants of 200 and 10?

b) Calculate the crystal nucleation rate (crystal/s) corresponding to diameter of 0.050 inch.

c) Derive a formula for r (crystal/s) in terms of D (inches).

Exercise 4

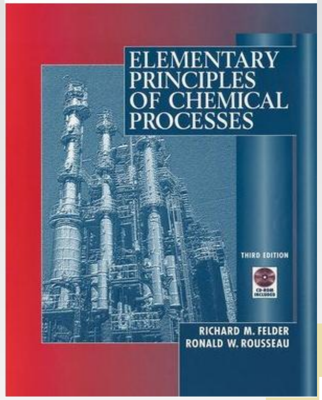
In biological systems, enzymes are used to accelerate the rates of certain biological reactions. Glucoamylase is an enzyme that aids in the conversion of starch to glucose (a sugar that cells use for energy). Experiments show that 1 µg mol of glucoamylase in a 4% starch solution results in a production rate of glucose of 0.6 µg mol /(mL)(min).

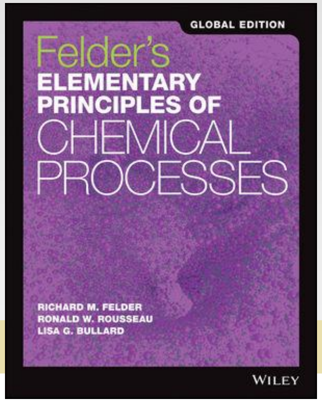
Determine the production rate of glucose for this system in the units of lb mol/(ft^3)(day).

Solution

$$\frac{0.6\ \cancel{\mu\text{g mol}}}{(\cancel{\text{mL}})(\cancel{\text{min}})}\Bigg|\frac{1\ \cancel{\text{g mol}}}{10^6\ \cancel{\mu\text{g mol}}}\Bigg|\frac{1\ \text{lb mol}}{454\ \cancel{\text{g mol}}}\Bigg|\frac{1000\ \cancel{\text{mL}}}{1\ \cancel{\text{L}}}\Bigg|\frac{1\ \cancel{\text{L}}}{3.531\times10^{-2}\ \text{ft}^3}\Bigg|\frac{60\ \cancel{\text{min}}}{\cancel{\text{hr}}}\Bigg|\frac{24\ \cancel{\text{hr}}}{\text{day}}$$

$$= 0.0539\frac{\text{lb mol}}{(\text{ft}^3)(\text{day})}$$





Elementary Principles of Chemical Processes,
3rd or 4th edition,
Wiley & Sons, Inc.
Richard M. Felder, Ronald W. Rousseau, & Lisa G. Bullard.

Student Sample Slides

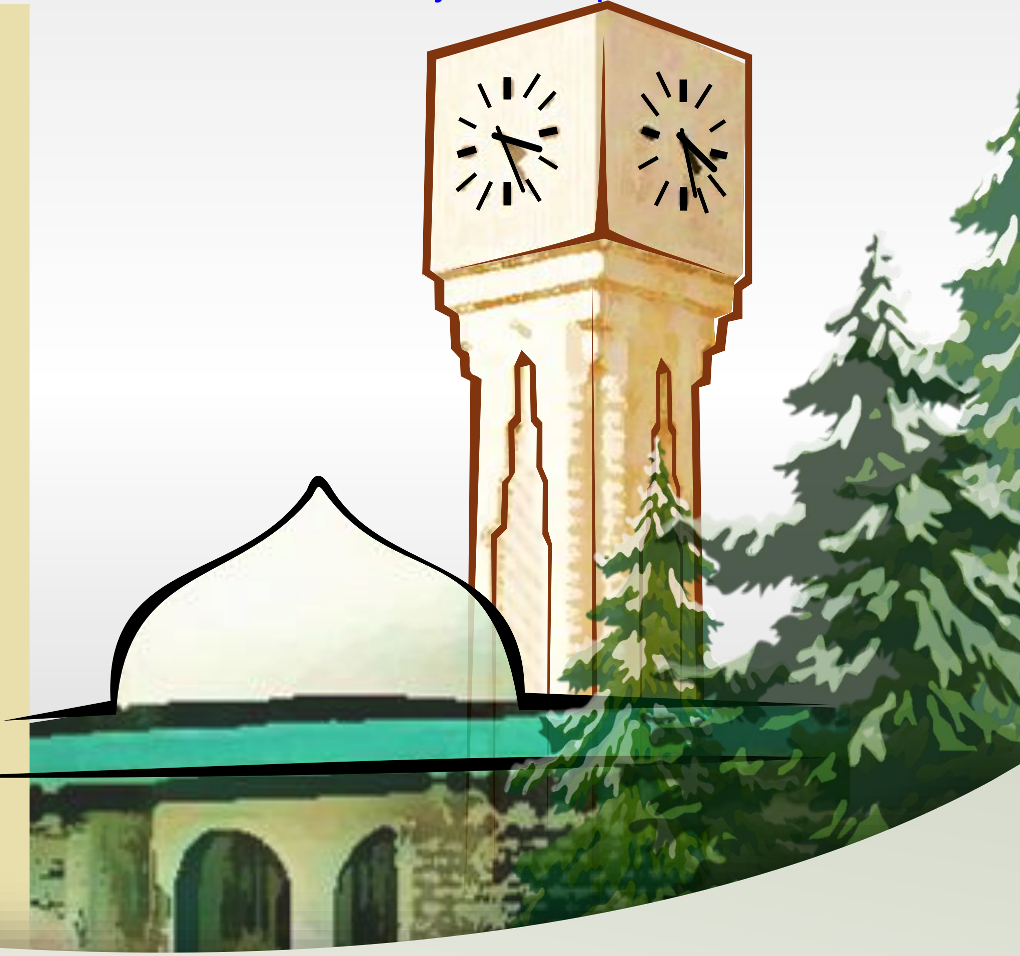
This only a sample of material. Refer to textbook for study of the topics

CHE 0905211

Chemical Engineering Principles 1

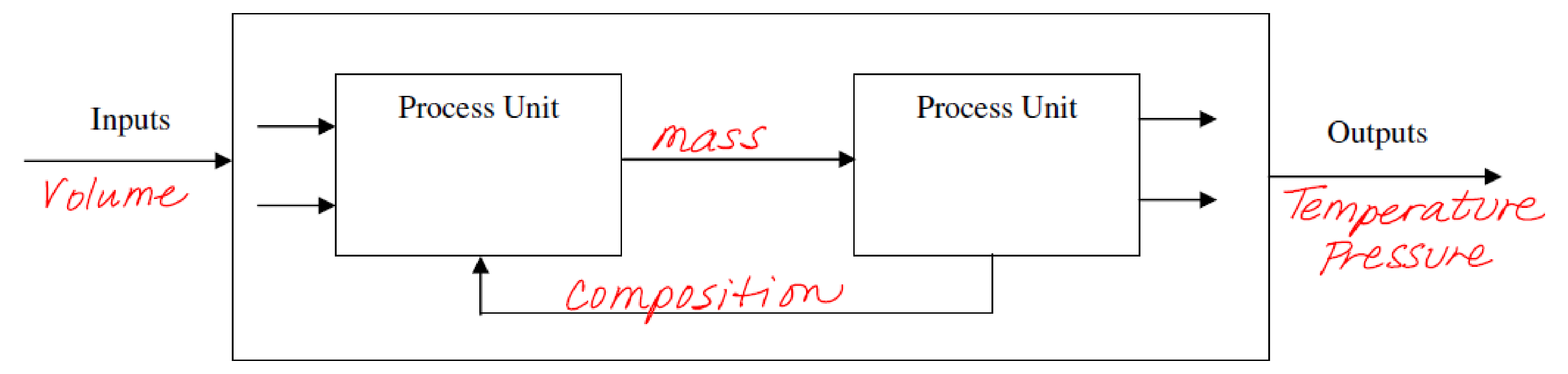
Fall 2025

Dr. Hatem Alsyouri	Chapter 3



The University of Jordan
Chemical Engineering Department

Introduction

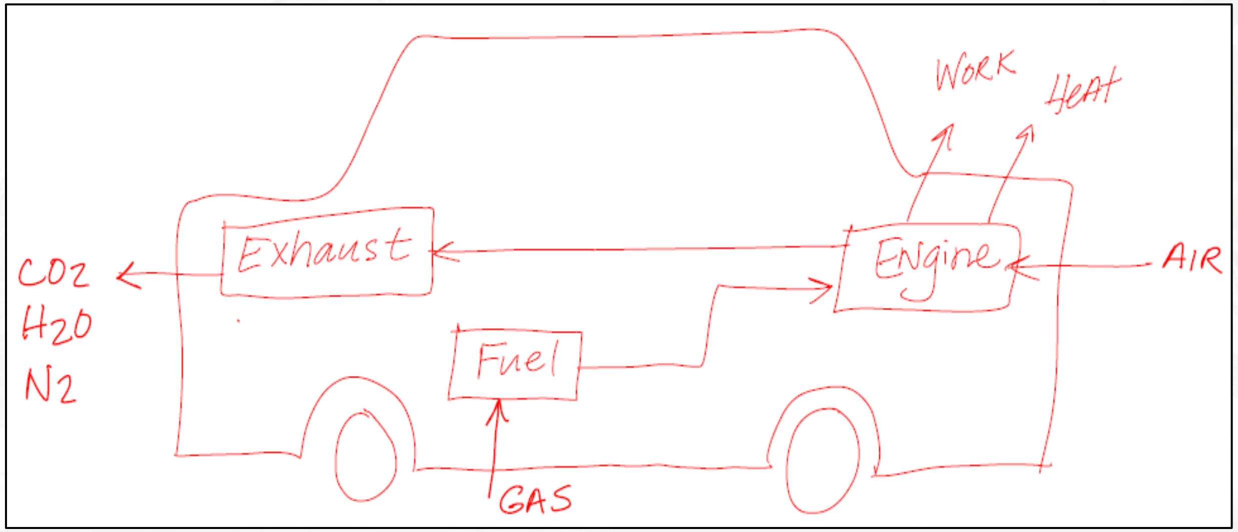


System =
a group of units

Process: any operation or series of operations by which a particular objective is accomplished. These operations can cause a physical or chemical change in a substance or mixture of substances.

Can you think of other processes?

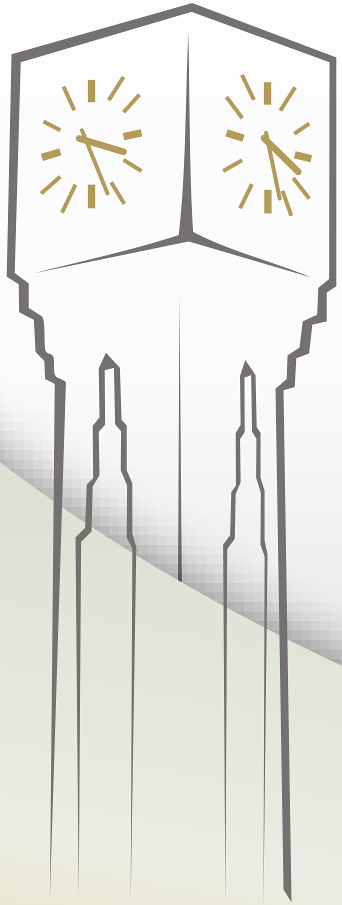
Consider a familiar "system": A car



Process Variables

Major process variables that will be covered in this course:

1. **Mass and Volume**
    a. Density
    b. Specific volume
    c. Specific gravity
2. **Flow rate**
    a. Mass flow rate
    b. Volumetric flow rate
3. **Chemical composition**
    a. Moles and molecular weight
    b. Mass fraction and mole fraction
    c. Concentration
4. **Pressure**
5. **Temperature**



3.1 Mass and Volume

This section will define the mass and volume variables and the associated physical properties such as density and specific gravity

3.1 Mass and Volume

Density (ρ = row): is the mass per unit volume of a material (pure compound, solution, mixture). SI unit (kg/m^3).

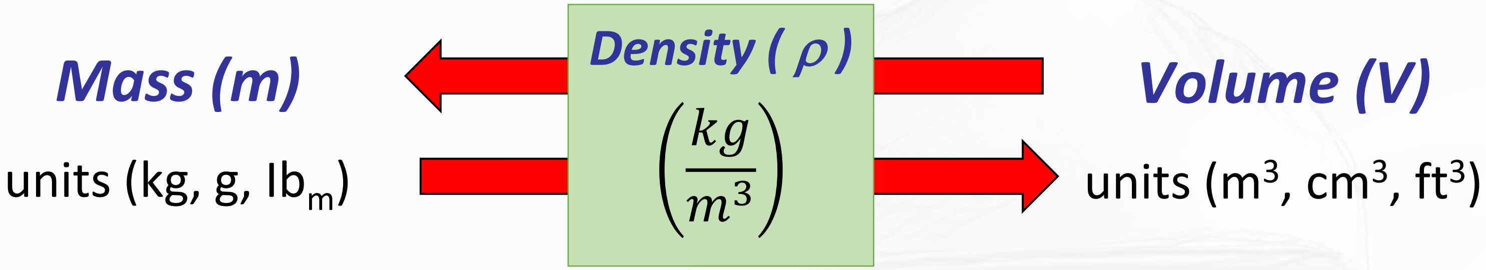
$\rho_{H2O(liq)}$ (4°C)

$= 1.000\ g / cm^3$

$= 1000\ kg / m^3$

$= 62.43\ lb_m / ft^3$

- Density varies with temperature and pressure.
- Density of liquids is independent of pressure but varies with temperature.
- Densities are reported at specific reference conditions in several resources.
- **Reference of water** is LIQUID phase and 4°C.



Mass (m)

units (kg, g, lb$_m$)

Density (ρ)

$\left(\frac{kg}{m^3}\right)$

Volume (V)

units (m^3, cm^3, ft^3)

Mass × 1 / Density = Volume

$$\frac{2\ kg}{\ } \cdot \frac{1\ m^3}{1000\ kg} = 0.002\ m^3$$

Density is a conversion factor between mass and volume

Volume × Density = Mass

$$\frac{5\ m^3}{\ } \cdot \frac{1000\ kg}{1\ m^3} = 5000\ kg$$

Specific Property*:* is the amount of property per unit mass of the substance (xx/ kg).

Specific volume $(\hat{V})$*:* is the volume occupied by unit mass of the substance (m^3/ kg).

Density (ρ)

$$\left(\frac{kg}{m^3}\right)$$

INVERSE

Specific Volume ($\hat{V}$)

$$\left(\frac{m^3}{kg}\right)$$

Specific gravity*:* is the ratio of the density ρ of the substance to the density ρ_{ref} of a reference at a specific condition *(water @ 4.0°C):*

$$SG = \frac{\rho}{\rho_{ref}}$$

- $\boldsymbol{\rho_{ref}}$ is the reference density = $\boldsymbol{\rho}$ of Liquid water at 4°C = 1000 kg/m^3.
- SG is the value used to obtain densities of several materials. SG is the conversion factor between $\boldsymbol{\rho}$ and $\boldsymbol{\rho_{ref}}$
- SG values are reported in Table B.1 Appendix B

Solution Strategy

This is a general procedure for solving problems

Plan the steps

Define the problem, identify knowns/unknown

Analyze the system

Apply principles (engineering, physical, chemical, etc.)

Choose tools & methods

Select equations, techniques, or software

Solve

Check & Interpret

Verify solution and interpret results

Exercises on Mass and Volume

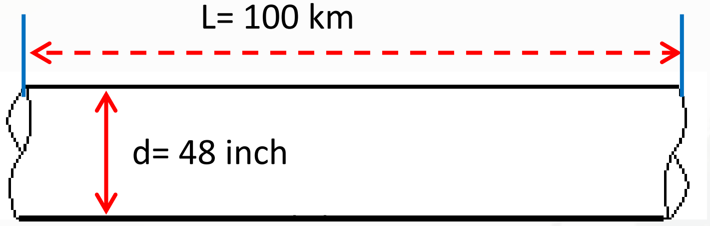
Problem. A pipeline transporting oil from a production site to a refinery is 48 inch diameter and 100 km long.

a. How many barrels of oil (volume unit) are required to fill the pipeline? (1 barrel = 42 gallon)

b. Find the mass in metric ton, assuming the specific gravity is 0.9 (light crude oil)

1 barrel = 42 gal ≈ 159 Lit

Answer



$$Volume = Area \times Length$$

$$V = \frac{\pi}{4} d^2 L$$

Math basics

a. Volume of oil in pipeline

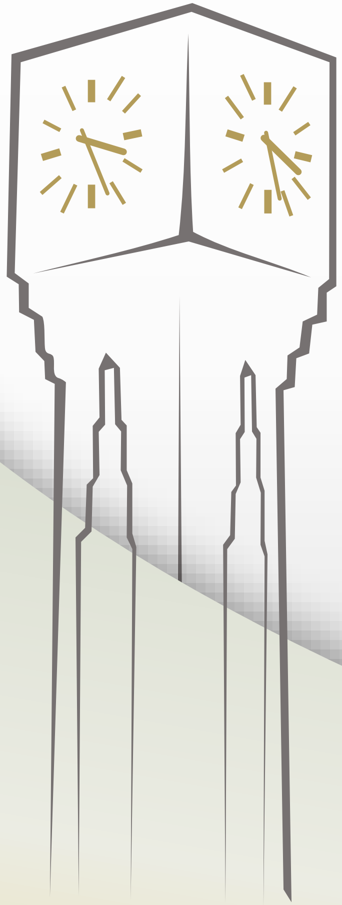
1. d (inch → m) … using known conversion factor (1 m = 39.37 in.) (ans. d= 1.22 m)
2. L (km → m) … using known multiples (1 km = 1000 m) (ans. L= 100,000 m)
3. Volume in (m^3) … using volume equation (ans. V= 116,899 m^3)
4. Volume (m^3 → gal → barrel) …. using conversion table (ans. V= 735,267 barrel)

$$V = \frac{\pi}{4} d^2\, L = \frac{\pi}{4} \times (d\ ft\ \to m)^2 \times L\ (km\ \to m) \times factor\ (m^3 \to gal \to barrel)$$

b. Mass of oil

1. Density in (kg/m^3) … using SG and density of water (ans. ρ_{oil}= 900 kg/m^3)
2. Mass in (kg) using Volume in (m^3) and density (kg/m^3) (ans. m_{oil} = 105,209,100 kg)
3. Mass in (m. ton) using conversion factor (1 m. ton = 1000 kg) (ans. m_{oil} = 105,209.1 metric ton)

What is the material of construction of oil pipelines?



3.2 Flow Rates

This section will define the variables that have a flow nature

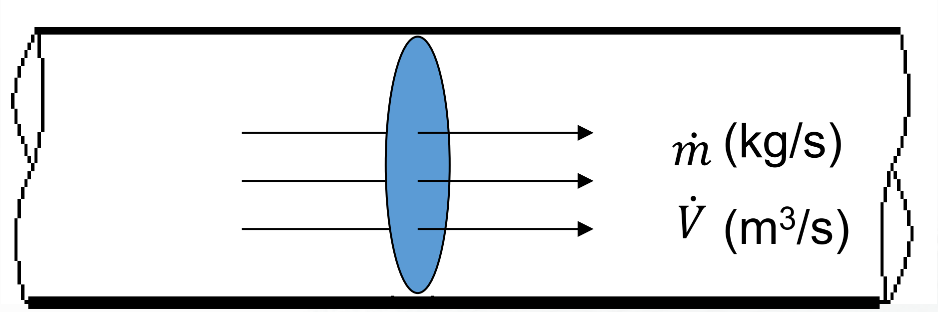
3.2 a. Mass and Volumetric Flow Rates

- **Flow rate:** the rate at which a material is transported through a process line. Unit of Rate is [property / time]

$$\boldsymbol{Mass}: \quad \boldsymbol{m} \quad \text{while} \quad \boldsymbol{Mass\ flow\ rate}: \quad \dot{\boldsymbol{m}} \quad \left(\frac{mass}{time}\right)$$

$$\boldsymbol{Volume}: \quad \boldsymbol{V} \quad \text{while} \quad \boldsymbol{Volumetric\ flow\ rate}: \quad \dot{\boldsymbol{V}} \quad \left(\frac{volume}{time}\right)$$

Flow in Pipe/tube/duct



$$Density: \quad \boldsymbol{\rho} = \frac{m}{V} = \frac{\dot{m}}{\dot{V}}$$

3.2 b. Flow Rate Measurements

Flowmeter: is a device mounted in a process line that provides a continuous reading of the flow rate in the line

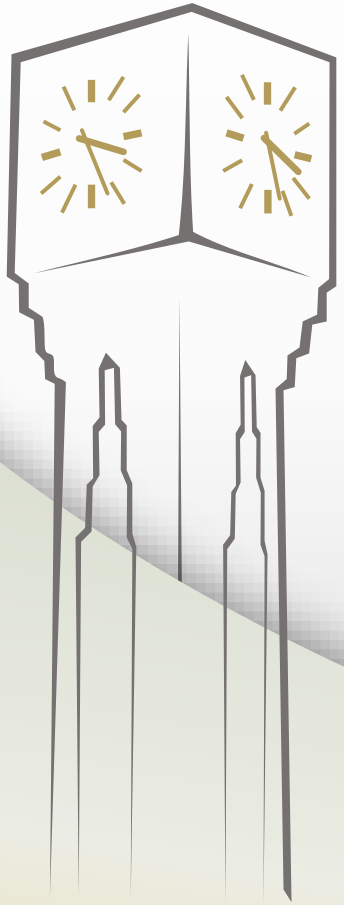
Refer to book for more details on flow measurement devices

Exercises on Flow Rates

Problem. Liquid butane enters a process. By measurement, it is found that 300 kg of butane pass into the process every 12 minutes. The density of liquid butane is 600 kg/m^3.

a. Calculate the mass flow rate (in kg/h) (ans. $\dot{m}$= 1500 kg/h)

b. Calculate the volumetric flow rate (in m^3/h) using the given density. (ans. $\dot{V}$= 2.5 m^3/h)



3.3 Chemical Composition

This section introduces the different ways to express the composition of a mixture in mass values, molar values, and concentration

3.3a Moles and Molecular Weight

Mole (n):

- The amount of a substance that contains 6.022×10^{23} entities.
- SI and CGS unit is (***g-mole*** = ***mol***). British unit is (***lb-mole***).
- Other multiples of mol is ***kg-mole*** = ***kmol***.
- Conversion between (g-mole) and (kg-mole) is as conversion between (g) and (kg). Similarly, convert (g-mole) to (lb-mole) by using (g) to (lb_m) conv. factor

Molecular Weight (M):

- the sum of the atomic weights of the atoms that constitute a molecule of the compound (same as molar mass).
- Units of ***M*** , i.e., (***g/mol***, kg/kmol, or lb_m/lb-mole).
- Values of M are available in Table B.1 for several species

Exercises on Moles and Molecular Weight

Problem. Liquid butane enters a process. By measurement, it is found that 300 kg of butane pass into the process every 12 minutes. The density of liquid butane is 600 kg/m³.

a. Calculate the mass flow rate (in kg/h) (ans. $\dot{m}$= 1500 kg/h)

b. Calculate the volumetric flow rate (in m³/h) using the given density. (ans. $\dot{V}$= 2.5 m³/h)

c. Calculate the molar flow rate (in kmol/h). Molecular weight of butane (M) = 58 kg/kmol

Answer

Parts (a) and (b) were solved earlier

c.

1. $\dot{m}$ = 1500 kg/h (kg → kmol) using Molecular weigh (kg/kmol) (ans. d= 1.22 m)

Where can you obtain molecular values from?

3.3b Mass and Mole Fractions and Average Molecular Weight

- Process streams occasionally contain one substance, but more often they consist of **mixtures** of more than one substance.
- Physical properties of a mixture depend strongly on the composition of mixture.
- To express the **Composition** of a mixture we use the fraction of a species (e.g., for substance A):

Fraction is always less than 1

Summation of all fractions is always 1

Fraction is unit-less

Mass fraction

$$x_A = \frac{mass\ of\ A}{total\ mass}\left(\frac{kg\ A}{kg\ total}\ or\ \frac{g\ A}{g\ total}\ or\ \frac{lb_m\ A}{lb_m\ total}\right)$$

(the mass percent of A is 100 $\boldsymbol{x_A}$)

Mole fraction

$$y_A = \frac{moles\ of\ A}{total\ moles}\left(\frac{kmol\ A}{kmol\ total}\ or\ \frac{mol\ A}{mol\ total}\ or\ \frac{lb-mol\ A}{lb-mole\ total}\right)$$

(the mole percent of A is 100 $\boldsymbol{y_A}$)

Average Molecular Weight of a Mixture $\bar{M}$

- Is used to convert between mass and moles of a mixture.
- The ratio of total mass of a mixture to the total number of moles.
- $\bar{M}$ unit (kg/kmol, g/mol, or lb_m/lb-mol).
- It can be calculated from mass fractions or mole fractions

Based on *mole* fraction (y_i)

$$\boxed{\bar{M} = y_1 M_1 + y_2 M_2 + \ldots = \sum_{all\ components} y_i M_i}$$

(y_i) is the mole fractions of component ***i***

(M_i) is the molecular weight of component ***i***

Based on *mass* fraction (x_i)

$$\boxed{\frac{1}{\bar{M}} = \frac{x_1}{M_1} + \frac{x_2}{M_2} + \ldots = \sum_{all\ components} \frac{x_i}{M_i}}$$

(x_i) is the mass fractions of component ***i***

Exercises on the average molecular weight

Problem. Calculate the average molecular weight of air:

a. From its approximate molar composition of 79% N2, 21% O2 (ans. $\bar{M}_{air}$= 29 g/mol)

b. From its approximate composition by mass of 76.7% N2 and 23.3% O2 (ans. $\bar{M}_{air}$= 29 g/mol)

Answer

a. ..

$$\bar{M} = \sum_{\text{all components}} y_i M_i \qquad \bar{M} = y_{N_2} M_{N_2} + y_{O_2} M_{O_2}$$

$$= \frac{0.79 \text{ kmol N}_2}{\text{kmol}} \left| \frac{28 \text{ kg N}_2}{\text{kmol}} \right. + \frac{0.21 \text{ kmol O}_2}{\text{kmol}} \left| \frac{32 \text{ kg O}_2}{\text{kmol}} \right.$$

$$\bar{\boldsymbol{M}}_{\boldsymbol{air}} = \boxed{29 \frac{\text{kg}}{\text{kmol}}} \left(= 29 \frac{\text{lb}_\text{m}}{\text{lb-mole}} = 29 \frac{\text{g}}{\text{mol}} \right)$$

b. ..

$$\frac{1}{\bar{M}} = \sum_{\text{all components}} \frac{x_i}{M_i} = \frac{x_{N_2}}{M_{N_2}} + \frac{x_{O_2}}{M_{O_2}} = \frac{0.767\, g\, N_2/g}{28\, g\, N_2/mol} + \frac{0.233\, g\, O_2/g}{32\, g\, O_2/mol} = 0.035 \frac{mol}{g}$$

$$\Rightarrow \bar{\boldsymbol{M}}_{\boldsymbol{air}} = 29 \text{ g/mol}$$

3.3c Concentration

Concentration: quantity of a component per unit volume of a mixture.

Mass Concentration: mass of a component per unit volume of the mixture (g/cm^3, lb$_m$/ft^3, kg/in^3, etc) ***= density***.

Molar Concentration: number of moles of the component per unit volume of the mixture (mol/L, kmol/m^3, lb-moles/ft^3).

Molarity of a solution: moles / Lit solution

$$C_A = \frac{n_A}{V}$$

Concentration is a conversion factor between mole and volume

Molar concentration is analogous to Density but in molar unit

Exercises on Concentration

Conversion between Mass, Molar, and Volumetric Flow Rates of a Solution

Problem.

A 0.50 molar aqueous solution of sulfuric acid (H_2SO_4) flows into a process unit at a rate of 1.25 m^3/min. The specific gravity of the solution is 1.03.

Mass concentration is the Density

a. Calculate the mass concentration of H_2SO_4 in kg/m^3.

b. Calculate the mass flow rate of H_2SO_4 in kg/s.

c. The mass fraction of H_2SO_4 (tricky)

Note: 0.5 molar solution, means the molarity of the solution is 0.5 molar = 0.5 mol H_2SO_4/L

Molecular weight (M) of H_2SO_4 is 98 g/mol

Answer

1. **The mass concentration of H_2SO_4 in kg/m^3.**

$$C_{\mathrm{H_2SO_4}}\left(\frac{\mathrm{kg\ H_2SO_4}}{\mathrm{m^3}}\right) = \begin{array}{c|c|c|c} 0.50\ \mathrm{mol\ H_2SO_4} & 98\ \mathrm{g} & 1\ \mathrm{kg} & 10^3\ \mathrm{L} \\ \hline \mathrm{L} & \mathrm{mol} & 10^3\ \mathrm{g} & 1\ \mathrm{m^3} \end{array}$$

$$= \boxed{49\ \frac{\mathrm{kg\ H_2SO_4}}{\mathrm{m^3}}}$$

2. **The mass flow rate of H_2SO_4 in kg/s.**

$$\dot{m}_{\mathrm{H_2SO_4}}\left(\frac{\mathrm{kg\ H_2SO_4}}{\mathrm{s}}\right) = \begin{array}{c|c|c} 1.25\ \mathrm{m^3} & 49\ \mathrm{kg\ H_2SO_4} & 1\ \mathrm{min} \\ \hline \mathrm{min} & \mathrm{m^3} & 60\ \mathrm{s} \end{array} = \boxed{1.0\ \frac{\mathrm{kg\ H_2SO_4}}{\mathrm{s}}}$$

Answer cont'd

3. The mass fraction of H_2SO_4. (tricky)

The mass fraction of H_2SO_4 equals the ratio of the mass flow rate of H_2SO_4 to the total mass flow rate, which can be calculated from the total volumetric flow rate and the solution density.

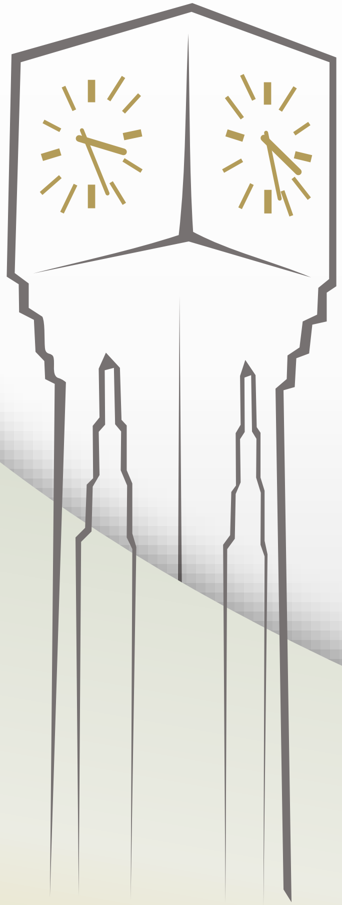
$$\rho_{\text{solution}} = (1.03)\left(\frac{1000\ \text{kg}}{\text{m}^3}\right) = 1030\ \frac{\text{kg}}{\text{m}^3}$$

$$\Downarrow$$

$$\dot{m}_{\text{solution}}\left(\frac{\text{kg}}{\text{s}}\right) = \begin{array}{c|c|c} 1.25\ \text{m}^3\ \text{solution} & 1030\ \text{kg} & 1\ \text{min} \\ \hline \text{min} & \text{m}^3\ \text{solution} & 60\ \text{s} \end{array} = 21.46\ \frac{\text{kg}}{\text{s}}$$

$$\Downarrow$$

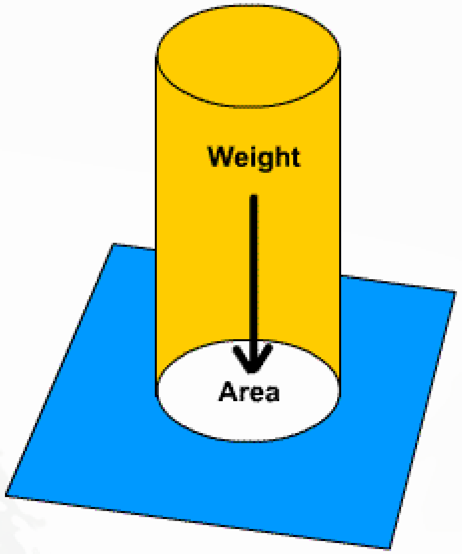
$$x_{H_2SO_4} = \frac{\dot{m}_{H_2SO_4}}{\dot{m}_{\text{solution}}} = \frac{1.0\ \text{kg}\ H_2SO_4/\text{s}}{21.46\ \text{kg solution/s}} = \boxed{0.048\ \frac{\text{kg}\ H_2SO_4}{\text{kg solution}}}$$



3.4 Pressure

This section defines the pressure variable, units, conversions between units, types of pressures, and measurement devices

Pressure (P): ratio of a NORMAL force to the area on which the force acts



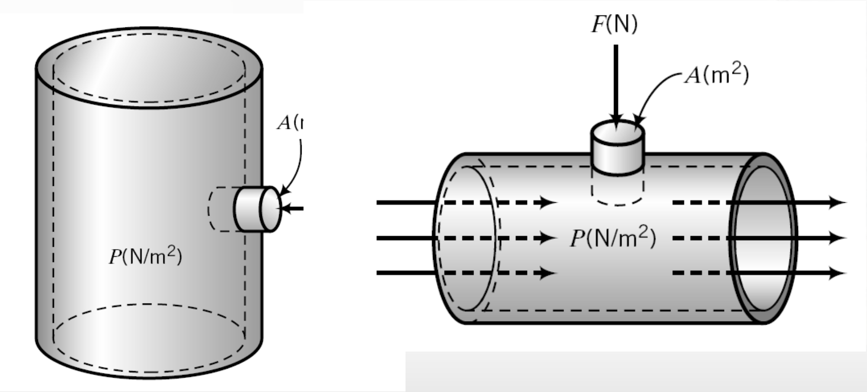
$$\boxed{P = \frac{Force}{Area} = \frac{F}{A}}$$

SI Unit ⟶ $\frac{N}{m^2} = Pa\ (pascal)$

CGS Unit ⟶ $\frac{dynes}{cm^2}$

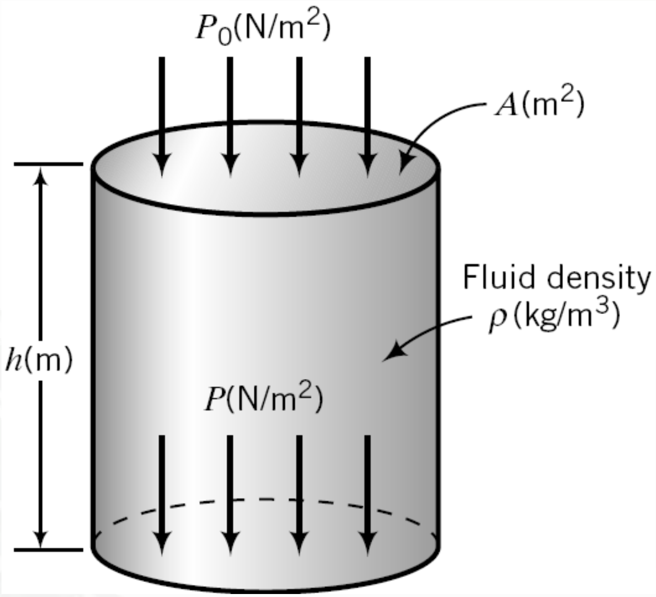
American Eng. Unit ⟶ $\frac{Ib_f}{in^2} = psi$

*(**p**ound force per **s**quare **i**nch)*



3.4a Fluid Pressure and Hydrostatic Head

Hydrostatic pressure: pressure of the fluid at the base of a column. It is the force (F) exerted on the base divided by the base area (A).



Fluid = gas or liquid

$$P = P_0 + \rho.g.h$$

$$(Pa) \quad (Pa) \quad \left(\frac{kg}{m^3}\cdot\frac{m}{s^2}\cdot m\right) = (Pa)$$

Prove that the term ($\rho \cdot g \cdot h$) has a pressure unit (Pa) or (N/m^2)

P: is the pressure exerted at bottom of column

P_0 is the pressure exerted on the top of the column (surface pressure), In most cases P_0 is the atmospheric pressure

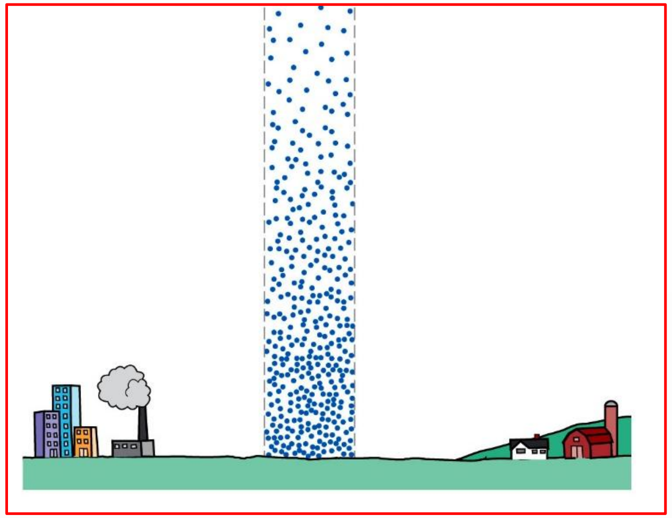
g is the acceleration of gravity.

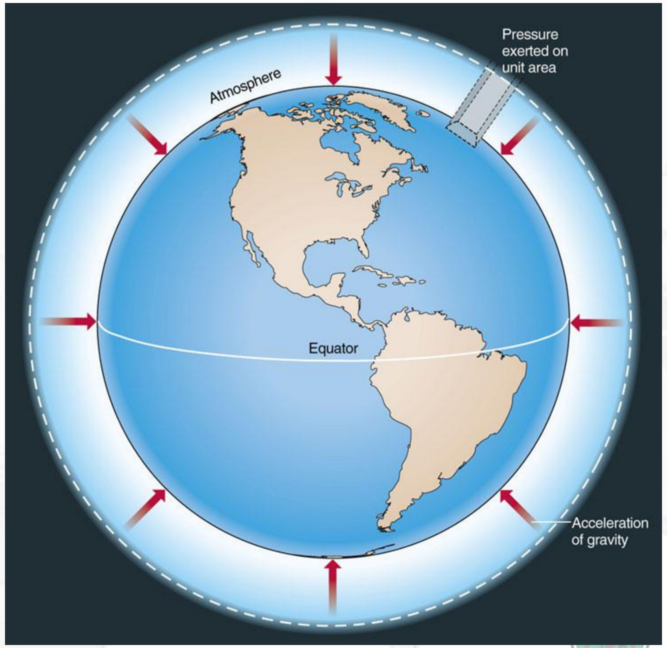
Atmospheric Pressure (P_{atm})

- The earth's atmosphere can be considered a very tall column of fluid (AIR). The pressure at the bottom of the column is atmospheric pressure (or barometric pressure).

It is useful to have a fixed reference value for atmospheric pressure. The sea-level value is used.

- At sea level, P_{atm} = 760 mm Hg.
- By definition ***P_{atm} = 760 mm Hg*** = ***1 atm*** = ***14.7 psi***
- See conversion table for other units





Question.

Would atmospheric pressure at the ski resort (mountain) be greater or less than the atmospheric pressure at sea level? Explain your answer

Answer. LESS atmospheric pressure because of shorter column of air at that height

3.4b. Types of Pressures

Types could be confusing to students

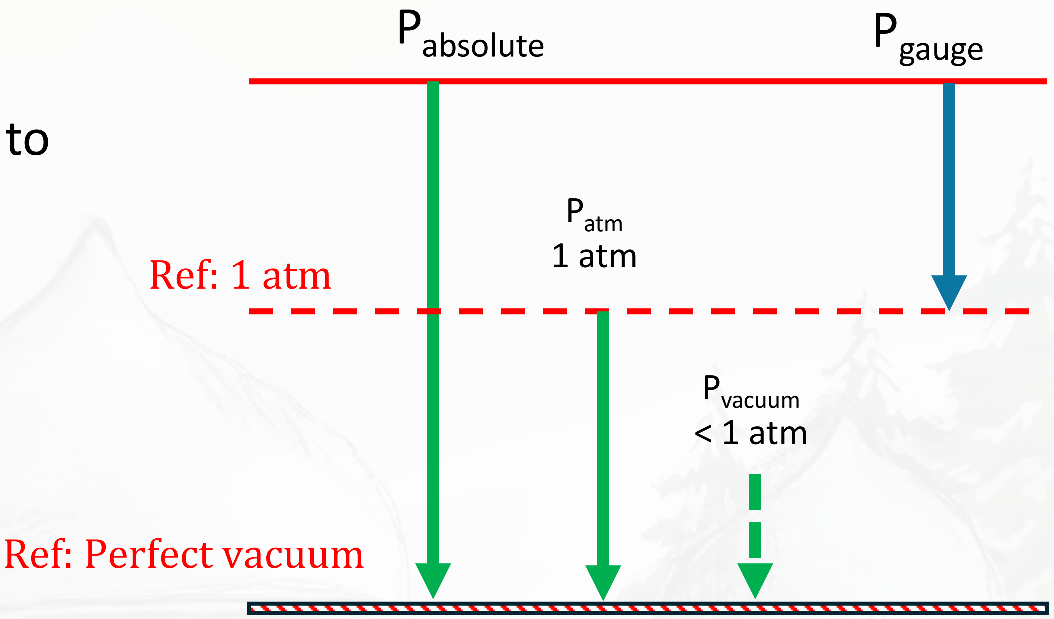
1. **Atmospheric pressure (P_{atm})**: is the pressure caused by the weight of atmosphere on surface of earth. (Barometric Pressure).

2. **Absolute pressure (P_{abs})**: is total pressure and relative to a perfect vacuum (P = 0).

3. **Gauge pressure (P_{gauge})**: is the pressure of the fluid relative to atmospheric pressure; it equals to P_{abs} minus P_{atm}.

$$\boxed{P_{gauge} = P_{absolute} - P_{atm}}$$

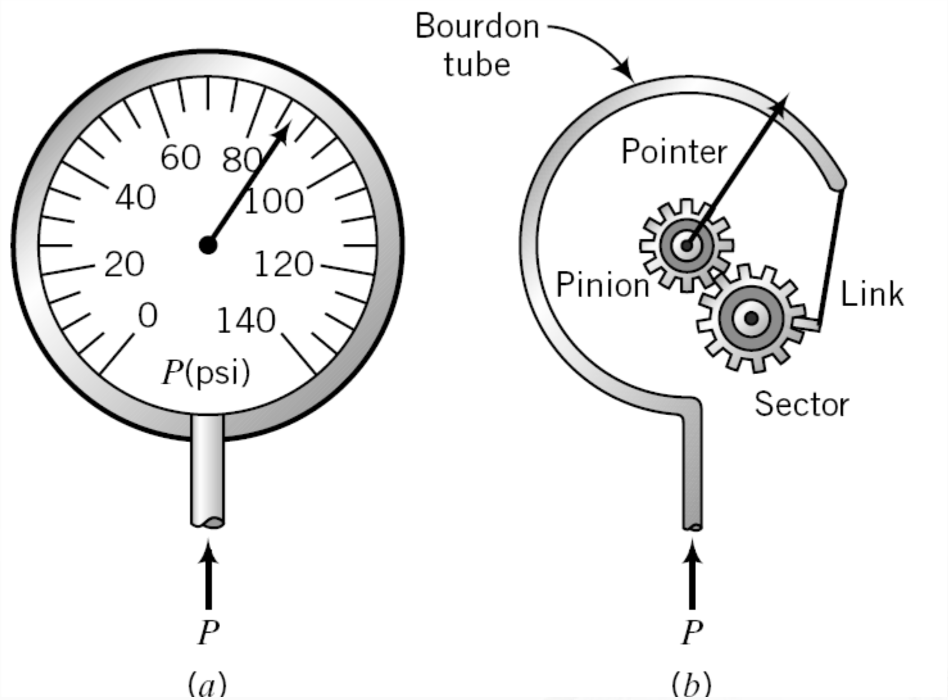
A gauge pressure of 0 indicates that the absolute pressure of the fluid is equal to atmospheric pressure.



4. ***Vacuum pressure (P_{vac})***: when pressure is below atmospheric value. Complete vacuum corresponds to zero pressure.

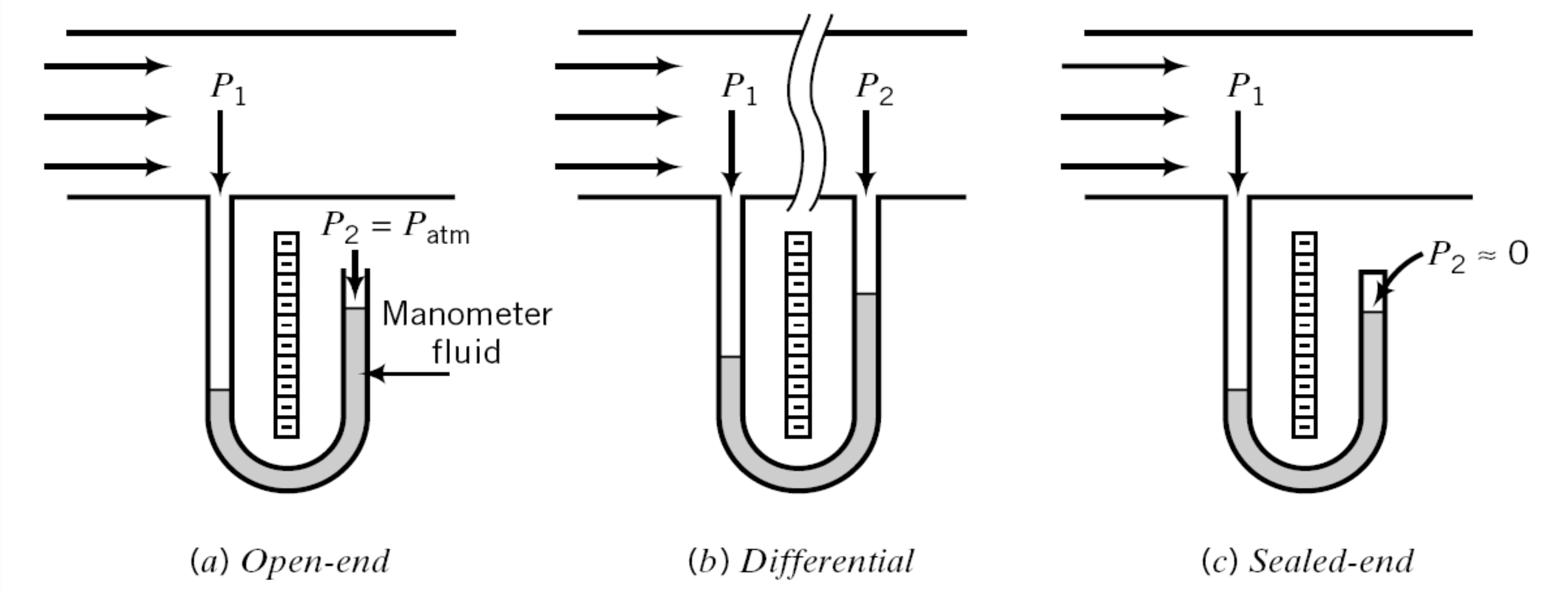
3.4c. Pressure measuring devices

Bourdon gauge



Refer to book for details the operation of this device

Manometers



(*a*) *Open-end* (*b*) *Differential* (*c*) *Sealed-end*

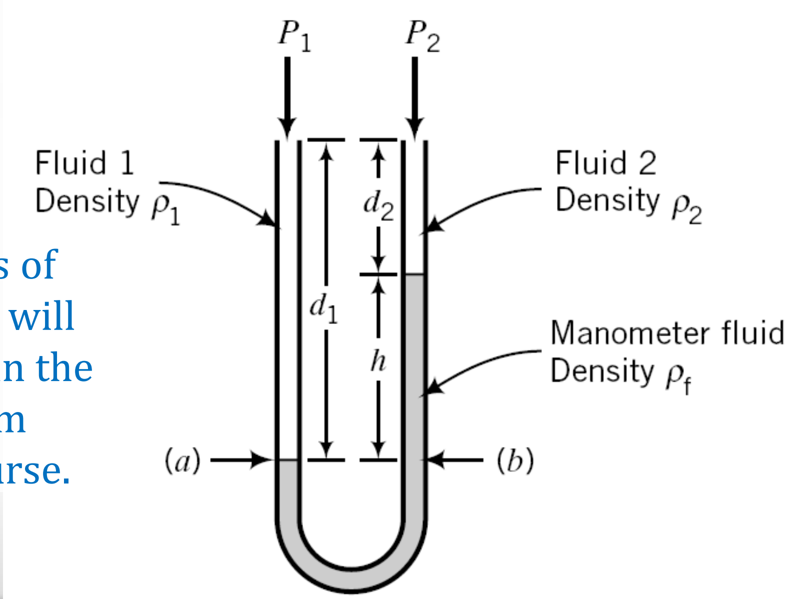
Measures pressure at one point

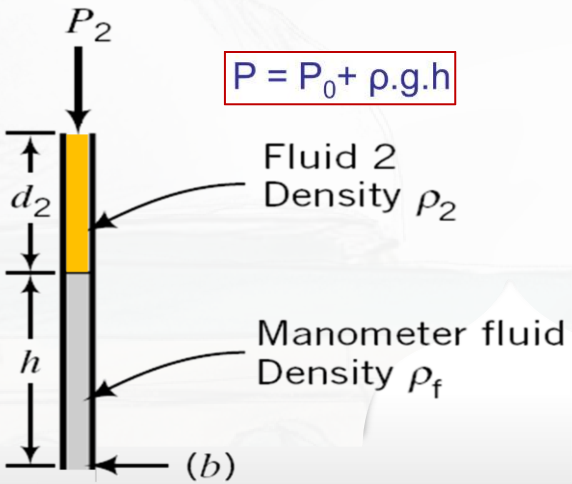
Measures pressure difference between two point in the line

P_2 = nearly vacuum ~ 0. If inlet end is exposed to atmosphere the unit is called Barometer (P_1 = 1 atm).

Manometers variables

Calculations of manometers will be discussed in the Momentum Transfer course.

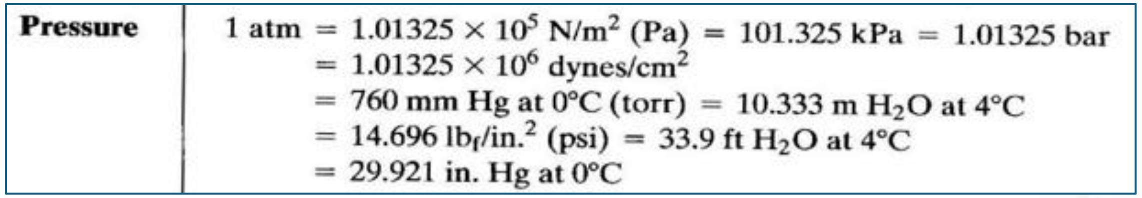




$$\boxed{P = P_0 + \rho.g.h}$$

Example 3.4-2 Pressure Below the Surface of a Fluid

What is the pressure 30.0 m below the surface of a lake? Atmospheric pressure (the pressure at the surface) is 10.4 m H_2O, and the density of water is 1000.0 kg/m³. Assume that g is 9.807 m/s².



Pressure	1 atm = 1.01325×10^5 N/m² (Pa) = 101.325 kPa = 1.01325 bar = 1.01325×10^6 dynes/cm² = 760 mm Hg at 0°C (torr) = 10.333 m H_2O at 4°C = 14.696 $\text{lb}_f/\text{in.}^2$ (psi) = 33.9 ft H_2O at 4°C = 29.921 in. Hg at 0°C

Solution **1)** By using $\boxed{P = P_0 + \rho g h}$

$$P_h = P_0 + \rho g h$$

$$\Downarrow$$

$$P_h = \begin{array}{c|c} 10.4\ \text{m H}_2\text{O} & 1.013 \times 10^5\ \text{N/m}^2 \\ \hline & 10.33\ \text{m H}_2\text{O} \end{array} + \begin{array}{c|c|c|c} 1000.0\ \text{kg/m}^3 & 9.807\ \text{m} & 30.0\ \text{m} & 1\ \text{N} \\ \hline & \text{s}^2 & & 1\ \text{kg}\cdot\text{m/s}^2 \end{array}$$

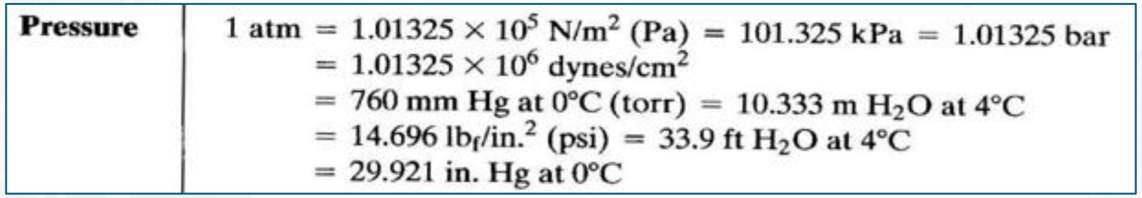
$$= \boxed{3.96 \times 10^5\ \text{N/m}^2(\text{Pa})}$$

By conversion and scientific notation ⇒ $\boxed{P_h = 396\ \text{kPa}}$

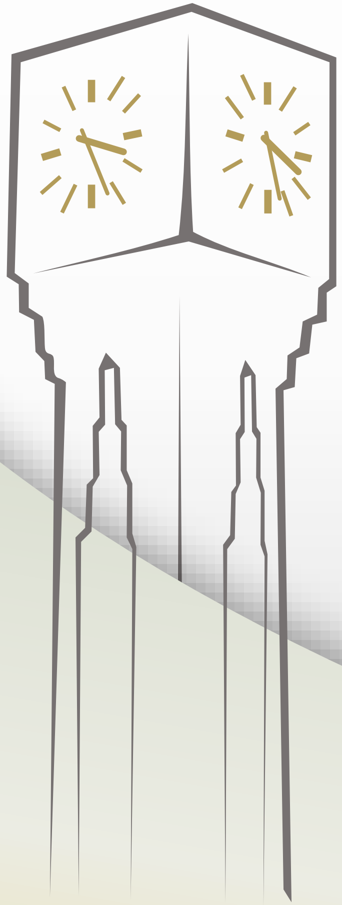
2) By using $\boxed{P_h(\text{mm Hg}) = P_0(\text{mm Hg}) + h(\text{mm Hg})}$ Replace Hg with H_2O

$$P_h = 10.4 \text{ m } H_2O + 30.0 \text{ m } H_2O = \boxed{40.4 \text{ m } H_2O}$$

Show that two calculated pressures are equivalent.



Pressure	1 atm $= 1.01325 \times 10^5$ N/m^2 (Pa) = 101.325 kPa = 1.01325 bar $= 1.01325 \times 10^6$ dynes/cm^2 = 760 mm Hg at 0°C (torr) = 10.333 m H_2O at 4°C = 14.696 lb$_f$/in.^{2} (psi) = 33.9 ft H_2O at 4°C = 29.921 in. Hg at 0°C



3.5 Temperature

This section defines the temperature variable, different scales and units, conversions between units, and measurement devices

3.5. Temperature

- Temperature is a measure of the average kinetic energy of the molecules of a substance.

- It is measured indirectly using a scale relative to a measureable physical property that depends on temperature (electrical resistance, voltage, radiation, etc).

Temperature Scales

- Can be defined in terms of any property or physical phenomena, e.g., volume of a fixed mass of fluid (thermometer), that takes place at a fixed temperature, e.g., freezing or boiling points..

- The two most common temperature scales are the **Fahrenheit** scale and the **Celsius** scale.

- They are defined using freezing temperature (T_f) and boiling temperature (T_b) of water at 1 atm at sea level.

Celsius or centigrade scale (degrees C, or °C)

- T_f is assigned a value of (0°C,) and T_b a value (100°C).
- **Absolute zero**: theoretically is the lowest temperature attainable in nature, where all molecular motion theoretically stops.
- On this scale, ***absolute zero*** falls at -273.15°C

Fahrenheit scale (°F)

- T_f is assigned a value of (32°F,) and T_b a value (212°F).
- ***Absolute zero*** falls at -459.67°F

Kelvin (K) and Rankine (°R) scales

- Are defined such that the **absolute zero** has a value of zero (**0**)
- In Kelvin scale, the size of degree Kelvin (K) is same as a °C.
- In Rankine scale, the size of degree Rankine (°R) is same as a °F.

Relation between temperature scales

$$\left.\begin{array}{l} T(\mathrm{K}) = T(^\circ\mathrm{C}) + 273.15 \\ T(^\circ\mathrm{R}) = T(^\circ\mathrm{F}) + 459.67 \\ T(^\circ\mathrm{F}) = 1.8\,T(^\circ\mathrm{C}) + 32 \\ T(^\circ\mathrm{R}) = 1.8\,T(\mathrm{K}) \end{array}\right\} \; y = a\,x + \mathrm{b}$$

These are the conversion factors between different temperature scales

Example. Convert 20°F into °C.

$$20^\circ\mathrm{F} = 1.8\,\mathrm{T}(^\circ\mathrm{C}) + 32 \Rightarrow \mathrm{T} = -6.67\ ^\circ\mathrm{C}$$

Temperature vs. Temp. Interval

- Consider heating from 20°C to 50°C
- 20°C is a temperature value, while 20°C to 50°C is an interval
- The interval value equals 50 – 20 = 30°C
- Temperature interval is any situation that can be described as ΔT

Conversion of units for a temperature value (T)

$$T(K) = T(°C) + 273.15$$

$$T(°R) = T(°F) + 459.67$$

$$T(°R) = 1.8\,T(K)$$

$$T(°F) = 1.8\,T(°C) + 32$$

Conversion of units for a temperature interval (ΔT)

$$\boxed{\frac{1.8°F}{1°C},\ \frac{1.8°R}{1\,K},\ \frac{1°F}{1°R},\ \frac{1°C}{1\,K}}$$

Show that
$R = 8.314\ m^3.Pa/mol.K$
equals to
$0.7302\ ft^3.atm/lb\text{-}mol.°R$

Example. How many °C are there in interval 20°F to 80°F?

ΔT = 80 - 20 = 60°F (interval).

$\Delta T(°C) = 60°F \times (1°C / 1.8°F) = 33.33°C$

What about:
$Q = m\,C\,\Delta T$?

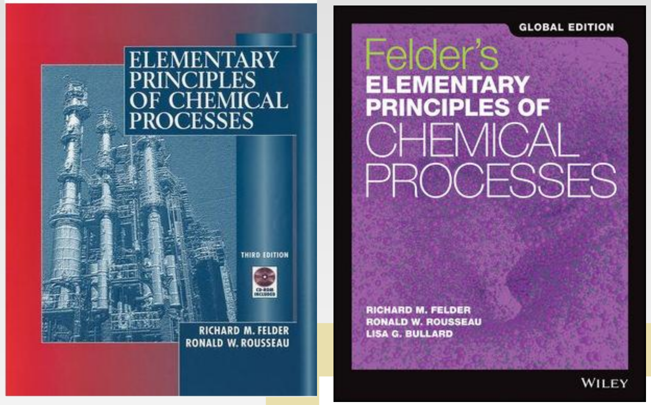
Example 3.5-3 Temperature Conversion and Dimensional Homogeneity

The heat capacity of ammonia, defined as the amount of heat required to raise the temperature of a unit mass of ammonia by precisely 1° at a constant pressure, is, over a limited temperature range, given by the expression

$$C_p\left(\frac{Btu}{lb_m \cdot \text{°F}}\right) = 0.487 + 2.29\ \times 10^{-4} T(\text{°F})$$

Determine the expression for C_p in $J/(g \cdot \text{°C})$ in terms of $T(\text{°C})$.

Solution



Elementary Principles of Chemical Processes,
3rd or 4th edition,
Wiley & Sons, Inc.
Richard M. Felder, Ronald W. Rousseau, & Lisa G. Bullard.

Student Sample Slides

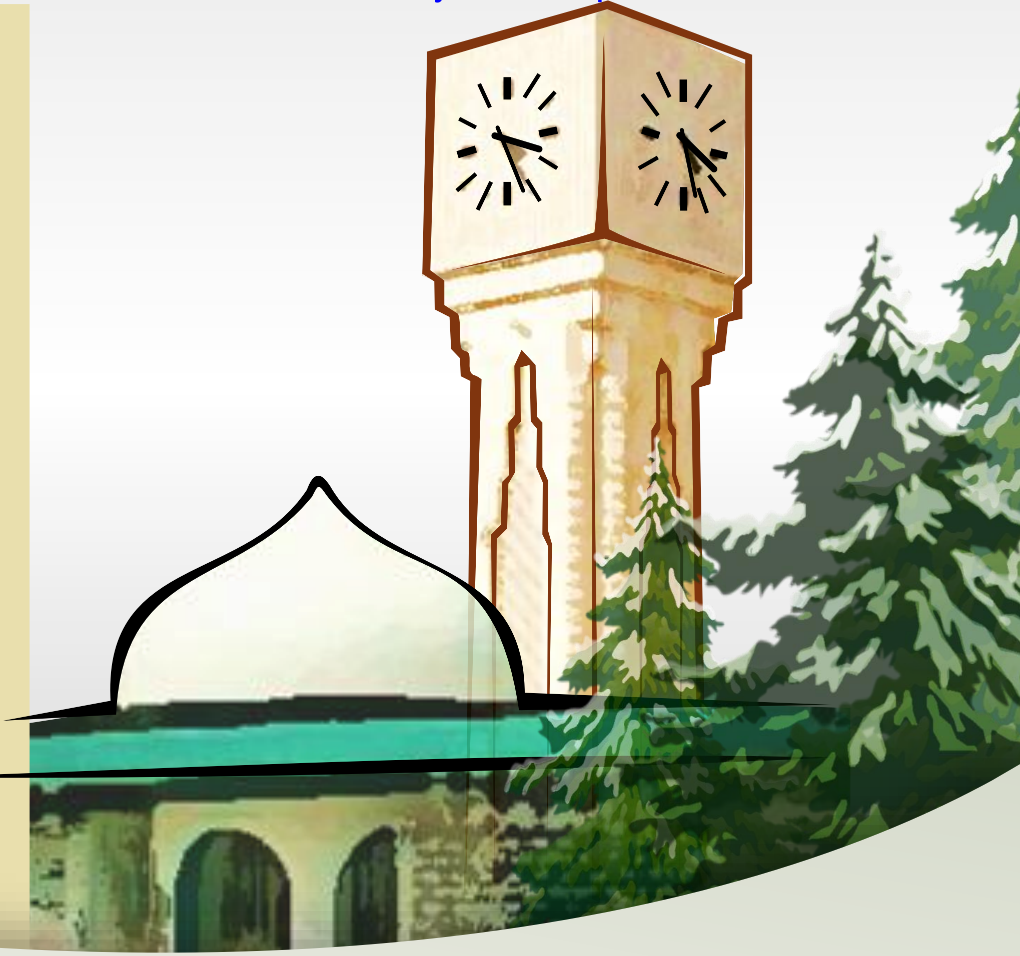
This only a sample of material. Refer to textbook for study of the topics

CHE 0905211

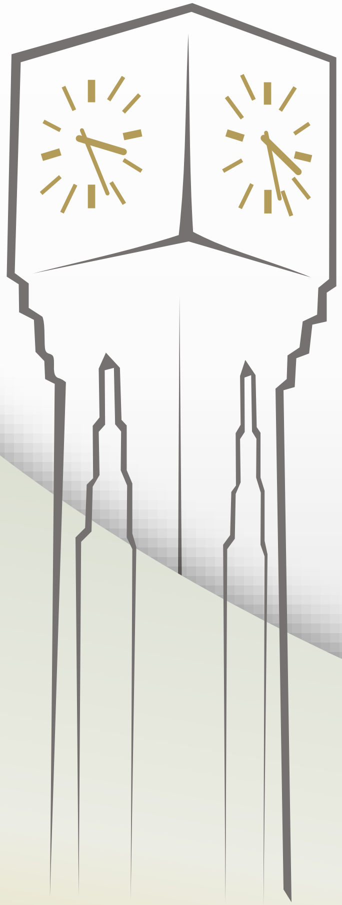
Chemical Engineering Principles 1

Fall 2025

Dr. Hatem Alsyouri	Chapter 4



The University of Jordan
Chemical Engineering Department

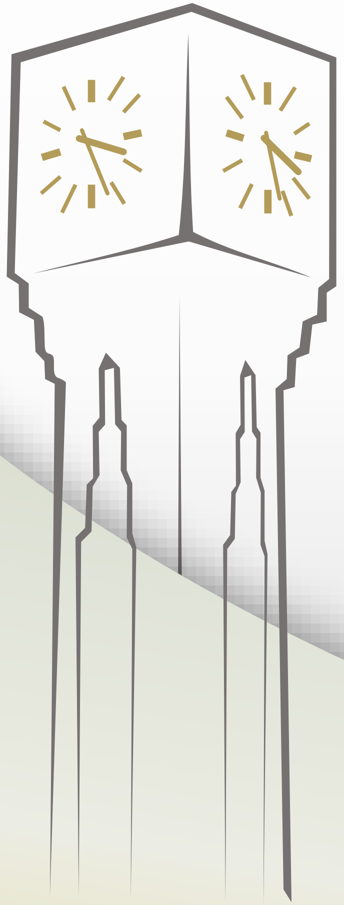


4.1 Process Classification

This section defines the classifications of chemical processes: batch, continuous, semi-batch as well as being open, closed, steady state and unsteady state.

Chapter 4: Fundamentals of Material Balances – Learning Objectives

1. Designing new process or analyzing existing one requires accounting for certain restrictions like law of conservation of mass (e.g., input to a reactor of 1000 g must produce an output mass of 1000 g)
2. **Law of conservation of mass** "mass can neither be created nor destroyed" is the basis for ***Mass balances*** or ***Material balances***
3. The mass or material balance states that ***Total Mass of Inputs = Total Mass of Outputs***. This means the inputs and outputs of the entire process and of each of individual unit satisfy balance equation.
4. Chapters 4, 5 and 6 outline of procedures for writing material balances on individual and multiple-unit processes.
5. Chapter 4 presents methods for organizing known information about process variables, setting up material balance equations, and solving these equations for unknown variables
6. Chapters 5 and 6, introduce various physical properties and law governing behavior of process materials and use them in formulating the balance equations.



4.1 Process Classification

This section defines the classifications of chemical processes: batch, continuous, semi-batch as well as being open, closed, steady state and unsteady state

4.1 Process Classifications

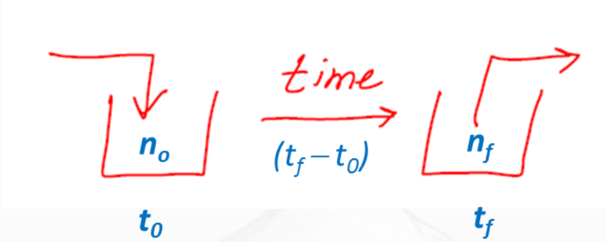
a) Types of systems

Open system

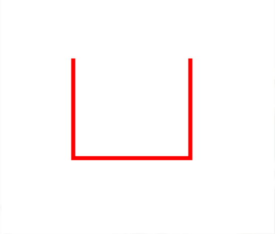
Material flows across the system boundary during the interval of time being studied

Closed system

No flows cross the system boundary, in or out.



no input or output during the operation time
$\Delta t = t_f - t_0$



b) Classification based on how the process varies with <u>time</u>

Steady state

Process variables (P, V, T, n, m) do not change with time.

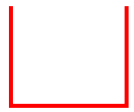
Unsteady state (transient)

Process variables change with time.

c) Classification based on how materials are added/removed

1. *Batch process*:

- Add content to system, then remove them later.
- Closed system (material transfer only during charging and product removal).
- Usually unsteady state
- Use amount units (kg, mol, etc)

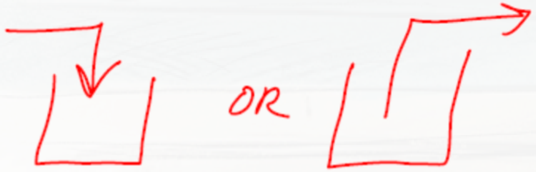


2. *Continuous process*:

- Materials are continuously added and removed
- System is open,
- Usually runs at steady state.
- Use flowrate units (kg/s, mol/h, etc)

3. *Semibatch process*:

- Neither batch nor continuous.
- Runs unsteady state



Exercises on Process Classification

Examples of processes.

Batch process:
1) Pharmaceutical manufacturing
2) Baking cakes
3) Soap making
4) Paint production

Continuous process:
1) Oil refining,
2) Electricity generation in power plants,
3) Plastic extrusion
4) Steel production

Semi-batch process
1) Fermentation in food processing
2) Polymerization,
3) Neutralization reactions,
4) Chemical reactions with gradual feed

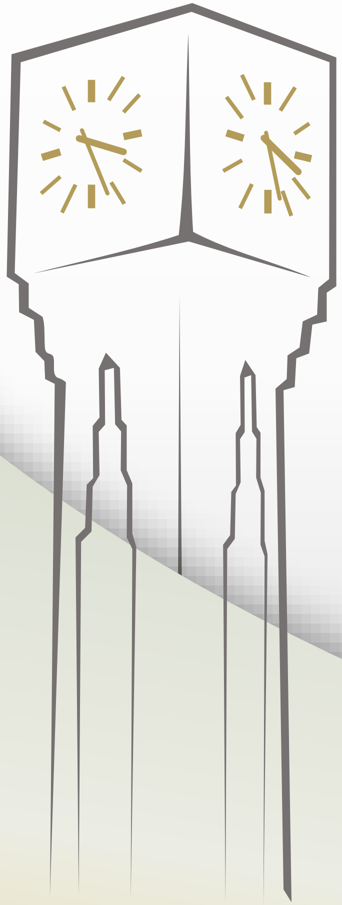
Ingredients are sometimes added during the process which involves batch and continuous characteristics (semi-batch). But process is not fully continuous

Problem. Classify these processes.

1. A balloon is filled with air at a constant rate of 2 g/min. (_______________) Semi-batch

2. Water is put in a closed flask then is boiled. (_______________) Semi-batch

3. Production of gasoline from crude oil. (_______________) Continuous



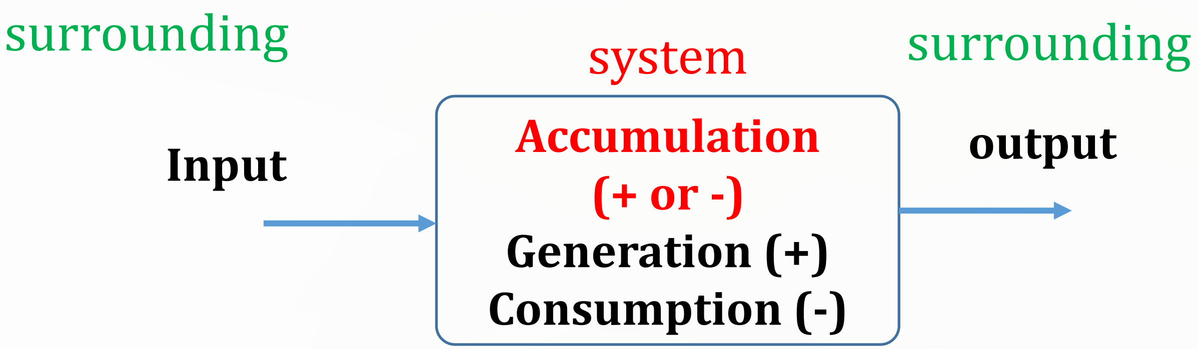
4.2 Balances

This section defines the General Material Balance Equation(GMBE) and explains how it is applied to different types of chemical processes to account for all species in the feed and product streams

4.2 Balances

4.2a General Balance Equation

It is based on the Law of Conservation of Mass, i.e. **Mass can neither be created nor destroyed**



[Units]
mass, or
mass/time

Input – Output + Generation – Consumption = Accumulation

$\left(\begin{array}{c}\text{Flow In}\\ \text{through system boundaries}\end{array}\right)$

$\left(\begin{array}{c}\text{Flow Out}\\ \text{through system boundaries}\end{array}\right)$

$\left(\begin{array}{c}\text{Generation}\\ \text{within system}\end{array}\right)$

$\left(\begin{array}{c}\text{Consumption}\\ \text{within system}\end{array}\right)$

$\left(\begin{array}{c}\text{Accumulation}\\ \text{within system}\end{array}\right)$

This **balance equation** applies to conserved quantities (total mass, mass of a particular species, energy, momentum, etc.) in a system (single unit, collection of units, or the entire process).

- ***Accumulation*** : is the rate of change of material with time within the system. It can be
  - i. Positive (material is increasing) (un-steady state or transient),
  - ii. Negative (material decreasing), (un-steady state or transient)
  - iii. Zero (steady state).

Differentiate between

Steady state
vs.
Un-steady state
(or transient)

Types of Balances

Differential balances

- Indicates what happen in the system at any instant in time.
- Each term in balance equation is a rate = property/time.
- Applies to continuous process.
- Expresses the property change at an instant in time

$$\frac{dm}{dt} = \dot{m}_{in} - \dot{m}_{out} + \dot{generation} - \dot{consumption}$$

Accumulation

Integral balances

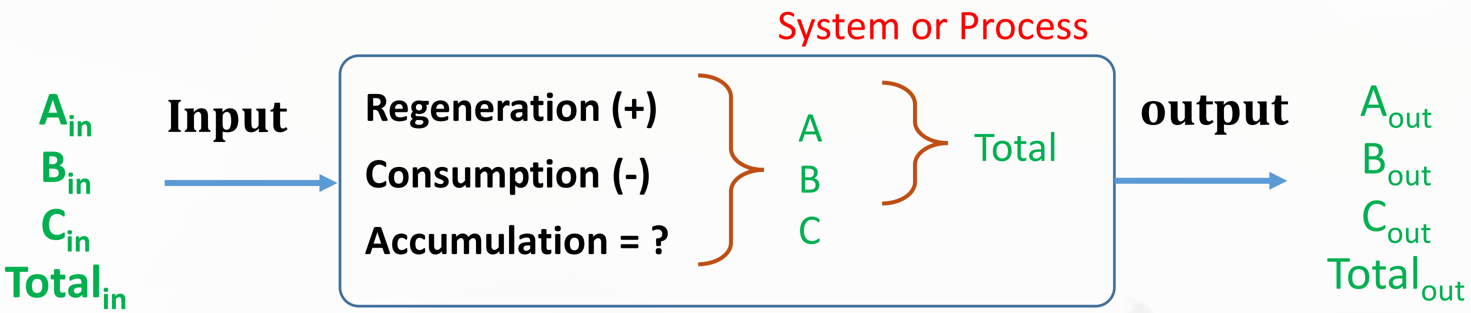
- Describes what happens between two instants of time.
- Each term in balance equation **amount** of property.
- Used for batch process.
- Expresses the property change **over a period of time** (t_0 to t_f)

$$\left(m(t_f) - m(t_0)\right) = \int_{t_0}^{t_f} \left(\dot{m}_{in} - \dot{m}_{out} + \dot{generation} - \dot{consumption}\right) dt$$

Accumulation

Material Balance Equation

- Applying the general material balance equation on masses of materials in a process leads to the **Material Balance Equation.** Two material balances are possible: ***Total Material Balance*** and ***Component Material Balance***



Input – Output + Generation – Consumption = Accumulation

$$\dot{m}_{in} - \dot{m}_{out} + \dot{r}_{gen} - \dot{r}_{cons} = \frac{dm}{dt}$$

Why 0? Because total mass is conserved

Total Material Balance $\quad Total_{in} - Total_{out} + \cancelto{0}{Total_{Gen}} - \cancelto{0}{Total_{Cons}} = Total_{Accum}$

Component Material Balance on A $\quad A_{in} - A_{out} + A_{Gen} - A_{Cons} = A_{Accum}$

Component Material Balance on B $\quad B_{in} - B_{out} + B_{Gen} - B_{Cons} = B_{Accum}$

Extra Exercises: General Material Balance Equation

Example 1. Differential balance with Generation (Air Pollution in a Room)

Consider a room where dust particles are generated by a machine at a rate of 100 g/min. A ventilation system is removing air from the room at a rate that carries away 40 g/min of dust. No dust enters the room from outside. Write a differential material balance for the mass of dust in the room, accounting for the generation and outflow.

Hints

- Unsteady state process
- Require the change in mass at an instant of time → use the differential method.
- No mass inflow of dust, so $\dot{m}_{in}$ = 0 g/min
- m_D(t) represents the mass of dust in the room at time t (in min)

Solution

Accumulation

$$\frac{dm_D}{dt} = \dot{m}_{in} - \dot{m}_{out} + \dot{generation} - \dot{consumption}$$

All elements of the equation has a consistent unit (kg/min)

$$\frac{dm_D}{dt} = \cancelto{0}{\dot{m}_{in}} - \dot{m}_{out} + \dot{generation} - \cancelto{0}{\dot{consumption}}$$

$$\frac{dm_D}{dt} = 0\,\frac{g}{min} - 40\ g/\min + 100\ g/\min - 0\ g/min$$

$$\boldsymbol{\frac{dm_D}{dt} = 60\,\frac{g}{min}}$$

This equation indicates that the mass of dust in the room is increasing at a rate of 60 g/min (or 0.06 kg/min) because the rate of dust generation is greater than the rate at which the ventilation system removes it.

Q. Calculate the dust accumulation rate in kg/h. [ans. 3.6 kg/h)

Extra Exercises: General Material Balance Equation

Example 2. Integral balance without Generation or Consumption (Tank Filling)

A tank initially contains 100 kg of water. Water flows into the tank at a rate of $\dot{m}_{in}$ =10 kg/s, and water flows out at $\dot{m}_{out}$ = 8 kg/s. Find the total mass of water in the tank after 60 seconds.

Hints

- Unsteady state process, because mass changes with time
- Require the change in mass over a period of time → use the Integral method
- Generation = consumption = 0
- $m(t_0)$ is mass of water at initial time = 100 kg
- $m(t_f)$ is mass of water after 60 sec. To be calculated

Solution

Accumulation (kg)

All terms of equation have unit of (kg) (e.g., $\dot{m}_{in}(kg/s)\ \times dt\ (s)$= (kg)

$$m(t_f) - m(t_0) = \int_{t_0}^{t_f} (\dot{m}_{in} - \dot{m}_{out} + gener\dot{a}tion - consu\dot{m}ption)\, dt$$

$$m(t_f) - m(t_0) = \int_{t_0}^{t_f} (\dot{m}_{in} - \dot{m}_{out} + \cancelto{0}{gener\dot{a}tion} - \cancelto{0}{consu\dot{m}ption})\, dt$$

$$m(t_f) - m(t_0) = \int_{t_0}^{t_f} (\dot{m}_{in} - \dot{m}_{out})\, dt$$

$$m(t_f) - m(t_0) = \int_{t_0}^{t_f} (10 - 8)\, dt$$

mass flow rates are constants, so take out of the integral

$$m(t_f) - m(t_0) = 2\int_{t_0=0}^{t_f=60} dt \quad \Rightarrow \quad m(t_f) - m(t_0) = 2\,(t_f - t_0)$$

$$m(t_f) - 100 = 2\,(60 - 0) \quad \Rightarrow \quad m(t_f) - 100 = 120$$

$$\boldsymbol{m(t_f) = 220\ kg}$$

120 kg is the change in mass over the time period (60 sec)

Extra Exercises: General Material Balance Equation

Example 3. Integral balance with Generation (Chemical Reaction in a Reactor)

A chemical reactor initially contains 300 kg of a reactant. The reactant is supplied at a rate of $\dot{m}_{in}$ = 5 kg/s and leaves at $\dot{m}_{out}$ = 4 kg/s. Inside the reactor, the reactant is consumed at a rate of 2 kg/s. Calculate the change of mass of the reactant in the reactor after 3 minutes.

Hints

- Unsteady state process
- Require the change in mass over a period of time → use the Integral method
- $m(t_0)$ is mass of water at initial time = 50 kg
- $m(t_1)$ is mass of water after 3 minutes (t_1= 3 min = 180 sec). To be calculated

Solution

$$m(t_1) - m(t_0) = \int_{t_0}^{t_1} \left(\dot{m}_{in} - \dot{m}_{out} + \cancelto{0}{\dot{generation}} - \cancelto{0}{\dot{consumption}}\right) dt$$

$$m(t_1) - m(t_0) = \int_{t_0}^{t_1} \left(\dot{m}_{in} - \dot{m}_{out} - \dot{consumption}\right) dt$$

$$\Delta m = \int_{t_0}^{t_1} (5 - 4 - 2)\, dt$$

mass flow rates are constants, so take out of the integral

$$\Delta m = (-1) \int_{t_0=0}^{t_1=180} dt$$

$$t_1 = \frac{3\ min}{} \times \frac{60\ sec}{1\ min} = 180\ sec$$

$$\Delta m = (-1)\,(t_1 - t_0)$$

$$\Delta m = (-1) \times\ (180 - 0)$$

The negative sign indicates that the mass inside the reactor is decreasing with time

$$\boldsymbol{\Delta m = -180\ kg}$$

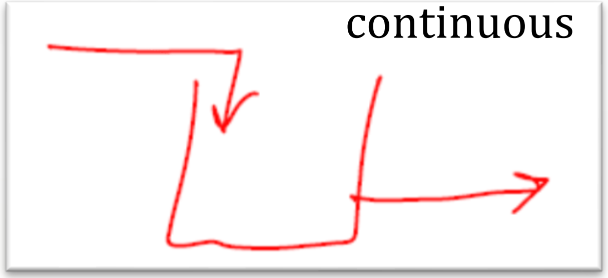
The mass of reactor decreased by 180 kg over the 3 min time period

Q. What is mass in reactor after 3 minutes? This is $m(t_1)$

Δm= $m(t_1) - m(t_0)$ ⇒ $-180 = m(t_1) - 300$ ⇒ $\boldsymbol{m(t_1)}$ **= 120 kg**

4.2b Material balance on continuous steady-state processes

- **Steady state** ⇒ **Accumulation = 0**



~~Accumulation~~ = In – Out + Generation – Consumption

$$\boxed{\text{Input + Generation = Output + Consumption}}$$

Mathematical form

$$\cancel{\frac{dm_A}{dt}} = \dot{m}_{A\,in} - \dot{m}_{A\,out} + \dot{Gen}._A - \dot{Cons}._A$$

All units are [**mass/time**]
Can be for any species (A, B, or total mass)

$$\boxed{0 = \dot{m}_{A\,in} - \dot{m}_{A\,out} + \dot{Gen}._A - \dot{Cons}._A} \Longrightarrow \boxed{\dot{m}_{A\,in} + \dot{Gen}._A = \dot{m}_{A\,out} + \dot{Cons}._A}$$

Steady state Reactive

- **(Special case).** If the steady state balance is **Non-reactive**

⇒ **Generation = 0** **and** **Consumption = 0**

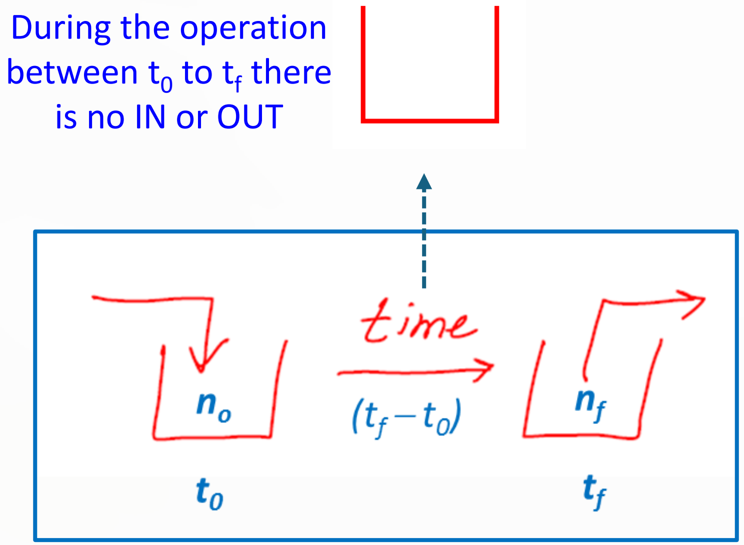
Input + ~~Generation~~ = Output + ~~Consumption~~

$$\boxed{\text{Input = Output}}$$

$$\dot{m}_{A\,in} + \cancel{\dot{Gen}._A} = \dot{m}_{A\,out} + \cancel{\dot{Cons}._A} \Longrightarrow \boxed{\dot{m}_{A\,in} = \dot{m}_{A\,out}}$$

Steady state, non-Reactive

4.2c Integral balances on batch processes



During the operation between t_0 to t_f there is no IN or OUT

Batch Reaction (Reactant→ Product)

- ✓ Consider balance on any species (reactant or product)
- ✓ Feed is charged into a system at time **t_0 = 0**, and thus the initial number of mole of species (reactant or product) is **n_o**
- ✓ When reaction is terminated at time **t_f ,** the species will be withdrawn at **n_f.**
- ✓ Between **t_o** and **t_f,** no species enters (input = 0) or leaves (output= 0)
- ✓ Over a period of time (batch) → use integral balance

Species balance

No input   No output

Accumulation = ~~Input~~ – ~~Output~~ + Generation – Consumption

Accumulation = Generation – Consumption ……. (1)

also Accumulation = Final output – Initial input ……. (2)

Equating (1) and (2)

Initial input+ Generation = Final output + Consumption

Same

Mathematical form

Accumulation

$$n_{Af}(t_f) - n_{A0}(t_0) = \int_{t_0}^{t_f} \left(\cancel{\dot{n}_{A\,in}} - \cancel{\dot{n}_{A\,out}} + G\dot{e}n_{.A} - C\dot{o}ns_{.A}\right) dt$$

$$n_{Af}(t_f) - n_{A0}(t_0) = \left(G\dot{e}n_{.A} - C\dot{o}ns_{.A}\right) \int_{t_0}^{t_f} dt$$

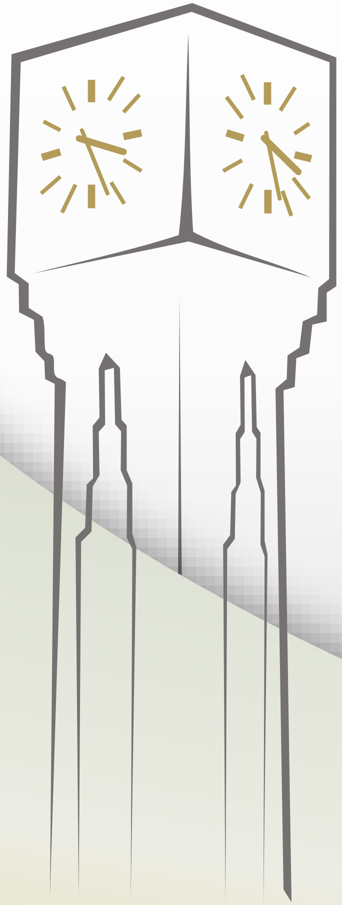
$$n_{Af}(t_f) - n_{A0}(t_0) = \left(G\dot{e}n_{.A} - C\dot{o}ns_{.A}\right) \times \Delta t$$

(mol) (mol) (mol/time)x(time) (mol/time)x(time)

$$n_{Af}(t_f) - n_{A0}(t_0) = G\dot{e}n_{.A} \times \Delta t - C\dot{o}ns_{.A} \times \Delta t$$

(mol) (mol) (mol) (mol)

$$\boxed{n_{Af}(t_f) - n_{A0}(t_0) = Gen_{.A} - Cons_{.A}}$$



4.3 Material Balance Calculations

a. Flowcharts

This section outlines a procedure for reducing and description of a process to a set of equations that can be solved for unknown process variables

4.3a. Flowcharts

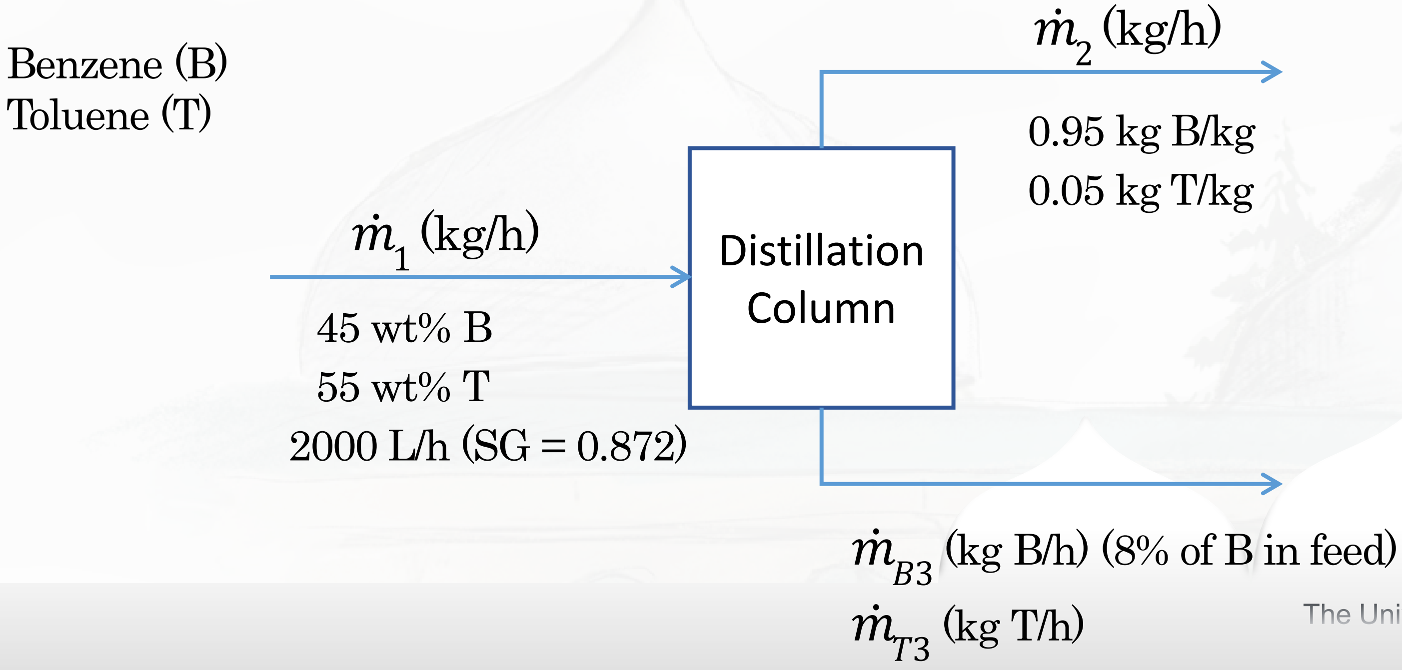
Process description

A chemical engineer should be able to draw a clear process flowchart from any written description and interpret flowcharts to understand the process operation, even when the system is complex..

Flowchart

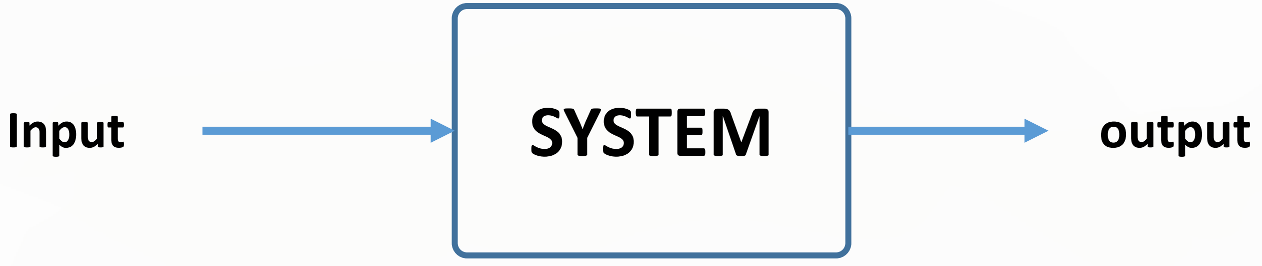
A liquid mixture containing 45.0 wt% benzene (B) and 55.0 wt% toluene (T) is fed to a ***distillation column*** (separation unit) operating at ***steady state***. Product streams leave from the top and bottom of the column. The top product stream contains 95.0 wt% B, and the bottom product contains 8% of the benzene fed to the column. The volumetric flow rate if the feed stream is 2000 liters/h and the specific gravity of the feed mixture is 0.872.

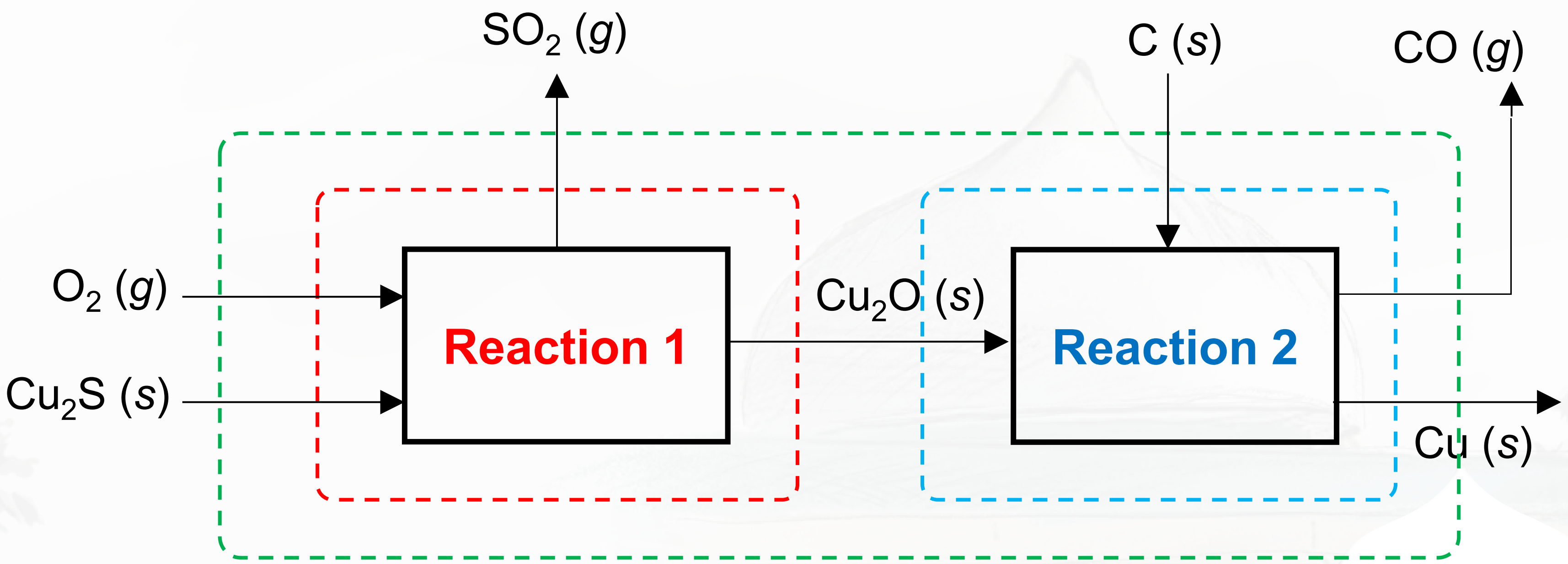
Determine the mass flow rate of the overhead product stream and the mass flow rate and composition (mass fraction) of the bottom product.



Simple flowcharts

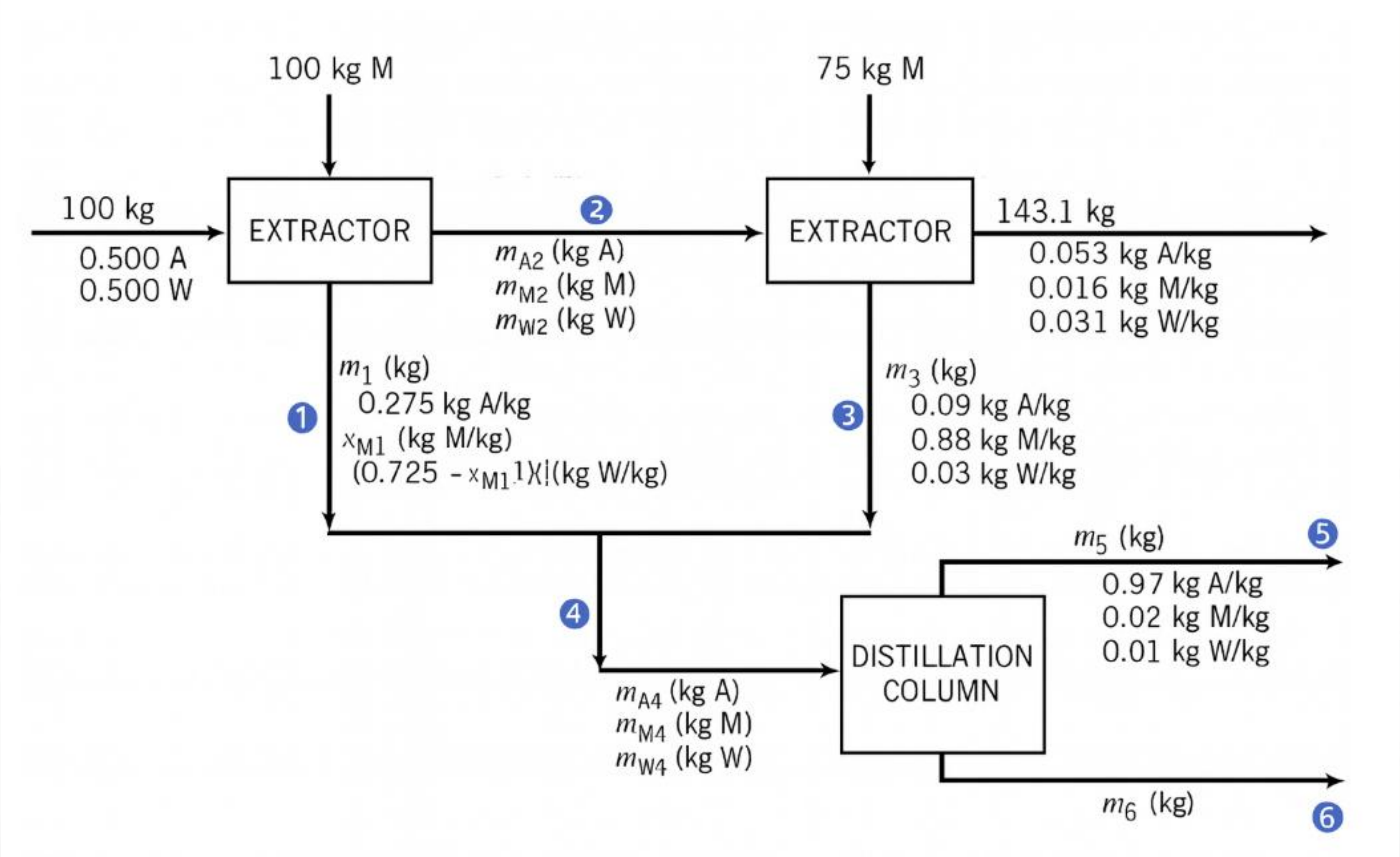
A flowchart is an illustration of the process using boxes or other symbols to represent process units and lines with arrows to represent inputs and outputs.





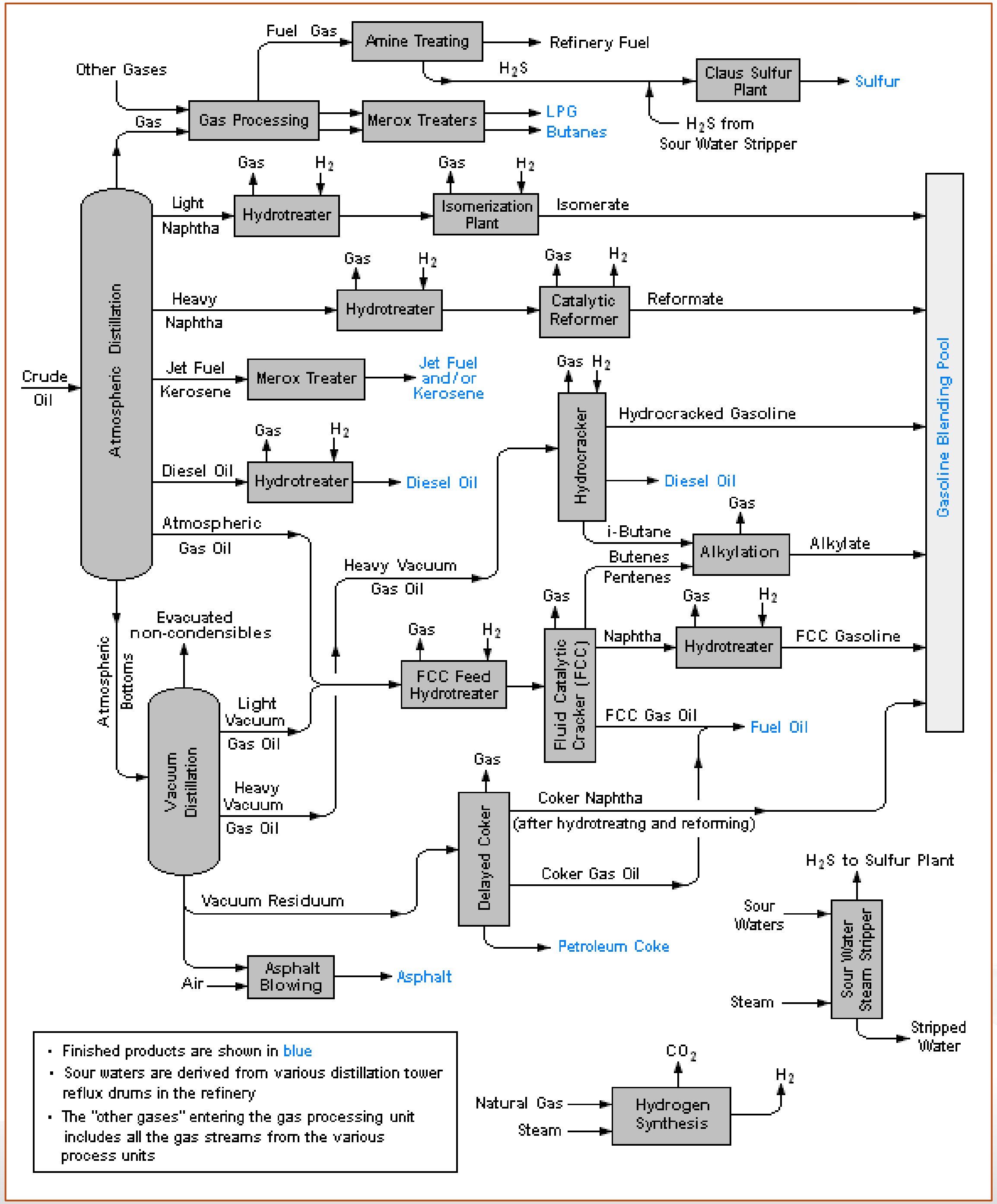
More complex flowcharts

Throughout this chapter, you will be to handle calculations of flowcharts like this for non-reactive and reactive processes



Detailed flowcharts

You will handle mass balance calculations for detailed process flow charts like this one during your **Graduation Project**

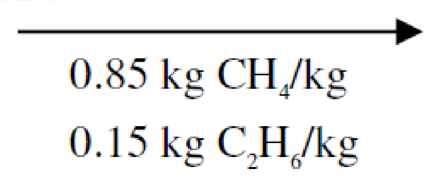


- Finished products are shown in blue
- Sour waters are derived from various distillation tower reflux drums in the refinery
- The "other gases" entering the gas processing unit includes all the gas streams from the various process units

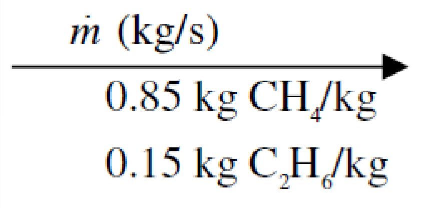
Drawing and Labelling Flowcharts

- Organize given process information in a convenient way called ***flowchart*** to have a typical problem for analysis and calculation. Flow chart must be ***completely labeled***.

- A stream on a flow chart is completely labeled when you can write an expression for the amount (batch) or flow rate (continuous) of each species in the stream in terms of numbers and variables written on the flow chart. A flow chart is completely labeled if every stream on it is completely labeled.



Not completely labelled. Why?



CH_4 flow rate= $0.85\ \dot{m}$

C_2H_6 flow rate= $0.15\ \dot{m}$

completely labelled

Rules of Labelling Flowcharts

1) Label either a total flow rate (or amount) and component mass or mole fractions, or individual component flow rates (amounts).

2) Label in the way that makes algebra easier

3) If volumes (or volumetric flow rates) of streams are either given or required, include labels both for them and for mass or molar quantities.

4) Use standard labels
   - (m) for mass, ($\dot{m}$) for mass flow rate
   - (n) for mole, ($\dot{n}$) for mole flow rate
   - (V) for volume, ($\dot{V}$) for volumetric flow rate
   - (x) for liquid composition
   - (y) for gas composition

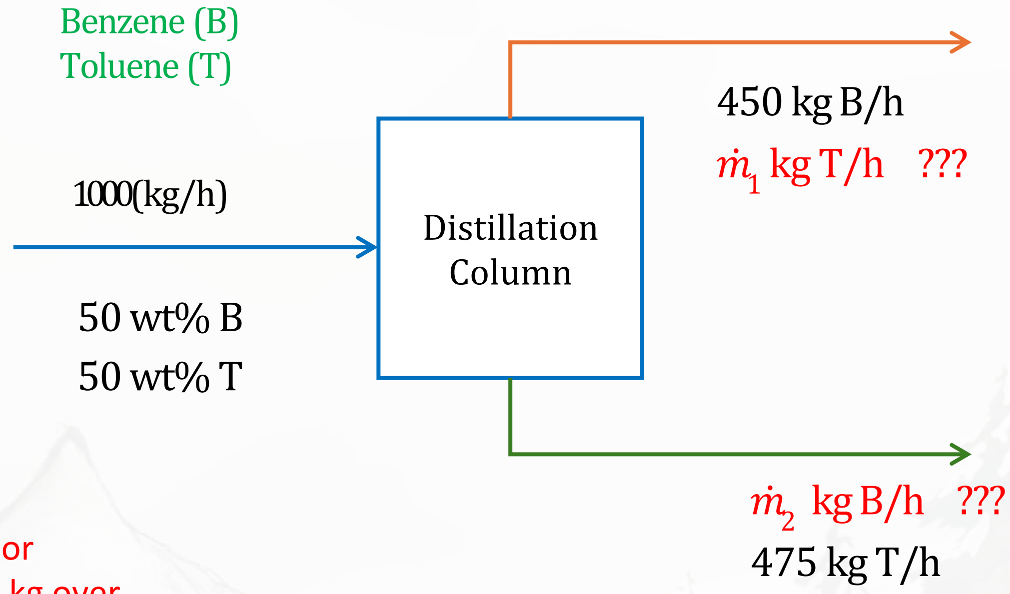
Don't use
random
A, B, C, etc.

Refer to book for more details and practice on labelling streams in a flow chart

Exercise on Material Balance on a Continuous Process

Example 4.2-2 Material Balances on a Continuous Distillation Process

One thousand kilogram **per hour** of a mixture of benzene (B) and toluene (T) containing 50% benzene by mass is separated by distillation unit into two fractions (streams). The mass flow rate of benzene in the top stream is 450 kg B/h and that of toluene in the bottom stream is 475 kg T/h. The operation is at **steady state**. Write balances on benzene and toluene to calculate the unknown component flow rate in the output streams ($\dot{m}_1$ and $\dot{m}_2$).



The mass of reactor decreased by 180 kg over the 3 min time period

Solution

Continuous steady state, no reaction

Input + ~~Generation~~ = Output + ~~Consumption~~

T- balances

$$T_{input} = T_{output}$$

$$0.5 \times 1000 = \dot{m}_1 + 475$$

B- balances

$$B_{input} = B_{output}$$

$$0.5 \times 1000 = 450 + \dot{m}_2$$

Solving 2 equations with 2 unknowns

solution

$$\dot{m}_1 = 25\ kg\ T/h$$

$$\dot{m}_2 = 50\ kg\ B/h$$

For solving 2 unknowns, you need 2 equations from any of the 3 balances:

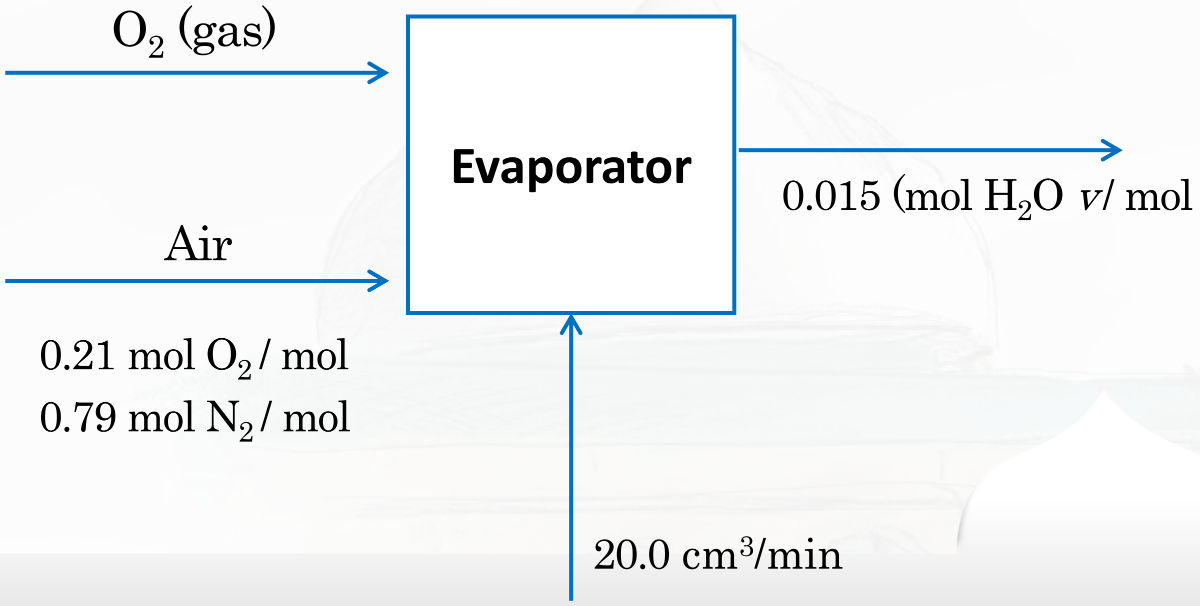
- Toluene (T)
- Benzene (B)
- Total

Exercise on Drawing and labeling Flowcharts

Example. Enriching Air with O_2

A stream of pure oxygen, a stream of air (21.0 mole% O_2, 79.0% N_2), and a stream of liquid water flowing at a rate of 20.0 cm^3/min, are fed to a steady-state evaporation chamber in which all of the liquid evaporates. The flow rate of the pure oxygen is 20% of the flow rate of the air. The emerging gas stream contains 1.5 mole% water vapor.

Completely label the flowchart (including the molar flow rate of the liquid water stream), following the rules!



O_2 (gas)

Air

0.21 mol O_2 / mol

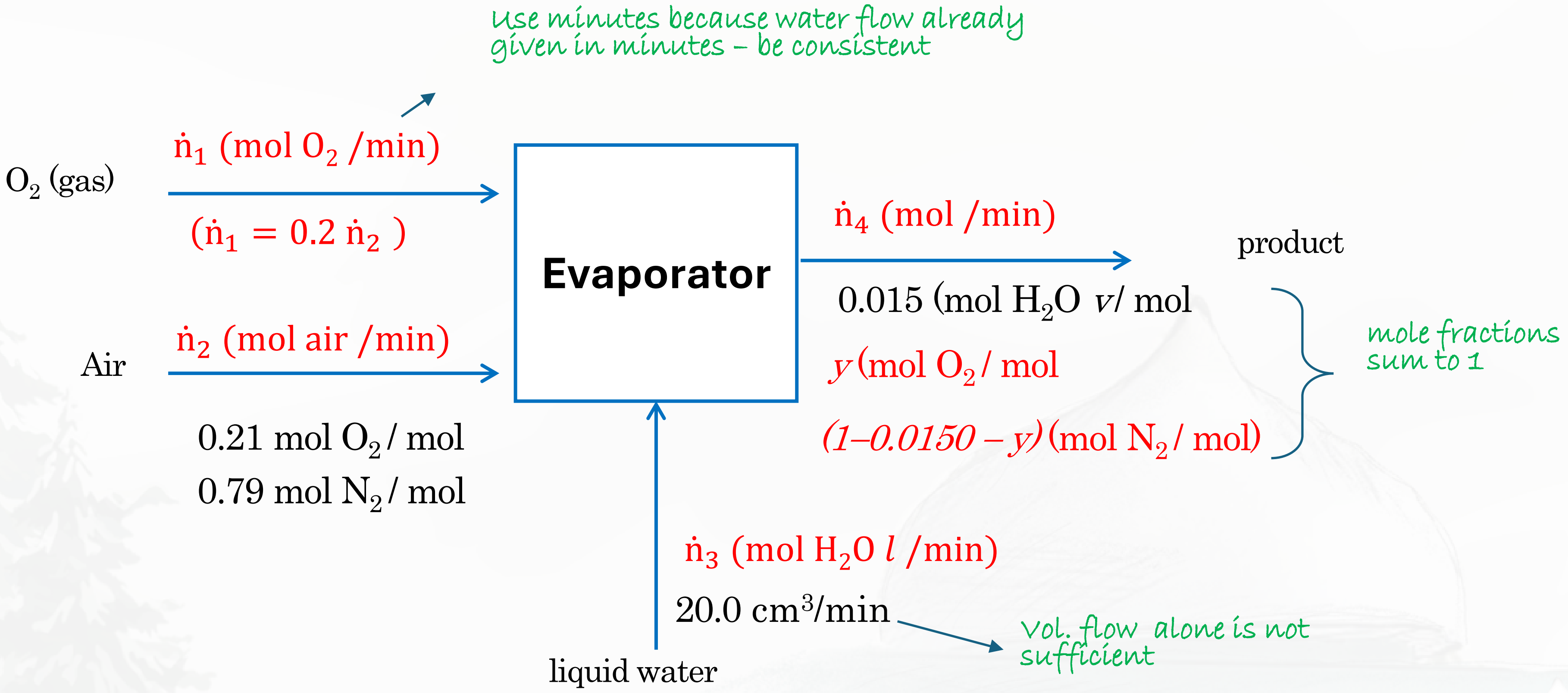
0.79 mol N_2 / mol

Evaporator

0.015 (mol H_2O v/ mol

20.0 cm^3/min

Solution – Enriching Air with O_2



Use minutes because water flow already given in minutes – be consistent

O_2 (gas)

$\dot{n}_1$ (mol O_2 /min)

($\dot{n}_1 = 0.2\ \dot{n}_2$)

Air

$\dot{n}_2$ (mol air /min)

0.21 mol O_2 / mol

0.79 mol N_2 / mol

Evaporator

$\dot{n}_4$ (mol /min)

product

0.015 (mol H_2O v/ mol

y (mol O_2 / mol

$(1 - 0.0150 - y)$ (mol N_2 / mol)

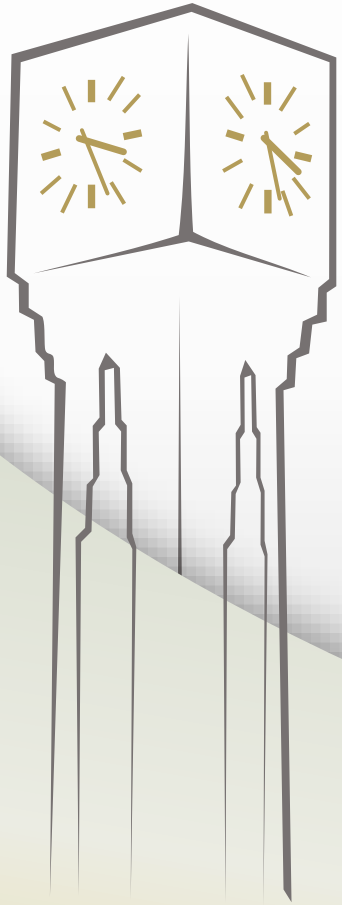
mole fractions sum to 1

$\dot{n}_3$ (mol H_2O l /min)

20.0 cm^3/min

Vol. flow alone is not sufficient

liquid water



4.3b. Flowchart Scaling and Basis of Calculation

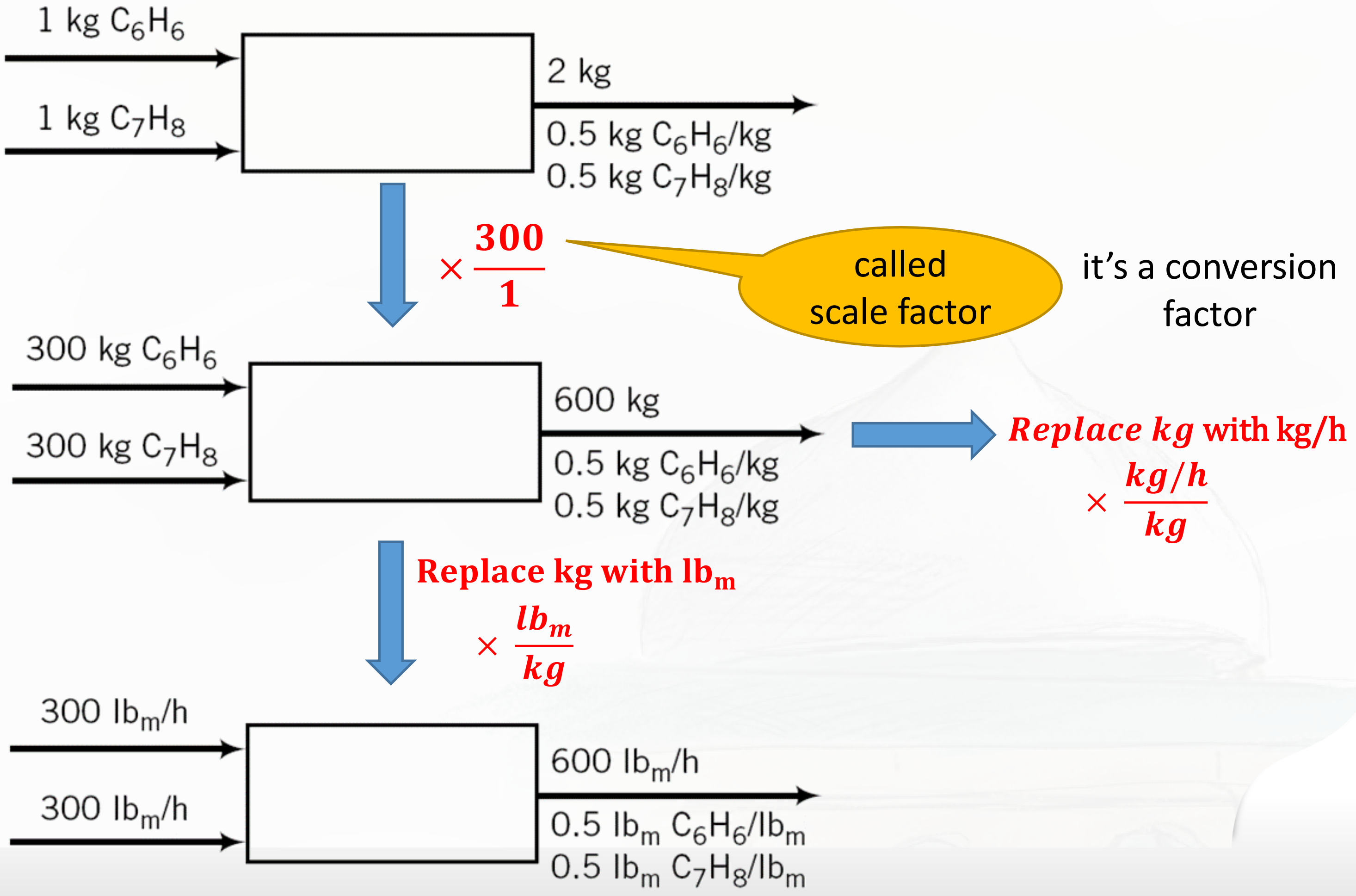
This section

4.3b Flowchart scaling and basis of calculation

Flow chart scaling

Scaling (up or down) is changing the values of all stream amounts (or flow rates) by proportional amounts while keeping stream compositions unchanged.

Refer to book for exercises on scaling



1 kg C_6H_6

1 kg C_7H_8

2 kg

0.5 kg C_6H_6/kg

0.5 kg C_7H_8/kg

$\times \frac{300}{1}$

called scale factor

it's a conversion factor

300 kg C_6H_6

300 kg C_7H_8

600 kg

0.5 kg C_6H_6/kg

0.5 kg C_7H_8/kg

Replace kg with kg/h

$\times \frac{kg/h}{kg}$

Replace kg with lb_m

$\times \frac{lb_m}{kg}$

300 lb_m/h

300 lb_m/h

600 lb_m/h

0.5 lb_m C_6H_6/lb_m

0.5 lb_m C_7H_8/lb_m

BASIS of Calculation

- At least one stream quantity or flow rate (mass, moles, volume) should be specified before any calculations are done.

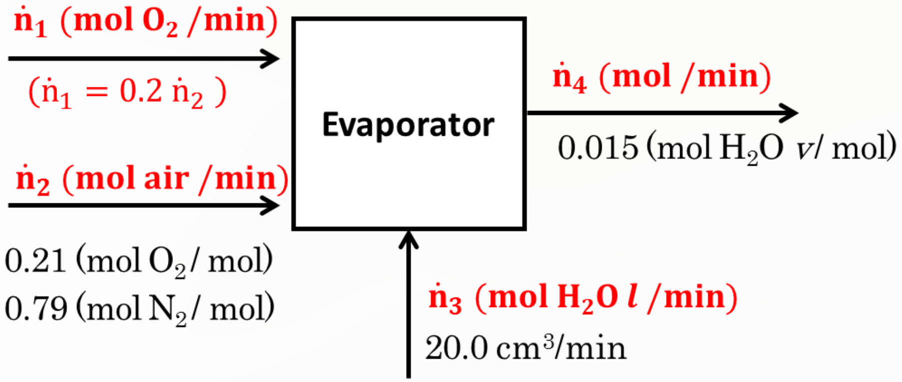
- If the problem statement does not specify any quantity, you should choose a convenient basis (an amount of a stream with known composition.)

  1. If a stream amount or flow rates is given in the problem statement, use it as the basis of calculation.
  2. If no stream amount or flow rates are known, assume a value for a stream, preferably a stream of known composition.
  3. If mass fractions are known, choose a total mass or mass flow rate of that stream (e.g., 100 kg or 100 kg/h)
  4. If mole fraction are known, choose a total number of moles or a molar flow rate (e.g., 100 mol or 100 mol/h).

Exercise on Flowcharts Basis

Example 2. Decide if we need to assume a basis for each flowchart.

No. Volume flow of input is given



$\dot{n}_1$ (mol O_2 /min)

($\dot{n}_1 = 0.2\ \dot{n}_2$)

$\dot{n}_2$ (mol air /min)

0.21 (mol O_2/ mol)
0.79 (mol N_2/ mol)

Evaporator

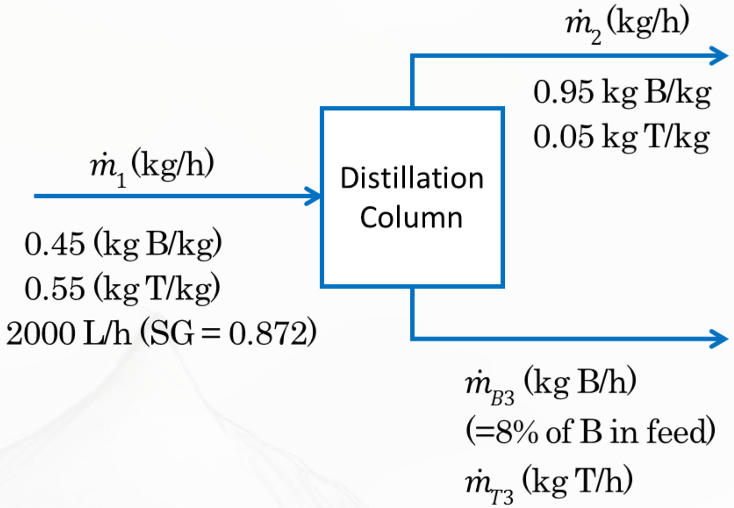
$\dot{n}_4$ (mol /min)

0.015 (mol H_2O v/ mol)

$\dot{n}_3$ (mol H_2O l /min)

20.0 cm^3/min

No. Volume flow of input is given



$\dot{m}_2$ (kg/h)

0.95 kg B/kg
0.05 kg T/kg

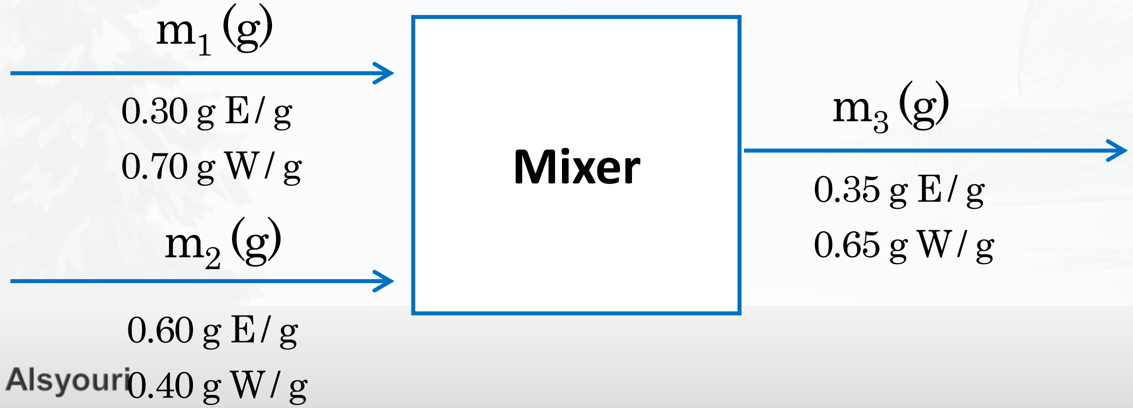
$\dot{m}_1$ (kg/h)

0.45 (kg B/kg)
0.55 (kg T/kg)
2000 L/h (SG = 0.872)

Distillation Column

$\dot{m}_{B3}$ (kg B/h)
(=8% of B in feed)
$\dot{m}_{T3}$ (kg T/h)

Yes. No quantity is specified for any stream



m_1 (g)

0.30 g E/ g
0.70 g W/ g

m_2 (g)

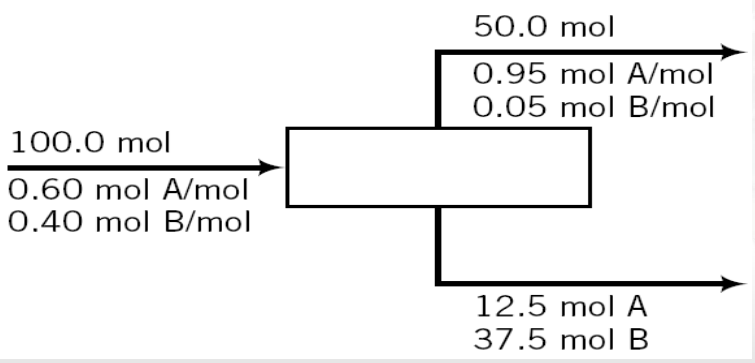
0.60 g E/ g
0.40 g W/ g

Mixer

m_3 (g)

0.35 g E/ g
0.65 g W/ g

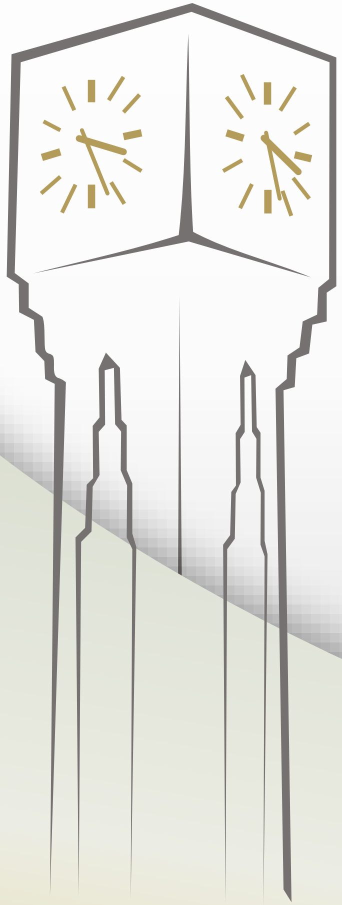
No. Moles are given



50.0 mol
0.95 mol A/mol
0.05 mol B/mol

100.0 mol
0.60 mol A/mol
0.40 mol B/mol

12.5 mol A
37.5 mol B



4.3 Material Balance Calculations

d. Degree-of-Freedom Analysis

This section outlines a procedure for reducing and description of a process to a set of equations that can be solved for unknown process variables

4.3d. Degree-of-freedom (DOF) analysis

DOF Analysis is an important tool for analysis of flowcharts. It determines whether you have enough information to solve the given problem.

Procedure:

1. Draw and completely label a flowchart.
2. Count the number of unknown variables in the chart ($n_{unknowns}$)
3. Count the number of independent equations relating to them ($n_{indep\ eqns}$)
4. Degrees of freedom of the process is (n_{df}) where

$$\boxed{n_{df} = \left(n_{unknowns} - n_{independent\ eqns}\right)}$$

Can be also called DOF

There are 3 possibilities for (n_{df}):

- $n_{df} = 0.0$ The system is completely defined (unique solution).
- $n_{df} > 0.0$ The system is under-defined (Infinite number of solutions)
- $n_{df} < 0.0$ The system is over-defined (Many boundaries).

What does a degree-of-freedom (DOF) analysis help determine in the context of flowcharts?

A. The number of unknown variables

B. The system is completely defined

C. Whether there is enough information to solve the problem

D. The number of independent equations

Answer

Correct answer:

Multiple Choice

In the context of process balancing, if the number of unknown variables exceeds the number of independent equations, what does that indicate?

A. You can easily solve the problem
B. You have sufficient equations
C. You missed a relation or the problem is under-defined
D. You need more inputs

Multiple Choice

The University of Jordan

If the degrees of freedom (ndf) is greater than 0, the system is considered _______.

💡 Answer

Source of Equations

1. Material balances (total and component) for a non-reactive process.
    - ✓ Number of material balance eqns = number of components (or species).
    - ✓ If you have 2 components, then you can make only 2 mass balance eqns.
2. Energy balances.
3. Process specifications given in the problem.
4. Physical properties and laws.
5. Physical constraints, for examples, for any stream (i)

$$\sum_i x_i = 1 \qquad \sum_i y_i = 1$$

6. Stoichiometric relations for reactive processes.

$$2\,H_2 + O_2 \rightarrow 2\,H_2O$$

$$\dot{n}_{O_2} = 0.5\,\dot{n}_{H_2}$$

$$\dot{n}_{H_2O} = \dot{n}_{H_2}$$

$$\dot{n}_{H_2O} = 2\,\dot{n}_{O_2}$$

fixed

4.3 Material Balance Calculations

e. General procedure for single-unit process

This section outlines a procedure to perform material balance calculations of a single-unit processes

4.3e General procedure for single-unit process material balance calculations

1. Choose as a basis of calculation an amount or flow rate of one of the process streams.
2. Draw a flowchart and fill in all known variable values, indicating the basis. Then label unknown stream variables on the chart.
3. Express what the problem statement asks you to determine in terms of labeled variables.
4. If you are given mixed mass and mole units for a stream, convert all quantities to one basis or the other using methods of chapter 2 and 3.
5. Do the degree of freedom (DOF) analysis.
6. Decide if the equations are to be solved manually or by an equation-solving software and write the equations in the desired order.
7. Check your solution by substituting the calculated variable values into any equations you did not use. Does the answer make sense?
8. Solve additional equations for quantities requested in the problem statement.
9. Scale up or down based on required result.

Keywords

- Basis of calculation
- Flowchart
- Fully-labeled streams
- Unknowns
- Amounts vs. flow rates
- Total vs. individual components
- Sources of equations
- DOF
- Logical reasoning
- Scale up/down

What is the first step in the general procedure for conducting material balance calculations in a single-unit process?

A. Draw the flowchart

B. Choose a basis of calculation

C. Perform a DOF analysis

D. Check your solution

Answer

Multiple Choice

What is the first step in the general procedure for single-unit process material balance calculations?

A. Perform a degree of freedom analysis.

B. Choose a basis of calculation.

C. Draw the flowchart.

D. Check the solution.

Multiple Choice

Exercise on DOF and material balance

Previous Exercise – Enriching Air with Water

SO1

Performance Indicators

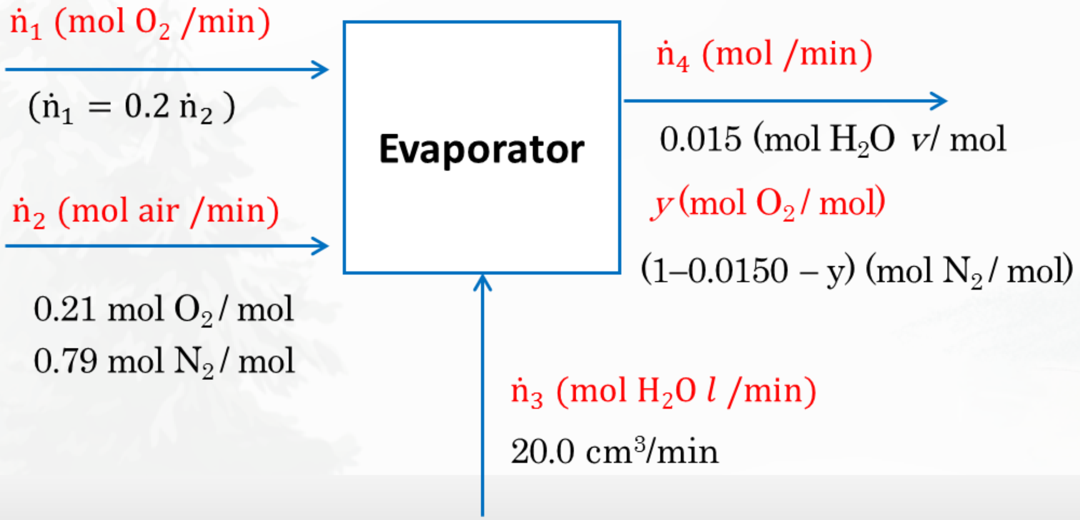
PI1a. Identify and define complex engineering problems.

PI1b. Model and formulate complex engineering problems by applying principles of engineering, science, and mathematics.

PI1c. Solve complex engineering problems by applying principles of engineering, science, and mathematics.

Use the flowchart drawn in a previous exercise to perform the following:

1) Analyze and define the system [PI1a]
2) Do degree of freedom analysis [PI1a]
3) Formulate the necessary equations [PI1b]
4) Solve for unknowns [PI1c]



1. Analyze and define the system [PI1a]

a. Type of System: Continuous steady state, no reaction

$\Rightarrow$ **Input = Output**

b. Basis of calculation

No need for Basis because flow rate of water stream is specified

c. Unknowns: 5 $(\dot{n}_1 , \dot{n}_2 , \dot{n}_3 , \dot{n}_4 , y)$

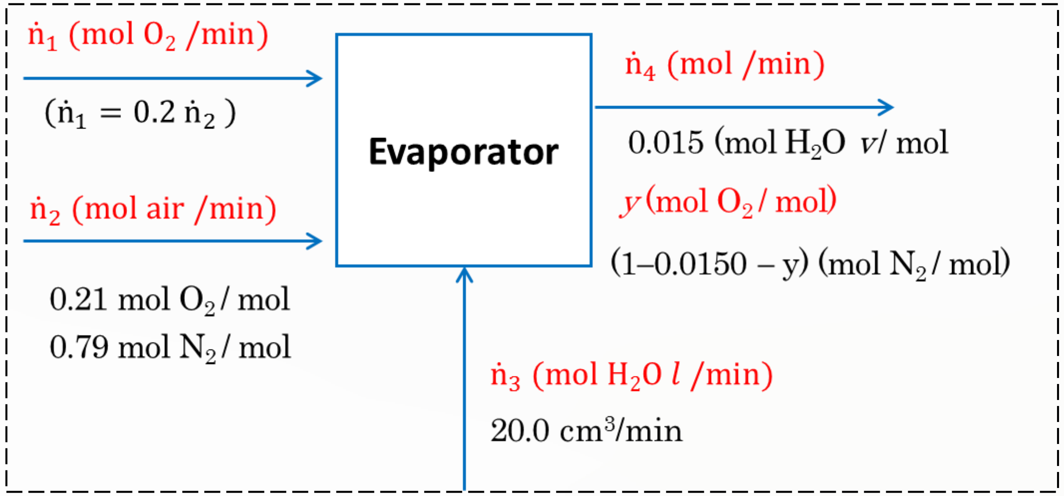
d. Number of components: 3 (O_2, N_2, H_2O)

$\Rightarrow$ We can write 3 material balance equations

e. Extra information: 2

Density relationship (for water stream)

Given specification in stream 1 $(\dot{n}_1 = 0.2\,\dot{n}_2)$



$\dot{n}_1$ (mol O_2 /min)

($\dot{n}_1 = 0.2\,\dot{n}_2$)

Evaporator

$\dot{n}_4$ (mol /min)

0.015 (mol H_2O *v*/ mol

y (mol O_2/ mol)

(1–0.0150 – y) (mol N_2/ mol)

$\dot{n}_2$ (mol air /min)

0.21 mol O_2/ mol

0.79 mol N_2/ mol

$\dot{n}_3$ (mol H_2O *l* /min)

20.0 cm³/min

2. Do degree of freedom analysis [PI1a]

$$\boxed{n_{df} = (n_{unknowns} - n_{indpendent\ eqns})}$$

Can be also called DOF

unknowns 5 ($\dot{n}_1, \dot{n}_2, \dot{n}_3, \dot{n}_4, y$)

Indep. equations -5
- 3 mass balance eqns
- 1 density eqns
- 1 given spec eqn

DOF = 5 – 5 = 0 ⇒ The problem is solvable

3. Formulate the necessary equations [PI1b]

 # unknowns: 5

Mass balance

3 components → 3 mass balances

Total balance $\dot{n}_1 + \dot{n}_2 + \dot{n}_3 = \dot{n}_4$ ❶

O_2 balance $\dot{n}_1 + 0.21\,\dot{n}_2 = y \cdot \dot{n}_4$ ❷

N_2 balance $0.79\,\dot{n}_2 = (0.985 - y) \cdot \dot{n}_4$ ❸

Independent equations

H_2O balance $\dot{n}_3 = 0.015\,\dot{n}_4$ dependent eqn (can't be used)

Additional equations

Density relationship $\dot{n}_3 = 20\left(\frac{cm^3}{min}\right) \times \frac{\rho_w\ (kg/cm^3)}{M_w\ (kg/kmol)}$ ❹ dep eqn

Given spec $\dot{n}_1 = 0.2\,\dot{n}_2$ ❺ dep eqn

4. Solve for unknowns [PI1c]

$\dot{n}_1 = 12.16$	$\dot{n}_2 = 60.80$	$\dot{n}_3 = 1.11$	$\dot{n}_2 = 74.07$	$y = 0.337$
mol/min	mol/min	mol/min	mol/min	kg/kg or [-]

Exercise on material balance calculations

Exercise 4.3-3 Balances on a mixing Unit

SO1	Performance Indicators	
		PI1a. Identify and define complex engineering problems.
		PI1b. Model and formulate complex engineering problems by applying principles of engineering, science, and mathematics.
		PI1c. Solve complex engineering problems by applying principles of engineering, science, and mathematics.

An aqueous solution of sodium hydroxide contains 20.0% NaOH by mass. It is desired to produce an 8.0% NaOH solution by diluting a stream of the 20% solution with a stream of pure water.

1. Identify an appropriate basis for the calculation of the dilution process. Explain why you selected this basis. [**PI1a**]
2. Define the dilution process by drawing a fully labeled flowchart. Determine the given key variables (mass, fraction, volume, etc.) and specify the required unknown variables. [**PI1a**]
3. Formulate the necessary equations for the dilution process by applying mass balance principles to solve for the unknowns. [**PI1b**]
4. Solve the formulated equations to calculate the mass and volume of water required for dilution and the mass of the product. Show all steps, including any necessary unit conversions. [**PI1c**]"
5. Calculate the following ratios [**PI1c**]:
   - liters H_2O / kg feed solution
   - kg product solution / kg feed solution

Solution

1. **Identify an appropriate basis for the calculation of the dilution process.** Explain why you selected this basis. [PI1a] this step can be also done after drawing the flowchart

The problem does not specify amounts for the input or output streams, so an appropriate basis must be chosen.

This can be either the amount or flow rate of any input or output stream.

Choose a basis of calculation

Amount or mass flow rate of one of the feed or output streams

a) **100 kg of the 20% feed solution**, or

b) a flow rate of 100 $\frac{lb_m}{min}$ of the 8% solution, or

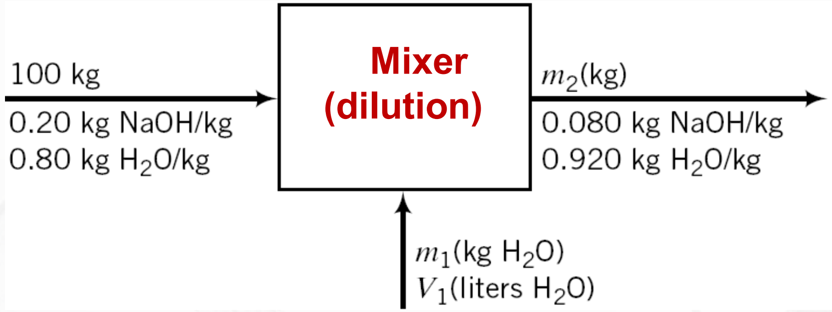
c) 10 tons of diluent water

Why the basis (a)? straightforward and is matching the units of given input variables. A mass flow rate in kg/h will be also appropriate

Process description

It is desired to produce a 8.0 wt% NaOH aqueous solution by diluting an input stream of concentrated 20 wt% NaOH solution with a stream of pure water.

2. **Define the dilution process by drawing a fully labeled flowchart.** Determine the given key variables (mass, fraction, volume, etc.) and specify the required unknown variables. [PI1a]



Given information:

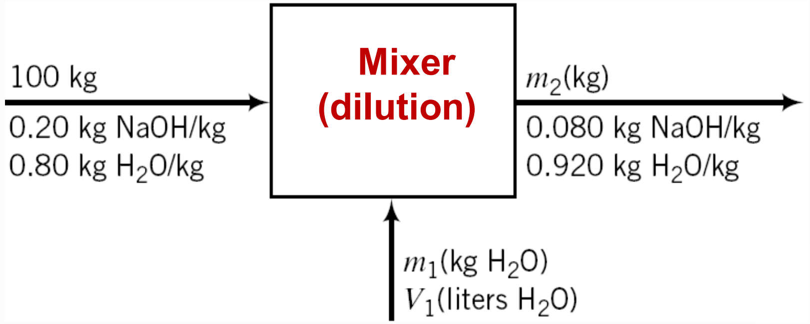
- Composition (or mass fraction) of input concentrated solution
- Composition (or mass fraction) of output diluted solution

Unknown variables

- m_1: mass of diluting water
- V_1: volume of diluting water
- m_2: mass of output diluted solution

Solution

3. Formulate the necessary equations for the dilution process by applying mass balance principles to solve for the unknowns. [PI1b]



Unknown variables = 3 m_1, m_2 and V_1

We need 3 equations to solve the 3 unknowns

Equations:

The system contains 2 species (NaOH, and H_2O) → we can write **2 mass balance equations.** The 3rd equation comes from the mass and density relationship

1) Total mass balance:

Batch non-reactive system

$$input = output$$

$$\boxed{100 + m_1 = m_2 \quad \text{... (1)}}$$

2) Component mass balance (NaOH)

$$input = output$$

$$\left(0.20\frac{kg\ NaOH}{kg}\right)(100\ kg) = \left(0.080\frac{kg\ NaOH}{kg}\right)m_2$$

$$\boxed{20 = 0.08\, m_2 \quad \text{... (2)}}$$

3) Diluent water volume:

(Density relation)

$$\boxed{V_1 = \frac{m_1}{\rho_w} = \frac{m_1\ kg}{1\ kg/L} \quad \text{... (3)}}$$

4. Solve the formulated equations to calculate the mass and volume of water required for dilution and the mass of the product. Show all steps, including any necessary unit conversions. [PI1c]

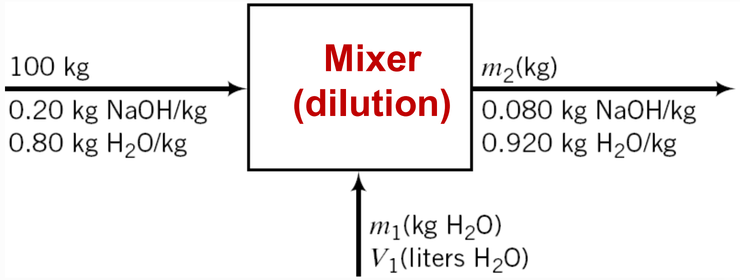
Solve the equations formulated in part (3)

Equation (2) $20 = 0.08\, m_2$ Solving → $\boldsymbol{m_2 = 250\ kg\ solution}$

Equation (1) $100 + m_1 = m_2$ Solving using m_2 → $\boldsymbol{m_1 = 150\ kg\ H_2O}$

Equation (3) $V_1 = \frac{m_1\ kg}{1\ kg/L}$ Solving using m_1 → $\boldsymbol{V_1 = 150\ L\ H_2O}$

Solution



$\boldsymbol{m_1 = 150\ kg\ H_2O}$

$\boldsymbol{V_1 = 150\ L\ H_2O}$

$\boldsymbol{m_2 = 250\ kg\ solution}$

5. Calculate the following ratios:

a) liters H_2O / kg feed solution
b) kg product solution / kg feed solution

a) liters H_2O / kg feed solution

$$Ratio_1 = \frac{V_1}{m_1} = \frac{150\ L}{100\ kg}$$

$$= 1.50\,\frac{L\ H_2O}{kg\ feed\ solution}$$

b) kg product solution / kg feed solution

$$Ratio_2 = \frac{m_2}{m_1} = \frac{250\ kg}{100\ kg}$$

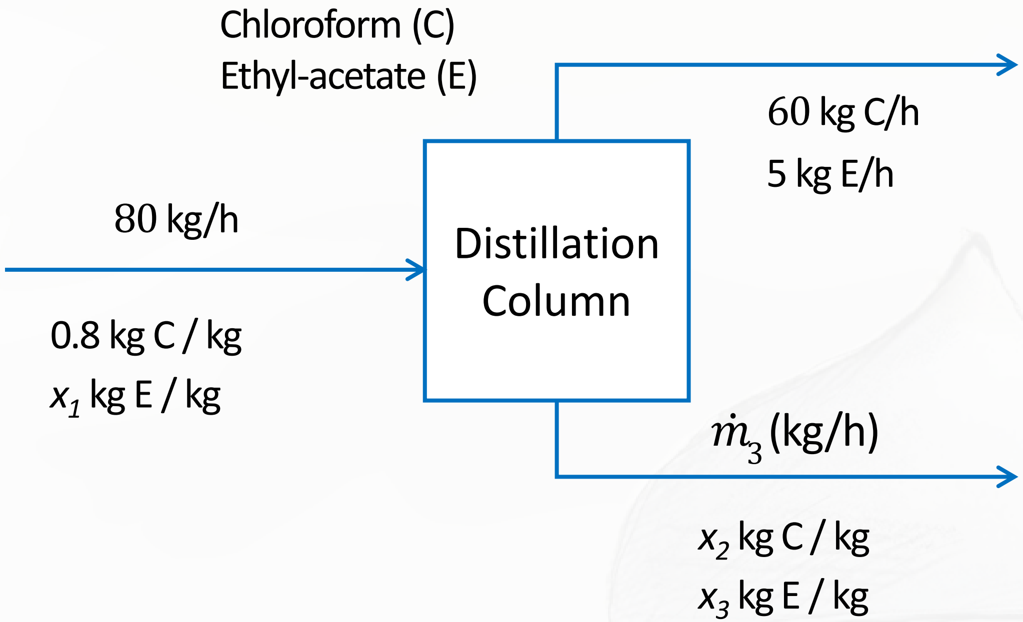
$$= 2.50\,\frac{kg\ product\ solution}{kg\ feed\ solution}$$

Problem 1: Flowchart Calculations

1. Use the flowchart to calculate required unknowns.
2. Calculate the values in the boxes for each stream

(1) calculate

$\dot{m}_C$
$\dot{m}_E$
$\dot{n}_C$
$\dot{n}_E$
y_C
y_E
$\bar{M}$



Chloroform (C)
Ethyl-acetate (E)

80 kg/h

0.8 kg C / kg
x_1 kg E / kg

Distillation Column

60 kg C/h
5 kg E/h

$\dot{m}_3$ (kg/h)

x_2 kg C / kg
x_3 kg E / kg

(2) calculate

$\dot{m}_{tot}$ (kg/h)
x_4
x_5
$\dot{n}_C$
$\dot{n}_E$
y_C
y_E
$\bar{M}$

(3) calculate

$\dot{m}_3$ (kg/h)
$\dot{m}_C$
$\dot{m}_E$
$\dot{n}_C$
$\dot{n}_E$
y_C
y_E
$\bar{M}$

Solution

Problem 2 – Flowchart Calculations

1. Use the flowchart to calculate the unknowns.
2. Calculate required properties in the boxes corresponding to each stream

(2) calculate

$\dot{m}_2$

x_W

x_I

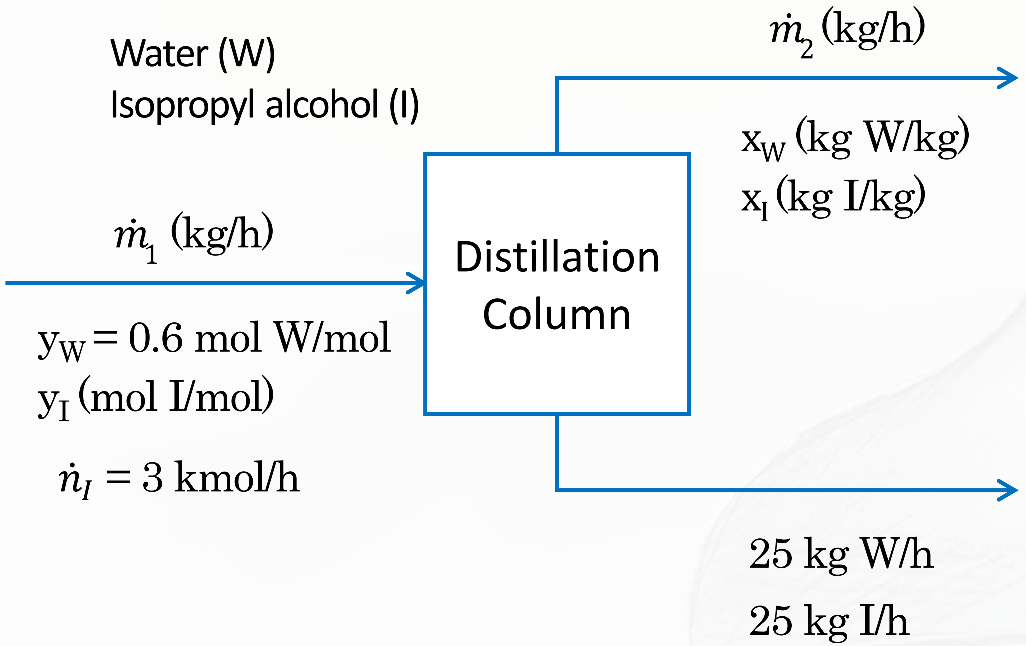
$\dot{n}_W$

$\dot{n}_I$

y_W

y_I

$\bar{M}$



Water (W)
Isopropyl alcohol (I)

$\dot{m}_1$ (kg/h)

$y_W = 0.6$ mol W/mol
y_I (mol I/mol)

$\dot{n}_I = 3$ kmol/h

Distillation Column

$\dot{m}_2$ (kg/h)

x_W (kg W/kg)
x_I (kg I/kg)

25 kg W/h
25 kg I/h

(1) calculate

$\dot{m}_1$ (kg/h)

x_W

x_I

$\dot{m}_W$

$\dot{m}_I$

$\dot{n}_W$

y_I

$\bar{M}$

(3) calculate

$\dot{m}_3$ (kg/h)

x_W

x_I

$\dot{n}_W$

$\dot{n}_I$

y_W

y_I

$\bar{M}$

Solution

Problem 3 – Flowchart and Material Balance on a Single Unit

The mixture of acetone (x_A=50%) and benzene (x_B=50%) enters a distillation column at 1 kg/s. The column separates the feed into two mixtures; one on the top (called light key) and the other at the bottom (called heavy key). The upper product is a mixture containing 80 mass % of more volatile component (it is the light component or the one with lower boiling point) which leaves at a mass flow rate of 0.6 kg/s. The column operates at steady state. Both products leave as a liquid phase.

a) Decide which component among Acetone (A) and Benzene (B) is more volatile (lighter) by comparing the boiling points found in Table B.1. The light component moves up in the top product, while the heavy stays in the bottom product.

b) Draw a completely labeled flowchart of this process.

c) Determine degree of freedom and analyze the situation.

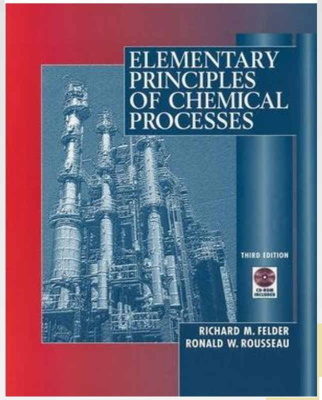
d) Determine the composition of the mixture on the top of the column

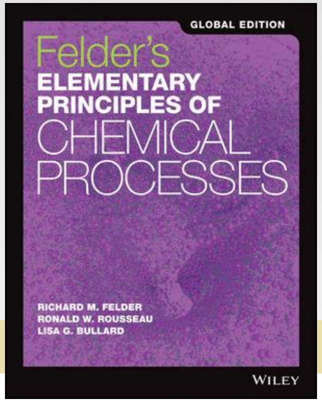
e) Determine the flow rates of each component in the mixture on top of the column

f) Determine the composition of the mixture on the bottom of the column

g) Determine the flow rates of each component in the mixture on the bottom of the column

Solution





Elementary Principles of Chemical Processes,
3rd or 4th edition,
Wiley & Sons, Inc.
Richard M. Felder, Ronald W. Rousseau, & Lisa G. Bullard.

Student Sample Slides

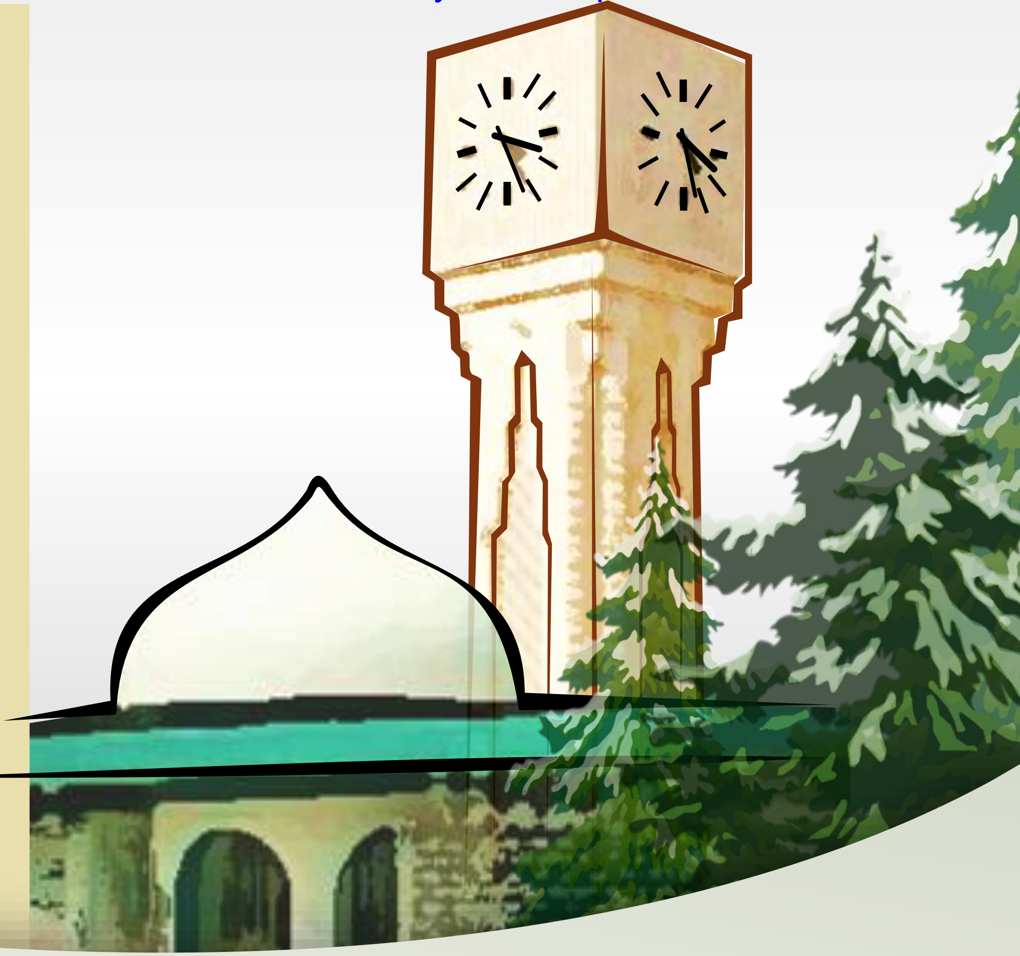
This only a sample of material. Refer to textbook for study of the topics

CHE 0905211

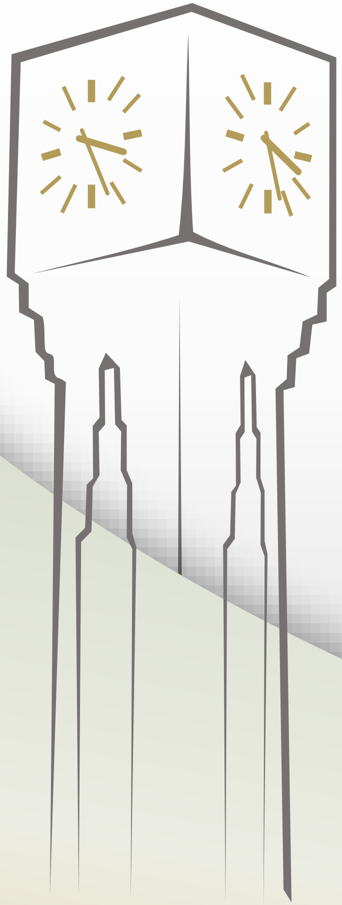
Chemical Engineering Principles 1

Fall 2025

Dr. Hatem Alsyouri	Chapter 4



The University of Jordan
Chemical Engineering Department



4.4 Balances on Multiple-Unit Processes

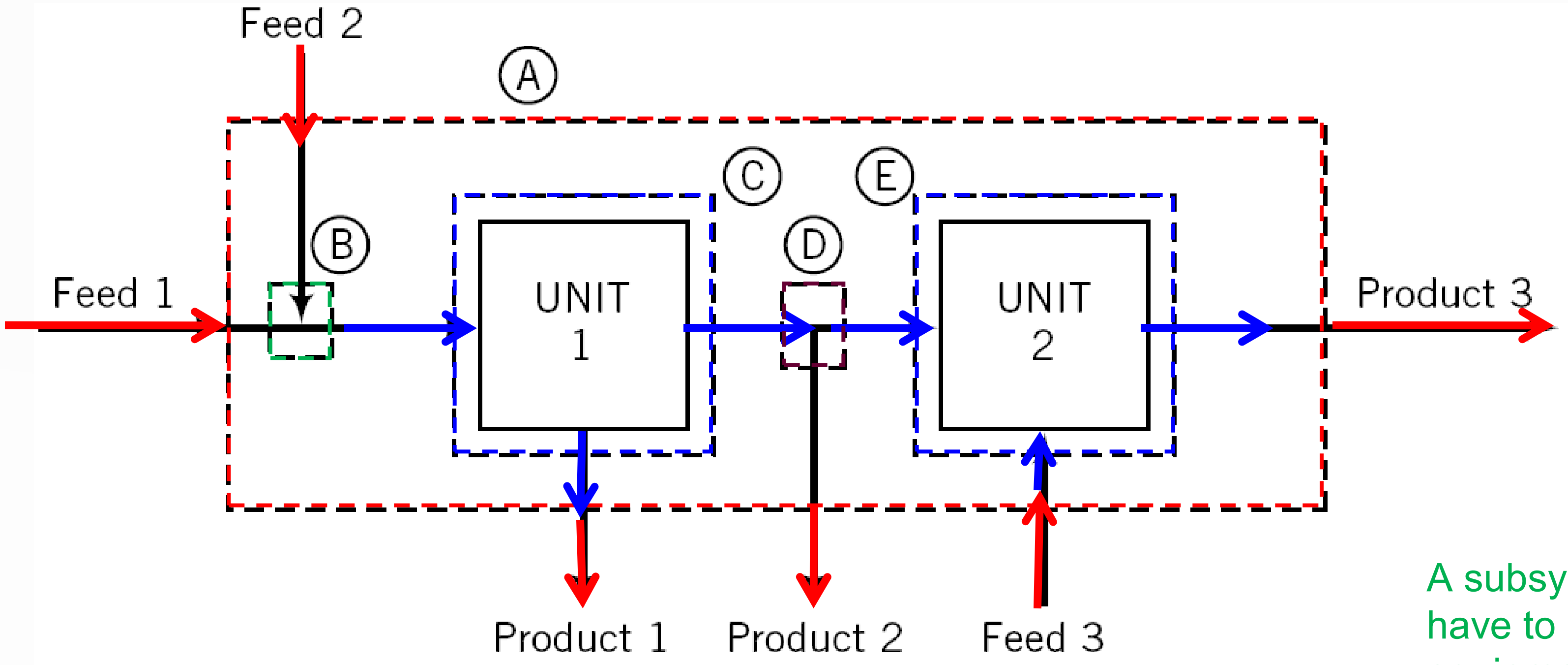
This section

4.4 Balances on Multiple-Unit Processes

- **Industrial process rarely involve only one process**
  - Chemical reactors are often present
  - Unit for mixing reactant
  - Blending products
  - Heating and cooling streams
  - Unit for product separation and hazards disposal

We need multiple-unit process

- **System:** is any portion of a process that can be enclosed within a boundary
- The inputs and outputs to a system are the process streams that intersect the system boundary



A subsystem doesn't have to be a piece of equipment; it might be a mixing point (pipe junction) or splitter

The system can be:

- The entire process: (Boundary A)
- Single process : (Boundary C, Boundary E)
- Point where two or more process streams combine: (Boundary B)
- One steam splits into branches : (Boundary D)
- Combination of process

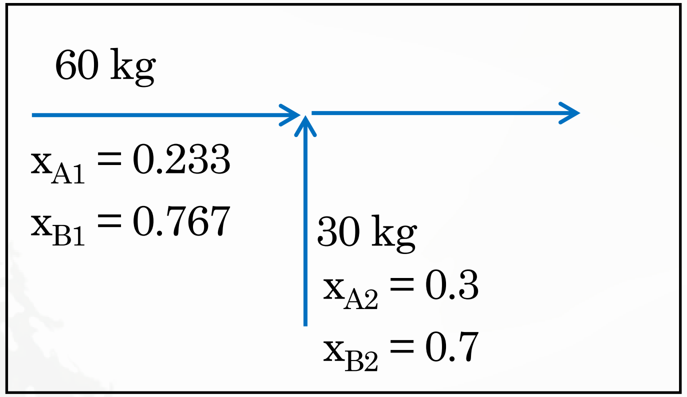
You can write material, component, and atom balances:

- Around the entire system, or
- Around any subsystem of the plant.

Mixing point and Split point

Mixing point

Two (or more) streams are combined into one stream. It's a mixing unit



60 kg

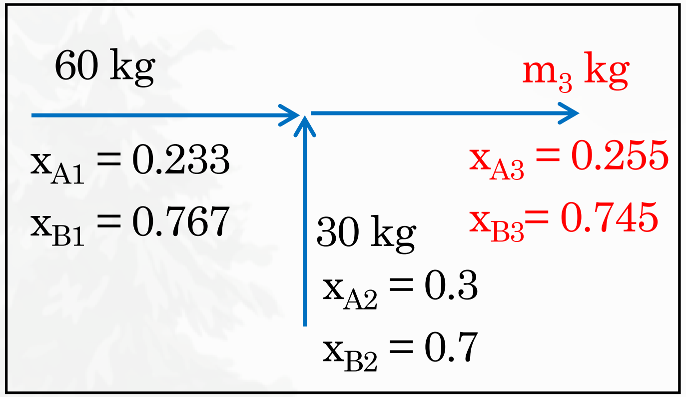
$x_{A1} = 0.233$

$x_{B1} = 0.767$

30 kg

$x_{A2} = 0.3$

$x_{B2} = 0.7$



60 kg

$x_{A1} = 0.233$

$x_{B1} = 0.767$

30 kg

$x_{A2} = 0.3$

$x_{B2} = 0.7$

m_3 kg

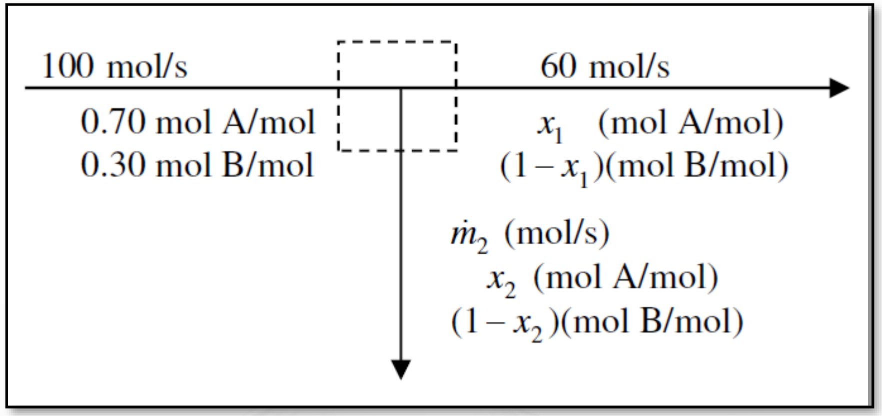
$x_{A3} = 0.255$

$x_{B3} = 0.745$

Split point

a stream is split into two streams.

It's not a separation unit



100 mol/s

0.70 mol A/mol

0.30 mol B/mol

60 mol/s

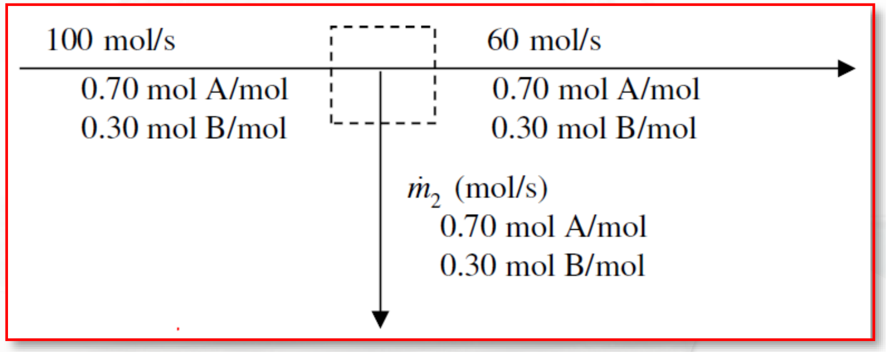
x_1 (mol A/mol)

$(1 - x_1)$(mol B/mol)

$\dot{m}_2$ (mol/s)

x_2 (mol A/mol)

$(1 - x_2)$(mol B/mol)



100 mol/s

0.70 mol A/mol

0.30 mol B/mol

60 mol/s

0.70 mol A/mol

0.30 mol B/mol

$\dot{m}_2$ (mol/s)

0.70 mol A/mol

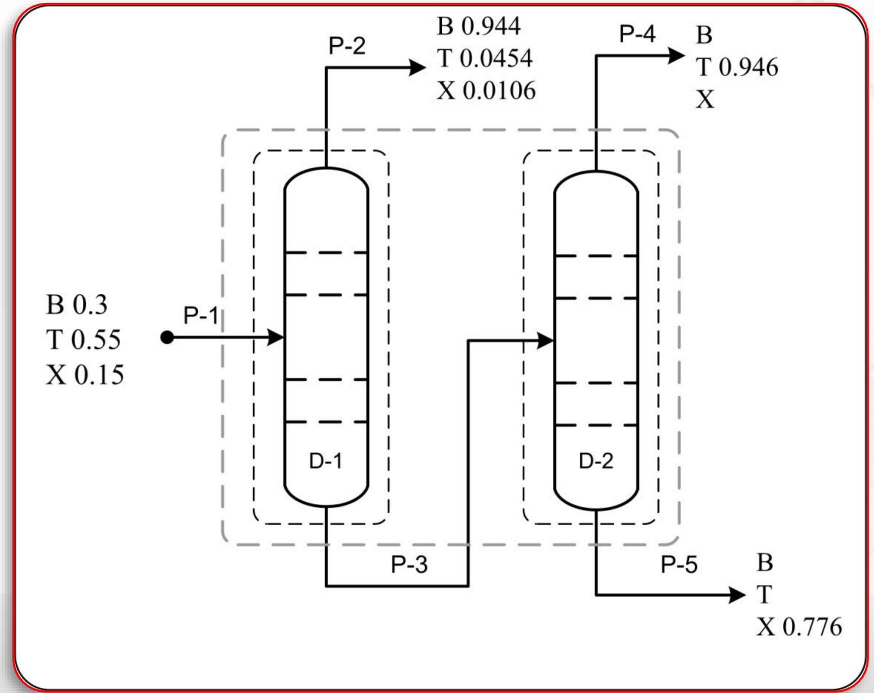
0.30 mol B/mol

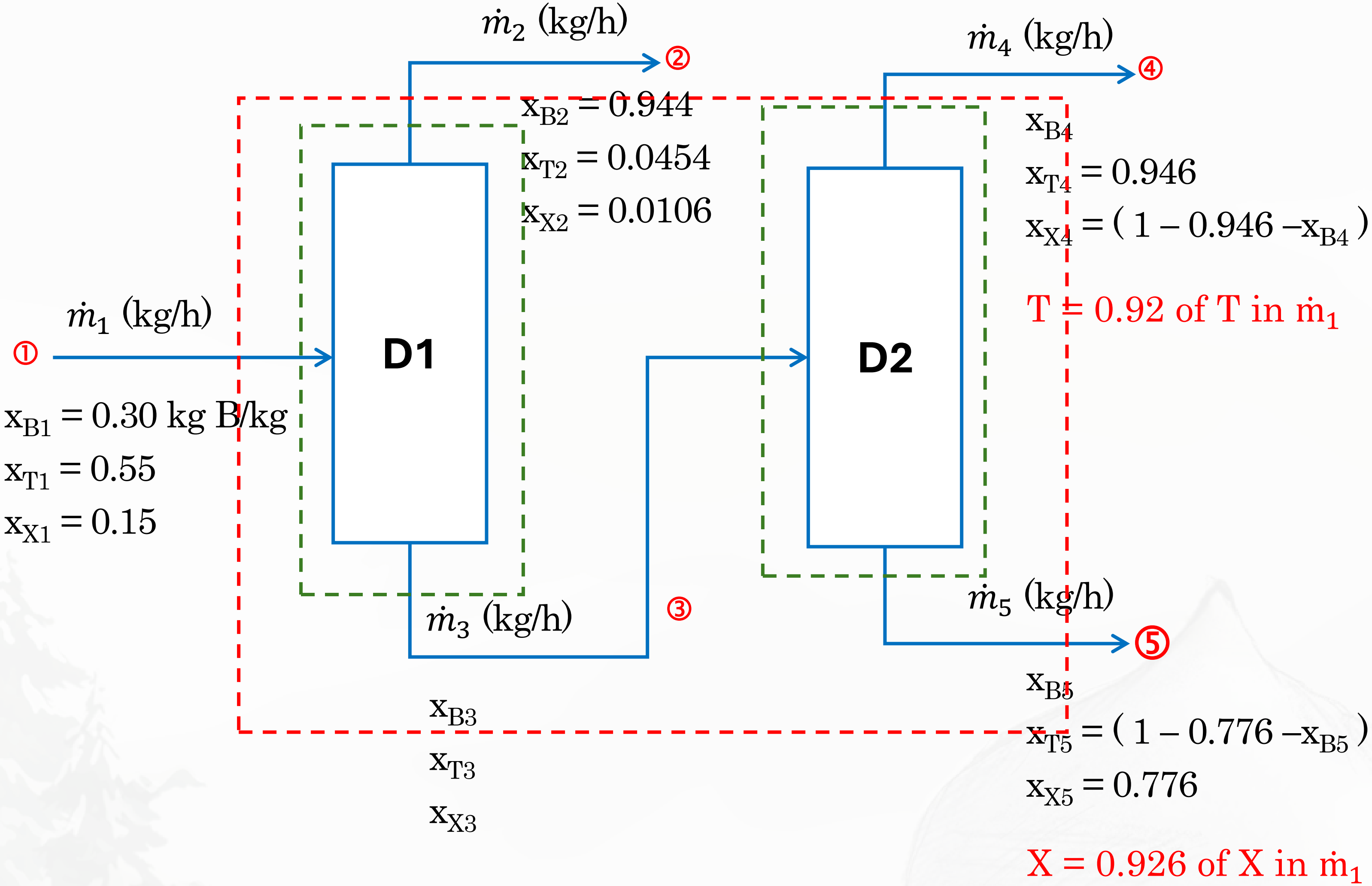
Example 1

Two columns in sequence are used to separate the components of a feed consisting of 30% benzene (B), 55% toluene (T), and 15% xylene (X) by mass. The analysis of the overhead stream from the first column is: 94.4%B, 4.54%T, 1.06%X by mass.

The second column is designed to recover 92% of the toluene in the **original feed** in the overhead stream at a composition of 0.946. The bottom stream is intended to contain 92.6% of xylene **of the original feed** at a composition of 0.776.

Compute the composition of all stream.





① $\dot{m}_1$ (kg/h)

$x_{B1} = 0.30$ kg B/kg

$x_{T1} = 0.55$

$x_{X1} = 0.15$

D1

② $\dot{m}_2$ (kg/h)

$x_{B2} = 0.944$

$x_{T2} = 0.0454$

$x_{X2} = 0.0106$

③ $\dot{m}_3$ (kg/h)

x_{B3}

x_{T3}

x_{X3}

D2

④ $\dot{m}_4$ (kg/h)

x_{B4}

$x_{T4} = 0.946$

$x_{X4} = (1 - 0.946 - x_{B4})$

T = 0.92 of T in $\dot{m}_1$

⑤ $\dot{m}_5$ (kg/h)

x_{B5}

$x_{T5} = (1 - 0.776 - x_{B5})$

$x_{X5} = 0.776$

X = 0.926 of X in $\dot{m}_1$

System	**Unknowns** (a)	**# species** (b)	**other specs** (c)	**DOF** (a-b-c)
Overall	6	3	2	1
D1	5	3	0	2
D2	7	3	0	4

The system can't be solved with the current information.

If we assume a basis, e.g., for m1, it can be solved.

Assume a basis

$\dot{m}_1$ = 100 kg/h

For each system, you count the unknowns in the input and output streams which cross the border of the system

Overall system

- Inputs: stream1, Outputs: streams 2, 4, 5
- Unknowns: stream 1 (m1), stream 2 (m2), stream 4 (m4, xB4), stream 5 (m5, xB5)
- Number of unknowns: 6

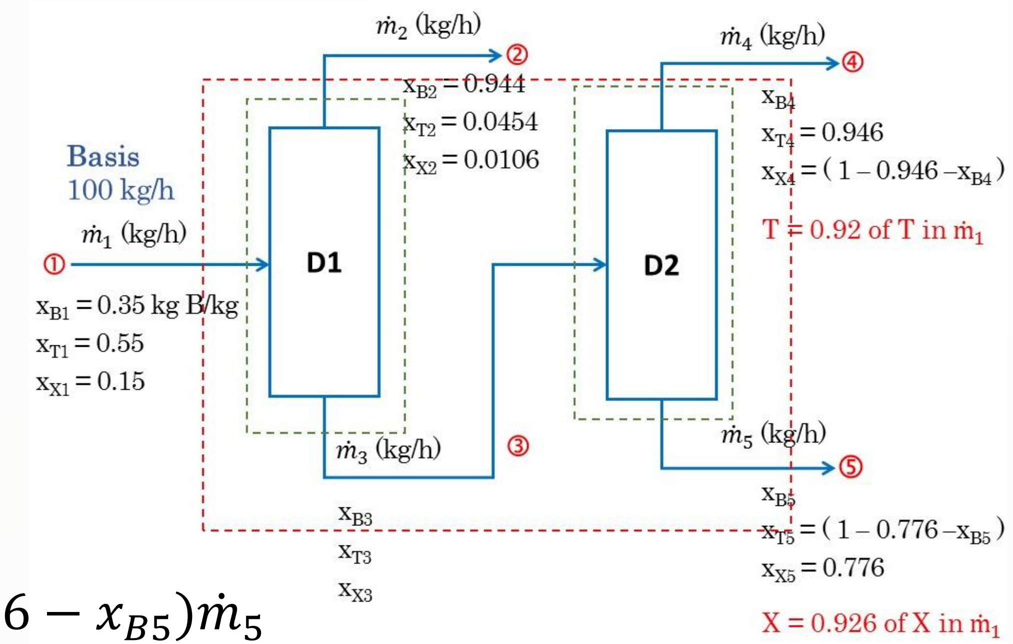
System Distillation 1

- Inputs: stream1, Outputs: streams 2, 3
- Unknowns: stream 1 (m1), stream 2 (m2), stream 3 (m3, xB3, xT3).
- ***Note 1****: xX3 is not counted because it is defined as (*1- xB3 - xT3)
- Number of unknowns: 5

System Distillation 2

- Inputs: stream3, Outputs: streams 4, 5
- Unknowns: stream 3 (m3, xB3, xT3), *see Note 1*, stream 4 (m4, xB4), stream 5 (m5, xB5)
- Number of unknowns: 7

Basis $\dot{m}_1$ **= 100 kg/h**



System: overall

Total mass balance:

$$100 = \dot{m}_2 + \dot{m}_4 + \dot{m}_5$$

Component mass balance:

$$B: (0.30)(100) = (0.944)\dot{m}_2 + x_{B4}\dot{m}_4 + x_{B5}\dot{m}_5$$
$$T: (0.55)(100) = (0.0454)\dot{m}_2 + (0.946)\dot{m}_4 + (1 - 0.776 - x_{B5})\dot{m}_5$$
$$X: (0.15)(100) = (0.0106)\dot{m}_2 + (1 - 0.946 - x_{B4})\dot{m}_4 + (0.776)\dot{m}_5$$

extra

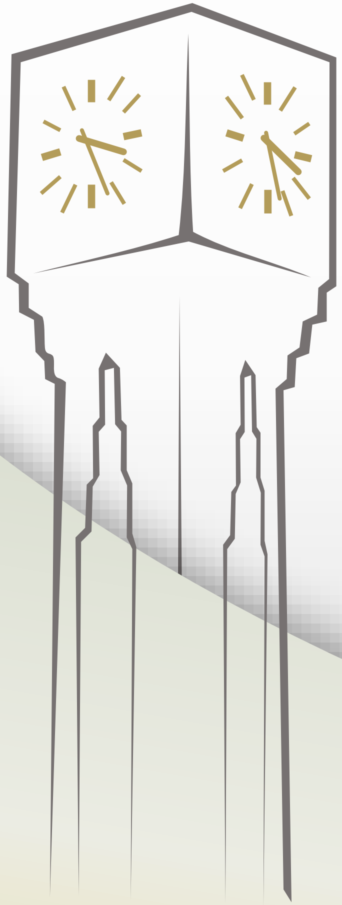
Other Equations:

$$(0.92)(0.55)(100) = (0.946)\dot{m}_4 \rightarrow \dot{m}_4 = 53.488 \text{ kg/h}$$
$$(0.926)(0.15)(100) = (0.776)\dot{m}_5 \rightarrow \dot{m}_5 = 17.90 \text{ kg/h}$$

Answer:

$$\dot{m}_2 = 28.612 \text{ kg/h}$$
$$x_{B5} = 0.0507$$
$$x_{B4} = 0.0389$$

Since $\dot{m}_1$ was assumed and $\dot{m}_2$ is calculated, DOF of Unit 1 turns to zero and $\dot{m}_3, x_{B3}, x_{T3}, and\ x_{X3}$ can be found.



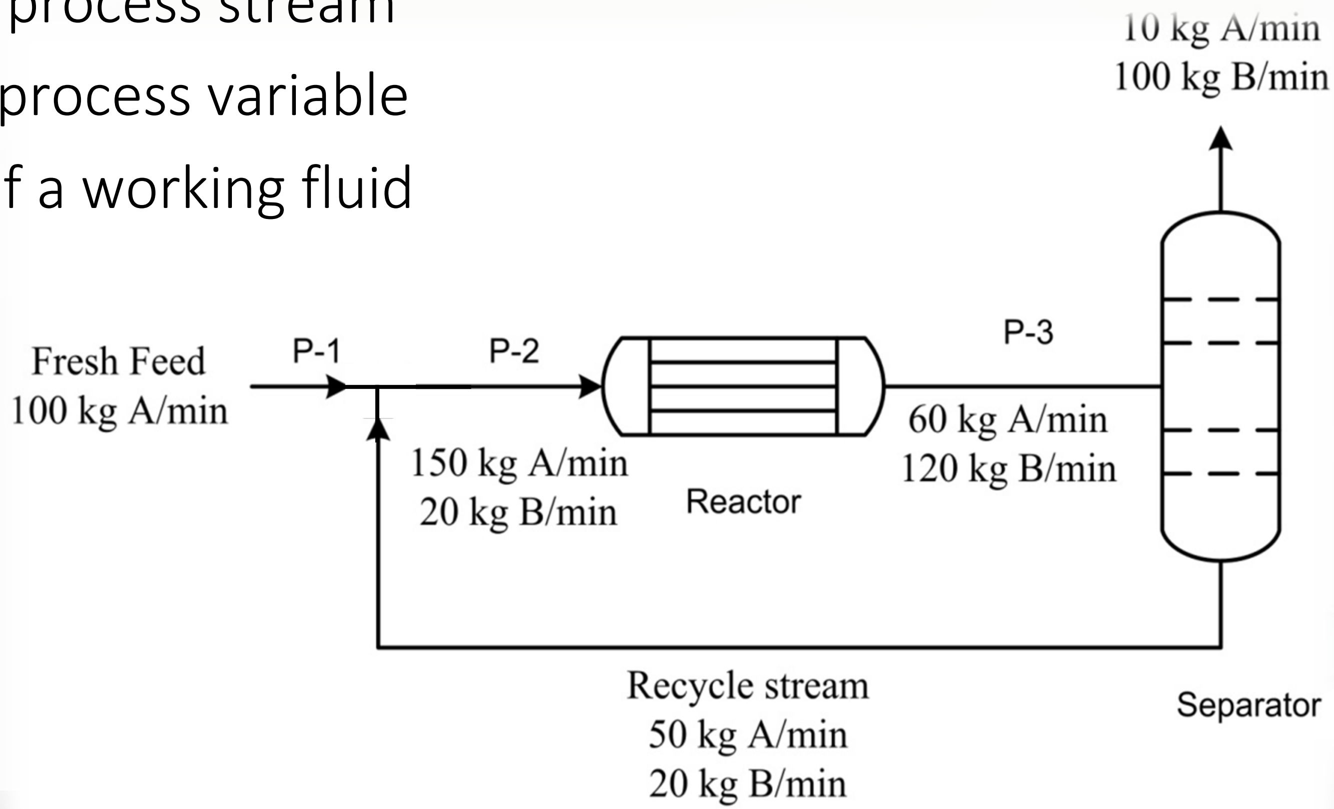
4.5 Recycle and Bypass

This section

Recycle: is a common practice of chemical process.

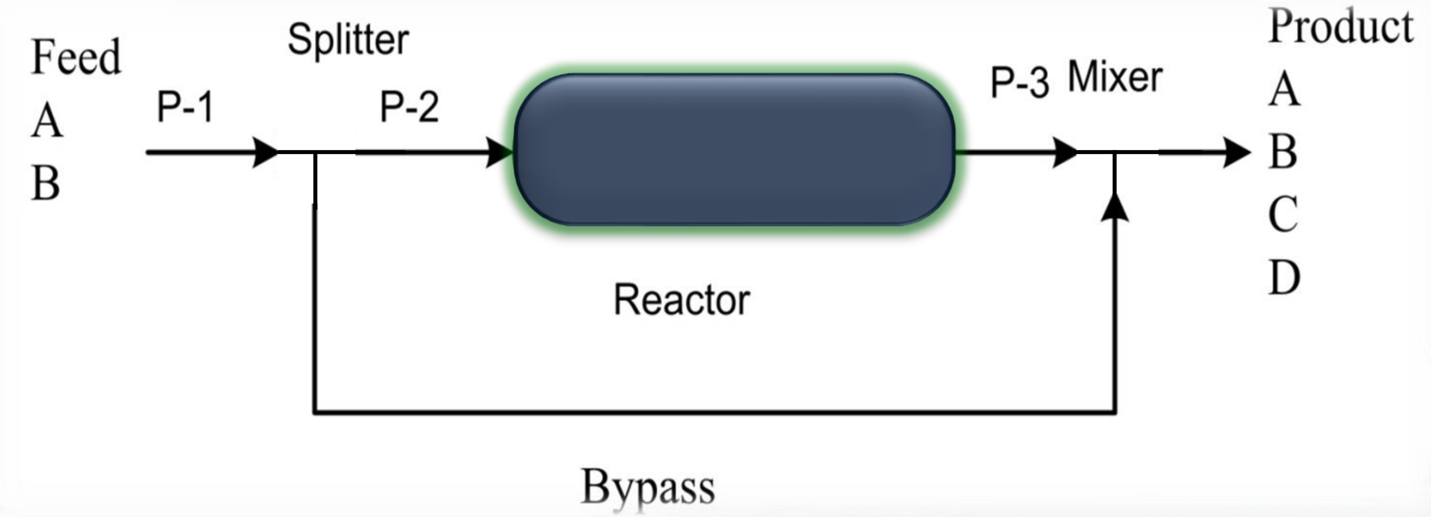
The reasons for using the recycle are:

1. Recovering and reusing unconsumed reactants
2. Recovery of catalyst
3. Dilution of a process stream
4. Control of a process variable
5. Circulation of a working fluid



Bypass

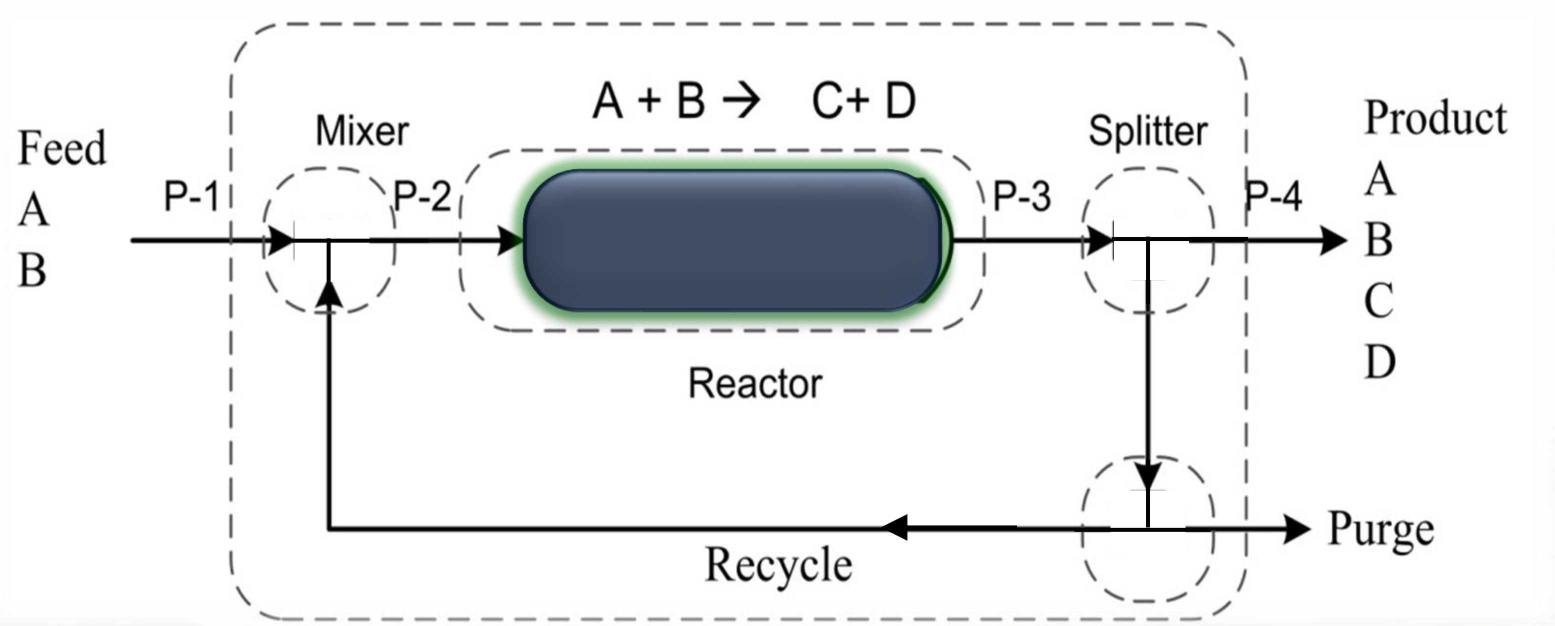
- Bypass: is a fraction of the feed to a process unit that is diverted around the unit and combined with the output stream. This allows to vary the composition and properties of the product stream.



Bypassing introduces a **splitting point** and a **mixing point**.

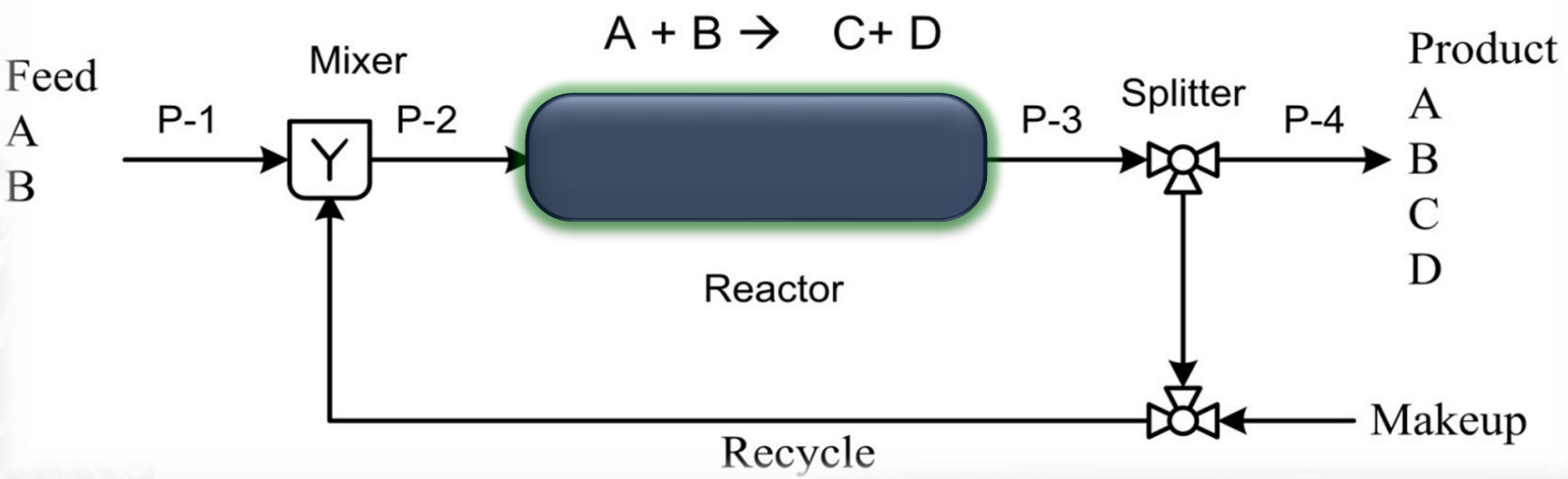
Purge

- A purge stream is a small stream bled off form a recycle loop to prevent building of inerts or impurities in the system
- It can be neglected because of the size



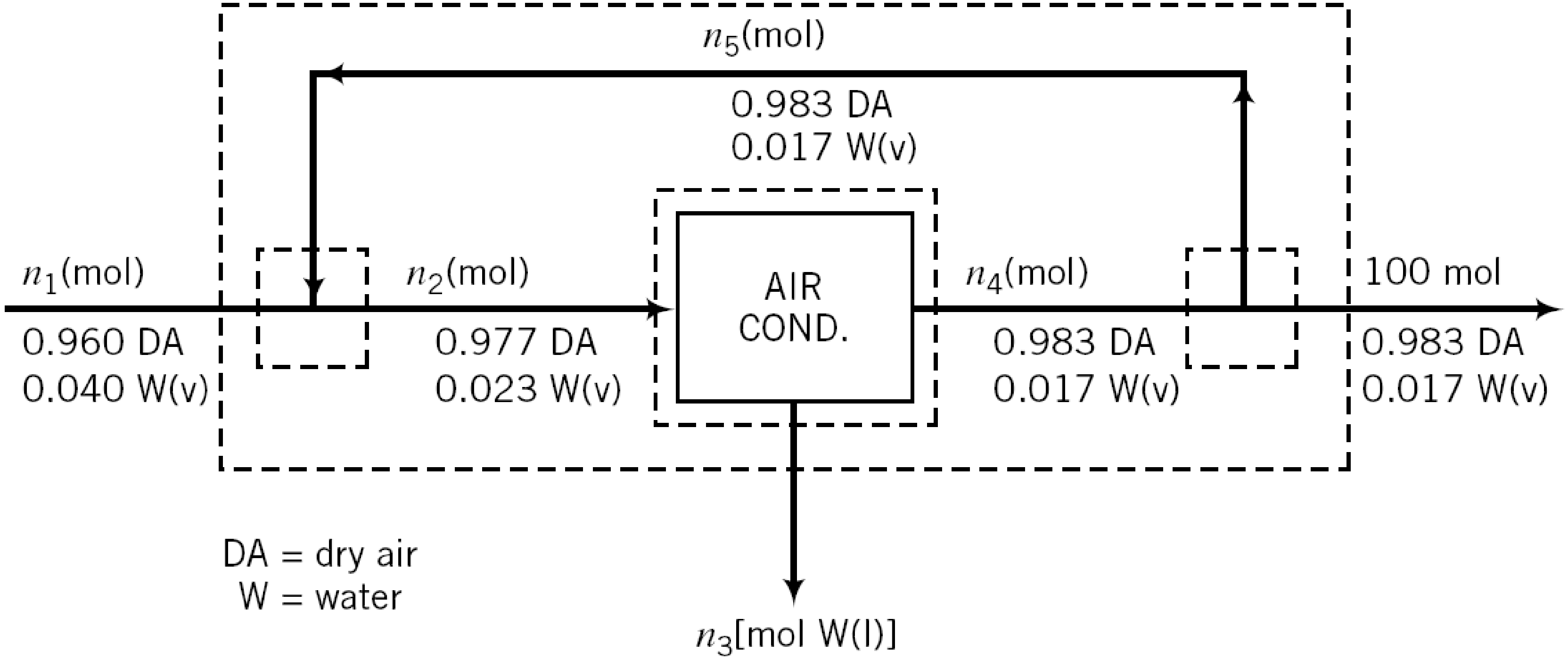
Make up

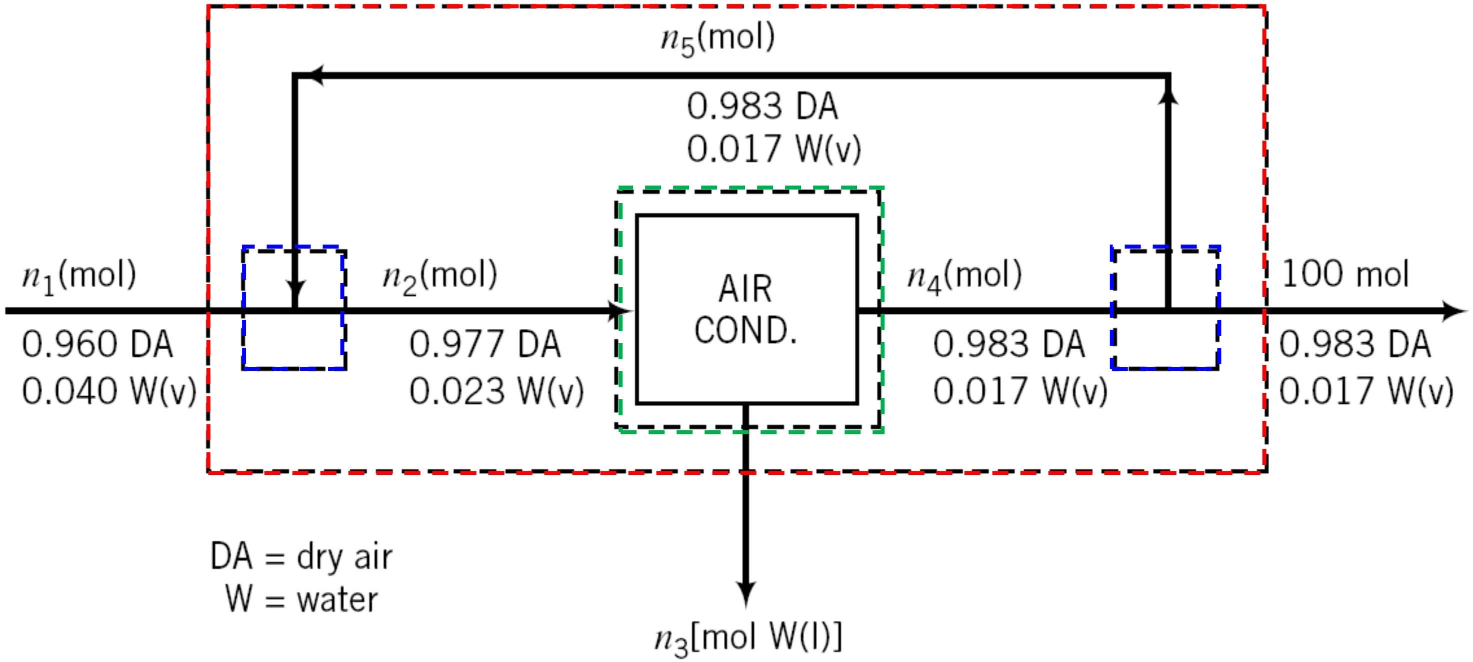
- A make up stream is required to replace losses to leaks, carryover, etc. within the recycle loop



Example 4.5-1 Material and Energy Balances on an Air Conditioner

Fresh air containing 4.00 mole% water vapor is to be cooled and dehumidified to a water content of 1.70 mole% H_2O. A stream of fresh air is combined with a recycle stream of previously dehumidified air and passes trough the cooler. The blended stream entering the unit contains 2.30 mole% H_2O. In the air conditioner, some of the water in the feed stream is condensed and removed as liquid. A fraction of the dehumidified air leaving the cooler is recycled and the remainder is delivered to a room. Taking 100 mol of dehumidified air delivered to the room as a basis of calculation, calculate the moles of fresh feed, moles of water condensed, and moles of dehumidified air recycled.





Degree-of-freedom analysis:

Overall System

2 variables (n_1, n_3) - 2 balance equations = 0 degrees of freedom

After solving for overall system

Mixing Point

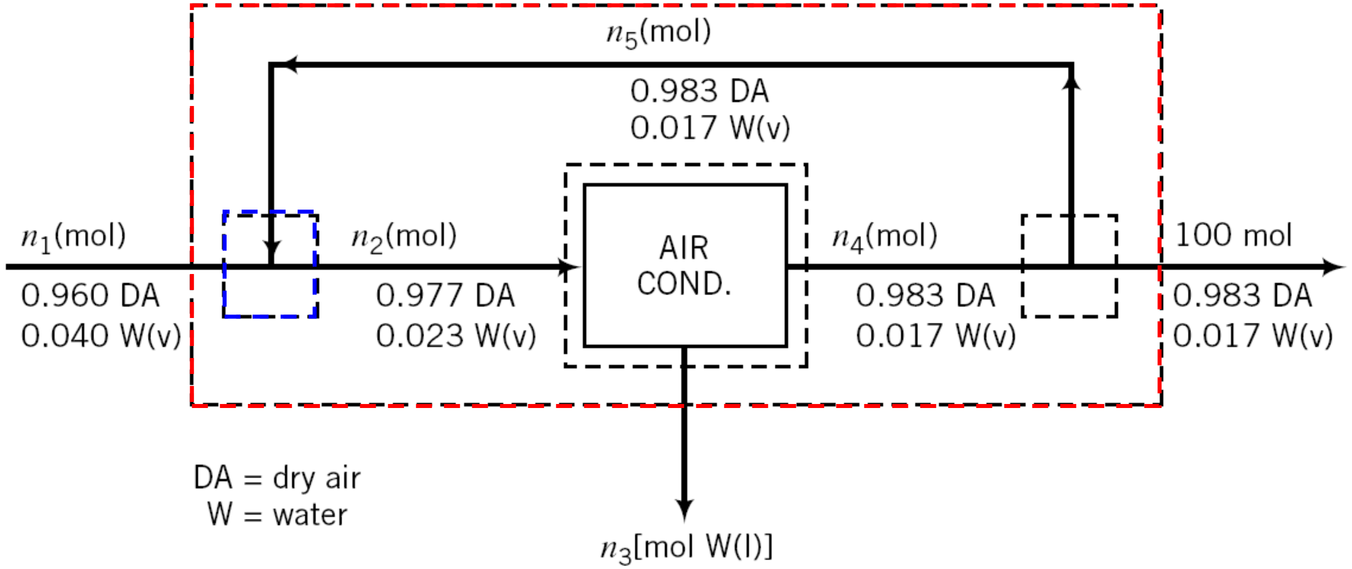
2 variables (n_2, n_5) - 2 balance equations = 0 degrees of freedom

Cooler

2 variables (n_2, n_4) - 2 balance equations = 0 degrees of freedom

Splitting Point

2 variables (n_4, n_5) - 1 balance = 1 degree of freedom



Overall dry air balance:

Input = Output

$$0.960n_1 = 0.983(100\ mol)$$

$n_1 = 102.4$ mol fresh feed

Overall mole balance:

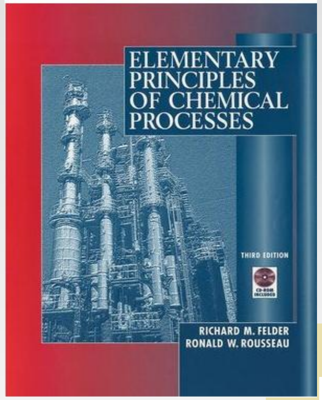
$$n_1 = n_3 + 100\ mol$$

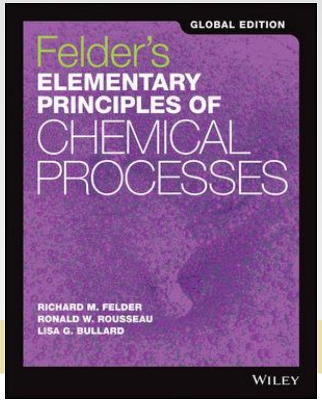
$n_3 = 2.4\ mol\ H_2O$ condensed

Mole balance on mixing point: $n_1 + n_5 = n_2$

Water balance on mixing point: $0.04n_1 + 0.017n_5 = 0.023n_2$

Solve simultaneously $n_2 = 392.5\ mol$ $n_5 = 290\ mol$ recycled





Elementary Principles of Chemical Processes,
3rd or 4th edition,
Wiley & Sons, Inc.
Richard M. Felder, Ronald W. Rousseau, & Lisa G. Bullard.

Student Sample Slides

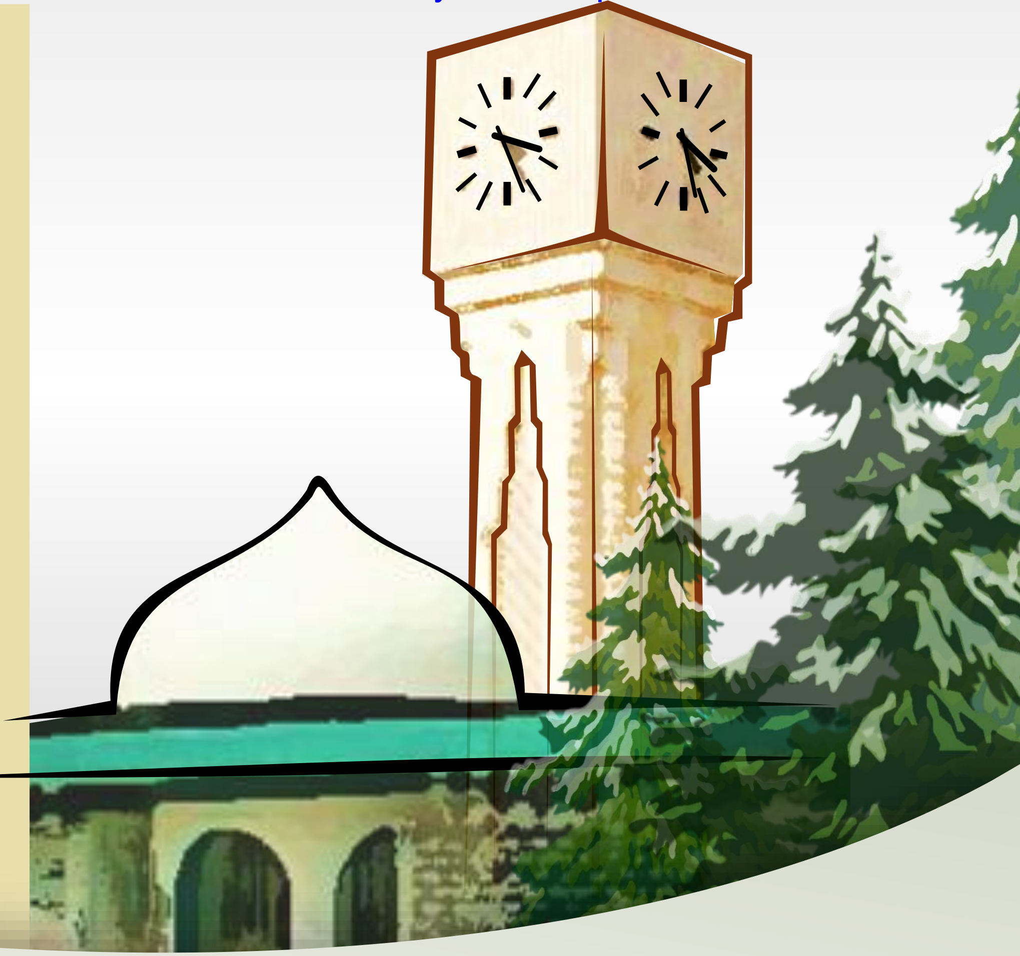
This only a sample of material. Refer to textbook for study of the topics

CHE 0905211

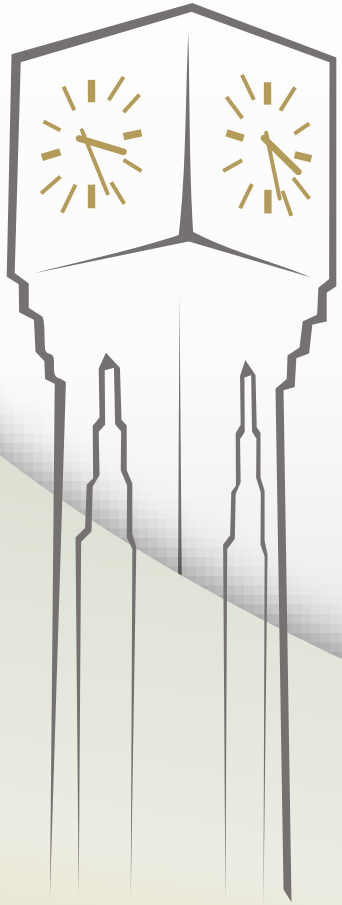
Chemical Engineering Principles 1

Fall 2025

Dr. Hatem Alsyouri	Chapter 4



The University of Jordan
Chemical Engineering Department



4.6 Chemical Reaction Stoichiometry

This section

4.6 Chemical Reaction Stoichiometry

4.6a Stoichiometry

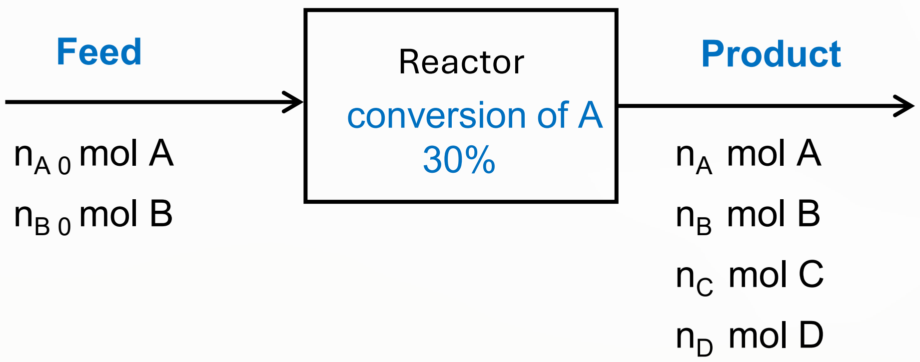
$$2\ SO_2 + 1\ O_2 \rightarrow 2\ SO_3$$

$$\frac{2\ mole\ SO_3\ generated}{1\ mole\ O_2\ consumed}$$

- Two reactants, A and B, are said to be present in ***stoichiometric proportion*** if the ratios (moles A present)/(moles B present) equals the stoichiometric ratio obtained from the balanced reaction equation.

Important terminology

$A + 2B \rightarrow C + 3D$



Feed

$n_{A\,0}$ mol A

$n_{B\,0}$ mol B

Reactor

conversion of A 30%

Product

n_A mol A

n_B mol B

n_C mol C

n_D mol D

		A	+	2 B	→	C	+	3 D	
1	Feed amount	n_{A0}		n_{B0}		n_{C0}		n_{D0}	*Notes*
2	Limiting/excess	Limiting		Excess					use 1
3	Stoichiometric amount	$n_{A\ stoic}$		$n_{B\ stoic}$					use 1 and rxn
4	%Excess	0		%Ex					use 1 and 3
5	Product amount	n_A		n_B		n_C		n_D	use extent
6	Conversion	f_A		f_B					use 1 and 5

$$Excess = \frac{n_{i0} - n_{i\ stoich}}{n_{i\ stoich}}$$

$$(n_i)_{out} = (n_i)_{in} \pm \nu_i \xi$$

$$n_i = n_{i0} \pm \nu_i \xi$$

$$f_i = 1 - \frac{n_i}{n_{i0}}$$

$$= \frac{amount\ reacted}{amount\ in\ feed} = \frac{n_{i0} - n_i}{n_{i0}}$$

4.6b Limiting and Excess reactants, Fractional Conversion, and Extent of reaction

- **Limiting reactant**

The reactant that would run out if a reaction proceeded to completion. (a reactant is limiting if it is present in less than its stoichiometric proportion relative to every other reactant).

- The other reactants are termed **excess reactants.**

- **Stoichiometric requirement of A** = $(n_A)_{stoich}$

the amount needed to react completely with the limiting reactant

- **Excess of the reactant** $(n_A)_{feed} - (n_A)_{stoich}$

is the amount of feed exceeding the stoichiometric requirement.

- **Fractional excess** of a reactant is the ratio of excess to the stoichiometric requirement;

$$\boxed{fractional\ excess\ of\ A = \frac{(n_A)_{feed} - (n_A)_{stoich}}{(n_A)_{stoich}}}$$

The Percentage excess of A is 100 times the fractional excess.

$n_{A0} = feed\ amount$

- **Fractional conversion (f)** of a reactant is the ratio:

$$\boxed{f = \frac{moles\ reacted}{moles\ fed} = \frac{n_{A0} - n_A}{n_{A0}} = 1 - \frac{n_A}{n_{A0}}}$$

Percentage unreacted is A is 100 times the fraction unreacted.

The Fraction Unreacted is accordingly 1- f

Extent of reaction (ξ: called Xi or Zai:)

Q: What is ξ?
A: It's a dummy variable that reflects how far each reaction proceeds. It reflects the stoichiometry of the reaction and helps us keep up with generation and consumption.

ξ
represents the amount converted from the limiting reactant

- Let ν_i be the stoichiometric coefficient of the ***i*** th species in a chemical reaction, making it negative for reactants and positive for products.

★
Important

$$\boxed{(n_i)_{out} = (n_i)_{in} \pm \nu_i \xi}$$

$\boldsymbol{\nu_i}$ is
Negative (-) for reactants and
Positive (+) for products.

Material Balance Equation

Input –output + gen –cons. = 0

output = Input + gen –cons.

$$(n_i)_{out} = (n_i)_{in} + \nu_i\xi \; - \nu_i\xi$$

$$\boldsymbol{(n_i)_{out} = (n_i)_{in} \pm \nu_i\xi}$$

Example: C_2H_2 + $2H_2$ → C_2H_6

Feed: 20 kmol 50 kmol 50 kmol

After some time 30.0 kmol H_2 has reacted.

$$\left.\begin{aligned} n_{H_2} &= (n_{H_2})_0 - 2 \times \xi \\ n_{C_2H_2} &= (n_{C_2H_2})_0 - 1 \times \xi \\ n_{C_2H_6} &= (n_{C_2H_6})_0 + 1 \times \xi \end{aligned}\right\}$$

ξ Is the same value for all components in the same reaction

Example 4.6-1 Reaction Stoichiometry

Train for midterm

Acrylonitrile is produced in the reaction of propylene, ammonia and oxygen:

$$C_3H_6 + NH_3 + 3/2\ O_2 \rightarrow C_3H_3N + 3\ H_2O$$

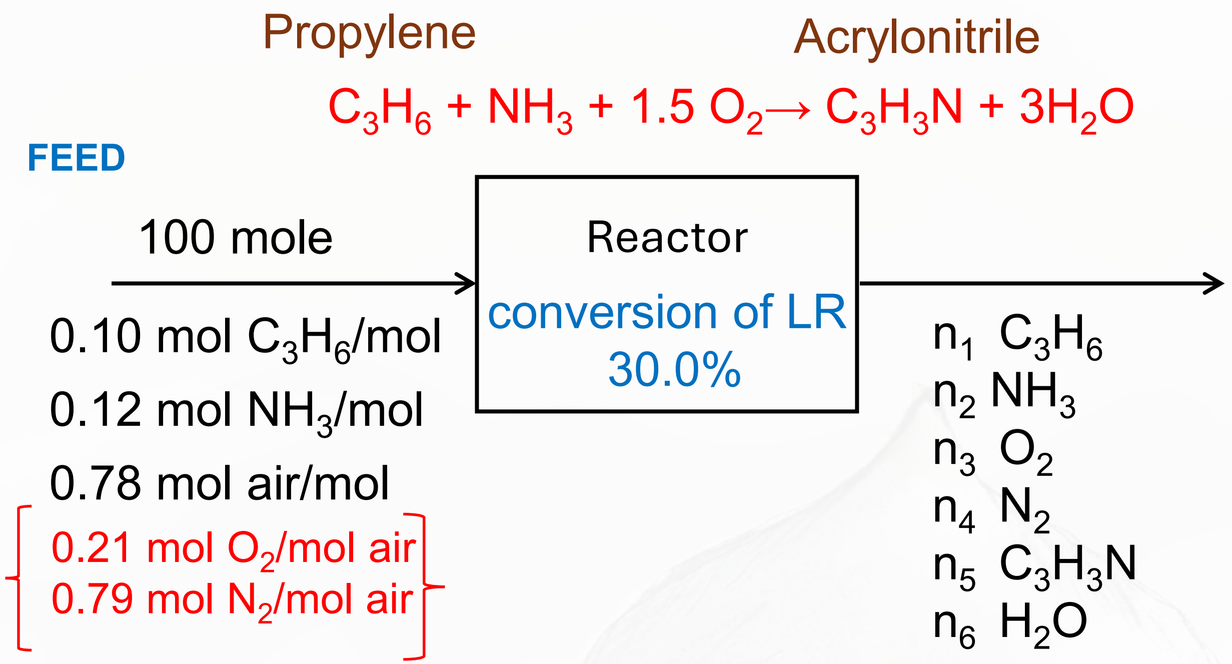
propylene   Acrylonitrile

The feed contains 10.0 mol% propylene, 12.0% ammonia, and 78.0% air. A fractional conversion of 30.0% of the limiting reactant is achieved. Taking 100 mol of feed as a basis, determine:

1. Which reactant is limiting?
2. The percentage by which each of the other reactants is in excess.
3. The molar amounts of all product gas constituents for a 30% conversion of the limiting reactant.

(Use the extent of reaction method)

Basis: 100 mol feed



Propylene Acrylonitrile

$C_3H_6 + NH_3 + 1.5\ O_2 \rightarrow C_3H_3N + 3H_2O$

FEED

100 mole

Reactor

conversion of LR 30.0%

0.10 mol C_3H_6/mol

0.12 mol NH_3/mol

0.78 mol air/mol

0.21 mol O_2/mol air
0.79 mol N_2/mol air

n_1 C_3H_6
n_2 NH_3
n_3 O_2
n_4 N_2
n_5 C_3H_3N
n_6 H_2O

1. Which reactant is limiting?
2. The percentage by which each of the other reactants is in excess.

$$C_3H_6 \quad + \quad NH_3 \quad + \quad 1.5\ O_2 \quad \rightarrow \quad C_3H_3N \quad + \quad 3H_2O$$

	C_3H_6	NH_3	$1.5\ O_2$
n_{feed}	10 mol	12 mol	16.4 mol
Limiting or excess	$\frac{10}{1}$	$\frac{12}{1}$	$\frac{16.4}{1.5}$
	$\boxed{10}$	12	10.9
	limiting	excess	excess
n_{stoich}	10	$10\times\frac{1}{1}=10$	$10\times\frac{1.5}{1}=15$
%Excess	$\frac{10-10}{10}$	$\frac{12-10}{10}$	$\frac{16.4-15}{15}\times 100\%$
	0%	20%	9.3%

all units are mol

mol

Example:

$$(n_{NH_3})_{stoich} = (10.0\ mol\ C_3H_6)\frac{1\ mol\ NH_3}{1\ mol\ C_3H_6} = 10.0\ mol$$

$$\%\,excess = \frac{(n_A)_{feed} - (n_A)_{stoich}}{(n_A)_{stoich}}$$

Example: $(\%\ excess)_{NH_3} = \frac{(NH_3)_0 - (NH_3)_{stoich}}{(NH_3)_{stoich}} \times 100\%$

$$= \frac{12.0-10.0}{10.0}\times 100\% \quad = \quad 20\%\ excess\ NH_3$$

3. Determine the molar amounts of all product gas constituents for a 30% conversion of the limiting reactant.

- Conversion of limiting reactant = 30.0% $\Rightarrow f_{C_3H_6} = 0.30$

$$0.30 = \frac{10 - n_1}{10} \quad \Rightarrow \quad \boxed{n_1 = 7.0 \text{ mol}}$$

$$\%conv = \frac{(n_A)_{feed} - (n_A)_{out}}{(n_A)_{feed}} x100$$

- Extent equations

$$(n_i)_{out} = (n_i)_{in} \quad \pm \quad \nu_i \xi$$

C_3H_6 $\quad 7 = 10 - 1 \times \xi \quad \Rightarrow \boxed{\xi = 3}$

NH_3 $\quad n_2 = 12 - 1 \times \xi \quad \Rightarrow \boxed{n_2 = 9 \text{ mol}}$

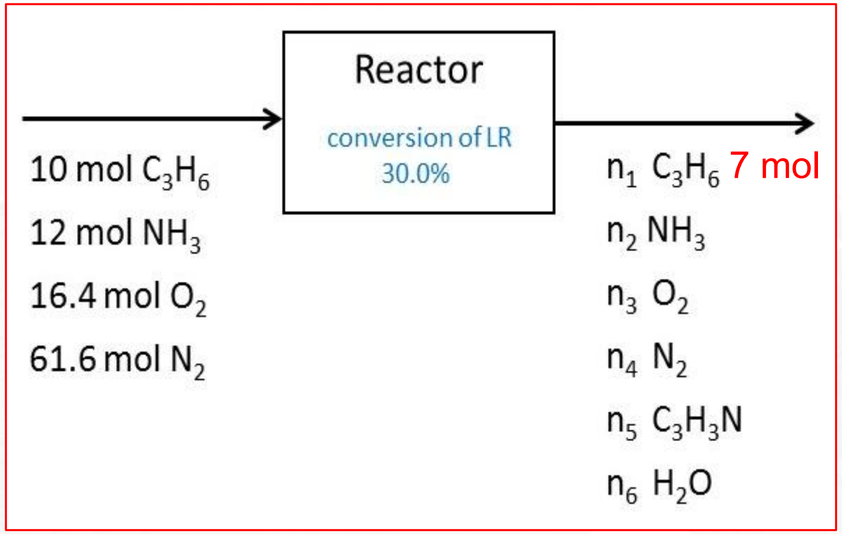
O_2 $\quad n_3 = 16.4 - 1.5 \times \xi \quad \Rightarrow \boxed{n_3 = 11.9 \text{ mol}}$

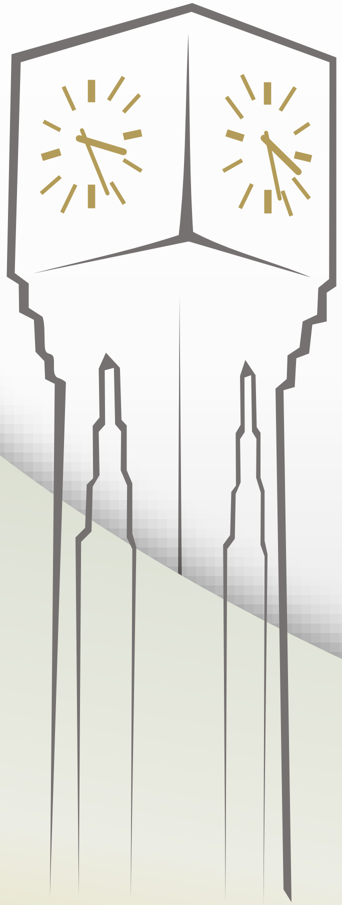
N_2 $\quad n_4 = 61.6 \quad \Rightarrow \boxed{n_4 = 61.6 \text{ mol}}$

C_3H_3N $\quad n_5 = 0 + 1 \times \xi \quad \Rightarrow \boxed{n_5 = 3 \text{ mol}}$

H_2O $\quad n_6 = 0 + 3 \times \xi \quad \Rightarrow \boxed{n_6 = 9 \text{ mol}}$

C_3H_6 + NH_3 + 1.5 O_2 → C_3H_3N + 3H_2O





4.7 Balances on Reactive Processes

This section outlines the procedures to calculate process variables involving a chemical reaction using molecular species balances, atomic species balances, and extent of reaction.

4.7 Balances on Reactive Processes

In a reactive system we have:

1. Molecular species (components)
2. Atomic species (atoms)
3. Chemical reaction(s)

Note: This method is not required. Self reading

Systems that involve chemical reactions may be analyzed using:

a) Molecular species balances (the approach always used for nonreactive systems).

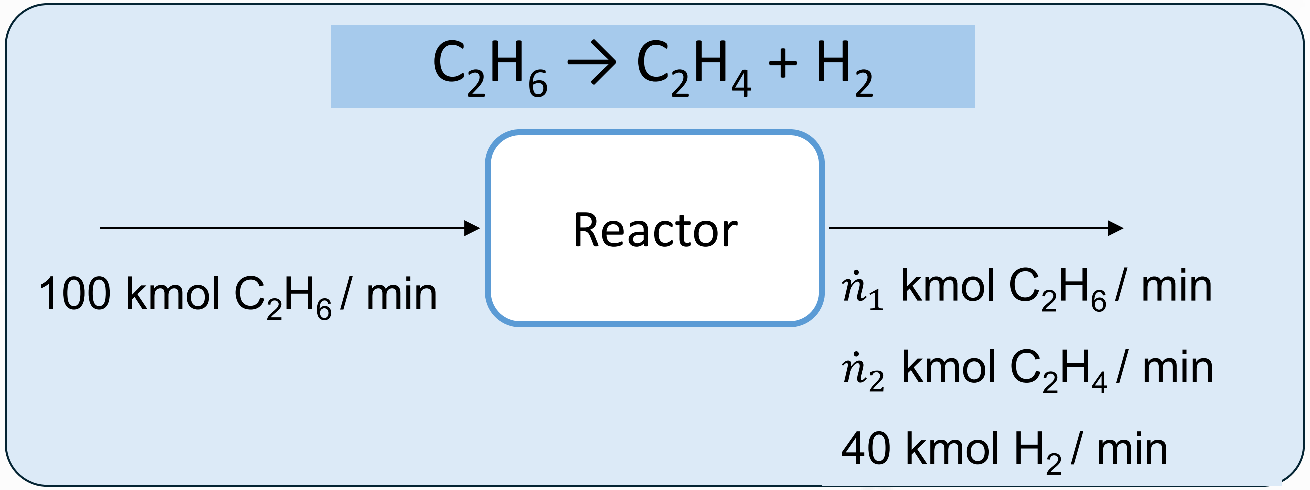
b) Atomic species balances, and

c) Extent of reaction (ξ).

easier

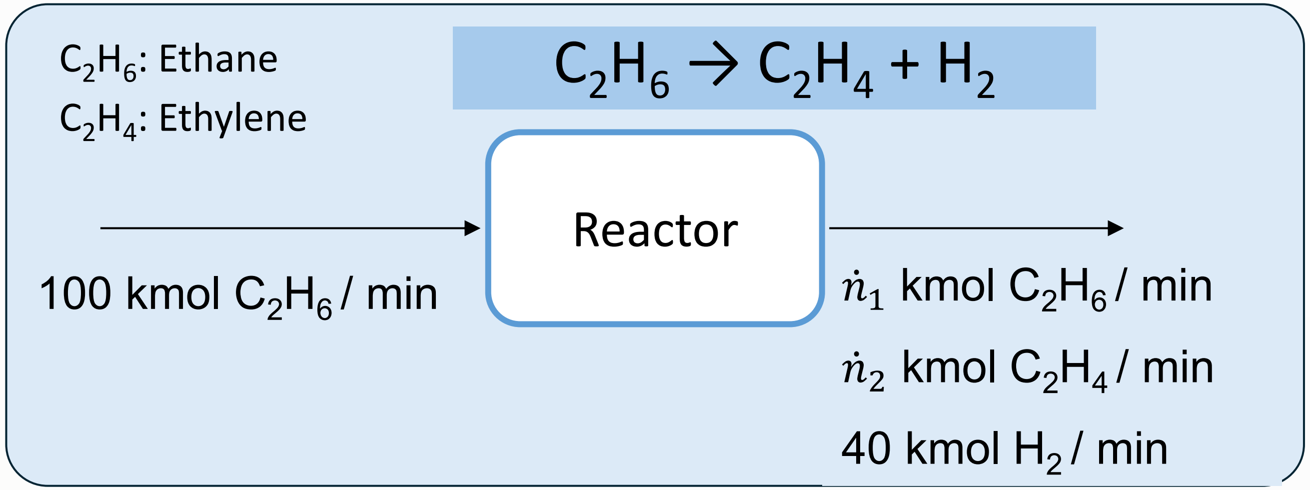
4.7a. Balances on Molecular and Atomic species

C_2H_6: Ethane
C_2H_4: Ethylene



- A number of different balances could be written on this process, including balances on total mass, $C_2H_6, C_2H_4, and\ H_2$.
- Balances on atomic species can be written *input = output*, since atoms can neither be created (generation = 0) nor destroyed (consumption = 0) in a chemical reaction.

Note: This method is not required. It's for self reading



C_2H_6: Ethane
C_2H_4: Ethylene

$$C_2H_6 \rightarrow C_2H_4 + H_2$$

Balance on Molecular Species

Input + Generation = Output + Consumption (continuous steady-state process)

Molecular H_2 Balance: generation = output

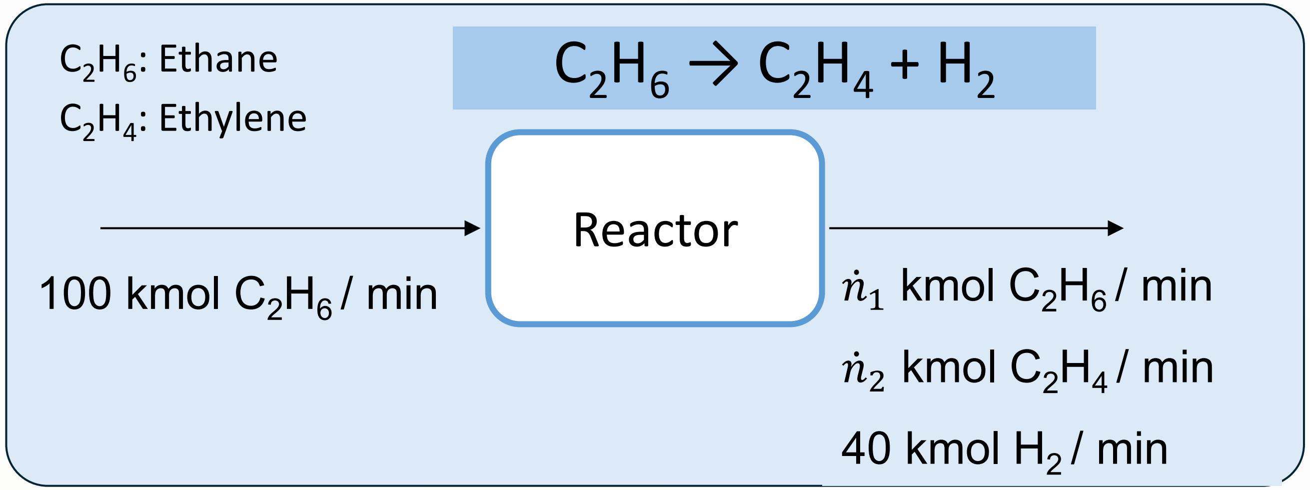
$$Gen_{H_2}\left(\frac{kmol\ H_2\ generated}{min}\right) = 40\ kmol/min$$

C_2H_6 Balance: input = output + consumption

$$\frac{100\ kmol\ C_2H_6}{min} = \dot{n}_1\left(\frac{kmol\ C_2H_6}{min}\right) + Cons_{C_2H_6}\left(\frac{kmol\ C_2H_6\ consumed}{min}\right)$$

C_2H_4 Balance: generation = output

$$Gen_{C_2H_4}\left(\frac{kmol\ C_2H_4\ generated}{min}\right) = \dot{n}_2\left(\frac{kmol\ C_2H_4}{min}\right)$$



C_2H_6: Ethane

C_2H_4: Ethylene

$$C_2H_6 \rightarrow C_2H_4 + H_2$$

Balance on Atomic Species

Input = Output (continuous steady-state process)

Atomic C Balance: input = output

$$\left(\frac{100\ kmol\ C_2H_6}{min}\right)\left(\frac{2\ kmol\ C}{1\ kmol\ C_2H_6}\right) = \left(\dot{n}_1\frac{kmol\ C_2H_6}{min}\right)\left(\frac{2\ kmol\ C}{1\ kmol\ C_2H_6}\right) + \left(\dot{n}_2\frac{kmol\ C_2H_4}{min}\right)\left(\frac{2\ kmol\ C}{1\ kmol\ C_2H_4}\right)$$

$$\Downarrow$$

$$200\ kmol\ C/\text{min} = 2\dot{n}_1 + 2\dot{n}_2$$

Atomic H Balance: input = output

$$\left(\frac{100\ kmol\ C_2H_6}{min}\right)\left(\frac{6\ kmol\ H}{1\ kmol\ C_2H_6}\right) = \left(\frac{40\ kmol\ H_2}{min}\right)\left(\frac{2\ kmol\ H}{1\ kmol\ H_2}\right) + \left(\dot{n}_1\frac{kmol\ C_2H_6}{min}\right)\left(\frac{6\ kmol\ H}{1\ kmol\ C_2H_6}\right) + \left(\dot{n}_2\frac{kmol\ C_2H_4}{min}\right)\left(\frac{4\ kmol\ H}{1\ kmol\ C_2H_4}\right)$$

$$\Downarrow$$

$$600\ kmol\ H/\text{min} = 80\ kmol\ H/min + 6\dot{n}_1 + 4\dot{n}_2$$

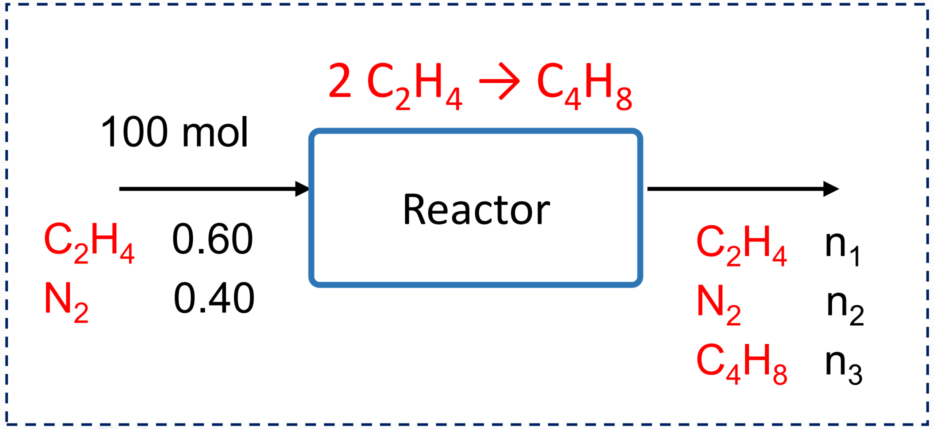
Example 1 - Reactive Processes

Identifying Molecular and Atomic species

SO1	Performance Indicators	**PI1a.** Identify and define complex engineering problems.
		PI1b. Model and formulate complex engineering problems by applying principles of engineering, science, and mathematics.
		PI1c. Solve complex engineering problems by applying principles of engineering, science, and mathematics.

Part 1.

Answer the following questions to identify the key variables and relationships in the presented reactive process. The questions help you define the reactor system and explain how these variables interact to affect the system's performance. [PI1a]



1) Molecular species (components) are C_2H_4, C_4H_8, N_2
2) Atomic species are C, H, N
3) What are the reactive species? C_2H_4, C_4H_8
4) What are the non-reactive species? N_2
5) How many chemical reactions are there? 1

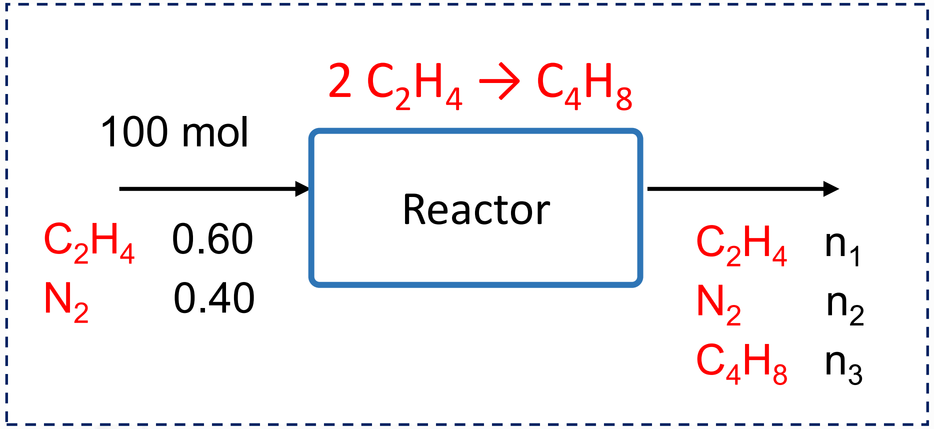
Example 1 - Reactive Processes [PI 1a]

Identifying Molecular and Atomic species

SO1	Performance Indicators	
		PI1a. Identify and define complex engineering problems.
		PI1b. Model and formulate complex engineering problems by applying principles of engineering, science, and mathematics.
		PI1c. Solve complex engineering problems by applying principles of engineering, science, and mathematics.

Part 2.

Formulate the necessary equations [PI1b] and calculate the following requirements [PI1c] in the reactive process



$2\ C_2H_4 \rightarrow C_4H_8$

100 mol

C_2H_4 0.60

N_2 0.40

Reactor

C_2H_4 n_1

N_2 n_2

C_4H_8 n_3

6) Ratio of C_2H_4 to N_2 in feed is $(0.6 \times 100) / (0.4 \times 100) = 6/4$.

7) Ratio of C_2H_4 to N_2 in output is n_1 / n_2.

8) Moles of C atom in feed is $2 \times (0.6 \times 100)$. Moles of N atom in feed is $2 \times (0.4 \times 100)$

9) Moles of H atom in input is $4 \times (0.6 \times 100)$. Moles of H atom in output is $4\ n_1 + 8\ n_3$.

10) Moles of C atom in output is $2\ n_1 + 4\ n_3$.

4.7b. Independent Equations/Species/Reactions

1. If two molecular species are in the same ratio to each other wherever they appear in a process and this ratio is incorporated in the flowchart labeling, balances on these species will not be independent equations.
2. If two atomic species occur in the same ratio wherever they appear in a process, balances on these species will not be independent equations.
3. Chemical reactions are independent if the stoichiometric equation of any one of them cannot be obtained by adding and subtracting multiples of the stoichiometric equations of the others.

Independent Reactions

Independent reactions:
Chemical reactions are independent if the stoichiometric equation of any one of them cannot be obtained by adding and subtracting multiples of the stoichiometric equations of the others.

$A \rightarrow B$ (1)
$2A \rightarrow 2B$ (2)

Reaction (2) = 2 × Reaction (1)

We have (2) reactions, one of them is dependent
⇒ Number of independent reactions = 1

Dependent Reactions:
Chemical reactions are not independent if we can get one in terms of the other by adding, subtracting and multiplying them.

$A \rightarrow 2B$ (1)
$B \rightarrow C$ (2)

$A \rightarrow 2C$ (3)

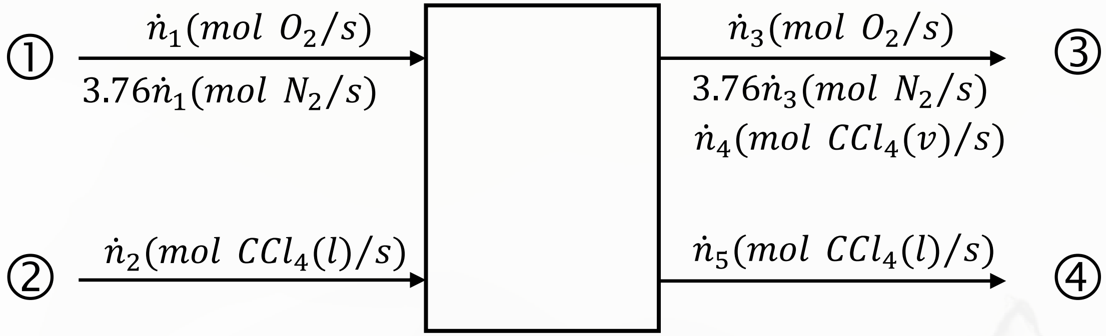
$$\begin{array}{l} A \rightarrow \cancel{2B} \\ +\ \cancel{2B} \rightarrow 2C \\ \hline A \rightarrow 2C \end{array}$$

Reaction (3) = Reaction (1) + 2 × Reaction (2)

We have 3 reactions, one of them is dependent
⇒ Number of independent reactions = 2

Example 2

Consider the following process in which carbon tetrachloride (CCl_4) is vaporized into a stream of air. Determine how many independent molecular species and independent atomic species are there.



① $\dot{n}_1(mol\ O_2/s)$, $3.76\dot{n}_1(mol\ N_2/s)$

② $\dot{n}_2(mol\ CCl_4(l)/s)$

③ $\dot{n}_3(mol\ O_2/s)$, $3.76\dot{n}_3(mol\ N_2/s)$, $\dot{n}_4(mol\ CCl_4(v)/s)$

④ $\dot{n}_5(mol\ CCl_4(l)/s)$

Molecular species

- Number of components = 3
- O_2, N_2, CCl_4
- Ratio of N_2 to O_2 in ① = 3.76
- Ratio of N_2 to O_2 in ③ = 3.76
- One of (N_2 and O_2) components is dependent
- Num. of independent molecular species = 3-1 = 2

Atomic species

- Number of atomic species = 4
- O, N, C, Cl
- Ratio of N to O in ① and ③ = 3.76
- One of (N and O) atoms is dependent
- Ratio of (Cl to C) in ② and ④ = 4
- One of (Cl and C) atoms is dependent
- Num. of independent atomic species = 4-2 = 2

4.7c. Molecular Species Balances

Note: This method is not required. It's for self reading

Degree of Freedom Analysis

+ No. unknown labeled variables

+ No. independent chemical reactions

− No. independent molecular species balances components in the process

− No. other equations relating unknown variables

____

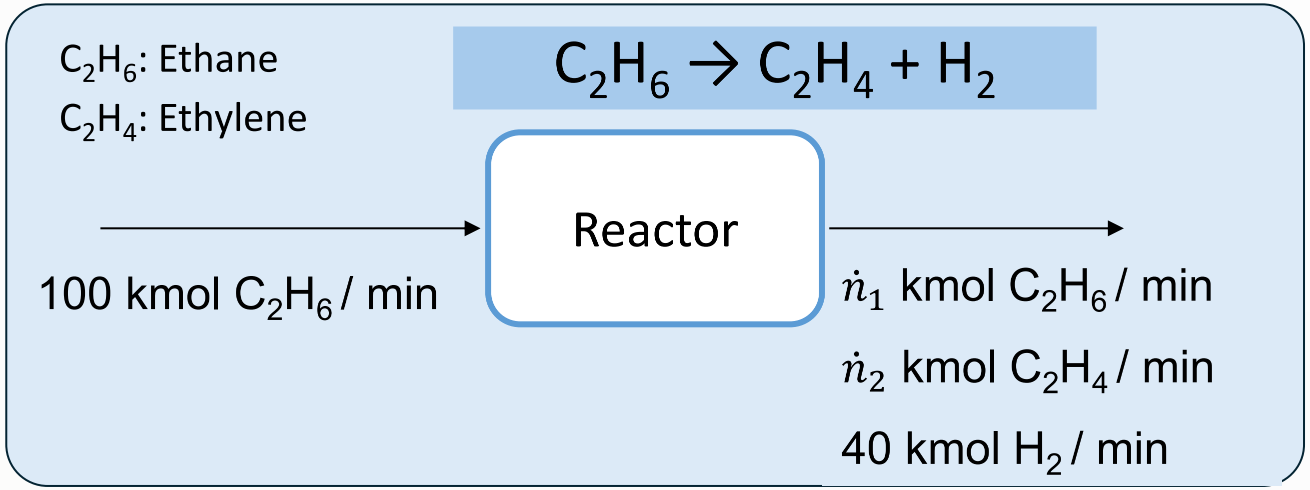
= Number of DOF (n_{DF})

Molecular species balances require more complex calculations than either of the other two approaches and should be used only for simple systems involving one reaction.

Example 3

1) Define the following reactor system by calculating the degrees of freedom using the *Molecular Species Balance* method. [PI1a]

Note: Not required. Self reading



C_2H_6: Ethane
C_2H_4: Ethylene

$C_2H_6 \rightarrow C_2H_4 + H_2$

Degree of Freedom Analysis [PI 1a]

No. unknown labeled variables
\+ No. independent chemical reactions
− No. independent molecular species balances
− No. other equations relating unknown variables

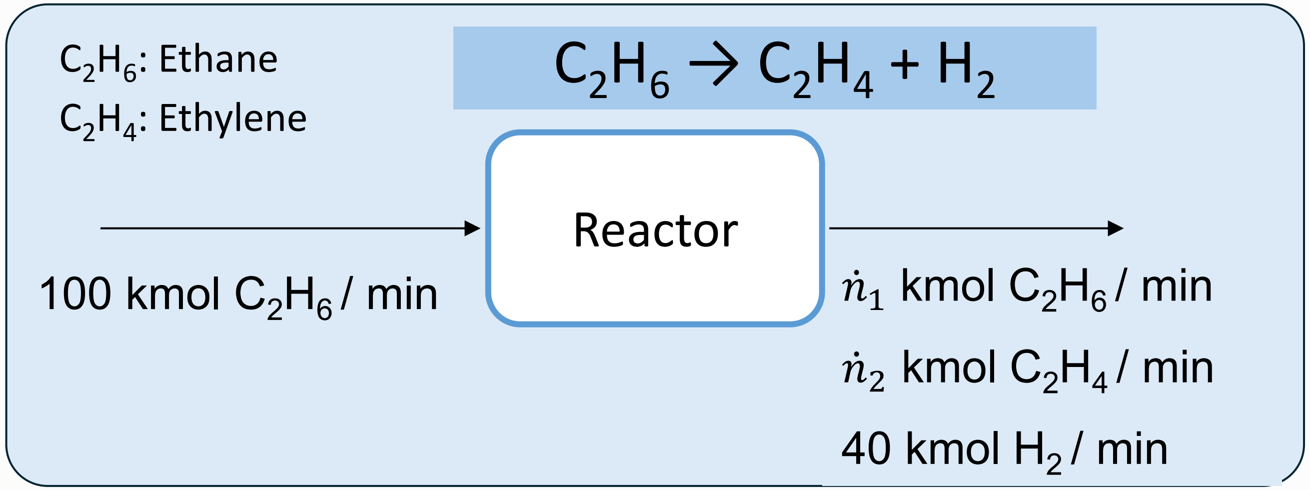
= Number of DOF

2 unknown labeled variables ($\dot{n}_1, \dot{n}_2$)
\+ 1 independent chemical reaction ($C_2H_6 \rightarrow C_2H_4 + H_2$)
− 3 independent molecular species balances (C_2H_6, C_2H_4, H_2)
− 0 other equations relating unknown variables

DOF = 0

Example 3

2) Formulate the necessary equations [PI1b] and calculate the unknown variables in the reactor output using the *Molecular Species Balance* method. [PI1c]



C_2H_6: Ethane
C_2H_4: Ethylene

$$C_2H_6 \rightarrow C_2H_4 + H_2$$

Brief discussion

Balance on Molecular Species

Input + Generation = Output + Consumption (continuous steady-state process)

Molecular H_2 Balance: generation = output

$$Gen_{H_2}\left(\frac{kmol\ H_2\ generated}{min}\right) = 40\ kmol\ H_2/min$$

C_2H_6 Balance: input = output + consumption

$$\frac{100\ kmol\ C_2H_6}{min} = \dot{n}_1\left(\frac{kmol\ C_2H_6}{min}\right) + \frac{40\ kmol\ H_2\ generated}{min}\left(\frac{1\ kmol\ C_2H_6\ consumed}{1\ kmol\ H_2\ generated}\right) \rightarrow \boldsymbol{\dot{n}_1 = 60\ kmol\ C_2H_6/min}$$

C_2H_4 Balance: generation = output

$$\frac{40\ kmol\ H_2\ generated}{min}\left(\frac{1\ kmol\ C_2H_4\ generated}{1\ kmol\ H_2\ generated}\right) = \dot{n}_2\left(\frac{kmol\ C_2H_4}{min}\right) \rightarrow \boldsymbol{\dot{n}_2 = 40\ kmol\ C_2H_4/min}$$

4.7d. Atomic species balances

Degree of Freedom Analysis

+ No. unknown labeled variables

− No. independent atomic species balances

Atoms in the process

− No. independent molecular species balances *on nonreactive species*

Non-Reactive components in the process

− No. other equations relating unknown variables

= Number of DOF (n_{DF})

Important

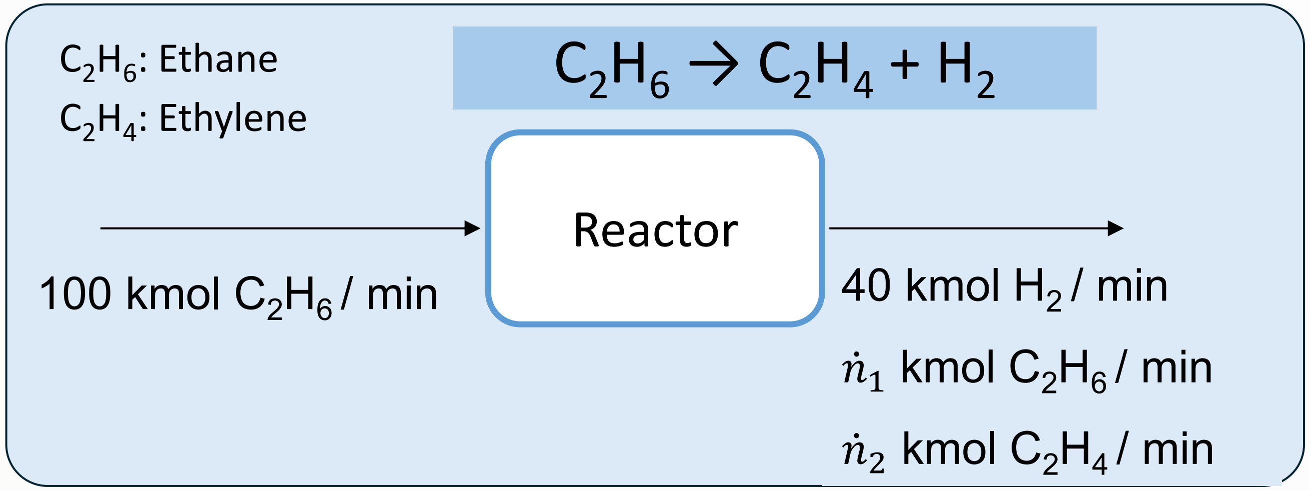
Balances on atomic species can be written as **INPUT = OUTPUT**

This is because atoms can neither be created (generation = 0) nor destroyed (consumption = 0) in a chemical reaction.

Atomic species balances generally lead to the most straightforward solution procedure, especially when more than one reaction is involved.

Example 4

1) Define the following reactor system by calculating the degrees of freedom using the *Atomic Species Balance* method. [PI1a]



C_2H_6: Ethane
C_2H_4: Ethylene

$C_2H_6 \rightarrow C_2H_4 + H_2$

Degree of Freedom Analysis [PI 1a]

No. unknown labeled variables
− No. independent atomic species balances
− No. independent molecular species balances on nonreactive species
− No. other equations relating unknown variables

____

= Number of DOF

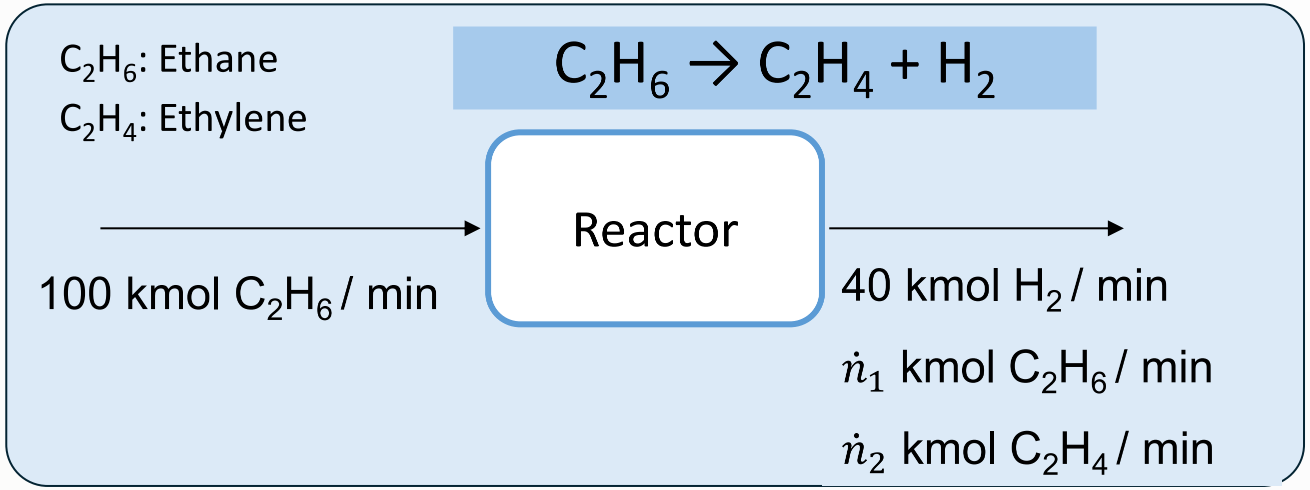
2 unknown labeled variables $(\dot{n}_1, \dot{n}_2)$
— 2 independent atomic species balances (C and H)
— 0 independent molecular species balances on non-reactive species
— 0 other equations relating unknown variables

____

DOF = 0

Example 4

2) Formulate the necessary equations [PI1b] and calculate the unknown variables in the reactor output using the *Atomic Species Balance* method. [PI1c]



C_2H_6: Ethane
C_2H_4: Ethylene

$C_2H_6 \rightarrow C_2H_4 + H_2$

Balance on Atomic Species

Input = Output (continuous steady-state process)

Atomic C Balance: input = output

$$\left(\frac{100\ kmol\ C_2H_6}{min}\right)\left(\frac{2\ kmol\ C}{1\ kmol\ C_2H_6}\right)=\left(\dot{n}_1\frac{kmol\ C_2H_6}{min}\right)\left(\frac{2\ kmol\ C}{1\ kmol\ C_2H_6}\right)+\left(\dot{n}_2\frac{kmol\ C_2H_4}{min}\right)\left(\frac{2\ kmol\ C}{1\ kmol\ C_2H_4}\right)$$

$$\Downarrow$$

$$200\ kmol\ C\,/\mathrm{min}=2\dot{n}_1+2\dot{n}_2$$

Atomic H Balance: input = output

$$\left(\frac{100\ kmol\ C_2H_6}{min}\right)\left(\frac{6\ kmol\ H}{1\ kmol\ C_2H_6}\right)=\left(\frac{40\ kmol\ H_2}{min}\right)\left(\frac{2\ kmol\ H}{1\ kmol\ H_2}\right)+\left(\dot{n}_1\frac{kmol\ C_2H_6}{min}\right)\left(\frac{6\ kmol\ H}{1\ kmol\ C_2H_6}\right)+\left(\dot{n}_2\frac{kmol\ C_2H_4}{min}\right)\left(\frac{4\ kmol\ H}{1\ kmol\ C_2H_4}\right)$$

$$\Downarrow$$

$$600\ kmol\ H\,/\mathrm{min}=\ 80\ kmol\ H/min+6\dot{n}_1+4\dot{n}_2$$

Solve simultaneously: $\boldsymbol{\dot{n}_1\ =\ 60\ kmol\ C_2H_6/min}$ and $\boldsymbol{\dot{n}_2\ =40\ kmol\ C_2H_4/min}$

4.7e. Extent of Reaction

Degree of Freedom Analysis

+ No. unknown labeled variables

+ No. independent reactions (one unknown ξ for each reaction)

Number of Reactions in process

− No. independent reactive species (one eqn for each species in terms of ξ)

− No. independent nonreactive species (one balance equation for each)

− No. other equations relating unknown variables

= Number of DOF (n_{DF})

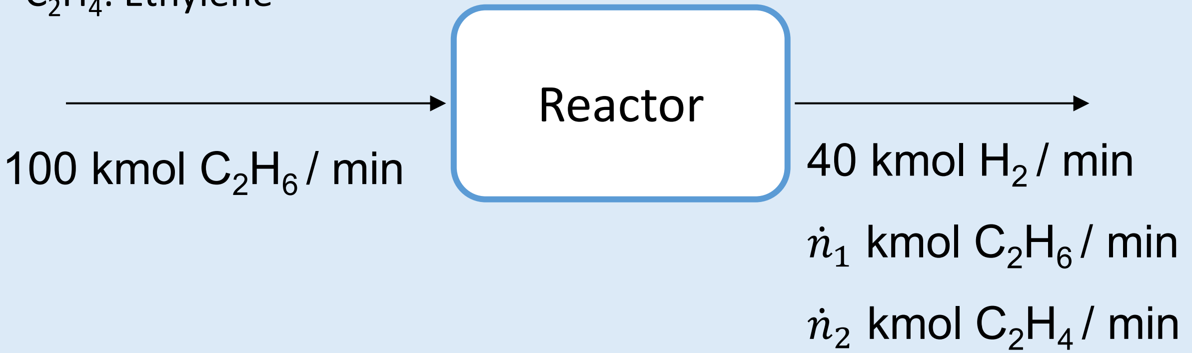
Extents of reaction are convenient for chemical equilibrium problems and when equation solving software is to be used.

Example 5

1) Define the following reactor system by calculating the degrees of freedom using the *Extent of Reaction* method. [PI1a]

C_2H_6: Ethane
C_2H_4: Ethylene

$$C_2H_6 \rightarrow C_2H_4 + H_2$$


Reactor

100 kmol C_2H_6 / min

40 kmol H_2 / min
$\dot{n}_1$ kmol C_2H_6 / min
$\dot{n}_2$ kmol C_2H_4 / min

Degree of Freedom Analysis [PI 1a]

+ No. unknown labeled variables
+ No. independent reactions
− No. independent reactive species
− No. independent nonreactive species
− No. other equations relating unknown variables

____

= Number of DOF

2 unknown labeled variables ($\dot{n}_1, \dot{n}_2$)
+ 1 independent reaction
− 3 independent reactive species (C_2H_6, C_2H_4, H_2)
− 0 independent nonreactive species
− 0 other equations relating unknown variables

____

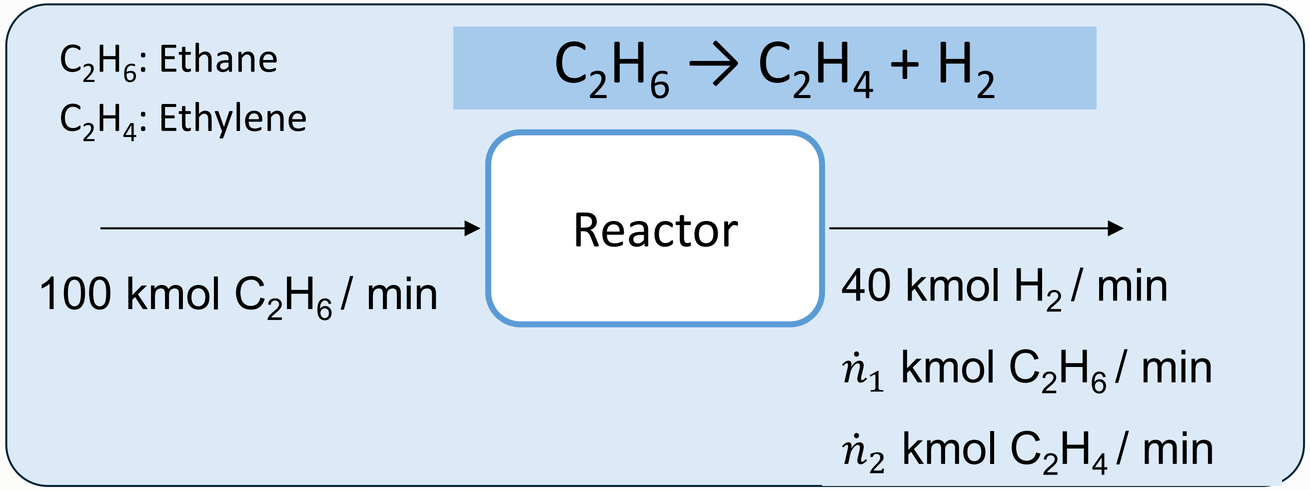
DOF = 0

Example 5

2) Formulate the necessary equations [PI1b] and calculate the unknown variables in the reactor output using the *Extent of Reaction* method. [PI1c]

$$\boldsymbol{n_i = n_{i0} \mp \nu_i \xi}$$ No flow systems

$$\boldsymbol{\dot{n}_i = \dot{n}_{i0} \mp \nu_i \dot{\xi}}$$ Flow systems



ν_i Stoichiometric coefficient of species i

ξ Extent of reaction (the amount converted from the limiting reactant)

H_2; Product; $(\nu = +1)$ → $\dot{n}_i = \dot{n}_{i0} + \nu_i \dot{\xi}$ → $40\ \text{kmol/h} = 0\ \text{kmol/h} + 1\left(\dot{\xi}\ \text{kmol/h}\right)$ → $\dot{\xi} = 40\ \text{kmol/h}$

Same for all species

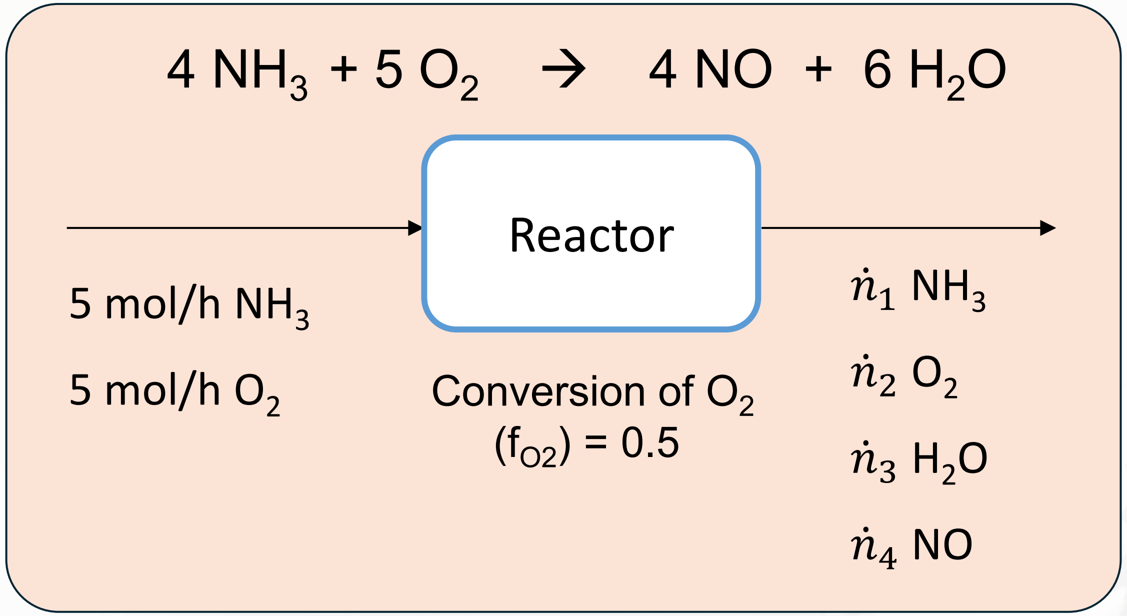
C_2H_6; Reactant; $(\nu = -1)$ → $\dot{n}_i = \dot{n}_{i0} - \nu_i \dot{\xi}$ → $\dot{n}_1 = 100 - 1\,(40)$ → $\dot{n}_1 = 60\ \text{kmol/h}$

C_2H_4; Product; $(\nu = +1)$ → $\dot{n}_i = \dot{n}_{i0} + \nu_i \dot{\xi}$ → $\dot{n}_2 = 0 + 1\,(40)$ → $\dot{n}_1 = 40\ \text{kmol/h}$

Example 6

Ammonia is burned to form nitric oxide. Fractional conversion of O_2 is 0.5. The inlet molar flow rates of NH_3 and O_2 are 5 mol/h. Calculate the exit component molar flow rates using:

a) Extent of reaction method.
b) Atomic balance approach.



$$4\ NH_3 + 5\ O_2 \rightarrow 4\ NO + 6\ H_2O$$

Reactor

5 mol/h NH_3

5 mol/h O_2

Conversion of O_2 (f_{O2}) = 0.5

$\dot{n}_1$ NH_3

$\dot{n}_2$ O_2

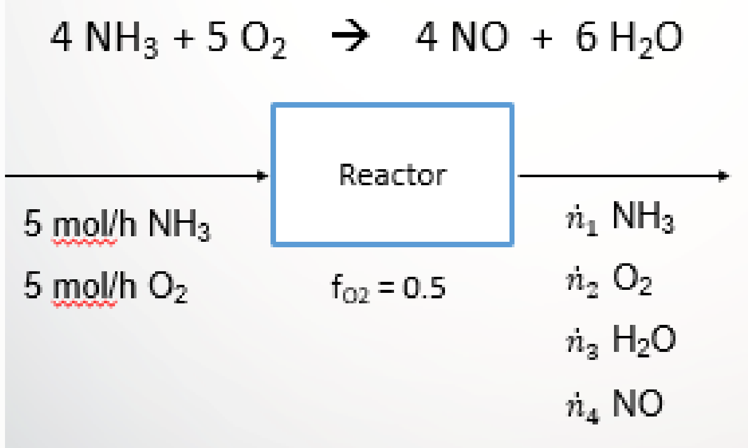
$\dot{n}_3$ H_2O

$\dot{n}_4$ NO

Solution

a) Extent of reaction method

- Unknowns: 4 ($\dot{n}_1, \dot{n}_2, \dot{n}_3, \dot{n}_4$)
- Reactions: 1 ($4\ NH_3 + 5\ O_2 \rightarrow 4\ NO + 6\ H_2O$)
- Reactive species: 4 (NH_3, O_2, NO, H_2O)
- Independent species? Yes
- Extent equations: 4 (one per species)
- Additional equations? Yes (conversion)



DOF analysis

4	unknown variables
+ 1	+ indep reactions
- 4	- indep reactive species
- 0	- indep nonreactive species
- 1	- other equations
0	= DOF

Extent of reaction balances

$$\dot{n}_i = \dot{n}_{io} \pm \nu_i \cdot \dot{\xi}$$

$$\nu_{NH3} = -4,\ \nu_{O2} = -5,\ \nu_{NO2} = 4,\ \nu_{H2O} = 6$$

- Balance of NH_3: $\dot{n}_1 = 5 - 4\,\xi$ ①
- Balance of O_2: $\dot{n}_2 = 5 - 5\,\xi$ ②
- Balance of H_2O: $\dot{n}_3 = 0 + 6\,\xi$ ③
- Balance of NO: $\dot{n}_4 = 0 + 4\,\xi$ ④

We can't solve without ξ … find it.

Conversion: $0.50 = 1 - \dot{n}_2/5$ ⑤

Find $\dot{n}_1$ from (5) then ξ from (2) then continue

⑤ Conversion: $0.50 = 1 - \dot{n}_2/5 \Rightarrow \dot{n}_2 = 2.5\ \text{mol/h}\ O_2$

② Balance of O_2: $\dot{n}_2 = 5 - 5\,\xi \Rightarrow 2.5 = 5 - 5\,\xi \Rightarrow \xi = 0.5\ \text{mol/h}$

① Balance of NH_3: $\dot{n}_1 = 5 - 4\,\xi \Rightarrow \dot{n}_1 = 5 - 4 \times 0.5 \Rightarrow \dot{n}_1 = 3.0\ \text{mol/h}\ NH_3$

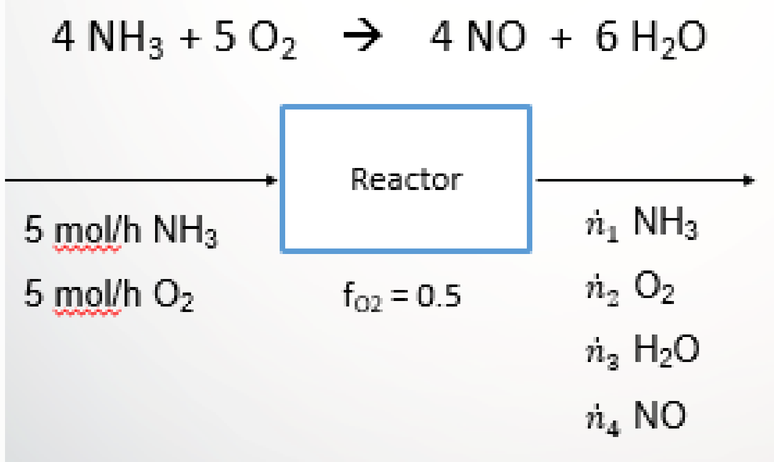
③ Balance of H_2O: $\dot{n}_3 = 0 + 6\,\xi \Rightarrow \dot{n}_3 = 0 + 6 \times 0.5 \Rightarrow \dot{n}_3 = 3.0\ \text{mol/h}$

④ Balance of NO: $\dot{n}_4 = 0 + 4\,\xi \Rightarrow \dot{n}_4 = 0 + 4 \times 0.5 \Rightarrow \dot{n}_4 = 2.0\ \text{mol/h}$

Solution

b) Atomic balance method

- Unknowns: 4 ($\dot{n}_1, \dot{n}_2, \dot{n}_3, \dot{n}_4$)
- Atomic species: 3 (N , H , O)
- Independent atoms? Yes
- # indep atomic balances: 3 (one per atom)
- Non reactive species? None
- Additional equations? Yes (conversion)



$4\,NH_3 + 5\,O_2 \rightarrow 4\,NO + 6\,H_2O$

DOF analysis

4 unknown variables
- 3 - indep atomic species balances
- 0 - indep nonreactive species
- 1 - other equations

0 = DOF

Atomic balances: $\boldsymbol{Input_i = Output_i}$

- ***N*** balance: $1 \times 5 = 1 \times \dot{n}_1 + 1 \times \dot{n}_4$

  $\dot{n}_1 + \dot{n}_4 = 5$ ①

- ***H*** Balance: $3 \times 5 = 3 \times \dot{n}_1 + 2 \times \dot{n}_3$

  $3\,\dot{n}_1 + 2\,\dot{n}_3 = 15$ ②

- ***O*** Balance: $2 \times 5 = 2 \times \dot{n}_2 + 1 \times \dot{n}_3 + 1 \times \dot{n}_4$

  $2\,\dot{n}_2 + \dot{n}_3 + \dot{n}_4 = 10$ ③

$0.50 = 1 - \dot{n}_2/5$ ④

$\dot{n}_1 + \dot{n}_4 = 5$ ①

$3\,\dot{n}_1 + 2\,\dot{n}_3 = 15$ ②

$2\,\dot{n}_2 + \dot{n}_3 + \dot{n}_4 = 10$ ③

$0.50 = 1 - \dot{n}_2/5$ ④

Solving 4 simultaneous equations:

$\dot{n}_1 = 3.0$ mol/h NH_3

$\dot{n}_2 = 2.5$ mol/h O_2

$\dot{n}_3 = 3.0$ mol/h H_2O

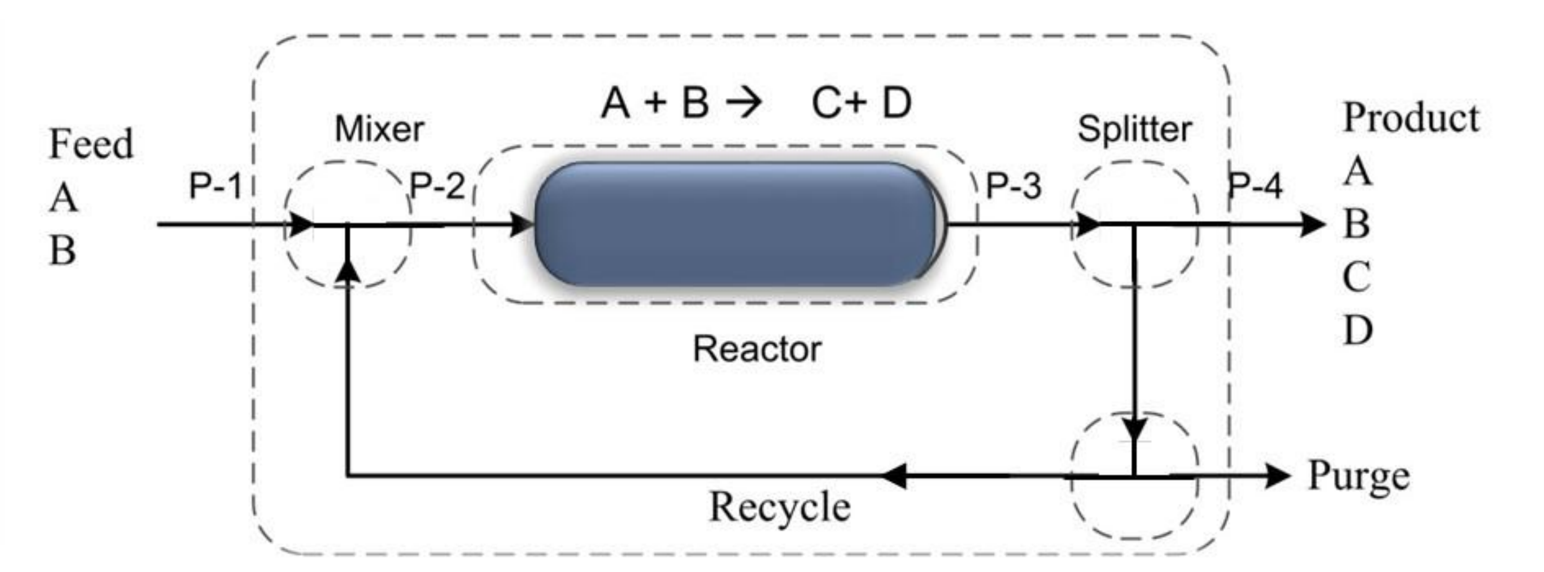
$\dot{n}_4 = 2.0$ mol/h NO

Same answers to extent of reaction method

4.7f. Product Separation and Recycle

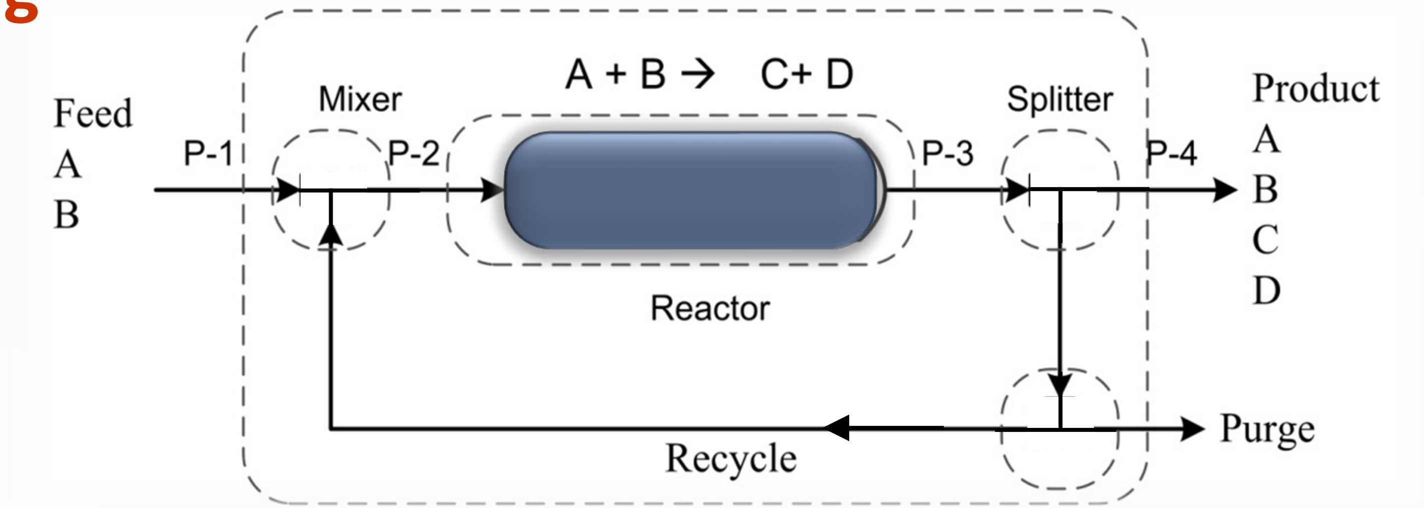
Overall Conversion: $$\frac{\text{reactant input to process} - \text{reactant ouput from process}}{\text{reactant input to process}}$$

Single-Pass Conversion: $$\frac{\text{reactant input to reactor} - \text{reactant ouput from reactor}}{\text{reactant input to reactor}}$$



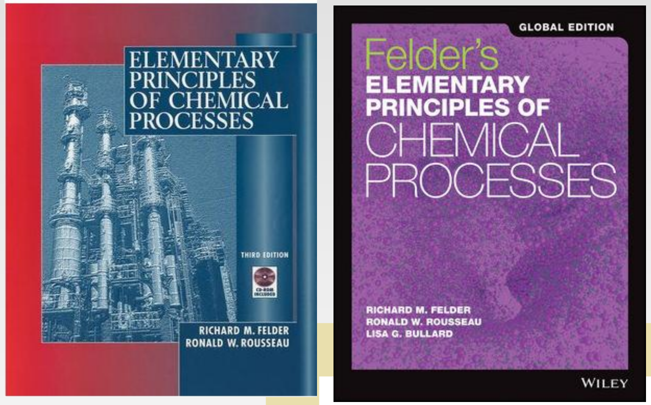
Refer to textbook for exercises on single pass and overall conversions

4.7g Purging



Why Purging is needed.

- Inert gases (e.g., nitrogen, argon, etc.) are used in processes because they do not undergo chemical reactions under given conditions.
- Using inert gas in a system prevents undesirable chemical reactions from occurring (e.g., oxidation, hydrolysis, combustion).
- Purging with nitrogen (N_2) minimizes hazards of residual solvents or process fluids.
- If an inert gas is introduced to the system and it doesn't react, it has to exit the system somewhere – otherwise, it builds up and would shut down the process.



Elementary Principles of Chemical Processes,
3rd or 4th edition,
Wiley & Sons, Inc.
Richard M. Felder, Ronald W. Rousseau, & Lisa G. Bullard.

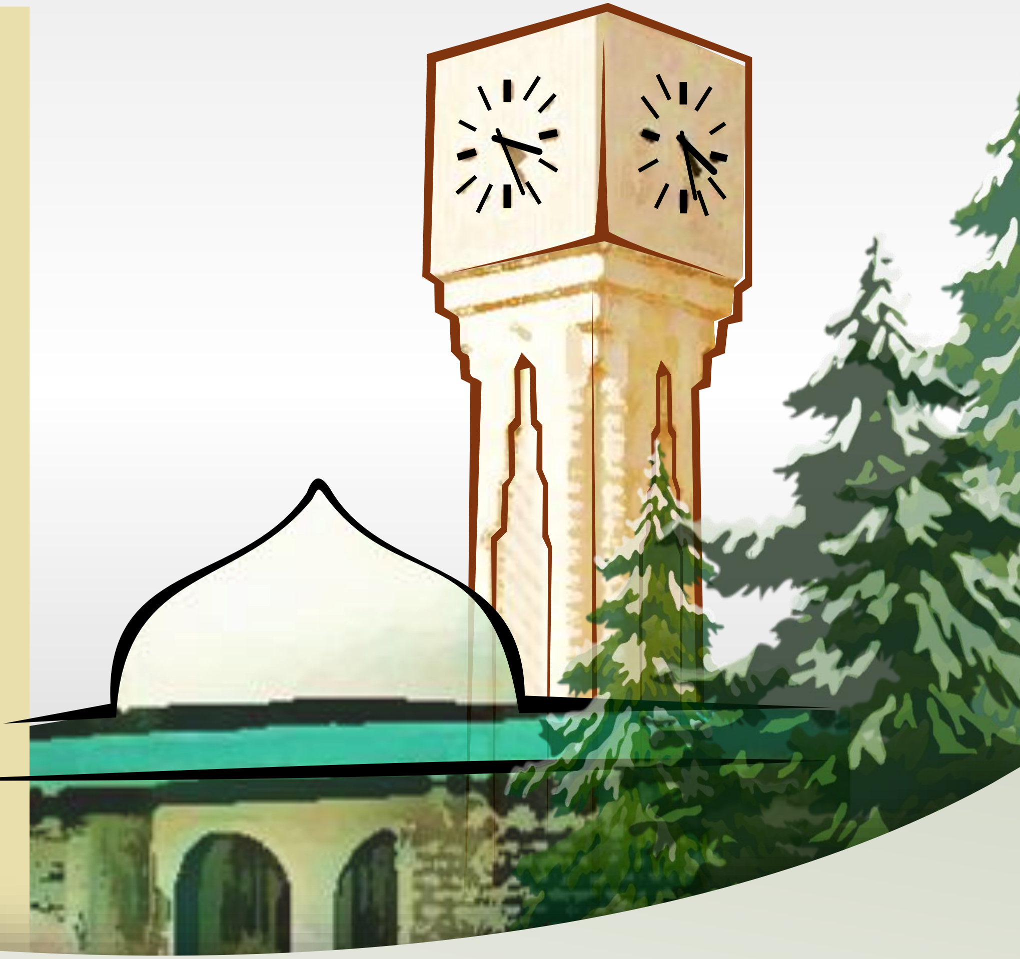
CHE 0905211

Chemical Engineering Principles 1

Fall 2025

Dr. Hatem Alsyouri	**Chapter 4**

The University of Jordan
Chemical Engineering Department



4.8 Combustion Reactions

Familiarize your self with the definitions of the following expressions:

- Combustion (definition and reaction chemistry)
- Fuel (types and example)
- Complete vs. Incomplete combustion
- Ratios of air component to each other
- Composition of gas on a Wet-basis and dry-basis
- Stack gas, exhaust gas or flue gas
- Theoretical and Excess Oxygen and Air

Example 4.8-2 Theoretical and Excess Air

100 mol/h of butane (C_4H_{10}) and 5000 mol/h of air are fed into a combustion reactor. Calculate the percent excess air.

The stoichiometric equation for complete combustion of butane:

$$C_4H_{10} + \frac{13}{2}O_2 \rightarrow 4CO_2 + 5H_2O$$

The theoretical air from the feed rate of fuel and the stoichiometric equation

$$(\dot{n}_{O_2})_{theoretical} = \frac{100\ mol\ C_4H_{10}}{h}\left|\frac{6.5\ mol\ O_2\ required}{mol\ C_4H_{10}}\right. = 650\,\frac{mol\ O_2}{h}$$

$$(\dot{n}_{air})_{theoretical} = \frac{650\ mol\ O_2}{h}\left|\frac{4.76\ mol\ air}{mol\ O_2}\right. = 3094\,\frac{mol\ air}{h}$$

$$\%\ excess\ air = \frac{(\dot{n}_{air})_{fed} - (\dot{n}_{air})_{theoretical}}{(\dot{n}_{air})_{theoretical}} \times 100\% = \frac{5000 - 3094}{3094} \times 100\% = 61.6\%$$

$$(\dot{n}_{air})_{fed} = 1.616(\dot{n}_{air})_{theoretical} = 1.616 \times 3094\,\frac{mol}{h} = 5000\,\frac{mol}{h}$$

Exercise 1: Incomplete Combustion of Methane

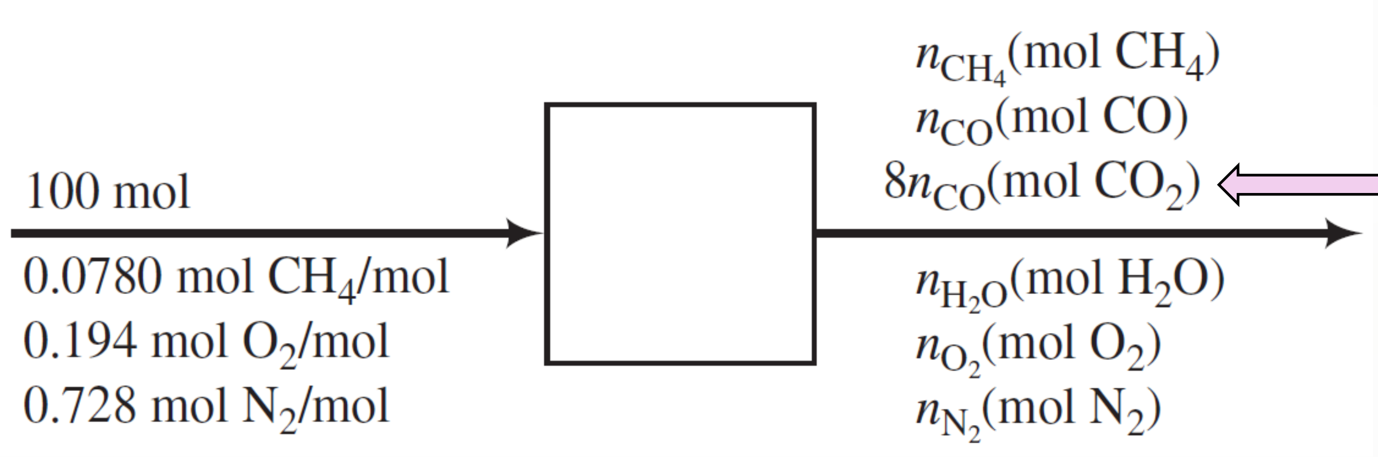
Methane is burned with air in a continuous steady-state combustion reactor to yield a mixture of carbon monoxide, carbon dioxide, and water. The reactions taking place are

$$CH_4 + \frac{3}{2}O_2 \rightarrow CO + 2H_2O \qquad (\mathbf{1})$$

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O \qquad (\mathbf{2})$$

The feed to the reactor contains 7.80 mole% CH_4, 19.4% O_2, and 72.8% N_2. The percentage conversion of methane is 90.0%, and the gas leaving the reactor contains 8 mol CO_2/mol CO. Carry out a dgree-of-freedom analysis on the process. Then calculate the molar composition of the product stream using molecular species balances, atomic species balances, and extents of reaction.

Basis: 100 mol Feed



This is the CO2 unknown output. It was represented by the extra equation given in statement. Therefore, the unknown and extra equations are not counted in the DOF

Degree-of-Freedom Analysis

- **Molecular species balances:** 5 unknown variables + 2 independent reactions – 6 independent molecular species balances (CH_4, O_2, N_2, CO, CO_2, H_2O) – 1 specified methane conversion = 0 degrees of freedom

- **Atomic species balances:** 5 unknown variables – 3 independent atomic species balances (C, H, O) – 1 nonreactive molecular species balance (N_2) – 1 specified methane conversion = 0 degrees of freedom

- **Extents of reaction:** 5 unknown variables + 2 independent reactions – 5 expressions for n_i (ξ) (i = CH_4, O_2, CO, CO_2, H_2O) – 1 nonreactive molecular species balance (N_2) – 1 specified methane conversion = 0 degrees of freedom

- ✓ The specified methane conversion can be used to determine n_{CH4}:

90% CH_4 Conversion: 10% remains unconverted

$$n_{CH_4} = 0.100(7.80\, mol\, CH_4\, fed) = 0.780\, mol\, CH_4$$

- ✓ Nitrogen balance to determine the nonreactive species in the process, n_{N2}:

N_2 Balance: input = output

$$n_{N_2} = 72.8\, mol\, N_2$$

- ➢ It remains to determine n_{CO}, n_{H2O} and n_{O2} by each of the indicated methods.

Molecular Species Balances (this method is not required)

This is the most cumbersome method when multiple reactions are involved. We strongly recommended against using it.

Each balance on a reactive species will contain generation and/or consumption terms.

$$C_{CH4,1}(mol\ CH_4)\ \rightarrow the\ consumption\ of\ methane\ in\ Reaction\ 1$$
$$G_{H2O,2}\ (mol\ H_2O) \rightarrow the\ generation\ of\ water\ in\ Reaction\ 2$$

Example:

$$G_{H2O,1}\ (mol\ H_2O\ generated\ in\ Reaction\ 1) = C_{O2,1}(mol\ O_2\ consumed\ in\ Reaction\ 1) \times \left(\frac{2\ mol\ H_2O\ generated}{1.5\ mol\ O_2\ consumed}\right)$$

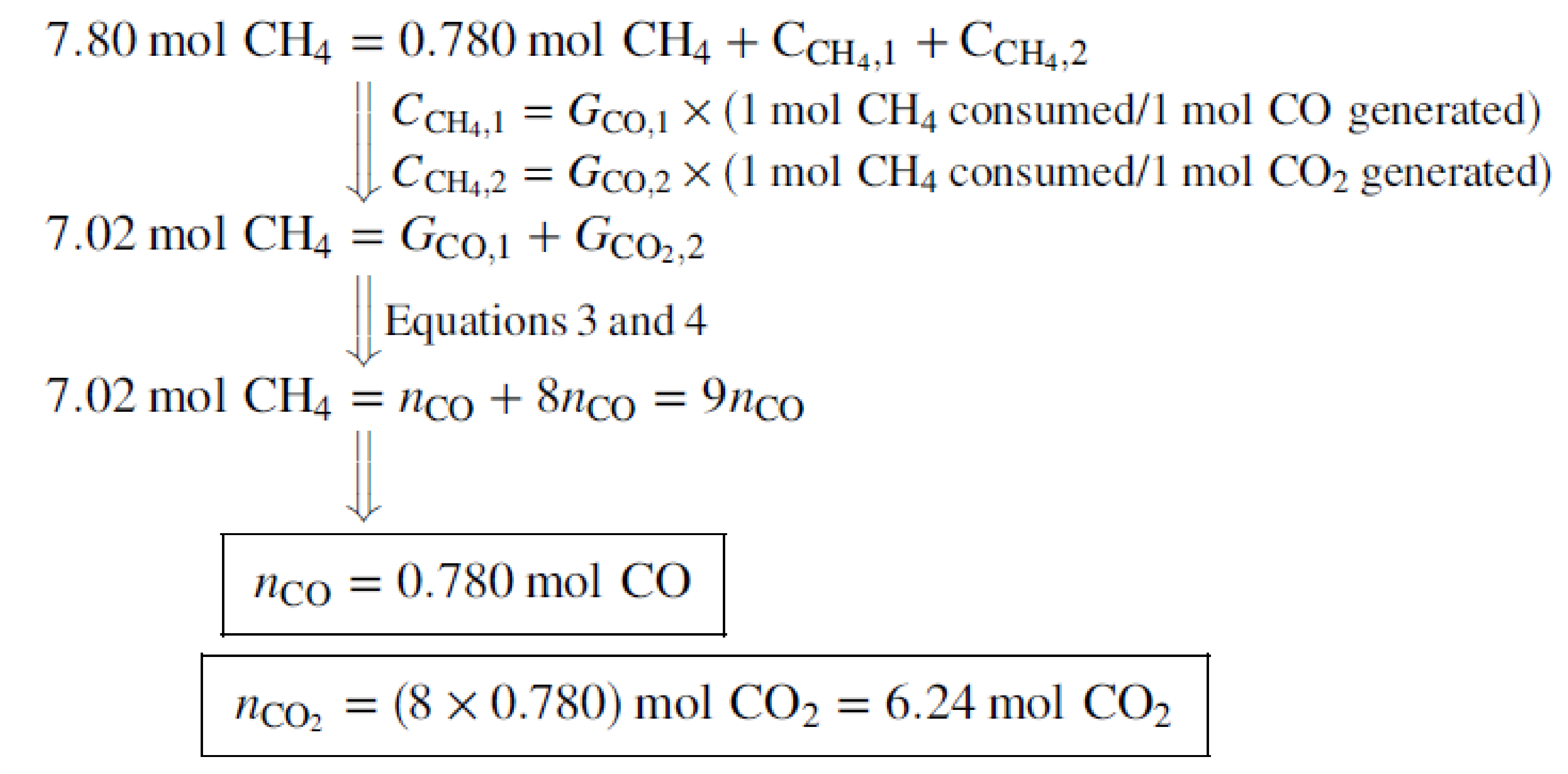
CO Balance: output = generation

$$n_{CO} = G_{CO,1}\ \ \mathbf{(3)}$$

CO$_2$ Balance: output = generation

$$8n_{CO} = G_{CO2,2}\ \mathbf{(4)}$$

CH_4 Balance: input = output + consumption



$$7.80 \text{ mol } CH_4 = 0.780 \text{ mol } CH_4 + C_{CH_4,1} + C_{CH_4,2}$$

$$\Big\Downarrow \begin{array}{l} C_{CH_4,1} = G_{CO,1} \times (1 \text{ mol } CH_4 \text{ consumed}/1 \text{ mol CO generated}) \\ C_{CH_4,2} = G_{CO,2} \times (1 \text{ mol } CH_4 \text{ consumed}/1 \text{ mol } CO_2 \text{ generated}) \end{array}$$

$$7.02 \text{ mol } CH_4 = G_{CO,1} + G_{CO_2,2}$$

$$\Big\Downarrow \text{Equations 3 and 4}$$

$$7.02 \text{ mol } CH_4 = n_{CO} + 8n_{CO} = 9n_{CO}$$

$$\Big\Downarrow$$

$$\boxed{n_{CO} = 0.780 \text{ mol CO}}$$

$$\boxed{n_{CO_2} = (8 \times 0.780) \text{ mol } CO_2 = 6.24 \text{ mol } CO_2}$$

$$n_{CO} = G_{CO,1} = 0.780 \; mol \; CO \; generated \qquad \mathbf{(5)}$$

$$8n_{CO} = G_{CO2,2} = 6.24 \; mol \; CO_2 \; generated \qquad \mathbf{(6)}$$

H_2O Balance: output = generation

$$n_{\mathrm{H_2O}} = G_{\mathrm{H_2O},1} + G_{\mathrm{H_2O},2}$$

$$= G_{\mathrm{CO},1}\left(\frac{2 \text{ mol } \mathrm{H_2O} \text{ generated}}{1 \text{ mol CO generated}}\right) + G_{\mathrm{CO_2},2}\left(\frac{2 \text{ mol } \mathrm{H_2O} \text{ generated}}{1 \text{ mol } \mathrm{CO_2} \text{ generated}}\right)$$

$$\Downarrow G_{\mathrm{CO},1} = 0.780 \text{ mol CO generated}, \; G_{\mathrm{CO_2},2} = 6.24 \text{ mol } \mathrm{CO_2} \text{ generated}$$

$$\boxed{n_{\mathrm{H_2O}} = 14.0 \text{ mol } \mathrm{H_2O}}$$

O_2 Balance: output = generation – consumption

$$n_{\mathrm{O_2}} = 19.4 \text{ mol } \mathrm{O_2} - C_{\mathrm{O_2},1} - C_{\mathrm{O_2},2}$$

$$= 19.4 \text{ mol } \mathrm{O_2} - G_{\mathrm{CO},1}\left(\frac{1.5 \text{ mol } \mathrm{O_2} \text{ consumed}}{1 \text{ mol CO generated}}\right) + G_{\mathrm{CO_2},2}\left(\frac{2 \text{ mol } \mathrm{O_2} \text{ consumed}}{1 \text{ mol } \mathrm{CO_2} \text{ generated}}\right)$$

$$\Downarrow G_{\mathrm{CO},1} = 0.780 \text{ mol CO generated}, \; G_{\mathrm{CO_2},2} = 6.24 \text{ mol } \mathrm{CO_2} \text{ generated}$$

$$\boxed{n_{\mathrm{O_2}} = 5.75 \text{ mol } \mathrm{O_2}}$$

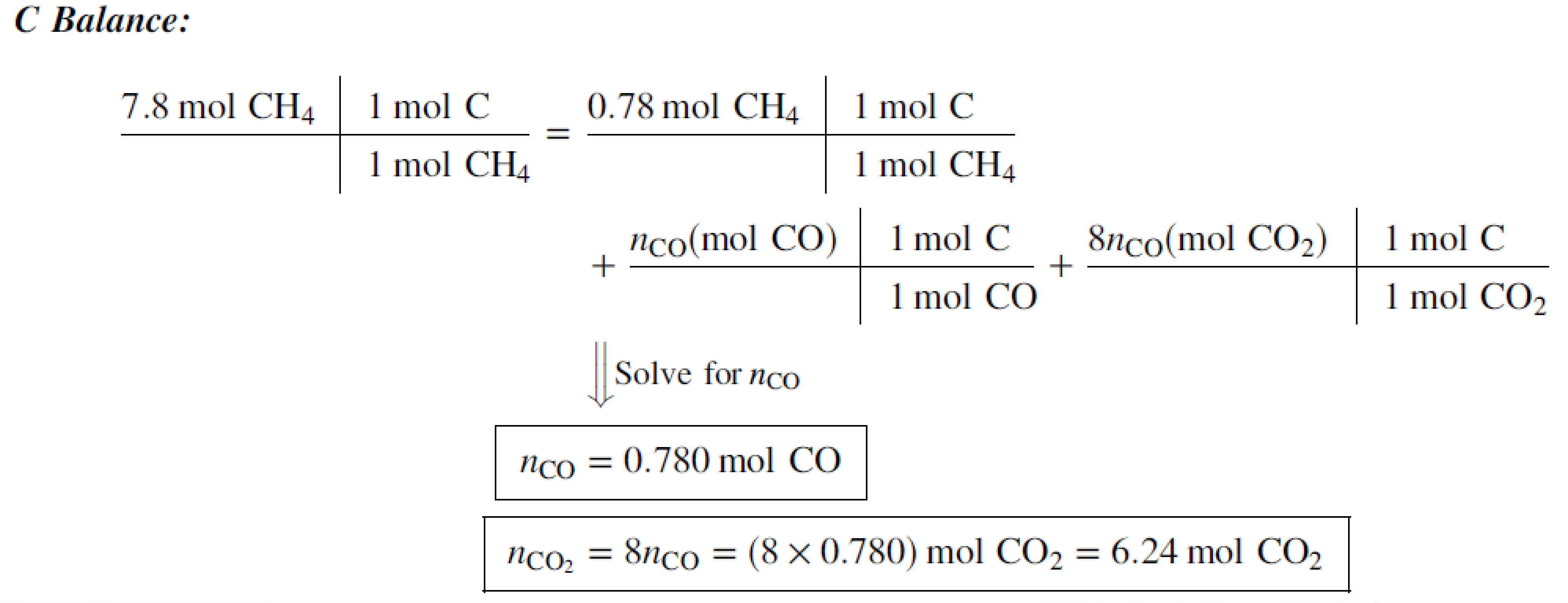
In summary, the stack gas contains 0.780 mol CH_4, 0.780 mol CO, 6.24 mol CO_2, 14.0 mol H_2O, 5.75 mol O_2, and 72.8 mol N_2. The molar composition of the gas is therefore

$$\boxed{0.78\% \; \mathrm{CH_4}, 0.78\% \; \mathrm{CO}, 6.2\% \; \mathrm{CO_2}, 14.0\% \; \mathrm{H_2O}, 5.7\% \; \mathrm{O_2}, \text{ and } 72.5\% \; \mathrm{N_2}}$$

Atomic Species Balances

We will write the C and H balances first (only one unknown), then the O balance to determine the remaining unknown.

All atomic species balances have the form ***input = output***.



C Balance:

$$\frac{7.8\text{ mol CH}_4}{} \left| \frac{1\text{ mol C}}{1\text{ mol CH}_4} \right. = \frac{0.78\text{ mol CH}_4}{} \left| \frac{1\text{ mol C}}{1\text{ mol CH}_4} \right.$$

$$+ \frac{n_{CO}(\text{mol CO})}{} \left| \frac{1\text{ mol C}}{1\text{ mol CO}} \right. + \frac{8n_{CO}(\text{mol CO}_2)}{} \left| \frac{1\text{ mol C}}{1\text{ mol CO}_2} \right.$$

$$\Downarrow \text{Solve for } n_{CO}$$

$$\boxed{n_{CO} = 0.780\text{ mol CO}}$$

$$\boxed{n_{CO_2} = 8n_{CO} = (8 \times 0.780)\text{ mol CO}_2 = 6.24\text{ mol CO}_2}$$

H Balance:

$$\begin{array}{c|c} 7.8\ \text{mol CH}_4 & 4\ \text{mol H} \\ \hline & 1\ \text{mol CH}_4 \end{array} = \begin{array}{c|c} 0.78\ \text{mol CH}_4 & 4\ \text{mol H} \\ \hline & 1\ \text{mol CH}_4 \end{array} + \begin{array}{c|c} n_{H_2O}(\text{mol H}_2\text{O}) & 2\ \text{mol H} \\ \hline & 1\ \text{mol H}_2\text{O} \end{array} \Longrightarrow \boxed{n_{H_2O} = 14.0\ \text{mol H}_2\text{O}}$$

O Balance:

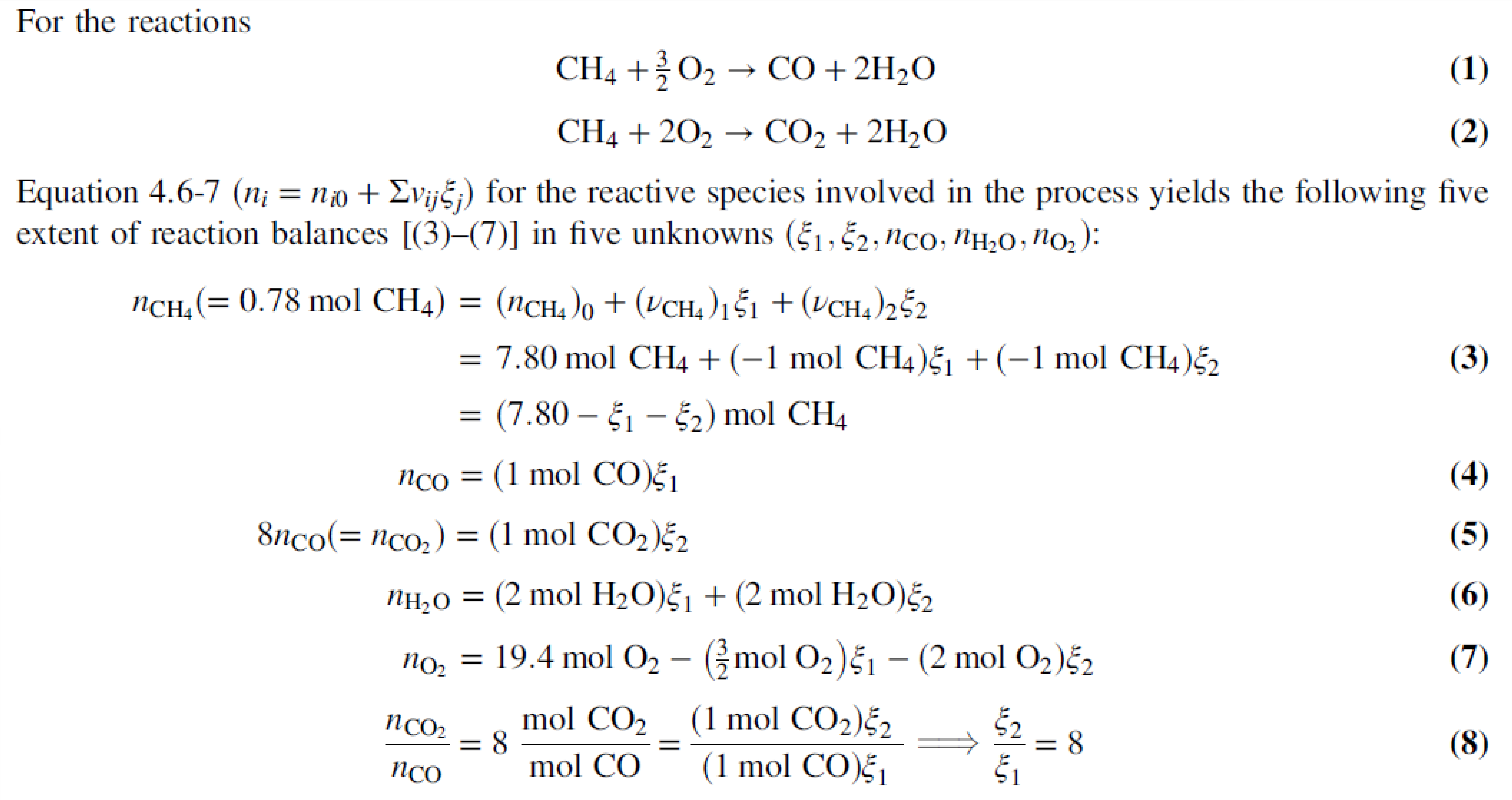
$$\begin{array}{c|c} 19.4\ \text{mol O}_2 & 2\ \text{mol O} \\ \hline & 1\ \text{mol O}_2 \end{array} = \begin{array}{c|c} n_{O_2}(\text{mol O}_2) & 2\ \text{mol O} \\ \hline & 1\ \text{mol O}_2 \end{array} + \begin{array}{c|c} 0.78\ \text{mol CO} & 1\ \text{mol O} \\ \hline & 1\ \text{mol CO} \end{array}$$

$$+ \begin{array}{c|c} 6.24\ \text{mol CO}_2 & 2\ \text{mol O} \\ \hline & 1\ \text{mol CO}_2 \end{array} + \begin{array}{c|c} 14.0\ \text{mol H}_2\text{O} & 1\ \text{mol O} \\ \hline & 1\ \text{mol H}_2\text{O} \end{array}$$

$$\Longrightarrow \boxed{n_{O_2} = 5.75\ \text{mol O}_2}$$

Same: $\boxed{0.78\%\ \text{CH}_4,\ 0.78\%\ \text{CO},\ 6.2\%\ \text{CO}_2,\ 14.0\%\ \text{H}_2\text{O},\ 5.7\%\ \text{O}_2,\ \text{and } 72.5\%\ \text{N}_2}$

Extents of Reaction



For the reactions

$$CH_4 + \tfrac{3}{2}O_2 \rightarrow CO + 2H_2O \qquad \textbf{(1)}$$

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O \qquad \textbf{(2)}$$

Equation 4.6-7 ($n_i = n_{i0} + \Sigma v_{ij}\xi_j$) for the reactive species involved in the process yields the following five extent of reaction balances [(3)–(7)] in five unknowns ($\xi_1, \xi_2, n_{CO}, n_{H_2O}, n_{O_2}$):

$$\begin{aligned} n_{CH_4}(= 0.78 \text{ mol } CH_4) &= (n_{CH_4})_0 + (\nu_{CH_4})_1\xi_1 + (\nu_{CH_4})_2\xi_2 \\ &= 7.80 \text{ mol } CH_4 + (-1 \text{ mol } CH_4)\xi_1 + (-1 \text{ mol } CH_4)\xi_2 \qquad \textbf{(3)} \\ &= (7.80 - \xi_1 - \xi_2) \text{ mol } CH_4 \end{aligned}$$

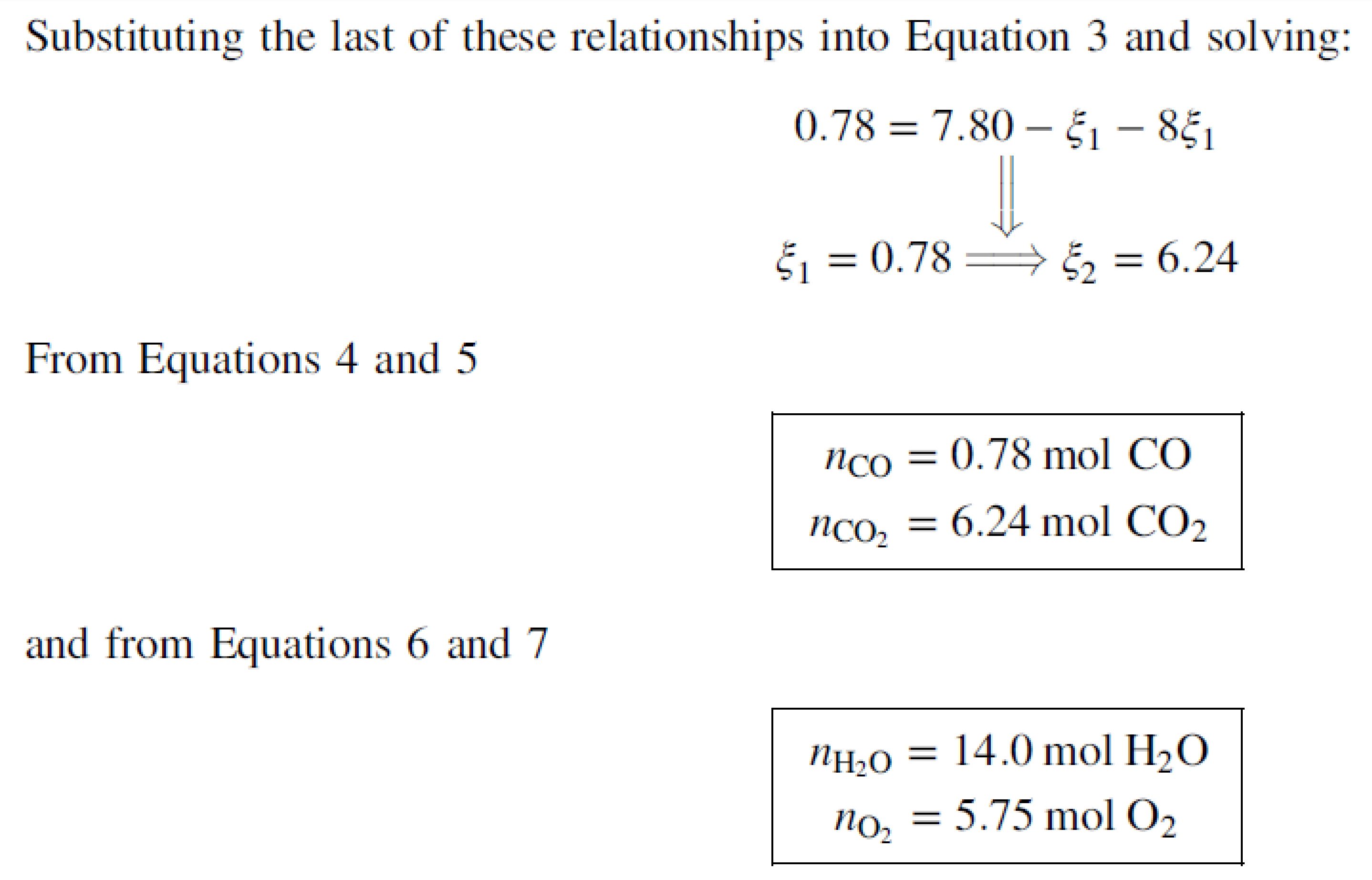
$$n_{CO} = (1 \text{ mol } CO)\xi_1 \qquad \textbf{(4)}$$

$$8n_{CO}(= n_{CO_2}) = (1 \text{ mol } CO_2)\xi_2 \qquad \textbf{(5)}$$

$$n_{H_2O} = (2 \text{ mol } H_2O)\xi_1 + (2 \text{ mol } H_2O)\xi_2 \qquad \textbf{(6)}$$

$$n_{O_2} = 19.4 \text{ mol } O_2 - \left(\tfrac{3}{2}\text{mol } O_2\right)\xi_1 - (2 \text{ mol } O_2)\xi_2 \qquad \textbf{(7)}$$

$$\frac{n_{CO_2}}{n_{CO}} = 8\,\frac{\text{mol } CO_2}{\text{mol } CO} = \frac{(1 \text{ mol } CO_2)\xi_2}{(1 \text{ mol } CO)\xi_1} \Longrightarrow \frac{\xi_2}{\xi_1} = 8 \qquad \textbf{(8)}$$



Substituting the last of these relationships into Equation 3 and solving:

$$0.78 = 7.80 - \xi_1 - 8\xi_1$$

$$\Downarrow$$

$$\xi_1 = 0.78 \Longrightarrow \xi_2 = 6.24$$

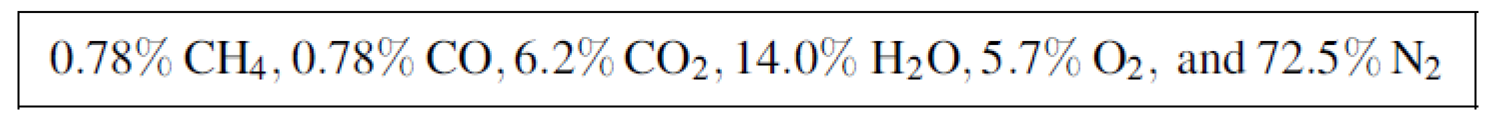
From Equations 4 and 5

$$\boxed{\begin{aligned} n_{CO} &= 0.78 \text{ mol CO} \\ n_{CO_2} &= 6.24 \text{ mol } CO_2 \end{aligned}}$$

and from Equations 6 and 7

$$\boxed{\begin{aligned} n_{H_2O} &= 14.0 \text{ mol } H_2O \\ n_{O_2} &= 5.75 \text{ mol } O_2 \end{aligned}}$$

Same:



$$\boxed{0.78\% \ CH_4, 0.78\% \ CO, 6.2\% \ CO_2, 14.0\% \ H_2O, 5.7\% \ O_2, \text{ and } 72.5\% \ N_2}$$

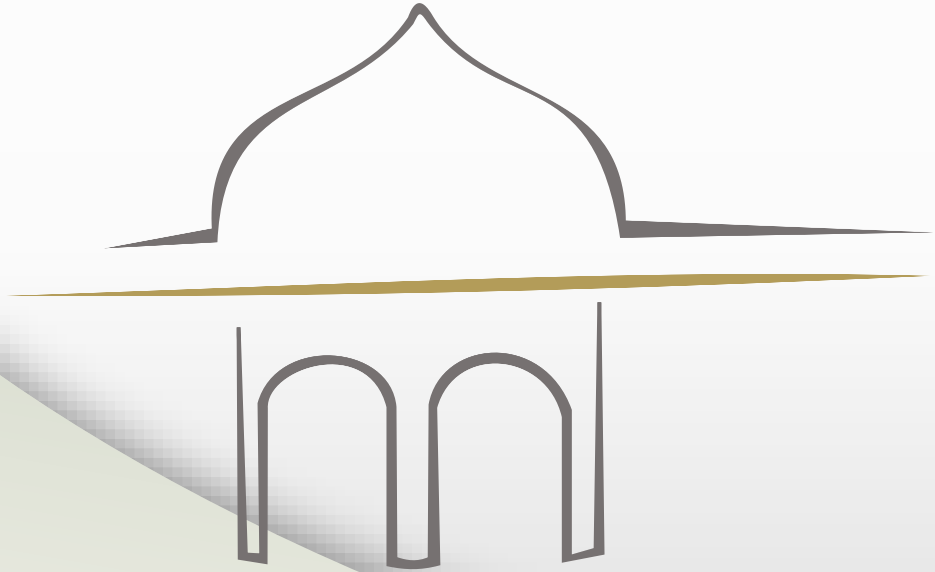
Which method is easy?

Important definitions from section 4.6

Yield and Selectivity

$$\text{Yield} = \frac{\text{moles of desired product formed}}{\substack{\text{moles that would be formed if there were no side reactions} \\ \text{and the limiting reactant were consumed completely}}} \times 100\% \qquad \textbf{(4.6-5)}$$

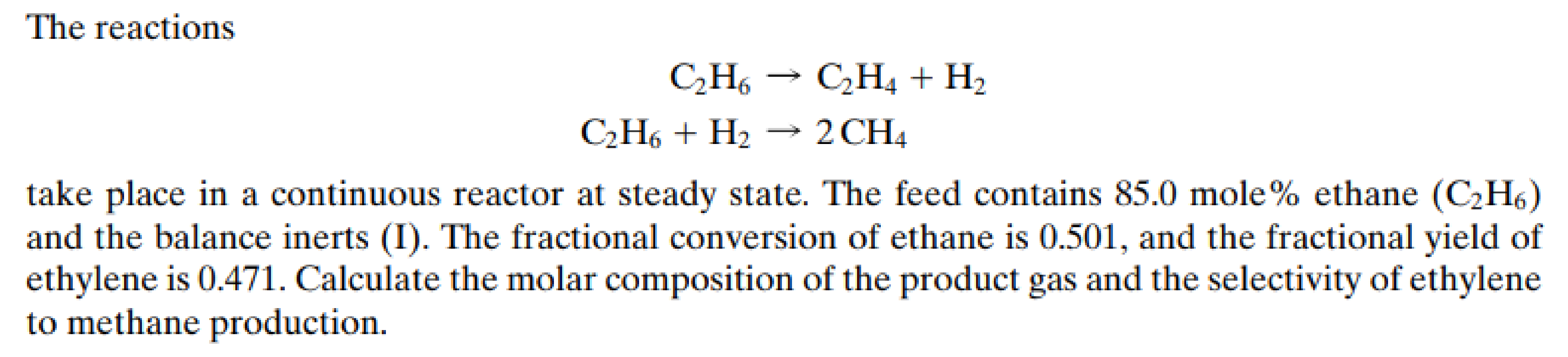
$$\text{Selectivity} = \frac{\text{moles of desired product formed}}{\text{moles of undesired product formed}} \qquad \textbf{(4.6-6)}$$



Problem Solving

Exercise 2:

Yield and selectivity in a dehydrogenation reactor



The reactions

$$C_2H_6 \rightarrow C_2H_4 + H_2$$
$$C_2H_6 + H_2 \rightarrow 2\,CH_4$$

take place in a continuous reactor at steady state. The feed contains 85.0 mole% ethane (C_2H_6) and the balance inerts (I). The fractional conversion of ethane is 0.501, and the fractional yield of ethylene is 0.471. Calculate the molar composition of the product gas and the selectivity of ethylene to methane production.

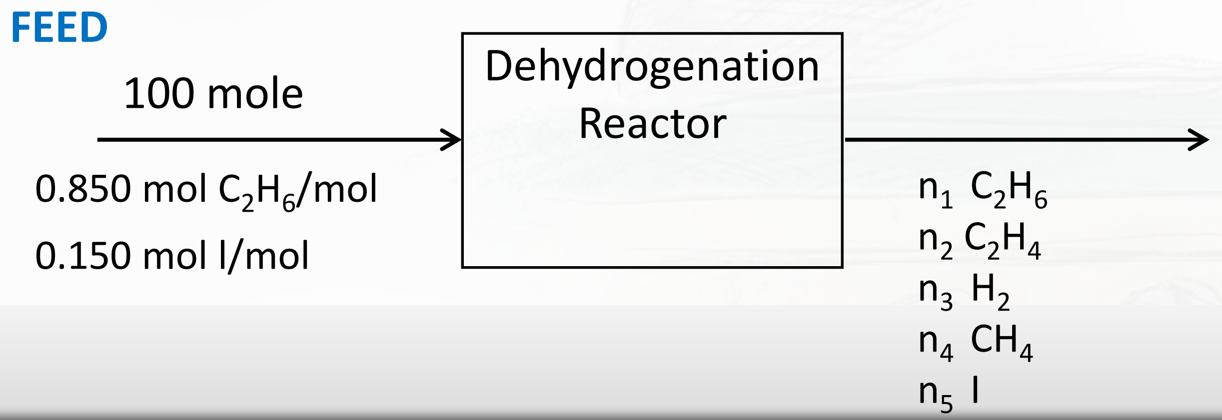
Basis: 100 mol feed

Ethane Ethylene

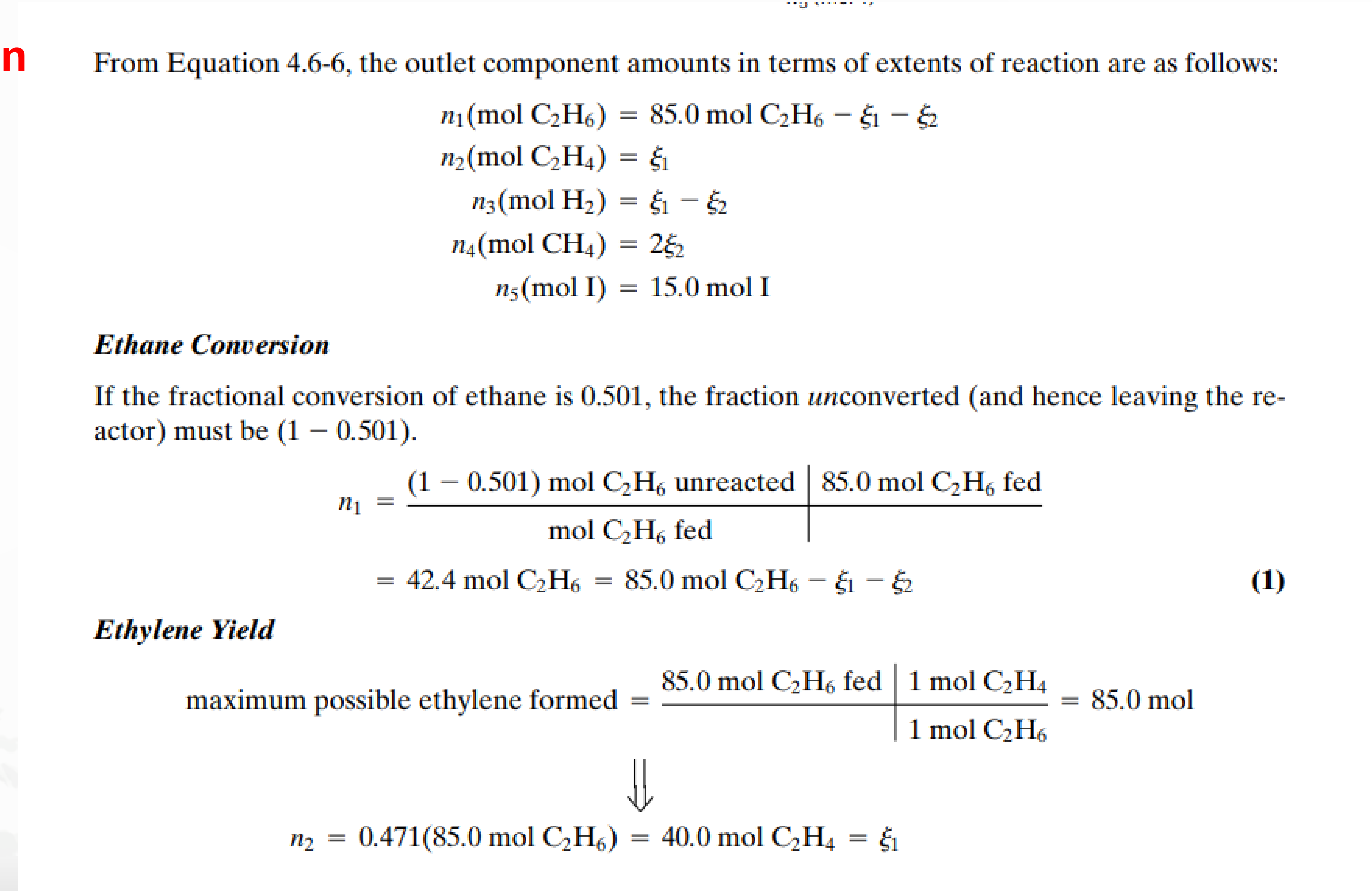
$C_2H_6 \rightarrow C_2H_4 + H_2$

Methane

$C_2H_6 + H_2 \rightarrow 2CH_4$



Solution



From Equation 4.6-6, the outlet component amounts in terms of extents of reaction are as follows:

$$\begin{aligned} n_1(\text{mol } C_2H_6) &= 85.0 \text{ mol } C_2H_6 - \xi_1 - \xi_2 \\ n_2(\text{mol } C_2H_4) &= \xi_1 \\ n_3(\text{mol } H_2) &= \xi_1 - \xi_2 \\ n_4(\text{mol } CH_4) &= 2\xi_2 \\ n_5(\text{mol I}) &= 15.0 \text{ mol I} \end{aligned}$$

Ethane Conversion

If the fractional conversion of ethane is 0.501, the fraction *un*converted (and hence leaving the reactor) must be (1 − 0.501).

$$n_1 = \frac{(1-0.501) \text{ mol } C_2H_6 \text{ unreacted}}{\text{mol } C_2H_6 \text{ fed}} \left| \frac{85.0 \text{ mol } C_2H_6 \text{ fed}}{} \right.$$

$$= 42.4 \text{ mol } C_2H_6 = 85.0 \text{ mol } C_2H_6 - \xi_1 - \xi_2 \qquad \textbf{(1)}$$

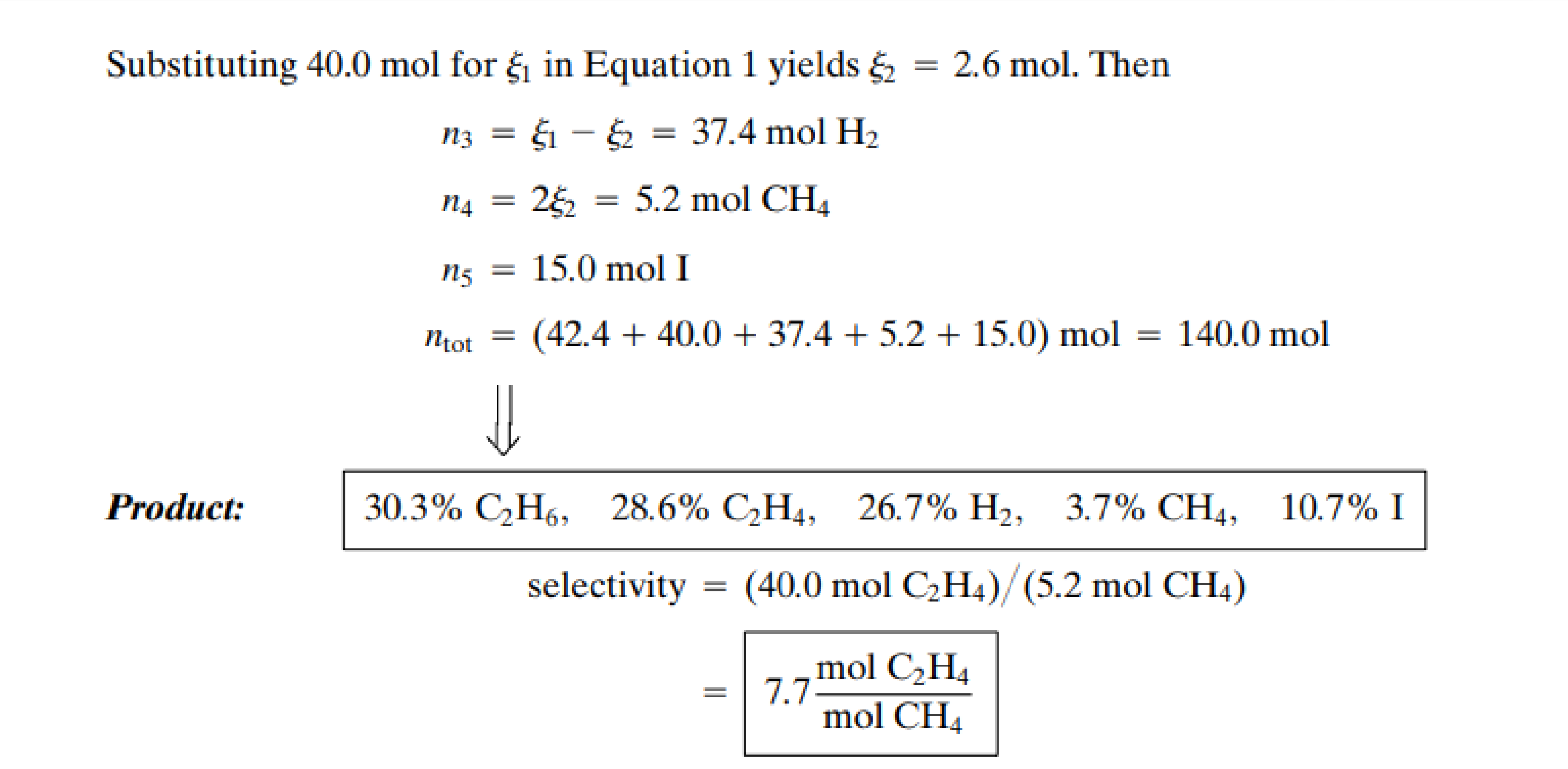
Ethylene Yield

$$\text{maximum possible ethylene formed} = \frac{85.0 \text{ mol } C_2H_6 \text{ fed}}{} \left| \frac{1 \text{ mol } C_2H_4}{1 \text{ mol } C_2H_6} \right. = 85.0 \text{ mol}$$

$$\Downarrow$$

$$n_2 = 0.471(85.0 \text{ mol } C_2H_6) = 40.0 \text{ mol } C_2H_4 = \xi_1$$

Solution



Substituting 40.0 mol for ξ_1 in Equation 1 yields $\xi_2 = 2.6$ mol. Then

$$n_3 = \xi_1 - \xi_2 = 37.4 \text{ mol } H_2$$

$$n_4 = 2\xi_2 = 5.2 \text{ mol } CH_4$$

$$n_5 = 15.0 \text{ mol I}$$

$$n_{tot} = (42.4 + 40.0 + 37.4 + 5.2 + 15.0) \text{ mol} = 140.0 \text{ mol}$$

$$\Downarrow$$

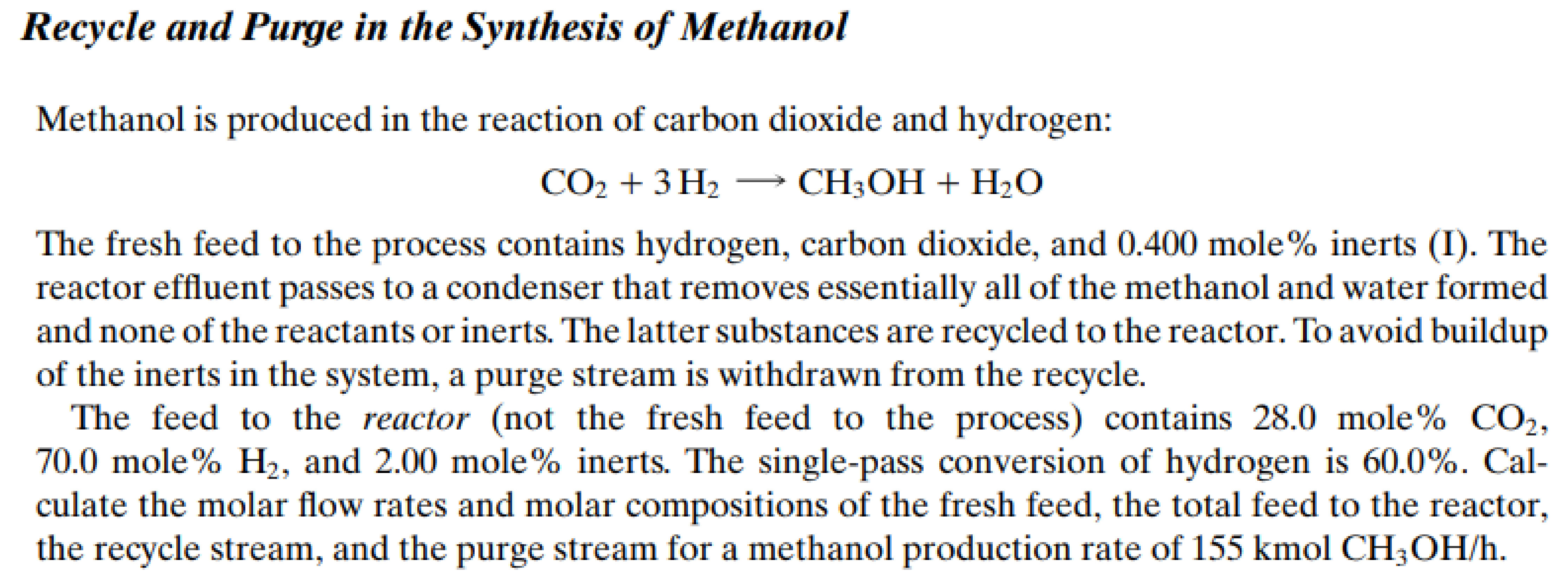
Product: $\boxed{30.3\%\ C_2H_6,\quad 28.6\%\ C_2H_4,\quad 26.7\%\ H_2,\quad 3.7\%\ CH_4,\quad 10.7\%\ I}$

$$\text{selectivity} = (40.0 \text{ mol } C_2H_4)/(5.2 \text{ mol } CH_4)$$

$$= \boxed{7.7 \frac{\text{mol } C_2H_4}{\text{mol } CH_4}}$$

Exercise 3: Recycle and purge in the synesis of Methanol

Presented in
an earlier
lecture



Recycle and Purge in the Synthesis of Methanol

Methanol is produced in the reaction of carbon dioxide and hydrogen:

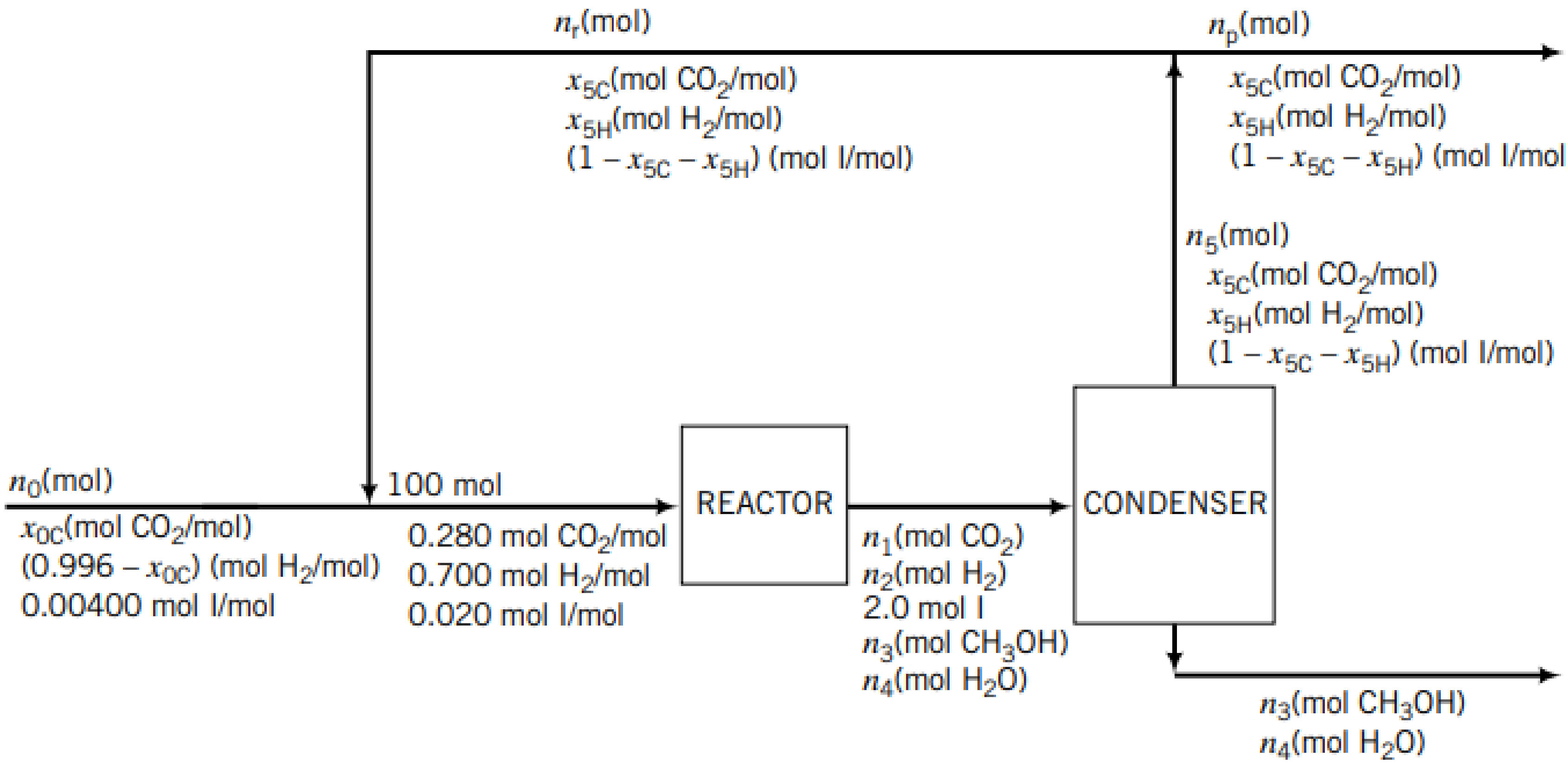
$$CO_2 + 3\,H_2 \longrightarrow CH_3OH + H_2O$$

The fresh feed to the process contains hydrogen, carbon dioxide, and 0.400 mole% inerts (I). The reactor effluent passes to a condenser that removes essentially all of the methanol and water formed and none of the reactants or inerts. The latter substances are recycled to the reactor. To avoid buildup of the inerts in the system, a purge stream is withdrawn from the recycle.

The feed to the *reactor* (not the fresh feed to the process) contains 28.0 mole% CO_2, 70.0 mole% H_2, and 2.00 mole% inerts. The single-pass conversion of hydrogen is 60.0%. Calculate the molar flow rates and molar compositions of the fresh feed, the total feed to the reactor, the recycle stream, and the purge stream for a methanol production rate of 155 kmol CH_3OH/h.

Exercise 3: Recycle and purge in the synesis of Methanol

Basis: 100 mol Combined Feed to the Reactor



n_r(mol)
x_{5C}(mol CO_2/mol)
x_{5H}(mol H_2/mol)
$(1 - x_{5C} - x_{5H})$ (mol I/mol)

n_p(mol)
x_{5C}(mol CO_2/mol)
x_{5H}(mol H_2/mol)
$(1 - x_{5C} - x_{5H})$ (mol I/mol)

n_5(mol)
x_{5C}(mol CO_2/mol)
x_{5H}(mol H_2/mol)
$(1 - x_{5C} - x_{5H})$ (mol I/mol)

n_0(mol)
x_{0C}(mol CO_2/mol)
$(0.996 - x_{0C})$ (mol H_2/mol)
0.00400 mol I/mol

100 mol
0.280 mol CO_2/mol
0.700 mol H_2/mol
0.020 mol I/mol

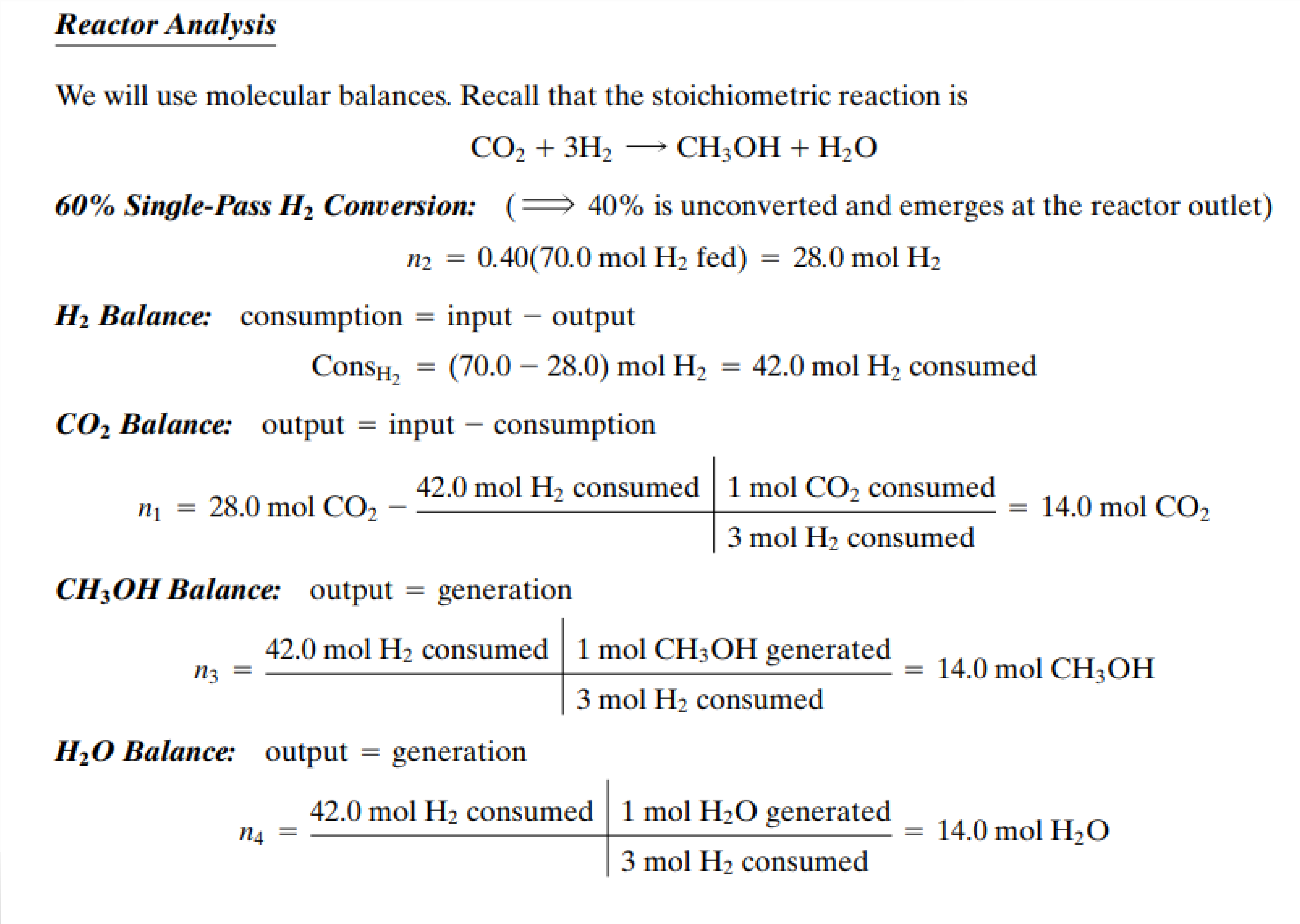
REACTOR

n_1(mol CO_2)
n_2(mol H_2)
2.0 mol I
n_3(mol CH_3OH)
n_4(mol H_2O)

CONDENSER

n_3(mol CH_3OH)
n_4(mol H_2O)

Solution



Reactor Analysis

We will use molecular balances. Recall that the stoichiometric reaction is

$$CO_2 + 3H_2 \longrightarrow CH_3OH + H_2O$$

60% Single-Pass H_2 Conversion: ($\Longrightarrow$ 40% is unconverted and emerges at the reactor outlet)

$$n_2 = 0.40(70.0 \text{ mol } H_2 \text{ fed}) = 28.0 \text{ mol } H_2$$

H_2 Balance: consumption = input − output

$$\text{Cons}_{H_2} = (70.0 - 28.0) \text{ mol } H_2 = 42.0 \text{ mol } H_2 \text{ consumed}$$

CO_2 Balance: output = input − consumption

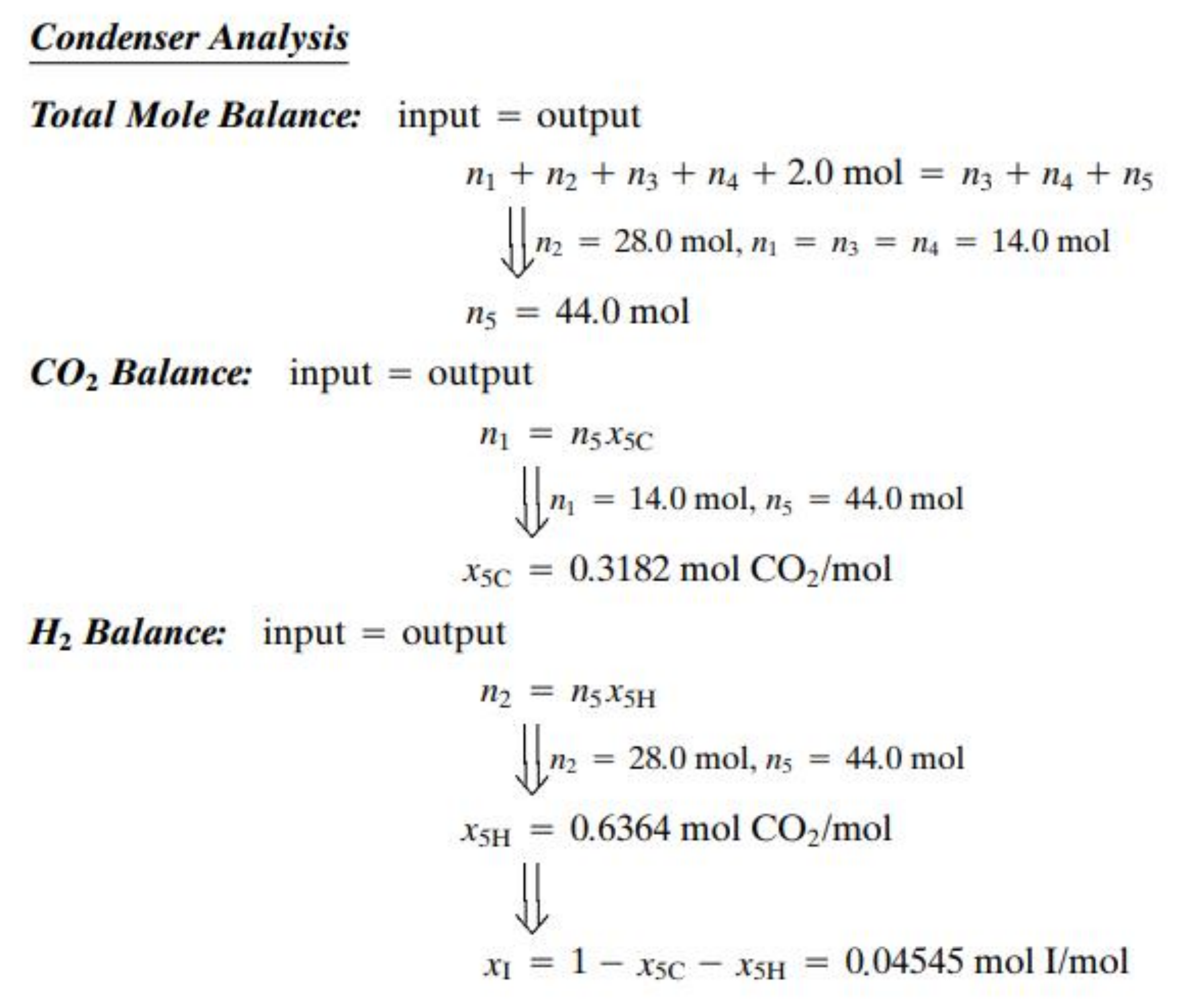
$$n_1 = 28.0 \text{ mol } CO_2 - \frac{42.0 \text{ mol } H_2 \text{ consumed} \,\big|\, 1 \text{ mol } CO_2 \text{ consumed}}{\big|\, 3 \text{ mol } H_2 \text{ consumed}} = 14.0 \text{ mol } CO_2$$

CH_3OH Balance: output = generation

$$n_3 = \frac{42.0 \text{ mol } H_2 \text{ consumed} \,\big|\, 1 \text{ mol } CH_3OH \text{ generated}}{\big|\, 3 \text{ mol } H_2 \text{ consumed}} = 14.0 \text{ mol } CH_3OH$$

H_2O Balance: output = generation

$$n_4 = \frac{42.0 \text{ mol } H_2 \text{ consumed} \,\big|\, 1 \text{ mol } H_2O \text{ generated}}{\big|\, 3 \text{ mol } H_2 \text{ consumed}} = 14.0 \text{ mol } H_2O$$



Condenser Analysis

Total Mole Balance: input = output

$$n_1 + n_2 + n_3 + n_4 + 2.0\text{ mol} = n_3 + n_4 + n_5$$

$$\Big\Downarrow\, n_2 = 28.0\text{ mol},\ n_1 = n_3 = n_4 = 14.0\text{ mol}$$

$$n_5 = 44.0\text{ mol}$$

CO_2 Balance: input = output

$$n_1 = n_5 x_{5C}$$

$$\Big\Downarrow\, n_1 = 14.0\text{ mol},\ n_5 = 44.0\text{ mol}$$

$$x_{5C} = 0.3182\text{ mol } CO_2/\text{mol}$$

H_2 Balance: input = output

$$n_2 = n_5 x_{5H}$$

$$\Big\Downarrow\, n_2 = 28.0\text{ mol},\ n_5 = 44.0\text{ mol}$$

$$x_{5H} = 0.6364\text{ mol } CO_2/\text{mol}$$

$$\Big\Downarrow$$

$$x_I = 1 - x_{5C} - x_{5H} = 0.04545\text{ mol I/mol}$$

Fresh Feed–Recycle Mixing Point Analysis

Total Mole Balance: input = output

$$n_0 + n_r = 100 \text{ mol}$$

I Balance: input = output

$$n_0(0.00400) + n_r(0.04545) = 2.0 \text{ mol I}$$

Solving these two equations simultaneously yields

$$n_0 = 61.4 \text{ mol fresh feed},\ n_r = 38.6 \text{ mol recycle}$$

CO_2 Balance: input = output

$$n_0 x_{0C} + n_r x_{5C} = 28.0 \text{ mol } CO_2$$

$$\Big\Downarrow n_0 = 61.4 \text{ mol},\ n_r = 38.6 \text{ mol},\ x_{5C} = 0.3182 \text{ mol } CO_2/\text{mol}$$

$$x_{0C} = 0.256 \text{ mol } CO_2/\text{mol}$$

$$\Big\Downarrow$$

$$x_{0H} = (1 - x_{0C} - x_{0I}) = 0.740 \text{ mol } H_2/\text{mol}$$

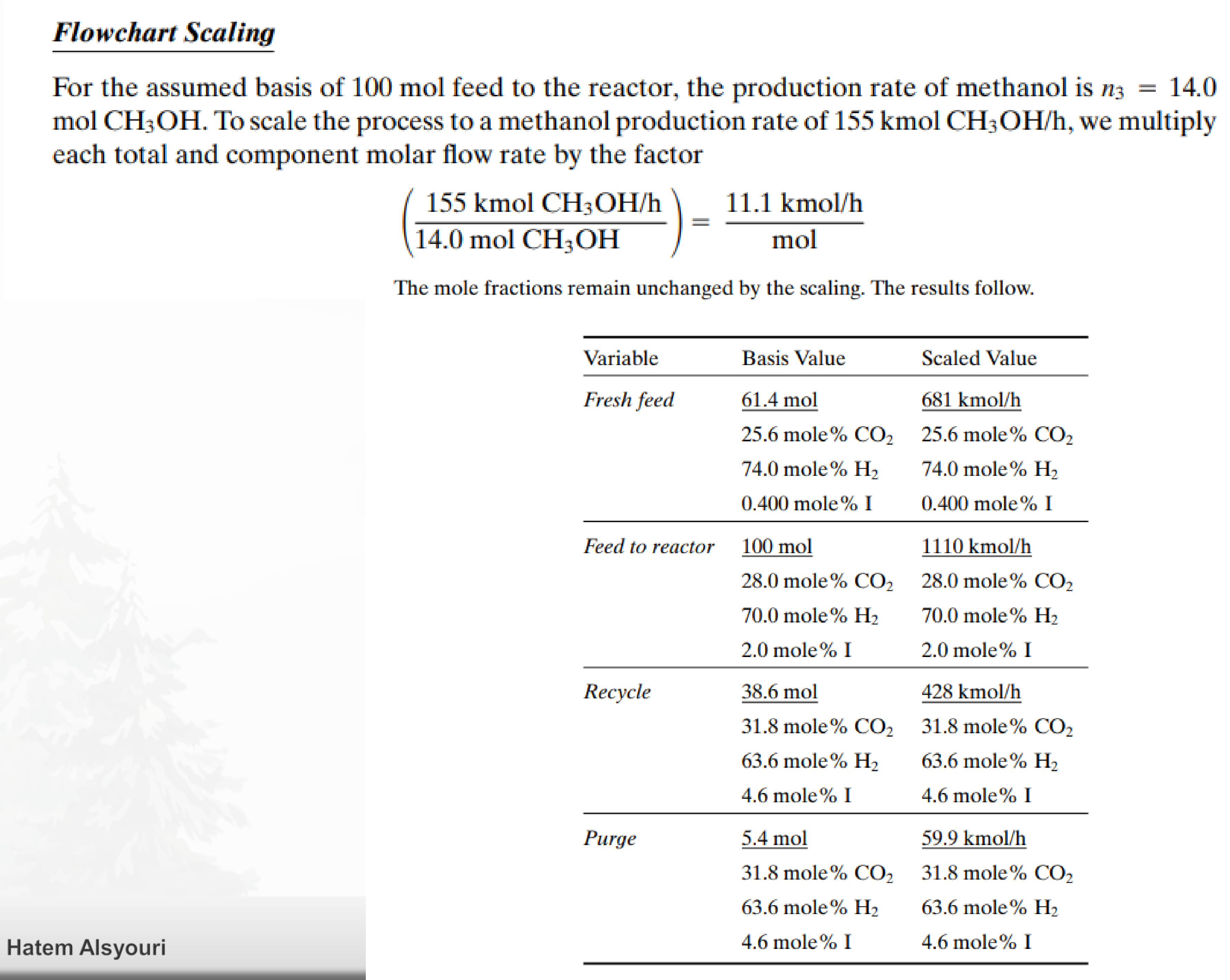
Recycle–Purge Splitting Point Analysis

Total Mole Balance: input = output

$$n_5 = n_r + n_p$$

$$\Big\Downarrow n_5 = 44.0 \text{ mol},\ n_r = 38.6 \text{ mol}$$

$$n_p = 5.4 \text{ mol purge}$$



Flowchart Scaling

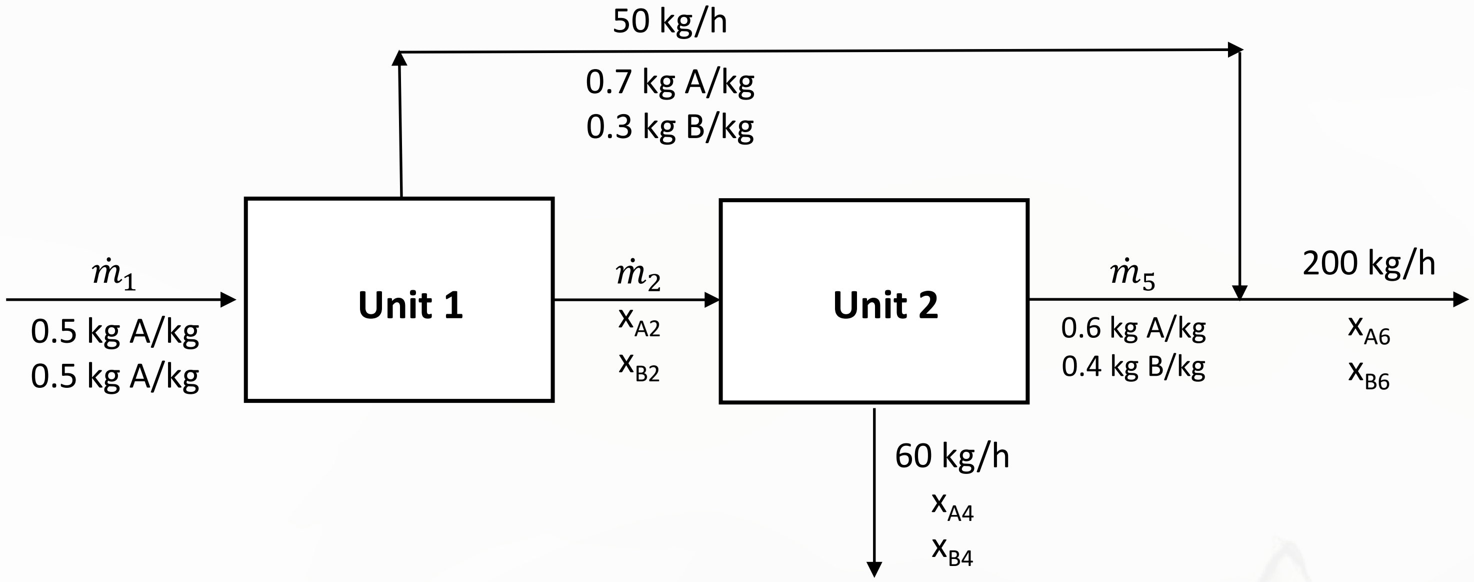
For the assumed basis of 100 mol feed to the reactor, the production rate of methanol is $n_3 = 14.0$ mol CH_3OH. To scale the process to a methanol production rate of 155 kmol CH_3OH/h, we multiply each total and component molar flow rate by the factor

$$\left(\frac{155 \text{ kmol } CH_3OH/h}{14.0 \text{ mol } CH_3OH}\right) = \frac{11.1 \text{ kmol/h}}{\text{mol}}$$

The mole fractions remain unchanged by the scaling. The results follow.

Variable	Basis Value	Scaled Value
Fresh feed	61.4 mol	681 kmol/h
	25.6 mole% CO_2	25.6 mole% CO_2
	74.0 mole% H_2	74.0 mole% H_2
	0.400 mole% I	0.400 mole% I
Feed to reactor	100 mol	1110 kmol/h
	28.0 mole% CO_2	28.0 mole% CO_2
	70.0 mole% H_2	70.0 mole% H_2
	2.0 mole% I	2.0 mole% I
Recycle	38.6 mol	428 kmol/h
	31.8 mole% CO_2	31.8 mole% CO_2
	63.6 mole% H_2	63.6 mole% H_2
	4.6 mole% I	4.6 mole% I
Purge	5.4 mol	59.9 kmol/h
	31.8 mole% CO_2	31.8 mole% CO_2
	63.6 mole% H_2	63.6 mole% H_2
	4.6 mole% I	4.6 mole% I

Exercise: Multiple unit process and recycle



Calculate:

1. DOF for the mixing point?
2. Mass flow for the stream 5 ($\dot{m}_5$)
3. Composition of the stream 6 (x_{A6} and x_{B6})
4. Mass flow for the stream 1 ($\dot{m}_1$)
5. Composition of the stream 4 (x_{A4} and x_{B4})
6. Mass flow for the stream 2 ($\dot{m}_2$)
7. Composition of the stream 2 (x_{A2} and x_{B2})

Exercise: Reactive Multiple units & combustion

A process for methanol synthesis is shown in the flowchart. The potential chemical reactions involved are

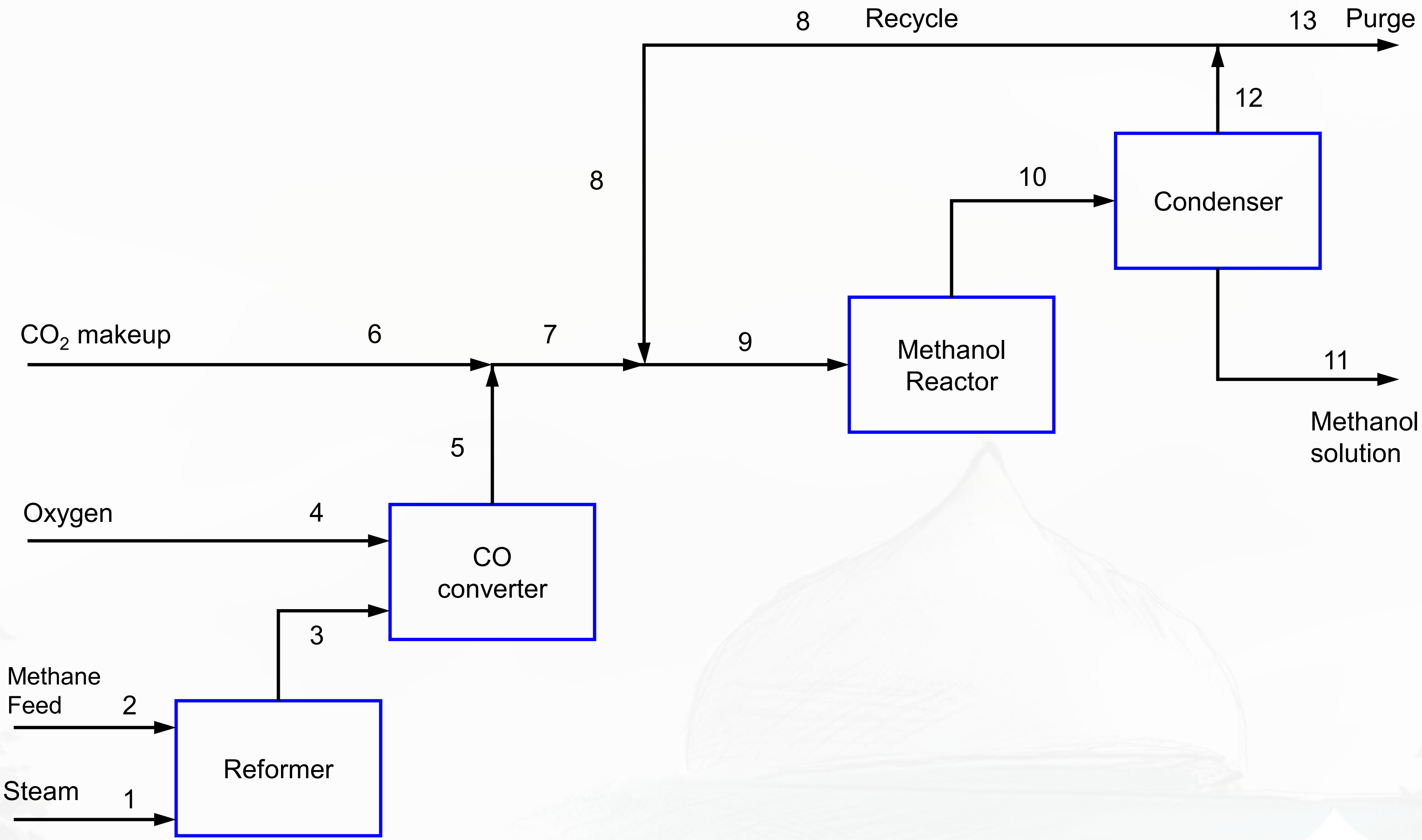
$CH_4 + 2H_2O \rightarrow CO_2 + 4H_2$	(main reformer reaction)	(a)
$CH_4 + H_2O \rightarrow CO + 3H_2$	(reformer side reaction)	(b)
$2CO + O_2 \rightarrow 2CO_2$	(CO converter reaction)	(c)
$CO_2 + 3H_2 \rightarrow CH_3OH + H_2O$	(methanol synthesis reaction)	(d)

Ten percent excess *steam*, based on reaction (a), is fed to the reformer, and conversion of methane is 100%, with a 90% yield of CO_2. Conversion in the methanol reactor is 55% on one pass through the reactor.
A stoichiometric quantity of oxygen is fed to the CO converter, and the CO is completely converted to CO_2. Additional makeup CO_2 is then introduced to establish a 3 to 1 ratio of H_2 to CO_2 in the feed stream to the methanol reactor.

The methanol reactor effluent is cooled to condense all the methanol and water, with non-condensible gases recycled to the methanol reactor feed. The H_2/CO_2 ratio in the recycle stream is also 3 to 1.
Because the methane feed contains 1% nitrogen as an impurity, a portion of the recycle stream must be purged as shown in the flowchart to prevent the accumulation of nitrogen in the system. The purge stream analyzes 5% nitrogen.

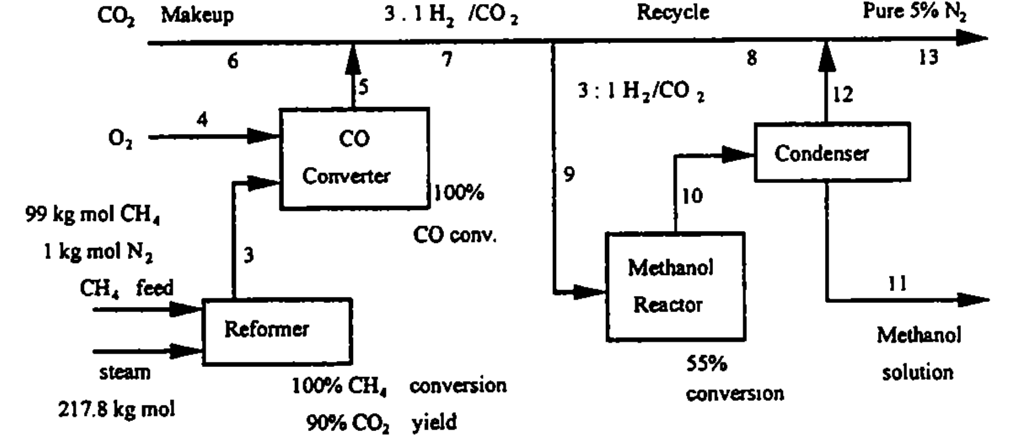
On the basis of 100 mol of methane feed (including the N_2), calculate:

i. How many moles of H_2 are lost in the purge
ii. How many moles of makeup CO_2 are required
iii. The recycle to purge ratio in mol/mol
iv. How much methanol solution (in kg) of what strength (weight percent) is produced.


8
Recycle
13
Purge
12
8
10
Condenser
CO$_2$ makeup
6
7
9
Methanol Reactor
11
Methanol solution
5
Oxygen
4
CO converter
3
Methane Feed
2
Reformer
Steam
1

12.25

Step 1, 2, 3 and 4:



Chemical Reactions

a) $CH_4 + 2H_2O \rightarrow CO_2 + 4H_2$ (main reformer rxn)

b) $CH_4 + H_2 \rightarrow CO + 3H_2$ (reformer side rxn)

c) $2CO + O_2 \rightarrow 2CO_2$ (CO converter rxn)

d) $CO_2 + 3H_2 \rightarrow CH_3OH + H_2O$ (methanol rxn)

CH_4 feed is 1% N_2 or 1 kg mol N_2

steam feed is 10% excess based on reaction (a).

$$99\text{ kg mol }CH_4\left(2\frac{\text{kg mol }H_2O}{\text{kg mol }CH_4}\right) = 198\text{ kg mol steam}$$

1.1 (198) = 217.8 kg mol steam

(continued)

Step 5: Basis: 100 kg mol CH_4 in feed

Steps 6 and 7: Unknowns:

3-reformer product

4-O_2 feed, stoichiometric

5-CO conv. products

6-CO_2 makeup

7-3:1 H_2/CO_2

8-recycle, H_2/CO_2=3

9-reactor feed, H_2/CO_2=3

10-reactor product

11-Methanol solution

12-condenser tops

13-purge, 5% N_2

Balances:

Reformer balance

CO conv. balance

CO_2 makeup balance

Feed/recycle balance

Methanol reactor balance

Condenser balance

purge/recycle balance

Steps 8 and 9: Solve balances serially.

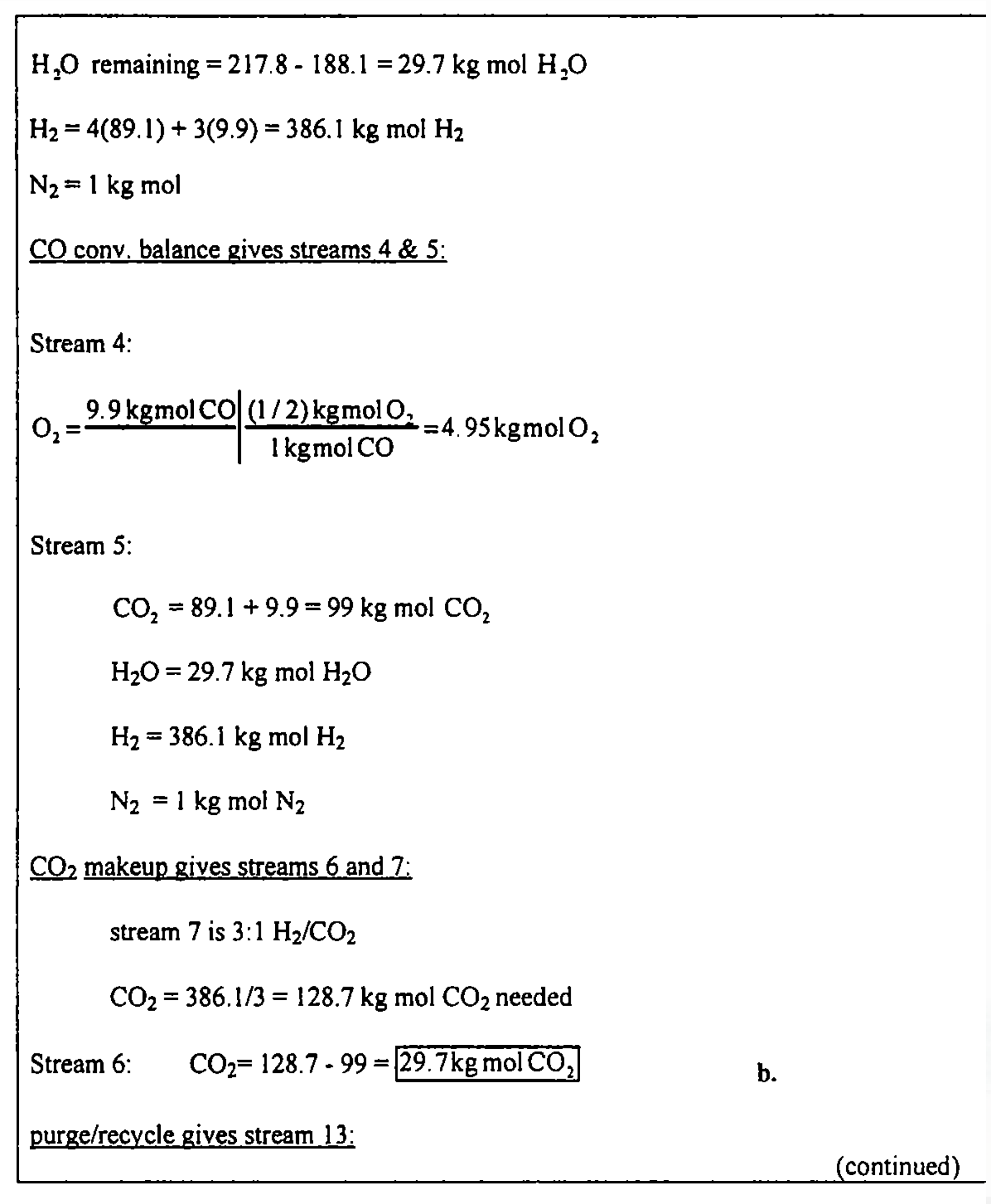
Reformer balance gives stream 3

$$CO_2 = \frac{99\text{ kgmol }CH_4\text{ conv.}}{}\left|\frac{0.9\text{ conv by (a)}}{1\text{ conv.}}\right|\frac{1\text{ kgmol }CO_2}{1\text{ kgmol }CH_4} = 89.1\text{ kgmol }CO_2$$

CO = 99(0.1) = 9.9 kg mol CO

$$H_2O\text{ reacted} = \frac{2\text{ kgmol }H_2O}{1\text{ kgmol }CO_2}\left|\frac{89.1\text{ kg mol }CO_2}{}\right.$$

$$+\frac{1\text{ kg mol }H_2O}{1\text{ kgmol }CO}\left|\frac{9.9\text{ kg mol }CO}{}\right. = 188.1\text{ kgmol }H_2O$$



H_2O remaining = 217.8 - 188.1 = 29.7 kg mol H_2O

H_2 = 4(89.1) + 3(9.9) = 386.1 kg mol H_2

N_2 = 1 kg mol

<u>CO conv. balance gives streams 4 & 5:</u>

Stream 4:

$$O_2 = \frac{9.9\,\text{kgmol CO}}{} \left| \frac{(1/2)\,\text{kgmol}\,O_2}{1\,\text{kgmol CO}} \right. = 4.95\,\text{kgmol}\,O_2$$

Stream 5:

CO_2 = 89.1 + 9.9 = 99 kg mol CO_2

H_2O = 29.7 kg mol H_2O

H_2 = 386.1 kg mol H_2

N_2 = 1 kg mol N_2

<u>CO_2 makeup gives streams 6 and 7:</u>

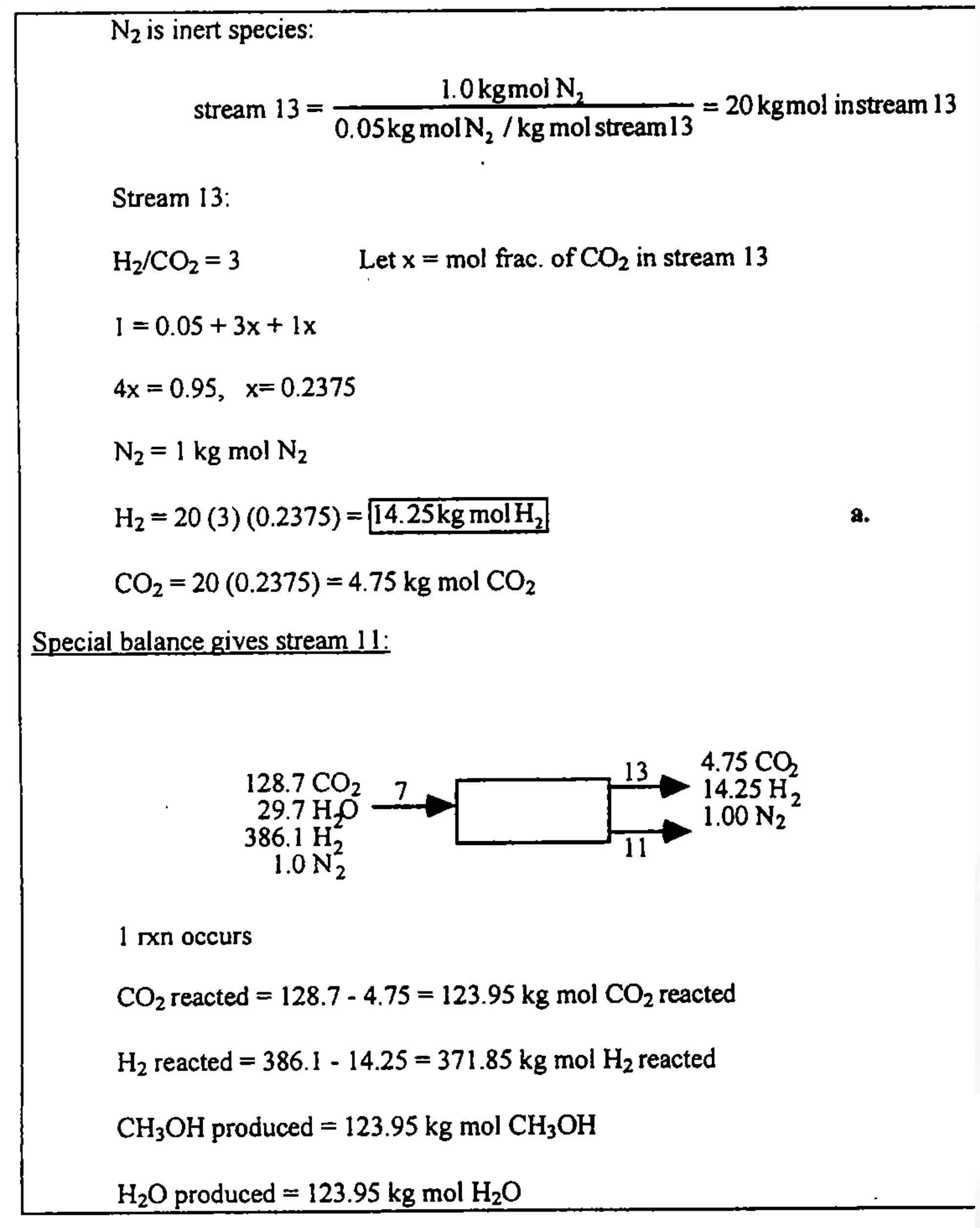
stream 7 is 3:1 H_2/CO_2

CO_2 = 386.1/3 = 128.7 kg mol CO_2 needed

Stream 6: CO_2= 128.7 - 99 = $\boxed{29.7\,\text{kg mol}\,CO_2}$ **b.**

<u>purge/recycle gives stream 13:</u>

(continued)



N_2 is inert species:

$$\text{stream 13} = \frac{1.0\,\text{kgmol}\,N_2}{0.05\,\text{kg mol}\,N_2\,/\,\text{kg mol stream 13}} = 20\,\text{kgmol in stream 13}$$

Stream 13:

$H_2/CO_2 = 3$ Let x = mol frac. of CO_2 in stream 13

$1 = 0.05 + 3x + 1x$

$4x = 0.95$, $x = 0.2375$

N_2 = 1 kg mol N_2

H_2 = 20 (3) (0.2375) = $\boxed{14.25\,\text{kg mol}\,H_2}$ **a.**

CO_2 = 20 (0.2375) = 4.75 kg mol CO_2

<u>Special balance gives stream 11:</u>

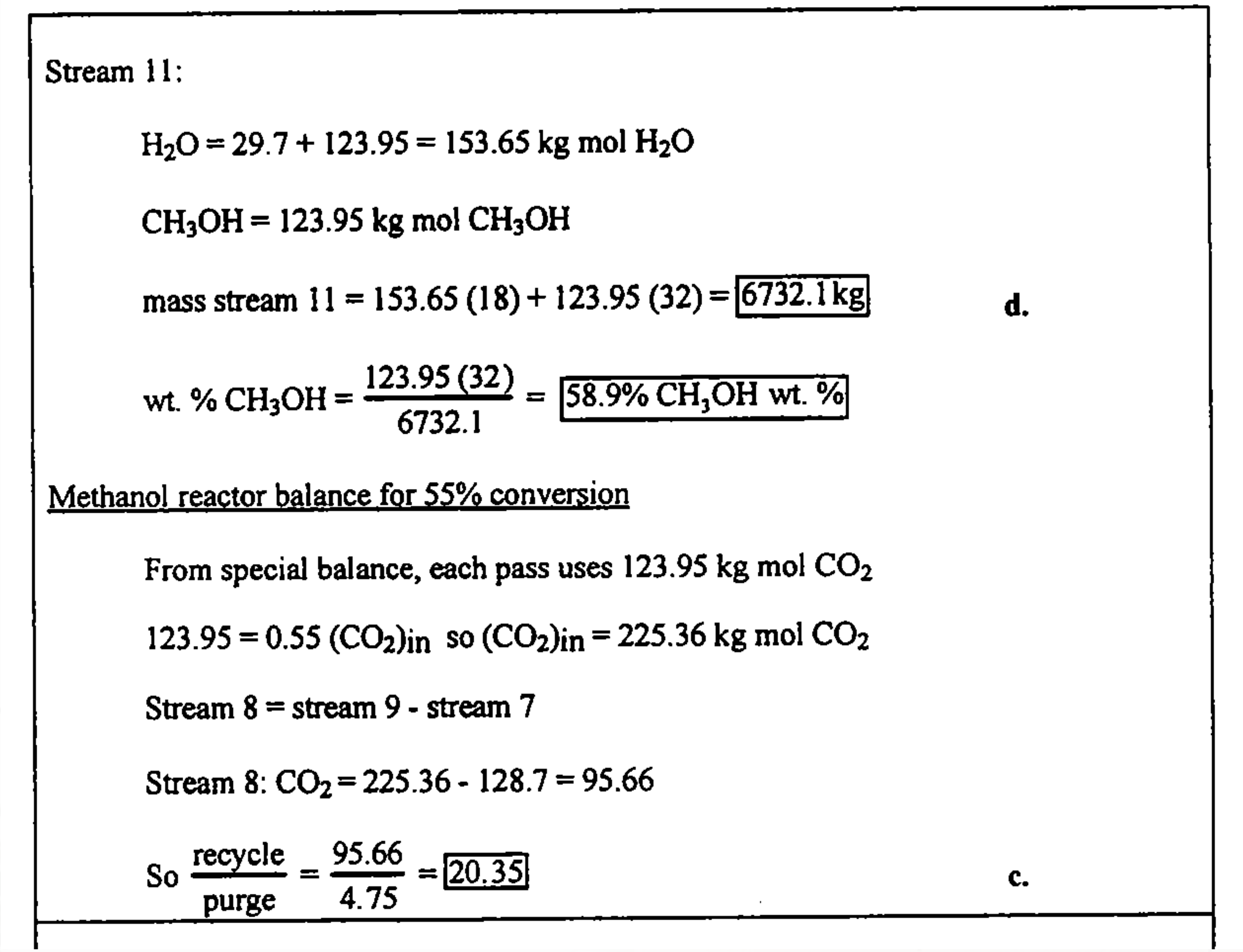
1 rxn occurs

CO_2 reacted = 128.7 - 4.75 = 123.95 kg mol CO_2 reacted

H_2 reacted = 386.1 - 14.25 = 371.85 kg mol H_2 reacted

CH_3OH produced = 123.95 kg mol CH_3OH

H_2O produced = 123.95 kg mol H_2O



Stream 11:

$H_2O = 29.7 + 123.95 = 153.65$ kg mol H_2O

$CH_3OH = 123.95$ kg mol CH_3OH

mass stream 11 = $153.65\,(18) + 123.95\,(32) = \boxed{6732.1\text{ kg}}$ **d.**

$$\text{wt. \% } CH_3OH = \frac{123.95\,(32)}{6732.1} = \boxed{58.9\%\ CH_3OH\text{ wt. \%}}$$

Methanol reactor balance for 55% conversion

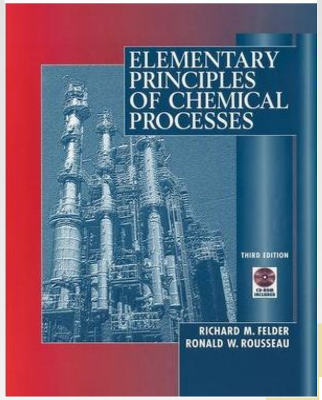
From special balance, each pass uses 123.95 kg mol CO_2

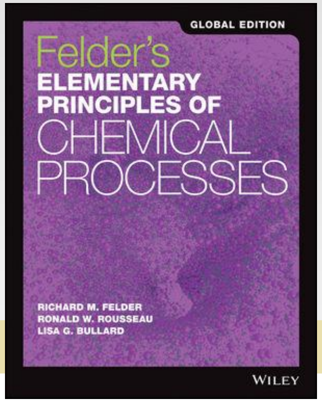
$123.95 = 0.55\,(CO_2)_{in}$ so $(CO_2)_{in} = 225.36$ kg mol CO_2

Stream 8 = stream 9 - stream 7

Stream 8: $CO_2 = 225.36 - 128.7 = 95.66$

$$\text{So } \frac{\text{recycle}}{\text{purge}} = \frac{95.66}{4.75} = \boxed{20.35}$$ **c.**





Elementary Principles of Chemical Processes,
3^{rd} or 4^{th} edition,
Wiley & Sons, Inc.
Richard M. Felder, Ronald W. Rousseau, & Lisa G. Bullard.

CHE 0905211

Chemical Engineering Principles 1

Fall 2025

Dr. Hatem Alsyouri	**Chapter 5**

The University of Jordan
Chemical Engineering Department

Week 9

Chapter 5 : Single-Phase Systems

Topics	**Lecture 1**	**5.1. Liquid and solid densities** **5.2. Ideal Gases** a. The ideal gas equation of state	Section 5.1 1, 2, 4
	Lecture 2	**5.2. Ideal Gases** b. Standard temperature and pressure	Section 5.2 a,b: 5, 7-9, 12, 14
	Lecture 3	**5.2. Ideal Gases** c. Ideal gas mixtures Problem solving	Section 5.2 c: 16, 18, 20, 22*, 25, 27, 30, 34*, 35, 39, 47
Learning Outcomes	LO11. Obtain and utilize physical property data for liquids, solids, and gases from reliable sources such as databases, handbooks, correlations, and experimental or literature data. (SO1) LO12. Perform pressure–volume–temperature calculations for ideal and non-ideal gases using appropriate equations of state and gas property charts. (SO1)		

Notes

This is only a sample material that does not cover the entire topics of the chapter.

Please refer to the textbook for full study, and solve the assigned exercises and suggested problems.

Refer to weekly lesson plan for details of covered topics

Introduction

- A gas enters a reactor at a rate of 255 ***SCMH***. What does that mean?
  standard vol flow rate → actual vol flow

- An orifice meter mounted in a process gas line indicates a flow rate of 24 ft^3/min. The gas temperature is 195^oF and the pressure is 62 psig. The gas is a mixture containing 70 mole% CO and the balance H_2. What is the mass flow rate of the hydrogen in the gas?
  vol flow + Temp + P_g → find mol flow → find mass flow

- A reactor feed stream consists of O_2 flowing at 32 kg/s. The gas is to be compressed from 37^oC and 2.8 atm absolute to 54^oC and 284 atm. What are the volumetric flow rates at the inlet and outlet (needed to rate the compressor)?
  mass flow + T1 + P1 → T2 + P2 → vol flow

- A pitot tube indicates that the velocity of a stack gas is 5.0 m/s at 175^oC. The stack diameter is 4.0 m. A continuous stack analyzer indicates an SO_2 level of 2500 ppm (2500 moles SO_2 per 10^6 moles gas). At what rate in kg/s is SO_2 being discharged into the atmosphere?
  Velocity + T + diameter + concentration → mass flow

- A 70.0 m^3 tank is rated at 2000 kPa. If 150 kg of helium is charged into the tank, what will the pressure be? How much more helium can be added before the rated pressure is attained?
  V + P + mass → P2

Answer **Need an equation of state (EOS)**

relationship between pressure (P), volume (V), number of moles (n), and temperature (T) of a gas.

5.2. Ideal Gases

ideal gas = perfect gas

5.2a. The ideal gas equation of state

The ideal gas (perfect gas) equation of state (relation between state variables) can be derived from the kinetic theory of gases by assuming that:

1. Gas molecules have a negligible volume,
2. Exert no forces on one another, and
3. Collide elastically with the walls of their container

assumptions of ideal gas

Ideal gas law $\boldsymbol{PV = nRT}$ or $\boldsymbol{P\dot{V} = \dot{n}RT}$

No need to know the type of gas

P = absolute pressure of a gas.

$V\ (\dot{V})$ = volume (or volumetric flow rate) of the gas.

$n\ (\dot{n})$ = number of moles (or molar flow rate) of the gas.

R = the gas constant, whose value depends on the units of P, V, n, and T.

T = absolute temperature of the gas.

Validity of equation: at high temperatures (> 0°C) and low pressures (~ 1 atm)

The gas constant (R)

Note
pressure x volume
= energy

Value of R depends on the units of P, V, n, and T

R =

$0.08206\ L \cdot atm/(mol.K)$	$8.314\ m^3 \cdot Pa/(mol.K)$	$10.73\ ft^3 \cdot psia/(lb-mole.°R)$
$1.987\ cal/(mol.K)$	$8.314\ J/(mol.K)$	$1.987\ Btu/(lb-mole.°R)$

Refer to book for more values of R

Specific molar volume ($\hat{V}$)

$\hat{V}$ = **the specific molar volume** = volume per unit mol

$$\hat{V} = \frac{V}{n} = \frac{\dot{V}}{\dot{n}}$$

The ideal gas can be written as

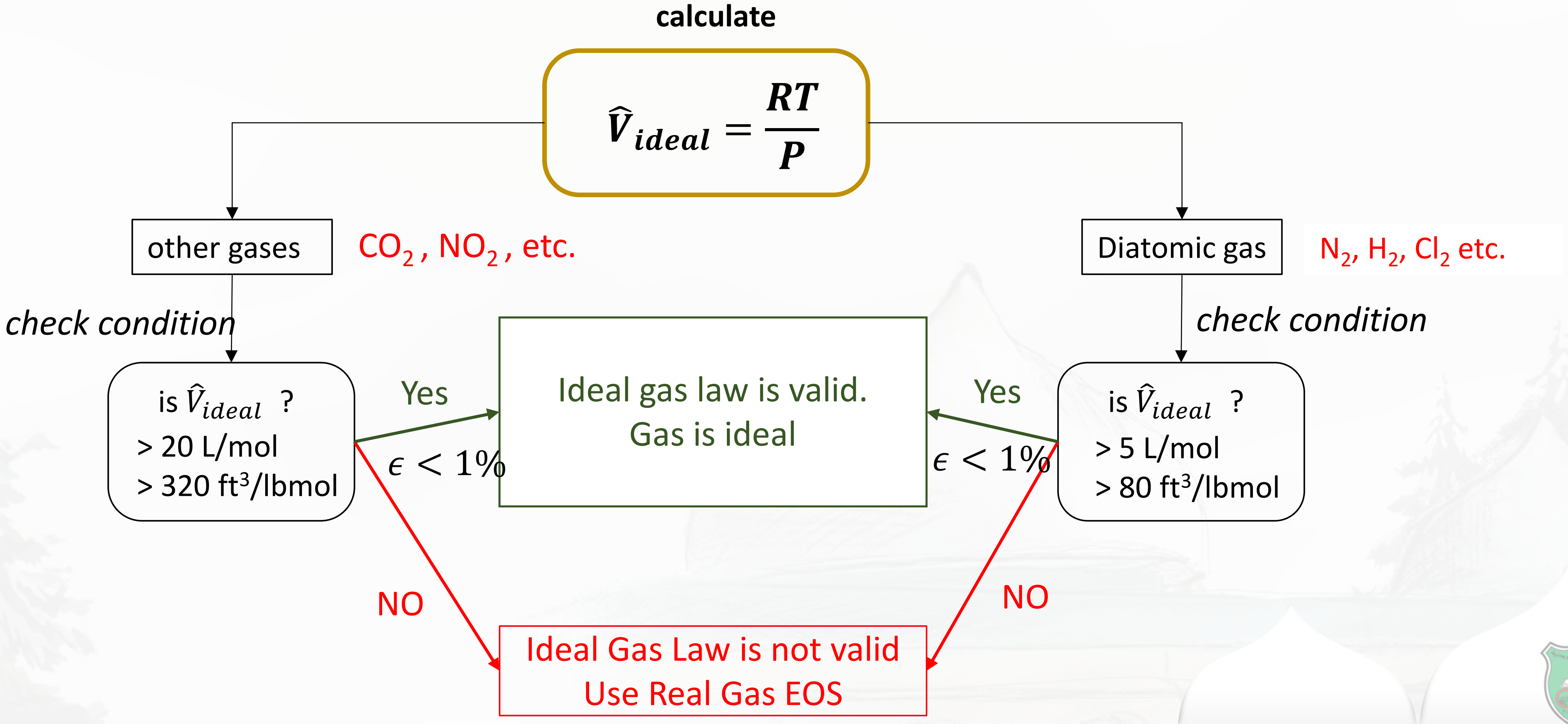
$$\boldsymbol{P \cdot V = n \cdot R \cdot T} \quad \Rightarrow \quad \boldsymbol{P \cdot \frac{V}{n} = R \cdot T} \quad \Rightarrow \quad \boldsymbol{P \cdot \hat{V} = R \cdot T}$$

Relative error (ϵ) of ideal gas law

$$\epsilon = \frac{X_{ideal} - X_{true}}{X_{true}} \times 100\%$$

A brief test to check validity of the ideal gas EOS

$\hat{V}_{ideal}$ = the ideal specific molar volume calculated using ideal gas law $P \cdot \hat{V} = R \cdot T$



calculate

$$\hat{V}_{ideal} = \frac{RT}{P}$$

other gases

CO_2 , NO_2 , etc.

check condition

is $\hat{V}_{ideal}$?
> 20 L/mol
> 320 ft^3/lbmol

Diatomic gas

N_2, H_2, Cl_2 etc.

check condition

is $\hat{V}_{ideal}$?
> 5 L/mol
> 80 ft^3/lbmol

Yes $\epsilon < 1\%$

Ideal gas law is valid.
Gas is ideal

NO

Ideal Gas Law is not valid
Use Real Gas EOS

Density of ideal gas

Brief discussion

starting from $\boldsymbol{P\,V = n\,R\,T}$

$$\boldsymbol{n} = \frac{m}{M} \quad \Rightarrow \quad P = \frac{m}{V \cdot M}\,R\,T \quad \Rightarrow \quad P = \frac{\boldsymbol{\rho}}{M}\,R\,T$$

$$\boxed{\boldsymbol{\rho} = \frac{P\,M}{R\,T}}$$

For ideal gas mixture

$$\boxed{\bar{\rho} = \frac{P\,\bar{M}}{R\,T}}$$

where $\bar{M} = \sum y_i M_i$

Example 5.2-1 The Ideal-Gas Equation of State

One hundred grams of nitrogen is stored in a container at 23.0 °C and 3.00 psig.

1. Assuming ideal gas behavior, calculate the container volume in liters.
2. Verify that the ideal gas equation of state is a good approximation for the given conditions.

Solution

1)

$$n = \frac{100.0\ g}{28.0\ g/mol} = 3.57\ mol, T = 296\ K, P = 17.7\ psia\ (P_{atm} = 14.7\ psia)$$

$$V(L) = \frac{nRT}{P}$$

$$V(L) = \frac{(3.57\ mol)(296\ K)}{17.7\ psia} \cdot \frac{R\ (L \cdot psia)}{(mol \cdot K)}$$

$$V(L) = \frac{(3.57\ mol)(296\ K)}{17.7\ psia} \cdot \frac{0.08206\ (L \cdot atm)}{(mol \cdot K)} \cdot \frac{14.7\ psia}{atm} = \boxed{72.0\ L}$$

2)

$$N_2\ is\ a\ diatomic\ gas\ \rightarrow \hat{V}_{ideal} = \frac{V}{n} = \frac{72.0\ L}{3.57\ mol} = 20.2\ L/mol\ > 5\ \ L/mol$$

$$The\ ideal\ gas\ equation\ of\ state\ should\ yield\ an\ error\ of\ less\ than\ 1\%.$$

5.2b Standard Temperature and Pressure

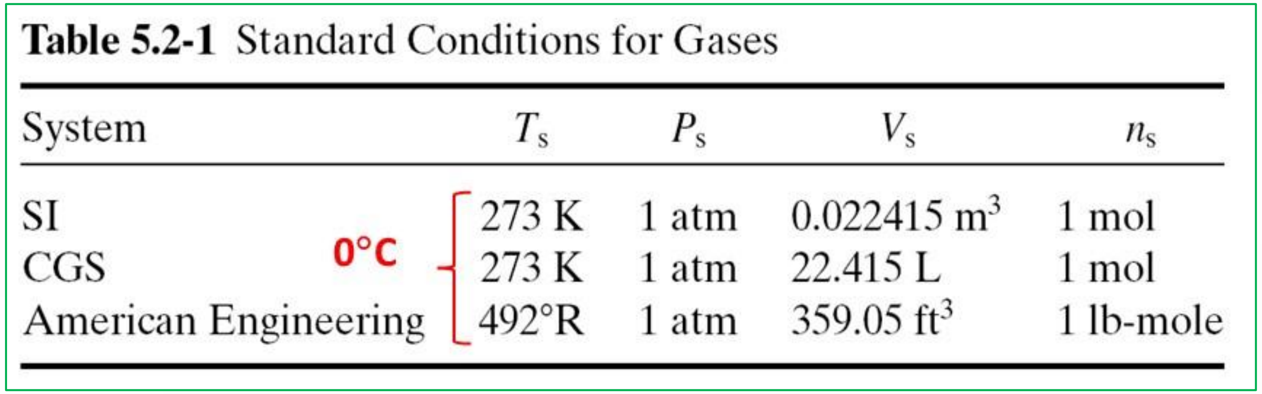


Table 5.2-1 Standard Conditions for Gases

System	T_s	P_s	V_s	n_s
SI	273 K	1 atm	0.022415 m^3	1 mol
CGS	273 K	1 atm	22.415 L	1 mol
American Engineering	492°R	1 atm	359.05 ft^3	1 lb-mole

0°C

- Standard Temperature (T_s) and pressure (P_s) are referred to as Standard Temperature and Pressure (or ***STP***)

$$273\ K, 1\ atm \Rightarrow \hat{V} = 0.022415\ m^3 = 22.415\ L$$

$$32\ °\text{F}, 1\ atm \Rightarrow \hat{V} = 359.05\ ft^3$$

$$\frac{PV}{P_s\hat{V}_s} = n\frac{T}{T_s}$$

- Standard Cubic Meters (or SCM) is often used to denote m^3(STP).
- Standard Cubic Feet (or SCF) denotes ft^3(STP).
- **SCMH** means Standard Cubic Meters per Hour (m^3 STP /h).
- A volumetric flow rate of 18.2 **SCMH** means 18.2 m^3/h at 0°C and 1 atm.

General calculations using Ideal gas law

1) Using R gas constant

$$\boldsymbol{P\,V = n\,R\,T}$$

$$P = \frac{n\,R\,T}{V} \qquad V = \frac{n\,R\,T}{P} \qquad n = \frac{P\,V}{R\,T} \qquad T = \frac{P\,V}{n\,R}$$

with selection of proper R value

2) Using relative method

Transfer from conditions (1) to condition (2)

$$\frac{P_2\,V_2}{P_1\,V_1} = \frac{n_2\,T_2}{n_1\,T_1}$$

Gas at conditions (2) relative to standard conditions

$$\frac{P_2\,V_2}{P_s\,V_s} = \frac{n_2\,T_2}{n_s\,T_s}$$

with knowledge of standard. Flexibility in units

3) Density calculations

Density of a pure gas

$$\rho = \frac{P\,M}{R\,T}$$

For ideal gas mixture

$$\bar{\rho} = \frac{P\,\bar{M}}{R\,T} \qquad \bar{M} = \sum y_i M_i$$

Exercises – Ideal Gas Law Calculations

1) How many pounds of H_2O are in 100 ft^3 of vapor at 15.5 mm Hg and 23C?
[ans. 0.0944 Ib H_2O]

2) One liter of a gas is under a pressure of 780 mmHg. What will be its volume at standard pressure, the temperature remaining constant? [ans. 1.026 L].

3) A gas occupying a volume of 1 m^3 under standard pressure is expanded to 1.200 m^3, the temperature remaining constant. What is the new pressure? [ans. 0.83 atm]

4) Determine the specific mass volume (volume per mass) and specific molar volume (volume per mole) for air at 78°F and 14.7 psia. [ans. 13.56 ft^3/Ibm and 392.7 ft^3/Ib-mol]

5) An oxygen cylinder used as standby source of oxygen contains 1.000 ft^3 of O_2 at 70°F and 200 psig. What will be the volume of this O_2 in a dry-gas holder at 90°F and 4.00 in. H_2O above atmospheric (i.e., p= 4 inH_2O + P atm)? The barometer reads 29.92 in. Hg. Note: Barometer is the device that reads the atmospheric pressure.
[ans. 15.0 ft^3].

6) You have 10 Ib of CO_2 in a 20-ft^3 fire extinguisher tank at 30°C. Assuming that the ideal gas law is valid, what will be the pressure gauge on the tank read in a test to see if the extinguisher is full? [ans P_2 = 66.6 psia = 51.9 psig].

Solution

1) How many pounds of H_2O are in 100 ft^3 of vapor at 15.5 mm Hg and 23C? [ans. 0.0944 lb H_2O]

$$n = \frac{PV}{RT} = \frac{15.5\ mm\ Hg}{760\ mm\ Hg} \cdot \frac{14.7\ psia}{10.73\ \frac{psia\ ft^3}{(lb\ mol)(°R)}} \cdot \frac{100\ ft^3}{(296)(1.8)°R} = \frac{(15.5)(14.7)(100)}{(760)(10.73)(533)}$$

$$= 0.00524\ lb\ mol$$

$$lb\ H_2O = (0.00524)(18) = \boxed{0.0944\ lb\ H_2O}$$

2) One liter of a gas is under a pressure of 780 mmHg. What will be its volume at standard pressure, the temperature remaining constant? [ans. 1.026 L].

$$\frac{P_1\ V_1}{P_s\ V_s} = \frac{n_1\ T_1}{n_s\ T_s} \qquad \frac{780\ mmHg\ x\ 1\ L}{760\ mmHg\ x\ V_s} = \frac{n_1\ T_1}{n_s\ T_s} = 1 \qquad V_s = 1.026\ L$$

$$n_1 = n_s \qquad T_1 = T_s$$

Solution

3) A gas occupying a volume of 1 m^3 under standard pressure is expanded to 1.200 m^3, the temperature remaining constant. What is the new pressure? [ans. 0.83 atm]

$$\frac{P_2\, V_2}{P_s\, V_s} = \frac{n_2\, T_2}{n_s\, T_s} \qquad \frac{P_2 \times 1.2\, m^3}{1\ atm \times 1 m^3} = \overset{\text{same}}{\frac{\cancel{n_2}\ \cancel{T_2}}{\cancel{n_s}\ \cancel{T_s}}} = 1 \qquad P_2 = \frac{1}{1.2} = 0.83\ atm$$

4) Determine the specific mass volume (volume per mass) and specific molar volume (volume per mole) for air at 78°F and 14.7 psia. [ans. 13.56 ft^3/lbm and 392.7 ft^3/lb-mol]

$$Specific\ molar\ volume: \hat{V} = \frac{RT}{P} \qquad R = 10.73\ \frac{ft^3 \cdot psia}{lb\ mole \cdot °R}, T = 78\ °F = 538\ °R, P = 14.7\ psia$$

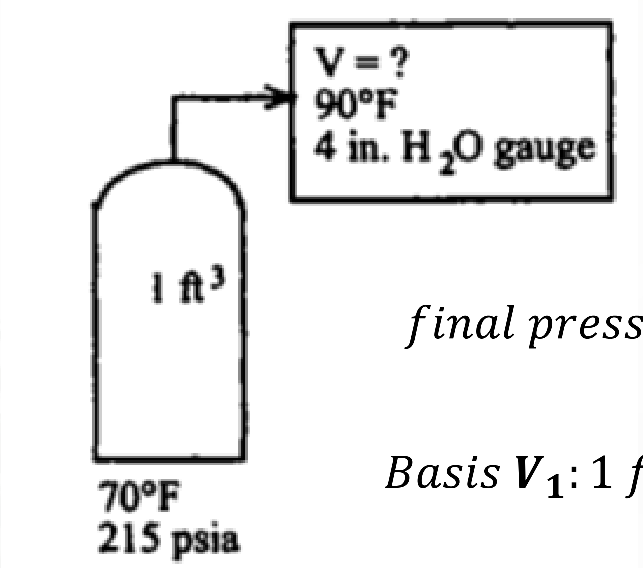
$$\hat{V} = \frac{RT}{P} = \frac{\left(10.73\ \frac{ft^3 \cdot psia}{lb\ mole \cdot °R}\right)(538\ °R)}{14.7\ psia} = \boxed{392.7\ \ ft^3/lb\ mole}$$

$$\hat{V}_m = \frac{\hat{V}}{MW} = \frac{392.7\ \ ft^3/lb\ mol}{28.97\ \ lb_m/lb\ mole} = \boxed{13.56\, ft^3/lb_m}$$

Solution

5) An oxygen cylinder, used as standby source of oxygen, contains 1.00 ft^3 of O_2 at 70°F and 200 psig. What will be the volume of this O_2 in a dry-gas holder at 90°F and 4.00 in. H_2O above atmospheric (i.e., p= 4 inH_2O + P atm)? The barometer reads 29.92 in. Hg. Note: Barometer is the device that reads the atmospheric pressure. [ans. 15.0 ft^3].

$$\boldsymbol{T_1} = 70\ °\mathrm{F} + 460 = 530\ °R \qquad \boldsymbol{T_2} = 90\ °\mathrm{F} + 460 = 550\ °R$$



$$atmospheric\ pressure = 29.92\ in.Hg = std\ atm = 14.7\ psia$$

$$initial\ pressure\ \boldsymbol{P_1} = (200 + 14.7)psia\left(\frac{29.92\ in.Hg}{14.7\ psia}\right) = \boldsymbol{437\ in.Hg}$$

$$final\ pressure\ \boldsymbol{P_2} = 29.92\ in.Hg + \left(\frac{4\ in.H_2O}{\frac{12\ in.H_2O}{ft\ H_2O}}\right)\left(\frac{29.92\ in.Hg}{33.91\ ft\ H_2O}\right) = 29.92 + 0.29 = \boldsymbol{30.21\ in.Hg}$$

$$Basis\ \boldsymbol{V_1}: 1\ ft^3\ of\ oxygen\ at\ 70\ °\mathrm{F}\ and\ 200\ psig$$

$$final\ volume\ \boldsymbol{V_2} = (1ft^3)\left(\frac{550\ °R}{530\ °R}\right)\left(\frac{437\ in.Hg}{30.21\ in.H_2O}\right) = \boldsymbol{15.0\ ft^3}\ at\ 90\ °\mathrm{F}\ and\ 4\ in.H_2O\ gauge$$

$$The\ same\ calculation\ can\ be\ made\ using\quad V_2 = V_1\left(\frac{P_1}{P_2}\right)\left(\frac{T_2}{T_1}\right)\ since\ n_1 = n_2$$

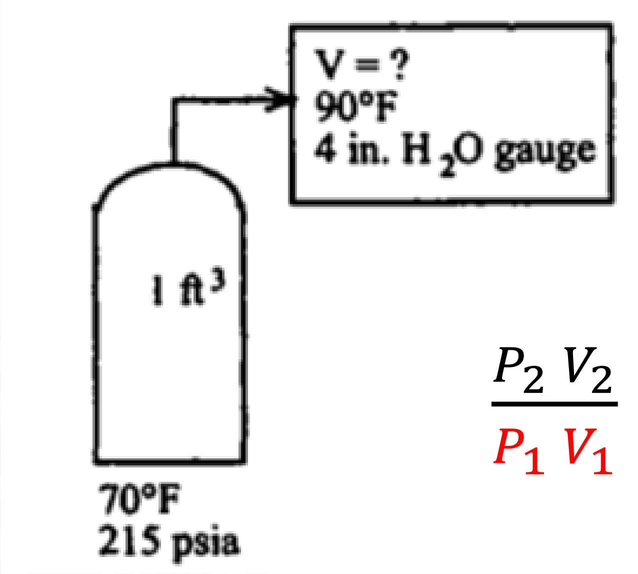
Solution

5) Solution by the ratio method

$$\boldsymbol{T_1} = 70\ °\mathrm{F} + 460 = 530\ °R \qquad \boldsymbol{T_2} = 90\ °\mathrm{F} + 460 = 550\ °R$$

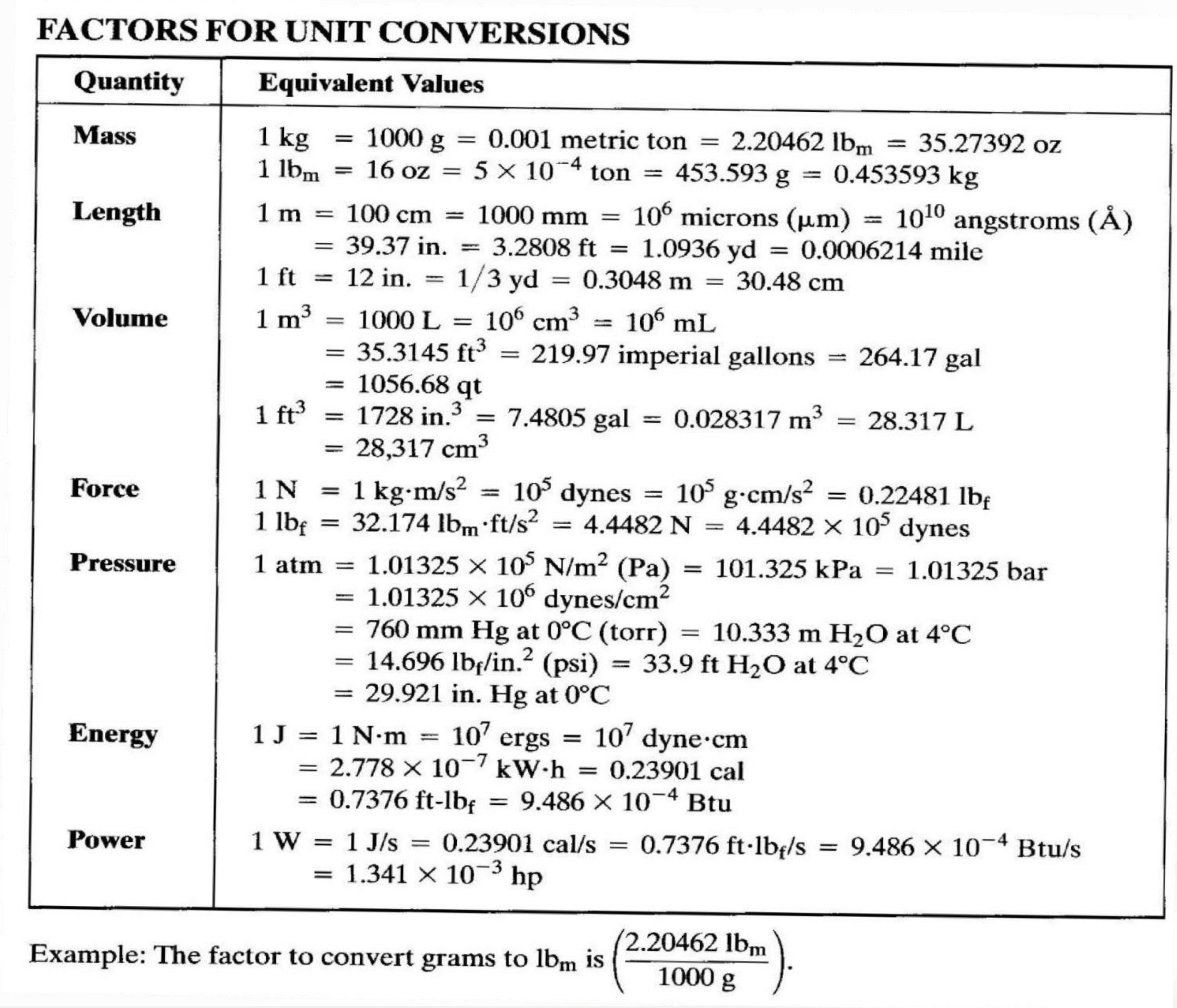
$$\boldsymbol{P_1 = 437\ in.Hg} \qquad \boldsymbol{P_2 = 30.21\ in.Hg}$$

$$\boldsymbol{V_1} = 1\ ft^3 \qquad \boldsymbol{V_2} = ??$$



$$\frac{P_2\, V_2}{P_1\, V_1} = \frac{\overset{\text{same}}{\cancel{n_2}}\, T_2}{\cancel{n_1}\, T_1} \qquad \frac{30.21\ inHg \times \boldsymbol{V_2}}{437\ inHg \times 1\ ft^3} = \frac{\overset{\text{same}}{\cancel{n_2}} \times 550R}{\cancel{n_s} \times 530\ R} \qquad V_2 =$$

Conversion Table



FACTORS FOR UNIT CONVERSIONS

Quantity	Equivalent Values
Mass	1 kg = 1000 g = 0.001 metric ton = 2.20462 lb_m = 35.27392 oz 1 lb_m = 16 oz = 5×10^{-4} ton = 453.593 g = 0.453593 kg
Length	1 m = 100 cm = 1000 mm = 10^6 microns (μm) = 10^{10} angstroms (Å) = 39.37 in. = 3.2808 ft = 1.0936 yd = 0.0006214 mile 1 ft = 12 in. = 1/3 yd = 0.3048 m = 30.48 cm
Volume	1 m^3 = 1000 L = 10^6 cm^3 = 10^6 mL = 35.3145 ft^3 = 219.97 imperial gallons = 264.17 gal = 1056.68 qt 1 ft^3 = 1728 in.^3 = 7.4805 gal = 0.028317 m^3 = 28.317 L = 28,317 cm^3
Force	1 N = 1 $\text{kg}\cdot\text{m/s}^2$ = 10^5 dynes = 10^5 $\text{g}\cdot\text{cm/s}^2$ = 0.22481 lb_f 1 lb_f = 32.174 $\text{lb}_m\cdot\text{ft/s}^2$ = 4.4482 N = 4.4482×10^5 dynes
Pressure	1 atm = 1.01325×10^5 N/m^2 (Pa) = 101.325 kPa = 1.01325 bar = 1.01325×10^6 dynes/cm^2 = 760 mm Hg at 0°C (torr) = 10.333 m H_2O at 4°C = 14.696 $\text{lb}_f/\text{in.}^2$ (psi) = 33.9 ft H_2O at 4°C = 29.921 in. Hg at 0°C
Energy	1 J = 1 N·m = 10^7 ergs = 10^7 dyne·cm = 2.778×10^{-7} kW·h = 0.23901 cal = 0.7376 ft-lb_f = 9.486×10^{-4} Btu
Power	1 W = 1 J/s = 0.23901 cal/s = 0.7376 ft·lb_f/s = 9.486×10^{-4} Btu/s = 1.341×10^{-3} hp

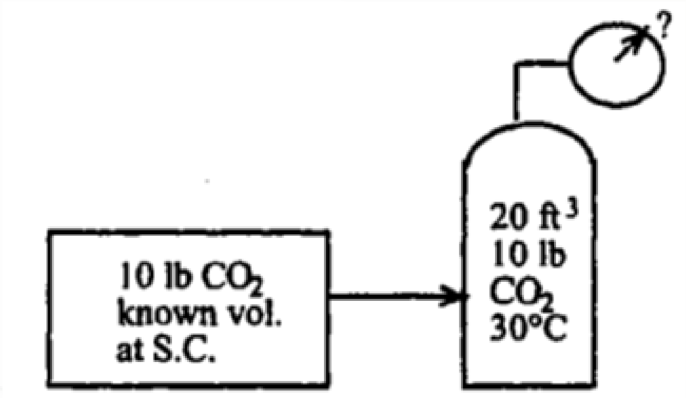
Example: The factor to convert grams to lb_m is $\left(\dfrac{2.20462\ \text{lb}_m}{1000\ \text{g}}\right)$.

Solution

6) You have 10 lb of CO_2 in a 20-ft^3 fire extinguisher tank at 30°C. Assuming that the ideal gas law is valid, what will be the pressure gauge on the tank read in a test to see if the extinguisher is full?

[ans P_2 = 66.6 psia = 51.9 psig].

$$\frac{P_1\,V_1}{P_s\,V_s} = \frac{n_1\,T_1}{n_s\,T_s}$$



$$V_s = 10\ lb\ CO_2 \cdot \frac{1\ lb\ mol\ CO_2}{44\ lb\ CO_2} \cdot \frac{359\ ft^3}{1\ lb\ mol}$$

same

$$\frac{P_1\,V_1}{P_s\,V_s} = \frac{n_1\,T_1}{n_s\,T_s}$$

$$P_1 = P_s\left(\frac{V_s}{V_1}\right)\left(\frac{T_1}{T_s}\right)$$

$$P_1 = (14.7\ psia)\left(\frac{10\ lb\ CO_2 \cdot \frac{1\ lb\ mol\ CO_2}{44\ lb\ CO_2} \cdot \frac{359\ ft^3}{1\ lb\ mol}}{20\ ft^3}\right)\left(\frac{303\ K}{273\ K}\right) = 66.6\ psia$$

$$P_{1,gauge} = 66.6 - 14.7 = \mathbf{51.9\ psig}$$

Example 5.2-2 Conversion from standard conditions

Butane (C_4H_{10}) at 360 °C and 3.00 atm absolute flows into a reactor at a rate of 1100 kg/h. Calculate the volumetric flow rate of this stream using conversion from standard conditions.

Solution

As always, molar quantities and absolute temperature and pressure must be used.

$$\dot{n} = \frac{1100\ kg/h}{58.1\ kg/kmol} = 19.0\ \ kmol/h\,, T = 633\ K, P = 3.00\ atm$$

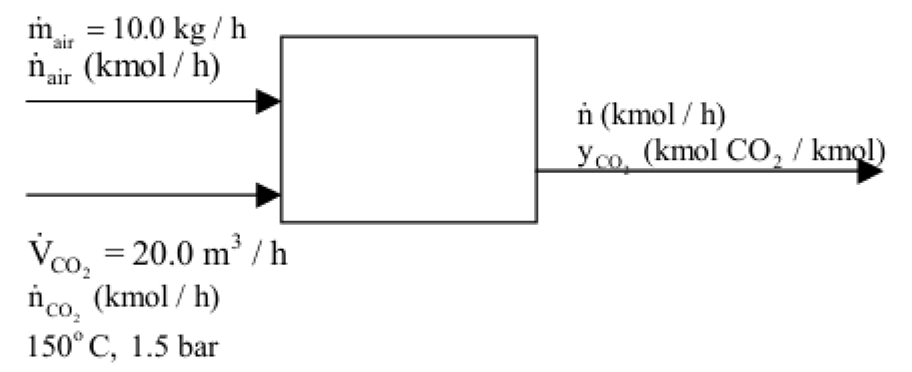
From $\dfrac{P\dot{V}}{P_s\hat{V}_s} = \dot{n}\dfrac{T}{T_s} \rightarrow \dot{V} = \dot{n}\hat{V}_s\dfrac{T}{T_s}\dfrac{P_s}{P}$

$$\dot{V} = \dot{n}\hat{V}_s\frac{T}{T_s}\frac{P_s}{P} = \left(\frac{19.0\ kmol}{h}\right)\left(\frac{22.4\ m^3(STP)}{kmol}\right)\left(\frac{633\ K}{273\ K}\right)\left(\frac{1.00\ atm}{3.00\ atm}\right) = \boxed{329\ \frac{m^3}{h}}$$

Problem 5.15 (3rd ed.): Mole Percent of CO_2 in a Mixed Gas Stream

A stream of air (21 mol% O_2, balance N_2) flows at **10.0 kg/h** and is mixed with a stream of **CO_2**. The CO_2 enters the mixer at **20.0 m³/h**, **150°C**, and **1.5 bar**.

Determine the **mole percent of CO_2** in the product gas stream. [answer: 71.2%]



Solution

Assume ideal gas behavior

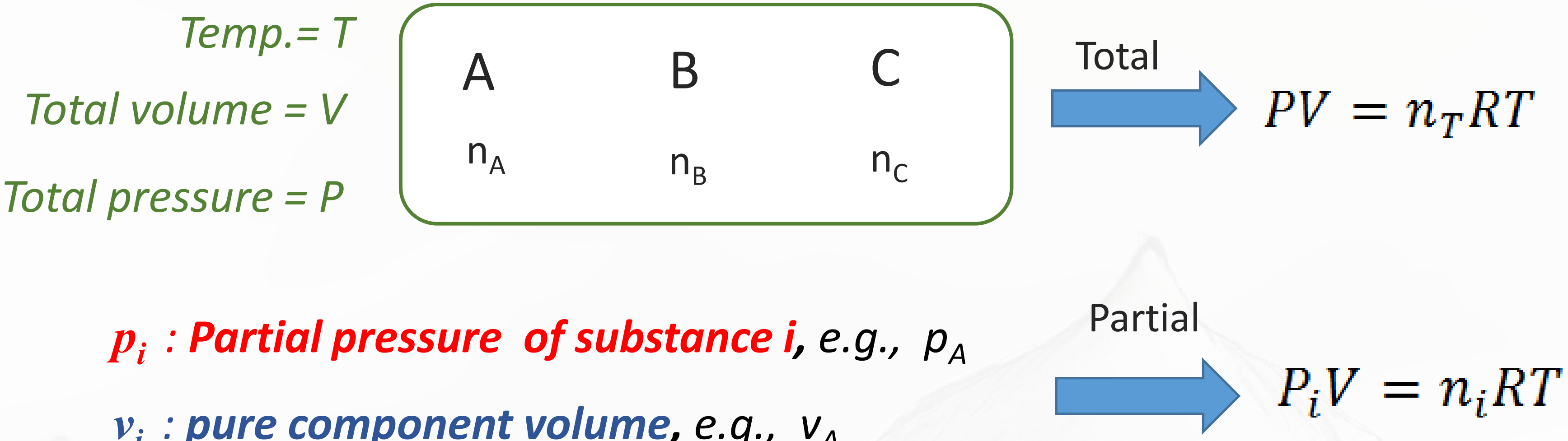
$$\dot{n}_{air} = \frac{10.0\text{ kg}}{\text{h}}\left|\frac{1\text{ kmol}}{29.0\text{ kg air}}\right. = 0.345\text{ kmol air / h}$$

$$\dot{n}_{CO_2} = \frac{P\dot{V}}{RT} = \frac{1.5\text{ bar}}{8.314\ \frac{\text{m}^3\cdot\text{kPa}}{\text{kmol}\cdot\text{K}}}\left|\frac{100\text{ kPa}}{1\text{ bar}}\right|\frac{20.0\text{ m}^3\text{ / h}}{423.2\text{ K}} = 0.853\text{ kmol CO}_2\text{ / h}$$

$$y_{CO_2} \times 100\% = \frac{0.853\text{ kmol CO}_2\text{ / h}}{(0.853\text{ kmol CO}_2\text{ / h} + 0.345\text{ kmol air / h})} \times 100\% = \underline{\underline{71.2\%}}$$

5.2c Ideal Gas Mixtures

- A mixture of ideal gases is itself an ideal gas,
- Suppose you have a mixture of gases, each is ideal, i.e. the mixture is ideal gas mixture, then



Temp.= T

Total volume = V

Total pressure = P

A n_A B n_B C n_C

Total

$$PV = n_T RT$$

***p_i : Partial pressure of substance i**, e.g., p_A*

***v_i : pure component volume**, e.g., v_A*

Partial

$$P_i V = n_i RT$$

p_A : the pressure that would be exerted by n_A moles of A alone in the same total volume *V* at the same temperature *T.*

v_A : the volume that would be occupied by n_A moles of A alone at the total pressure P and temperature *T of the mixture.*

Partial pressure of component

$$\frac{P_i V = n_i RT}{PV = n_T RT} \rightarrow \frac{P_i}{P} = \frac{n_i}{n_T} = y_i \rightarrow \boxed{p_i = y_i P}$$

For species A, B and C in the mixture,

$$n_T = n_A + n_B + n_C \rightarrow n_T = y_A n_T + y_B n_T + y_C n_T$$

$$\boxed{P = p_A + p_B + p_C} \rightarrow P = y_A P + y_B P + y_C P$$

Dalton's Law

Pure component volume

$$\frac{P v_i = n_i RT}{PV = n_T RT} \rightarrow \boxed{\frac{v_i}{P} = \frac{n_i}{n_T} = y_i} \rightarrow \boxed{v_i = y_i V}$$

For A, B and C ideal gas mixture: $\boxed{V = v_A + v_B + v_C}$ **Amagat's Law**

Problem 5.25 (3^{rd} ed.) – Ideal Gas Mixture

An ideal gas mixture contains 35% helium, 20% methane, and 45% nitrogen by volume at 2.00 atm absolute and 90°C. Calculate:

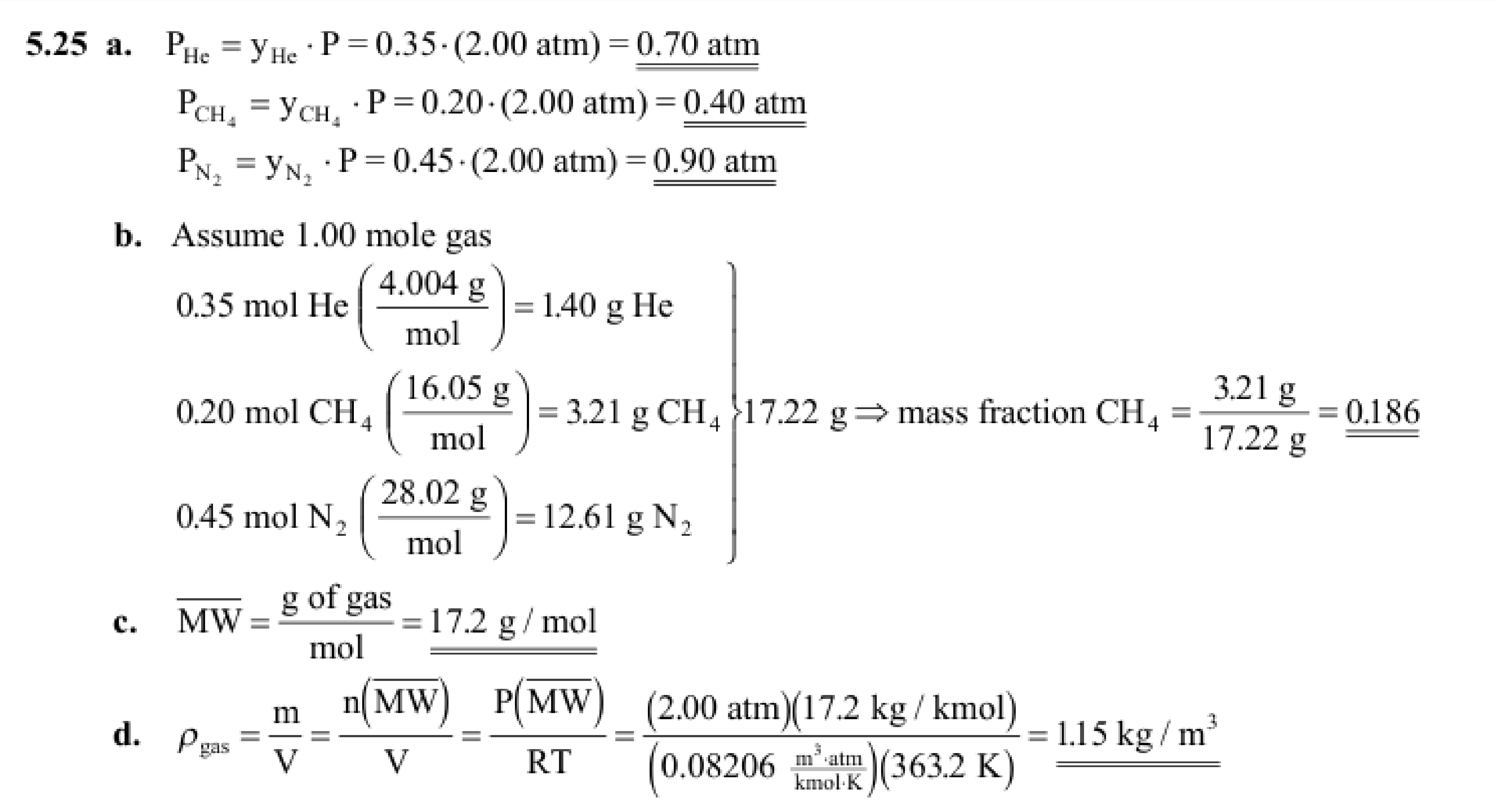
(a) the partial pressure of each component [answer: 0.7 atm, 0.4 atm, 0.9 atm]

(b) the mass fraction of methane [answer: 0.186]

(c) the average molecular weight of the gas [answer: 17.2]

(d) the density of the gas in kg/m³. [answer: 1.15 kg/m3]

Solution 5.25 (3^{rd} ed.)



5.25 a. $P_{He} = y_{He} \cdot P = 0.35 \cdot (2.00 \text{ atm}) = \underline{\underline{0.70 \text{ atm}}}$

$P_{CH_4} = y_{CH_4} \cdot P = 0.20 \cdot (2.00 \text{ atm}) = \underline{\underline{0.40 \text{ atm}}}$

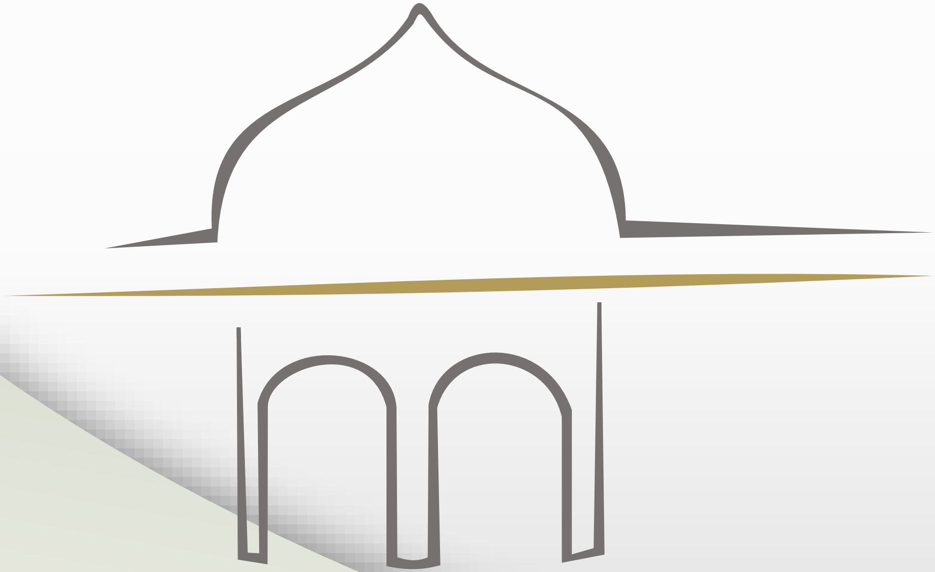
$P_{N_2} = y_{N_2} \cdot P = 0.45 \cdot (2.00 \text{ atm}) = \underline{\underline{0.90 \text{ atm}}}$

b. Assume 1.00 mole gas

$$\left.\begin{array}{l} 0.35 \text{ mol He}\left(\dfrac{4.004 \text{ g}}{\text{mol}}\right) = 1.40 \text{ g He} \\ 0.20 \text{ mol CH}_4\left(\dfrac{16.05 \text{ g}}{\text{mol}}\right) = 3.21 \text{ g CH}_4 \\ 0.45 \text{ mol N}_2\left(\dfrac{28.02 \text{ g}}{\text{mol}}\right) = 12.61 \text{ g N}_2 \end{array}\right\} 17.22 \text{ g} \Rightarrow \text{mass fraction CH}_4 = \frac{3.21 \text{ g}}{17.22 \text{ g}} = \underline{\underline{0.186}}$$

c. $\overline{MW} = \dfrac{\text{g of gas}}{\text{mol}} = \underline{\underline{17.2 \text{ g/mol}}}$

d. $$\rho_{gas} = \frac{m}{V} = \frac{n\left(\overline{MW}\right)}{V} = \frac{P\left(\overline{MW}\right)}{RT} = \frac{(2.00 \text{ atm})(17.2 \text{ kg/kmol})}{\left(0.08206 \frac{\text{m}^3\cdot\text{atm}}{\text{kmol}\cdot\text{K}}\right)(363.2 \text{ K})} = \underline{\underline{1.15 \text{ kg/m}^3}}$$



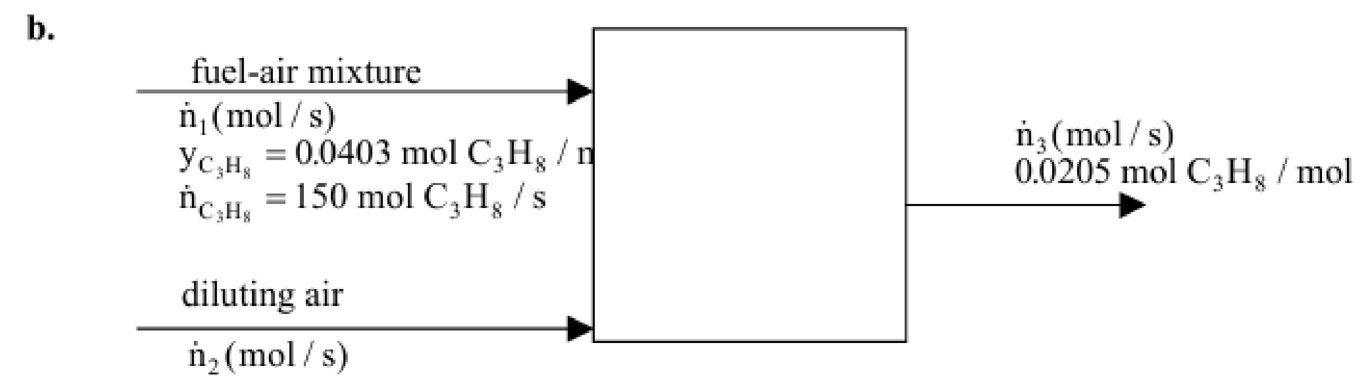
Problem Solving

Problem 5.26 (3rd ed.): Flammability Limits of Propane–Air Mixtures

- LFL of propane in air at 1 atm: **2.05 mol% C_3H_8**
- UFL of propane in air at 1 atm: **11.4 mol% C_3H_8**

Mixtures with propane concentration:

- **Below 2.05%** → *too lean* to ignite
- **Between 2.05% and 11.4%** → flammable
- **Above 11.4%** → *too rich* to ignite



Questions:

a) Which is safer to release into the atmosphere — a mixture that is *too lean* or *too rich*? Explain.

b) A propane–air mixture containing **4.03 mol% C_3H_8** feeds a furnace.
To avoid accidental ignition, the mixture is diluted with pure air.
If propane enters at **150 mol C_3H_8/s**, what is the **minimum molar flow rate of the diluting air**?

c) The actual diluting-air molar flow rate is **130%** of the minimum.
Given the furnace feed conditions (fuel mixture at **125°C & 131 kPa**, air at **25°C & 110 kPa**), calculate:

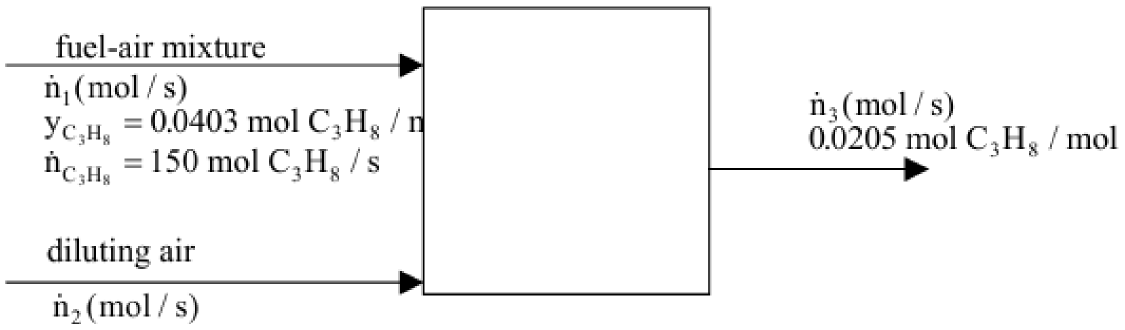
- The volumetric flow ratio *(m³ diluting air)/(m³ fuel gas)*
- The mole percent propane in the diluted mixture

(d) Give several reasons why operating the air valve at a rate **greater** than the calculated minimum is advisable.

Solution 5.26 (3^{rd} ed.)

a. It is safer to release a mixture that is too lean to ignite.
If a mixture that is rich is released in the atmosphere, it can diffuse in the air and the C_3H_8 mole fraction can drop below the UFL, thereby producing a fire hazard.

b.



fuel-air mixture

$\dot{n}_1 (\text{mol/s})$

$y_{C_3H_8} = 0.0403 \text{ mol } C_3H_8 / \text{n}$

$\dot{n}_{C_3H_8} = 150 \text{ mol } C_3H_8 / \text{s}$

diluting air

$\dot{n}_2 (\text{mol/s})$

$\dot{n}_3 (\text{mol/s})$

$0.0205 \text{ mol } C_3H_8 / \text{mol}$

$$\dot{n}_1 = \frac{150 \text{ mol } C_3H_8}{\text{s}} \left| \frac{\text{mol}}{0.0403 \text{ mol } C_3H_8} \right. = 3722 \text{ mol/s}$$

Propane balance: $150 = 0.0205 \cdot \dot{n}_3 \Rightarrow \dot{n}_3 = 7317 \text{ mol/s}$

Total mole balance: $\dot{n}_1 + \dot{n}_2 = \dot{n}_3 \Rightarrow \dot{n}_2 = 7317 - 3722 = 3595 \text{ mol air/s}$

c. $\dot{n}_2 = 1.3(\dot{n}_2)_{min} = 4674 \text{ mol/s}$

$$\dot{V}_2 = \frac{4674 \text{ mol/s}}{} \left| \frac{8.314 \text{ m}^3 \cdot \text{Pa}}{\text{mol} \cdot \text{K}} \right| \frac{398.2 \text{ K}}{131{,}000 \text{ Pa}} = 118 \text{ m}^3/\text{s}$$

$$\dot{V}_1 = \frac{3722 \text{ mol}}{\text{s}} \left| \frac{8.314 \text{ m}^3 \cdot \text{Pa}}{\text{mol} \cdot \text{K}} \right| \frac{298.2 \text{ K}}{110000 \text{ Pa}} = 83.9 \text{ m}^3/\text{s}$$

$$\frac{\dot{V}_2}{\dot{V}_1} = 1.41 \underline{\underline{\frac{\text{m}^3 \text{ diluting air}}{\text{m}^3 \text{ fuel gas}}}}$$

$$y_2 = \frac{150 \text{ mol/s}}{\dot{n}_1 + \dot{n}_2} = \frac{150 \text{ mol/s}}{(3722 \text{ mol/s} + 4674 \text{ mol/s})} \times 100\% = \underline{\underline{1.8\%}}$$

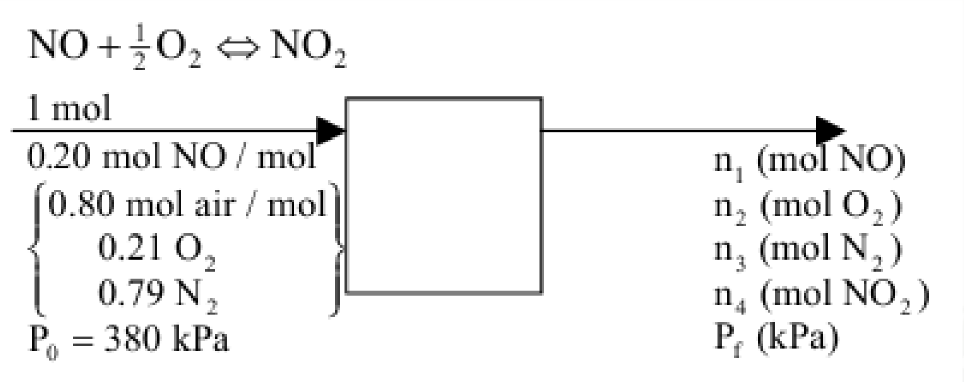
d. The incoming propane mixture could be higher than 4.03%.
If $\dot{n}_2 = (\dot{n}_2)_{min}$, fluctuations in the air flow rate would lead to temporary explosive conditions.

Problem 5.32 (3rd ed.):
Oxidation of Nitric Acid: Batch Reactor & Equilibrium Analysis

The oxidation of nitric oxide

$$\text{NO} + \frac{1}{2}O_2 \rightleftharpoons NO_2$$

takes place in an isothermal batch reactor. The reactor is charged with a mixture containing 20.0 volume percent NO and the balance air at an initial pressure of 380 kPa (absolute).



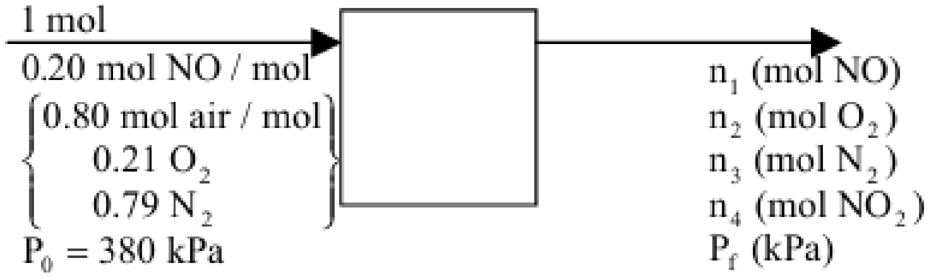
(a) Assuming ideal gas behavior, determine the composition of the mixture (component mole fractions) and the final pressure (kPa) if the conversion of NO is 90%.

(b) Suppose the pressure in the reactor eventually equilibrates (levels out) at 360 kPa. What is the equilibrium percent conversion of NO? Calculate the reaction equilibrium constant at the prevailing temperature, $K_p\left[(atm)^{-0.5}\right]$,defined as:

$$K_p = \frac{\left(p_{NO_2}\right)}{\left(p_{NO}\right)\left(p_{O_2}\right)^{0.5}}$$

Solution: Problem 5.32 (3rd ed.)

$NO + \frac{1}{2}O_2 \Leftrightarrow NO_2$



1 mol

0.20 mol NO / mol

0.80 mol air / mol

$0.21\ O_2$

$0.79\ N_2$

$P_0 = 380$ kPa

n_1 (mol NO)

n_2 (mol O_2)

n_3 (mol N_2)

n_4 (mol NO_2)

P_f (kPa)

a. Basis: 1.0 mol feed

90% NO conversion: $n_1 = 0.10(0.20) = 0.020$ mol NO $\Rightarrow$ NO reacted $= 0.18$ mol

O_2 balance: $n_2 = 0.80(0.21) - \frac{0.18\text{ mol NO}}{} \left| \frac{0.5\text{ mol }O_2}{\text{mol NO}} \right. = 0.0780\text{ mol }O_2$

N_2 balance: $n_3 = 0.80(0.79) = 0.632$ mol N_2

$$n_4 = \frac{0.18\text{ mol NO}}{} \left| \frac{1\text{ mol }NO_2}{1\text{ mol NO}} \right. = 0.18\text{ mol }NO_2 \Rightarrow n_f = n_1 + n_2 + n_3 + n_4 = 0.91\text{ mol}$$

$$y_{NO} = \frac{0.020\text{ mol NO}}{0.91\text{ mol}} = \underline{\underline{0.022\frac{\text{mol NO}}{\text{mol}}}}$$

$$y_{O_2} = \underline{\underline{0.086\frac{\text{mol }O_2}{\text{mol}}}} \quad y_{N_2} = \underline{\underline{0.695\frac{\text{mol }N_2}{\text{mol}}}} \quad y_{NO_2} = \underline{\underline{0.198\frac{\text{mol }NO_2}{\text{mol}}}}$$

$$\frac{P_f V}{P_0 V} = \frac{n_f RT}{n_0 RT} \Rightarrow P_f = P_0\frac{n_f}{n_0} = 380\text{ kPa}\left(\frac{0.91\text{ mol}}{1\text{ mol}}\right) = \underline{\underline{346\text{ kPa}}}$$

b. $n_f = n_0\frac{P_f}{P_0} = (1\text{ mol})\frac{360\text{ kPa}}{380\text{ kPa}} = 0.95\text{ mol}$

$$n_i = n_{i0} + \upsilon_i\xi$$

$$\Downarrow$$

n_1 (mol NO) $= 0.20 - \xi$

n_2 (mol O_2) $= (0.21)(0.80) - 0.5\xi$

n_3 (mol N_2) $= (0.79)(0.80)$

n_4 (mol NO_2) $= \xi$

$n_f = 1 - 0.5\xi = 0.95 \Rightarrow \xi = \underline{\underline{0.10}}$

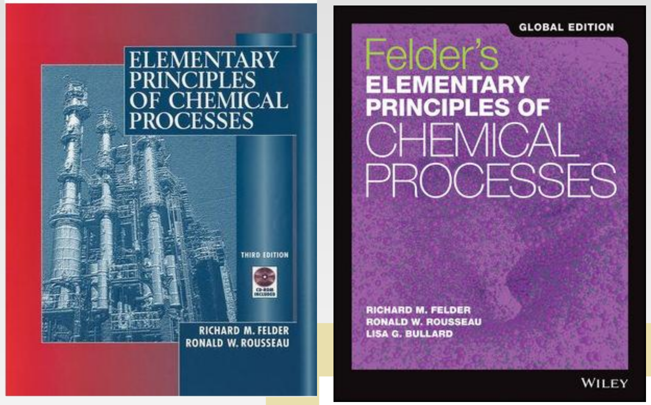
$\Rightarrow n_1 = 0.10$ mol NO, $n_2 = 0.118$ mol O_2, $n_3 = 0.632$ mol N_2,

$n_4 = 0.10$ mol $NO_2 \Rightarrow y_{NO} = 0.105$, $y_{O_2} = 0.124$, $y_{N_2} = 0.665$, $y_{NO_2} = 0.105$

$$\underline{\text{NO conversion}} = \frac{(0.20 - n_1)}{0.20} \times 100\% = \underline{\underline{50\%}}$$

$$P\text{ (atm)} = \frac{360\text{ kPa}}{101.3\ \frac{\text{kPa}}{\text{atm}}} = 3.55\text{ atm}$$

$$K_p = \frac{(y_{NO_2}P)}{(y_{NO}P)(y_{O_2}P)^{0.5}} = \frac{(y_{NO_2})}{(y_{NO})(y_{O_2})^{0.5}P^{0.5}} = \frac{0.105}{(0.105)(0.124)^{0.5}(3.55)^{0.5}} = \underline{\underline{1.51\text{ atm}^{\frac{1}{2}}}}$$



ELEMENTARY PRINCIPLES OF CHEMICAL PROCESSES
THIRD EDITION
RICHARD M. FELDER
RONALD W. ROUSSEAU

GLOBAL EDITION
Felder's
ELEMENTARY PRINCIPLES OF CHEMICAL PROCESSES
RICHARD M. FELDER
RONALD W. ROUSSEAU
LISA G. BULLARD
WILEY

Elementary Principles of Chemical Processes,
3rd or 4th edition,
Wiley & Sons, Inc.
Richard M. Felder, Ronald W. Rousseau, & Lisa G. Bullard.

CHE 0905211

Chemical Engineering Principles 1

Fall 2025

Dr. Hatem Alsyouri	**Chapter 5**

The University of Jordan
Chemical Engineering Department

Chapter 5

Chapter 5 : Single-Phase Systems

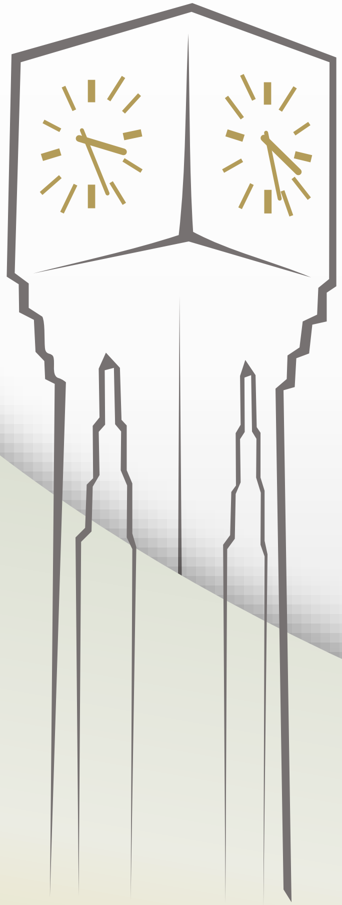
Topics		**5.3 Equations of State for Non-Ideal Gases** (brief of no-ideality and EOS models) **5.4 The compressibility factor equation of state** a. Compressibility factor tables b. The law of corresponding states and compressibility charts c. Non-ideal gas mixtures	Sections 5.4 ab: 64, 66, 69*, 73
		Problem Solving	
Learning Outcomes	LO12. Perform pressure–volume–temperature calculations for ideal and non-ideal gases using appropriate equations of state and gas property charts. (SO1)		

Notes

This is only a sample material that does not cover the entire topics of the chapter.

Please refer to the textbook for full study, and solve the assigned exercises and suggested problems.

Refer to weekly lesson plan for details of covered topics

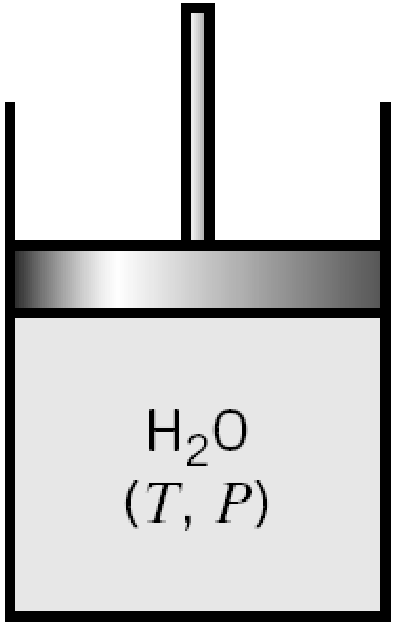


5.3 Compressibility Factor Equation

5.3 Equations of State for Nonideal Gases

- The ideal gas is the basis of the simplest and most convenient equation of state. However, it can be seriously inaccurate at a sufficiently low temperature and/or a sufficiently high pressure.
- For real "nonideal" gases several more complex but more accurate equations of state for single species exist:
  1. the virial equation.
  2. the van der Waals equation.
  3. the Soave–Redlich–Kwong equation.
- Another approach to nonideal gas analysis that makes use of the law of corresponding states and *compressibility factors*.

5.3a Critical Temperature and Pressure

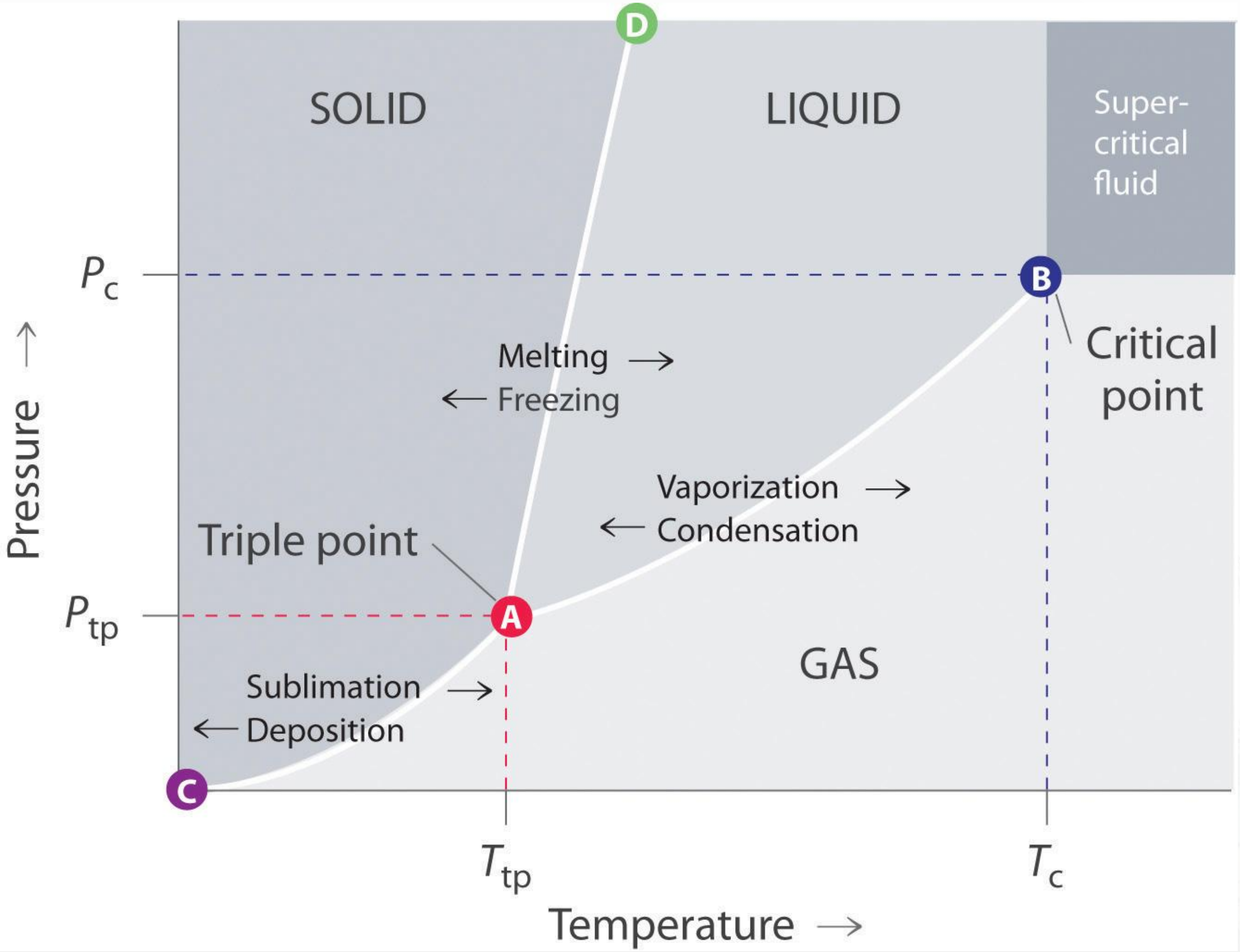


- How well or poorly the ideal gas equation of state PVT data for a species often depends on the values of the system temperature and pressure relative to two physical properties of the species- the **critical temperature (T_c)** and **critical pressure (P_c).**

- Suppose a quantity of water is kept in a closed piston-fitted cylinder.
- Initially, all the water is vapor.
- the water is compressed at constant temperature by lowering the piston until a drop of liquid water appears.
- Report $P_{cond}(atm), \rho_v\left(\frac{kg}{m^3}\right), \rho_l\left(\frac{kg}{m^3}\right)$.

Refer to book to for details and examples of this section

General Phase diagram (P vs. T)



Refer to book to for details and examples of this section

5.3b Virial Equations of State

5.3b. Only the concepts in final exam. No calculations

$$\frac{P\hat{V}}{RT} = 1 + \frac{B}{\hat{V}} + \frac{C}{\hat{V}^2} + \frac{D}{\hat{V}^3} + \cdots$$

Expresses the quantity $(P\hat{V}/RT)$ as a power series in the inverse of specific volume in the gas region (single phase system)

B, ***C***, and ***D*** are known as the second, third, and fourth Virial coefficients, respectively. They are functions of temperature.

Since theoretical and experimental data are not readily available for viral coefficients higher than the second one, the equation is often used in truncated (short) form.

$$\boxed{\frac{P\hat{V}}{RT} = 1 + \frac{B}{\hat{V}}}$$

and

$$B = \frac{RT_c}{P_c}(B_0 + \omega B_1)$$

$$\frac{P\hat{V}}{RT} = 1 + \frac{B}{\hat{V}}$$

$$B = \frac{RT_c}{P_c}(B_0 + \omega B_1)$$

where

$$B_0 = 0.083 - \frac{0.422}{T_r^{1.6}}$$

$$B_1 = 0.139 - \frac{0.172}{T_r^{4.2}}$$

$$T_r = T/T_c$$

T_r = The reduced temperature

ω: is Pitzer acentric factor, a parameter that reflects the geometry and polarity of a molecule

ω

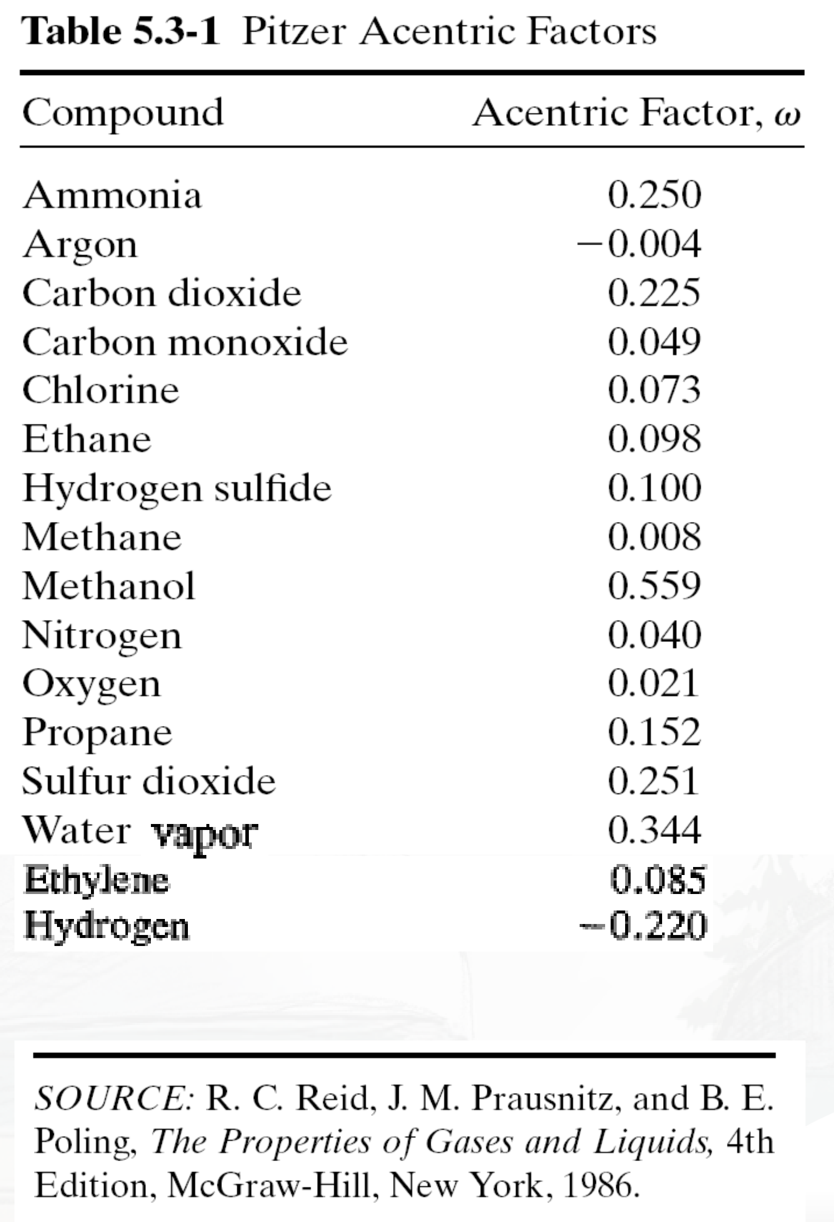


Table 5.3-1 Pitzer Acentric Factors

Compound	Acentric Factor, ω
Ammonia	0.250
Argon	−0.004
Carbon dioxide	0.225
Carbon monoxide	0.049
Chlorine	0.073
Ethane	0.098
Hydrogen sulfide	0.100
Methane	0.008
Methanol	0.559
Nitrogen	0.040
Oxygen	0.021
Propane	0.152
Sulfur dioxide	0.251
Water vapor	0.344
Ethylene	0.085
Hydrogen	−0.220

SOURCE: R. C. Reid, J. M. Prausnitz, and B. E. Poling, *The Properties of Gases and Liquids,* 4th Edition, McGraw-Hill, New York, 1986.

Background knowledge

Example

Two gram-moles of nitrogen is placed in a 3 liter tank at -150.8°C.
Estimate the tank pressure using the ideal gas equation of state and then using the virial equation of state (truncated form). Calculate the percentage error that results from the use of the ideal gas equation at the system conditions assuming the virial estimate is accurate.

$$T = (-150.8 + 273.2)\ \mathrm{K} = 122.4\ \mathrm{K},$$

n = 2 g-moles = 2 mol N_2 ***V = 3 L***

$$\hat{V} = \frac{V}{n} = 3.00\ \mathrm{L}/2.00\ \mathrm{mol} = 1.50\ \mathrm{L/mol}$$

Using the ideal gas equation of state

$$P_{\mathrm{ideal}} = \frac{RT}{\hat{V}} = \frac{0.08206\ \mathrm{L\cdot atm}}{\mathrm{mol\cdot K}} \left| \frac{123\ \mathrm{K}}{} \right| \frac{1\ \mathrm{mol}}{1.50\ \mathrm{L}} = 6.73\ \mathrm{atm}$$

Using the virial equation equation of state

$$\frac{P\hat{V}}{RT} = 1 + \frac{B}{\hat{V}}$$

Background knowledge

The critical properties

$$(T_c)_{N_2} = 126.2\ \text{K},\ (P_c)_{N_2} = 33.5\ \text{atm}$$

Table B.1

$$\omega_{N_2} = 0.040$$

Table 5.3-1

$$T_r = \frac{T}{T_c} = \frac{122.4\ \text{K}}{126.2\ \text{K}} = 0.970$$

$$\boxed{B_0 = 0.083 - \frac{0.422}{T_r^{1.6}}} \rightarrow B_0 = 0.083 - \frac{0.422}{0.970^{1.6}} = -0.36$$

$$\boxed{B_1 = 0.139 - \frac{0.172}{T_r^{4.2}}} \rightarrow B_1 = 0.139 - \frac{0.172}{0.970^{4.2}} = -0.056$$

$$\boxed{B = \frac{RT_c}{P_c}(B_0 + \omega B_1)}$$

$$\rightarrow B = \frac{\left(0.08206\ \dfrac{\text{L}\cdot\text{atm}}{\text{mol}\cdot\text{K}}\right)(126.2\ \text{K})}{33.5\ \text{atm}}[-0.36 + 0.040(-0.056)]$$

$$= -0.113\ \text{L/mol}$$

$$P = \frac{RT}{\hat{V}}\left(1 + \frac{B}{\hat{V}}\right) \qquad = \frac{\left(0.08206 \frac{\text{L}\cdot\text{atm}}{\text{mol}\cdot\text{K}}\right)(122.4\ \text{K})}{1.50\ \text{L/mol}}\left(1 + \frac{-0.113\ \text{L/mol}}{1.50\ \text{L/mol}}\right) = \boxed{6.19\ \text{atm}}$$

% error in the pressure

$$Error\ (\in) = \frac{estimated\ - true}{true} \times 100\%$$

$$\epsilon = \frac{P_{\text{ideal}} - P}{P} \times 100\% = \boxed{8.7\%\ \text{error}}$$

5.3c Cubic Equation of State

5.3c. Only the concepts in final exam. No calculations

- Virial equations cannot represent thermodynamic systems where both liquid and vapor are present.
- A "cubic" EOS is need to do this.
- **Cubic Equations of State** are PVT relationships when expanded, results in third-order equations for the specific volume.
- Two Cubic types: (1) Van der Waals and (2) Soave-Redlich-Kwong (SRK)

Van der Waals equation of state:

$$P = \frac{RT}{\hat{V} - b} - \frac{a}{\hat{V}^2}$$

Or

$$p = \frac{nRT}{V - nb} - \frac{n^2 a}{V^2}$$

where

$$a = \frac{27 R^2 T_c^2}{64 P_c}$$

$$b = \frac{R T_c}{8 P_c}$$

the term $a/\hat{V}^2$ accounts for attractive forces between molecules

and b is a correction accounting for the volume occupied by the molecules themselves

Soave-Redlich-Kwong (SRK) equation:

$$P = \frac{RT}{\hat{V} - b} - \frac{\alpha a}{\hat{V}(\hat{V} + b)}$$

where $a = 0.42747 \frac{(RT_c)^2}{P_c}$ $b = 0.08664 \frac{RT_c}{P_c}$

the *a* is a molecular interaction parameter, while the *b* term is a volume correction

$$\alpha = \left[1 + m\left(1 - \sqrt{T_r}\right)\right]^2$$

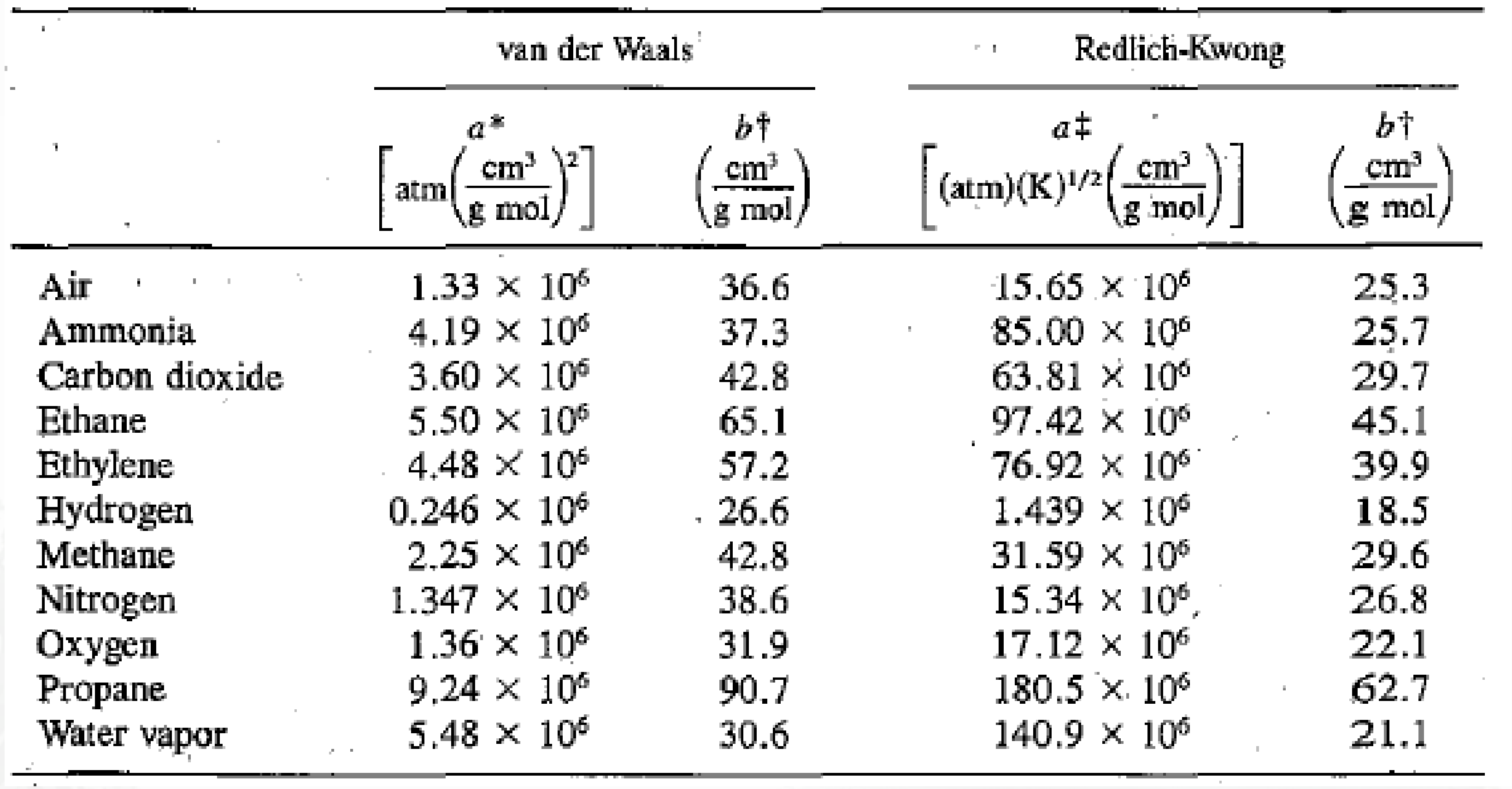
$m = 0.48508 + 1.55171\omega - 0.1561\omega^2$ $T_r = T/T_c$

ω: is Pitzer acentric factor, a parameter that reflects the geometry and polarity of a molecule

Solving the cubic equation typically requires an iterative solution

"TRIAL-AND- ERROR"

Constants for the Van der Waals and Redlich-Kwong Equations "Calculated From the Listed Values of the Critical Constants"



	van der Waals		Redlich-Kwong	
	a^* $\left[\text{atm}\left(\frac{\text{cm}^3}{\text{g mol}}\right)^2\right]$	$b^\dagger$ $\left(\frac{\text{cm}^3}{\text{g mol}}\right)$	$a^\ddagger$ $\left[(\text{atm})(\text{K})^{1/2}\left(\frac{\text{cm}^3}{\text{g mol}}\right)\right]$	$b^\dagger$ $\left(\frac{\text{cm}^3}{\text{g mol}}\right)$
Air	1.33×10^6	36.6	15.65×10^6	25.3
Ammonia	4.19×10^6	37.3	85.00×10^6	25.7
Carbon dioxide	3.60×10^6	42.8	63.81×10^6	29.7
Ethane	5.50×10^6	65.1	97.42×10^6	45.1
Ethylene	4.48×10^6	57.2	76.92×10^6	39.9
Hydrogen	0.246×10^6	26.6	1.439×10^6	18.5
Methane	2.25×10^6	42.8	31.59×10^6	29.6
Nitrogen	1.347×10^6	38.6	15.34×10^6	26.8
Oxygen	1.36×10^6	31.9	17.12×10^6	22.1
Propane	9.24×10^6	90.7	180.5×10^6	62.7
Water vapor	5.48×10^6	30.6	140.9×10^6	21.1

Example

A gas cylinder with a volume of 2.50 m^3 contains 1.00 kmol of carbon dioxide at T = 300 K. Use the SRK equation of state to estimate the gas pressure in atm.

The specific molar volume

$$\hat{V} = \frac{V}{n} = \frac{2.5\ \text{m}^3}{1.00\ \text{kmol}}\bigg|\frac{10^3\ \text{L}}{1\ \text{m}^3}\bigg|\frac{1\ \text{kmol}}{10^3\ \text{mol}} = 2.50\,\frac{\text{liter}}{\text{mol}}$$

The critical properties

$$T_c = 304.2\ \text{K and } P_c = 72.9\ \text{atm.}$$

$$\omega = 0.225.$$

The constants become

$$a = 0.42747\,\frac{\{[0.08206\ \mathrm{L\cdot atm/(mol\cdot K)}](304.2\ \mathrm{K})\}^2}{72.9\ \mathrm{atm}}$$

$$= 3.654\ \mathrm{L^2\cdot atm/mol^2}$$

$$b = 0.08664\,\frac{[0.08206\ \mathrm{L\cdot atm/(mol\cdot K)}](304.2\ \mathrm{K})}{72.9\ \mathrm{atm}}$$

$$= 0.02967\ \mathrm{L/mol}$$

$$m = 0.8263$$

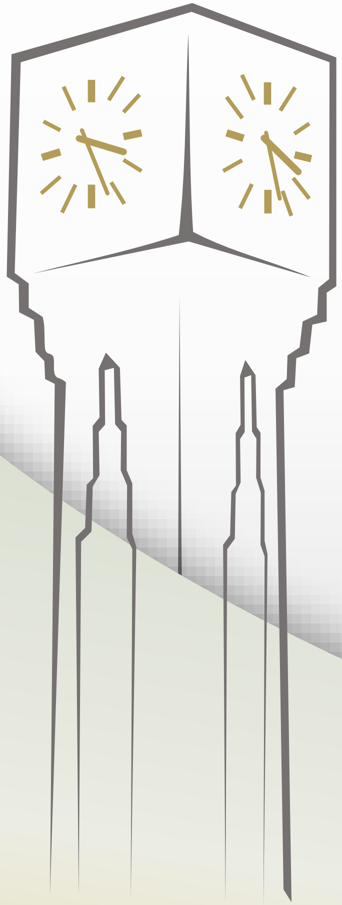
$$T_r = 0.986$$

$$\alpha = 1.0115$$

$$P = \frac{RT}{\hat{V} - b} - \frac{\alpha a}{\hat{V}(\hat{V} + b)}$$

$$= \frac{[0.08206\ \mathrm{L\cdot atm/(mol\cdot K)}](300\ \mathrm{K})}{[(2.50 - 0.02967)\mathrm{L/mol}]} - \frac{1.0115(3.654\ \mathrm{L^2\cdot atm/mol^2})}{(2.50\ \mathrm{L/mol})[(2.50 + 0.02967)\ \mathrm{L/mol}]}$$

$$= \boxed{9.38\ \mathrm{atm}}$$



5.4 Compressibility Factor Equation

5.4 Compressibility Factor Equation

- The compressibility factor of a gaseous species is defined as the ratio

$$\boxed{z = \frac{P\hat{V}}{RT}}$$

- For ideal gas z = 1, the extent to which z differs from 1 is a measure of the extent to which the gas is behaving non-ideally.
- The compressibility factor equation of state

$$\boxed{P\hat{V} = zRT \qquad PV = znRT \qquad P\dot{V} = z\dot{n}RT}$$

- The compressibility factor is a function of temperature and pressure

$$z = f(T, P)$$

- Values are available in references like: Perry's Chemical Engineers' Handbook

for air, argon, CO_2, CO, H_2, CH_4, N_2, O_2, steam,

Refer to book to for details and examples of this section

The procedure for using the generalized compressibility chart for PVT calculations is as follows:

1. Determine the critical temperature, T_c , and critical pressure, P_c , of the species "Table B.1".
2. If the gas is either hydrogen or helium, determine adjusted critical constants from the empirical formulas:

$$T_c^a = T_c + 8\,\mathrm{K}$$

$$P_c^a = P_c + 8\,\mathrm{atm}$$

3. Calculate reduced values of the two known variables (temperature and pressure, temperature and volume, or pressure and volume) using the definitions:

All temperatures and pressures used must be absolute.

$$T_r = \frac{T}{T_c}$$

$$P_r = \frac{P}{P_c}$$

$$V_r^{\text{ideal}} = \frac{P_c\hat{V}}{RT_c}$$

1. Use the compressibility charts to determine the compressibility factor, and then solve for the unknown variable from the compressibility-factor equation of state.

$$z = \frac{P\hat{V}}{RT}$$

Generalized compressibility factor chart

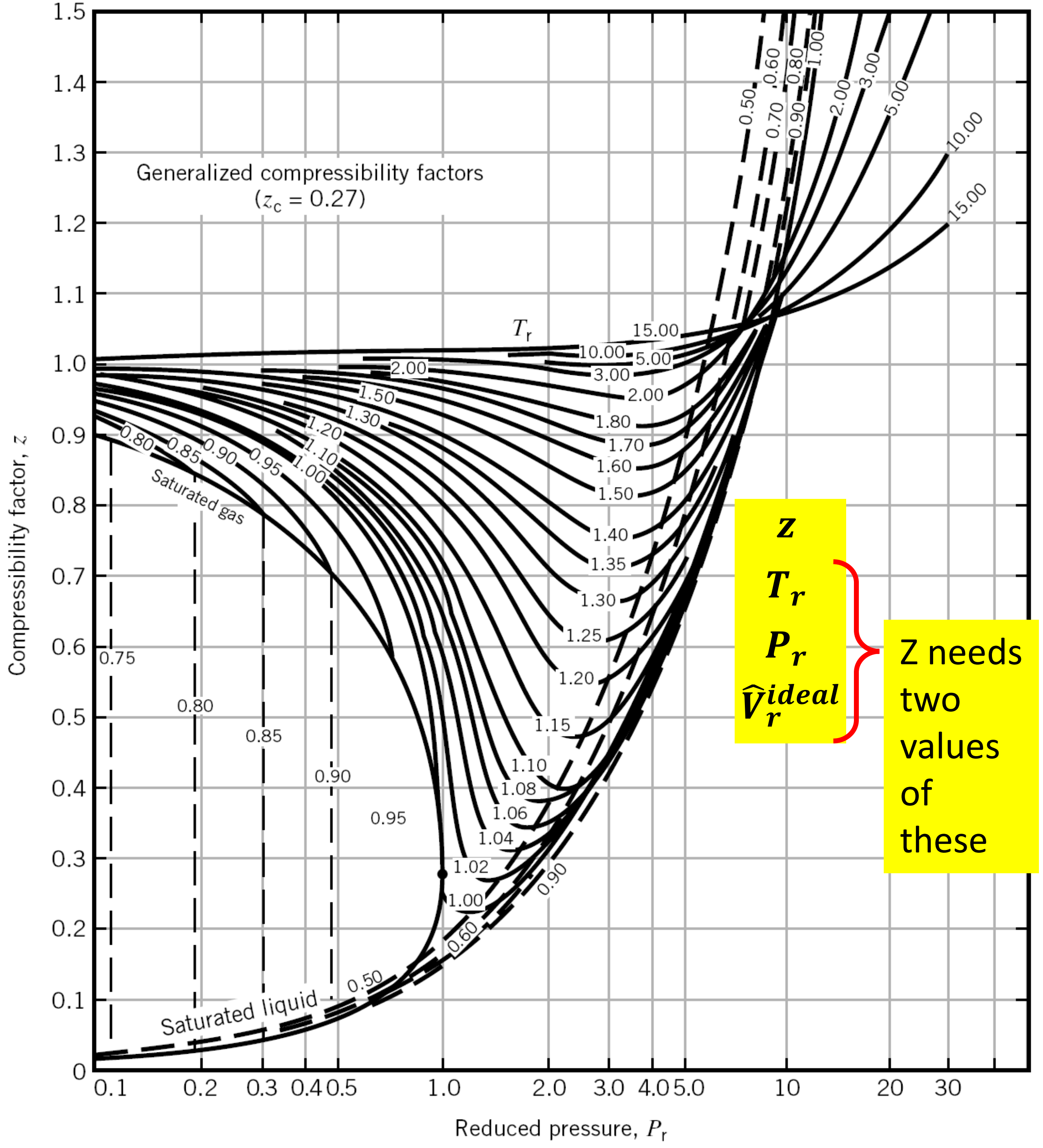
Figure 5.4-1

high pressures

Difficult to read some (Z) values accurately in some pressure ranges

Pressure ranges

Low	**P_r: 0 to 1**
Medium	**P_r: 0 to 10**
High	**P_r: 0 to 40**



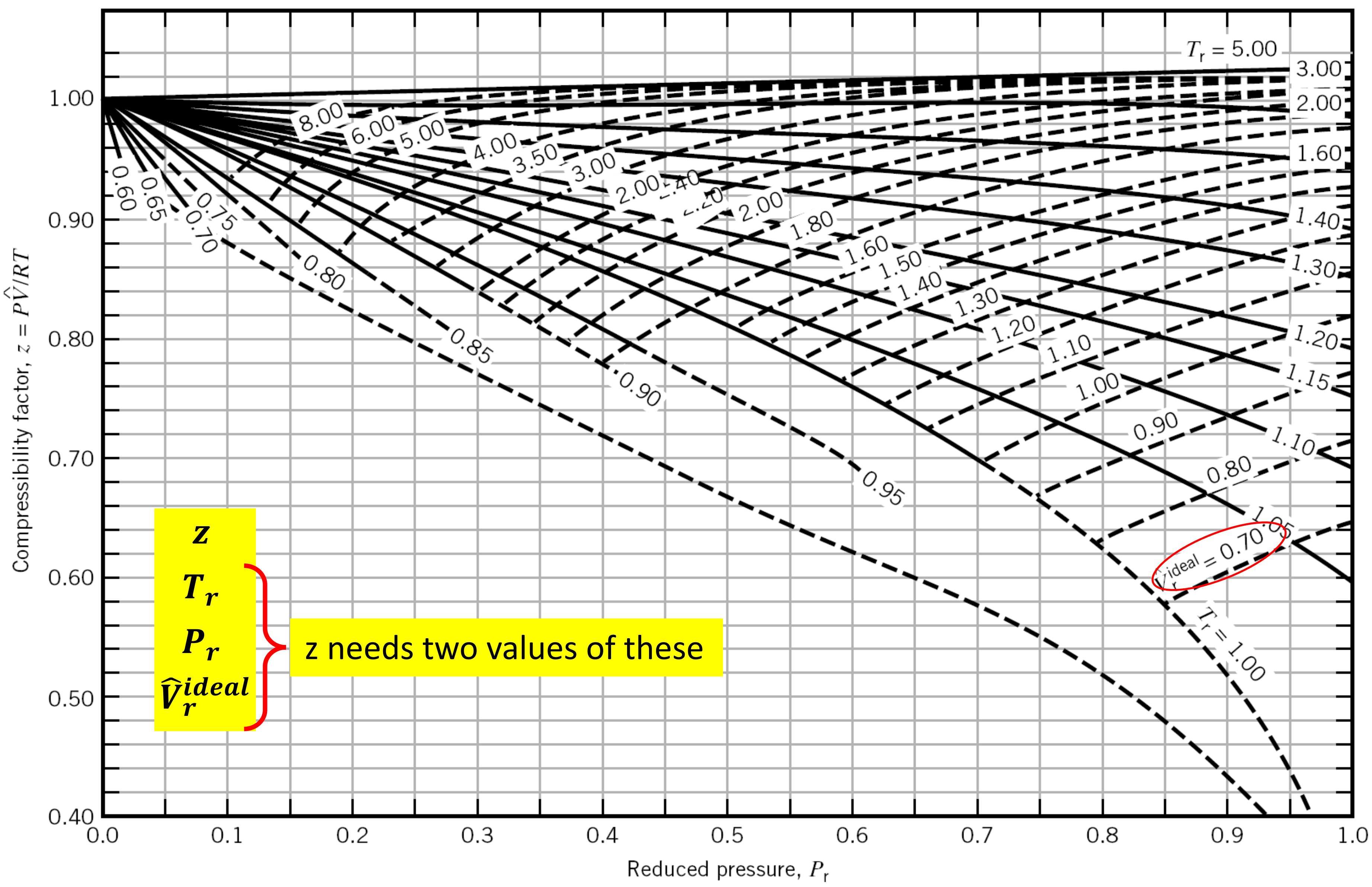
Z

T_r

P_r

$\hat{V}_r^{ideal}$

Z needs two values of these



z

T_r

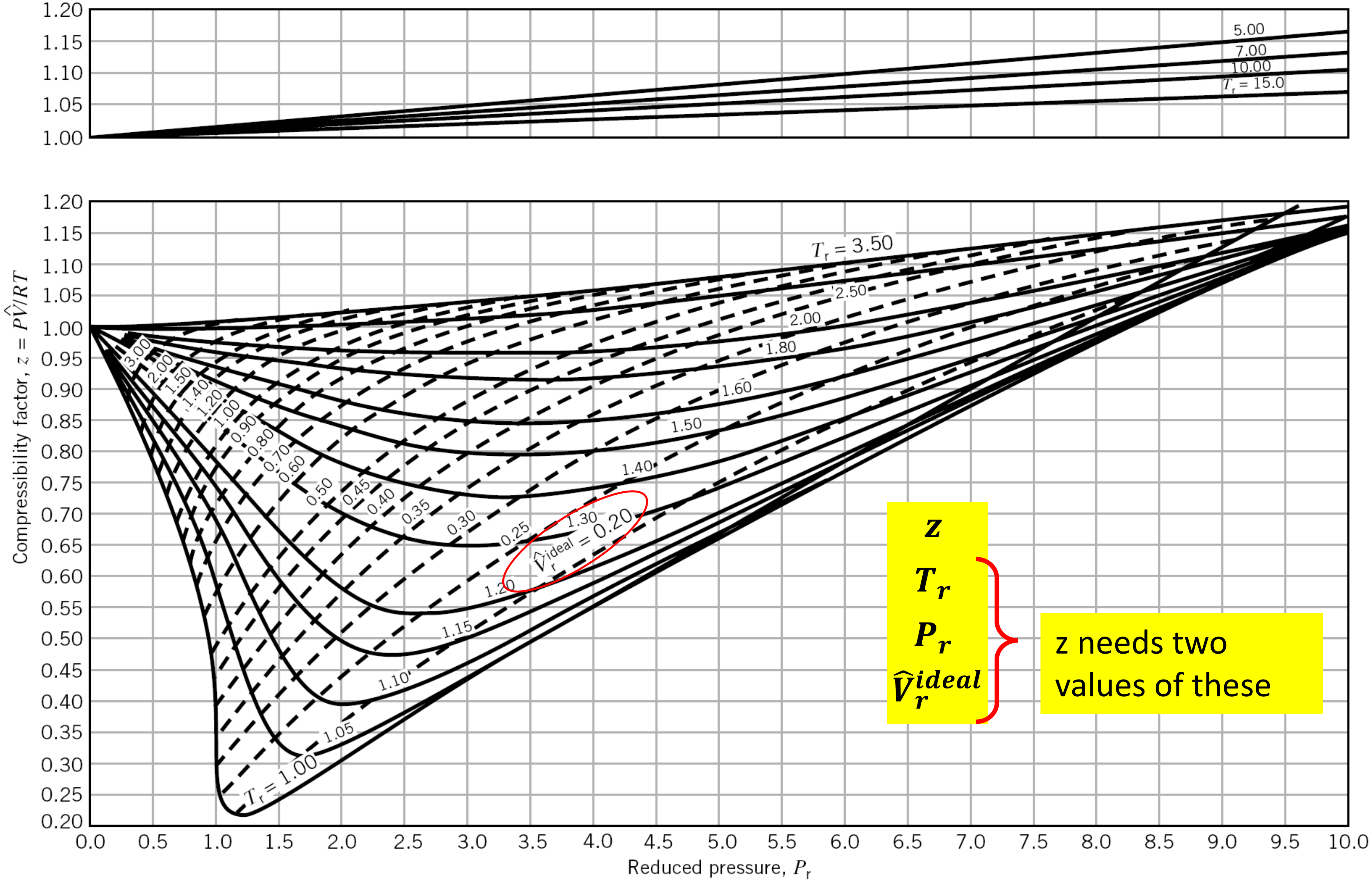
P_r

$\hat{V}_r^{ideal}$

z needs two values of these

Figure 5.4-2 (p. 209)

Generalized compressibility chart, **low pressures (P_r: 0 to 1)**



z

T_r

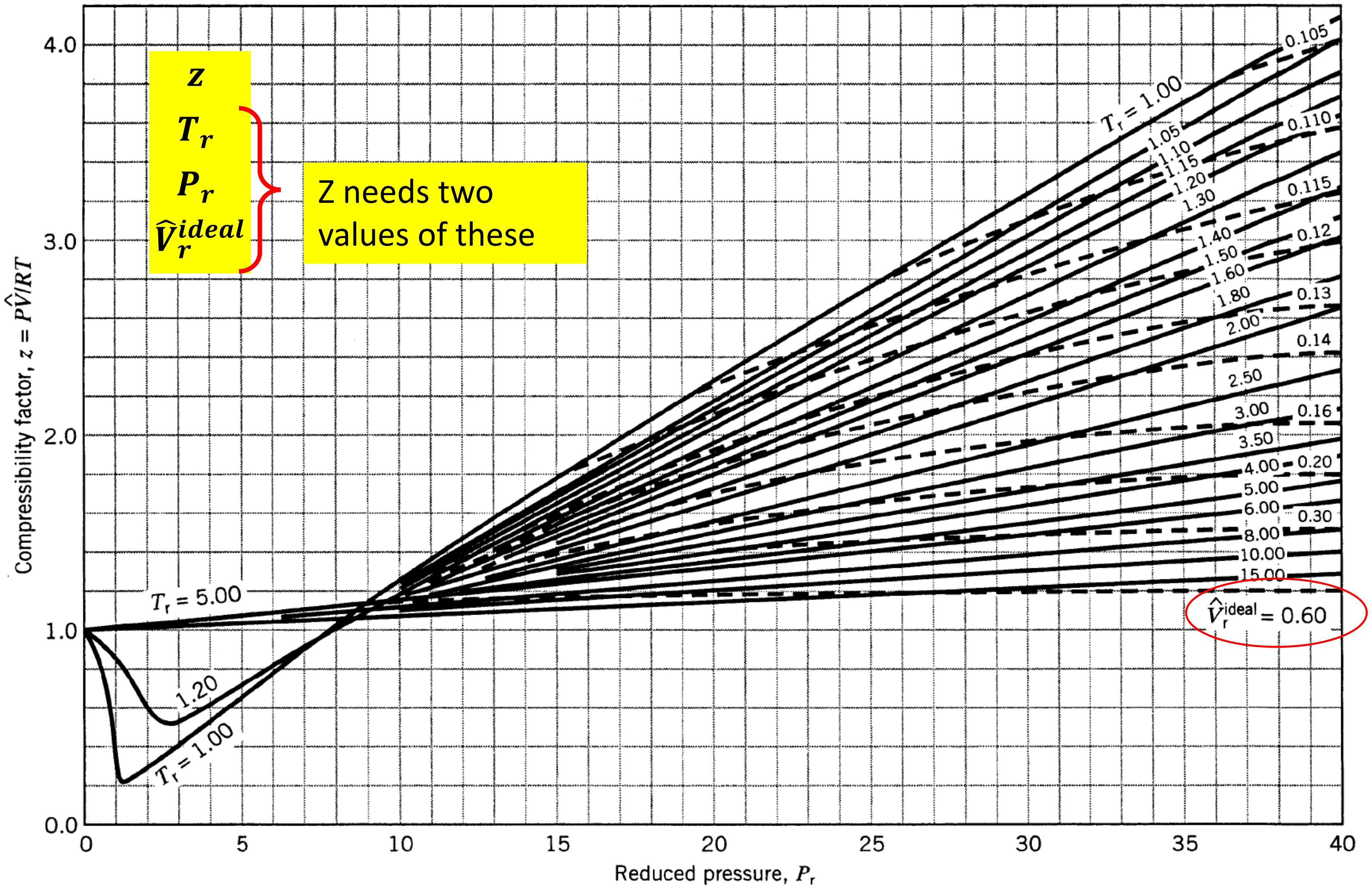
P_r

$\hat{V}_r^{ideal}$

z needs two values of these

Figure 5.4-3 (p. 210)

Generalized compressibility chart, **medium pressures (P_r: 0 to 10)**



z

T_r

P_r

$\hat{V}_r^{ideal}$

Z needs two values of these

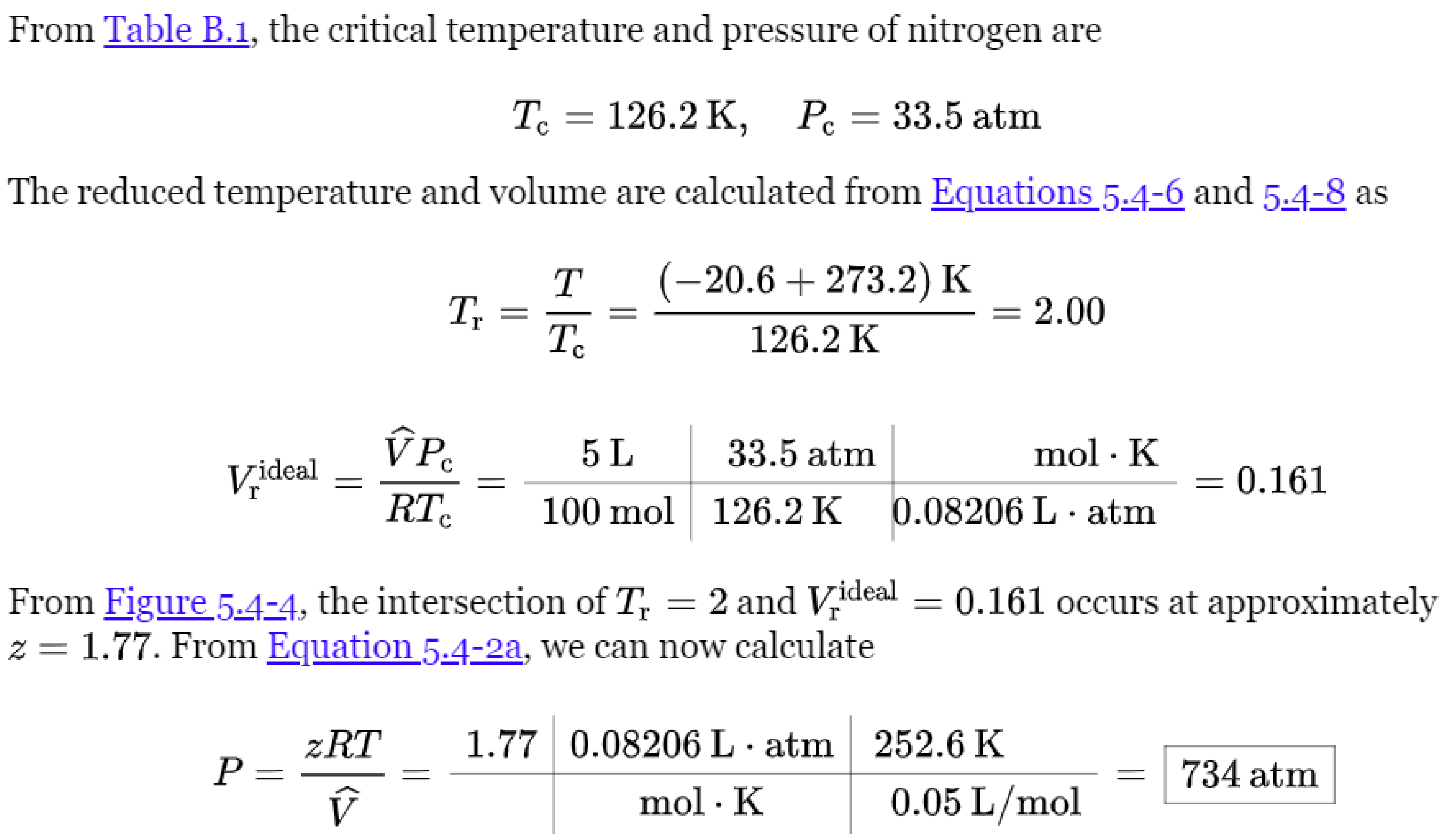
Figure 5.4-4

Generalized compressibility chart, **high pressures (P_r: 0 to 40)**

Example 5.4-1

One hundred gram-moles of nitrogen is contained in a 5.00-liter vessel at -20.6 ˚C. Estimate the pressure in the cylinder.

Solution



From Table B.1, the critical temperature and pressure of nitrogen are

$$T_\text{c} = 126.2\,\text{K}, \quad P_\text{c} = 33.5\,\text{atm}$$

The reduced temperature and volume are calculated from Equations 5.4-6 and 5.4-8 as

$$T_\text{r} = \frac{T}{T_\text{c}} = \frac{(-20.6 + 273.2)\,\text{K}}{126.2\,\text{K}} = 2.00$$

$$V_\text{r}^\text{ideal} = \frac{\hat{V} P_\text{c}}{RT_\text{c}} = \begin{array}{c|c|c} 5\,\text{L} & 33.5\,\text{atm} & \text{mol}\cdot\text{K} \\ \hline 100\,\text{mol} & 126.2\,\text{K} & 0.08206\,\text{L}\cdot\text{atm} \end{array} = 0.161$$

From Figure 5.4-4, the intersection of $T_\text{r} = 2$ and $V_\text{r}^\text{ideal} = 0.161$ occurs at approximately $z = 1.77$. From Equation 5.4-2a, we can now calculate

$$P = \frac{zRT}{\hat{V}} = \begin{array}{c|c|c} 1.77 & 0.08206\,\text{L}\cdot\text{atm} & 252.6\,\text{K} \\ \hline & \text{mol}\cdot\text{K} & 0.05\,\text{L/mol} \end{array} = \boxed{734\,\text{atm}}$$

5.4c Nonideal Gas Mixtures

- Use the generalized compressibility charts after estimating the *pseudocritical properties* (Kay's Rule):

$$Pseudocritical\ Temperature: \quad T_c' = y_A T_{cA} + y_B T_{cB} + y_C T_{cC} + \ldots..$$

$$Pseudocritical\ \ pressure: \quad P_c' = y_A P_{cA} + y_B P_{cB} + y_C P_{cC} + \ldots$$

$$Pseudoreduced\ Temperature: T_r' = \frac{T}{T_c'}$$

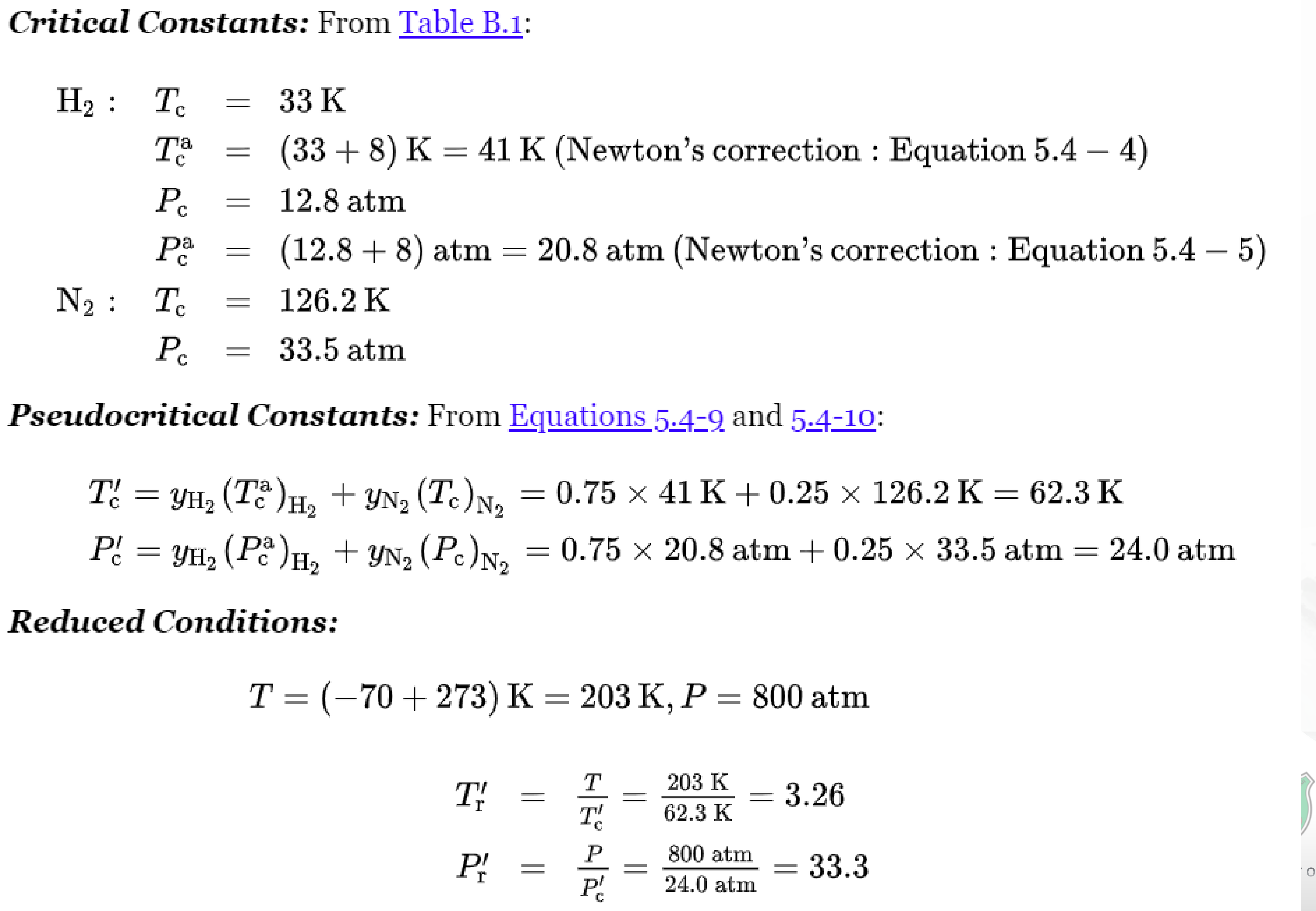
$$Pseudoreduced\ \ pressure: P_r' = \frac{P}{P_c'}$$

$$V = \frac{z_m RT}{P}$$

Example 5.4-2 Kay's Rule

A mixture of 75% H_2 and 25% N_2 (molar basis) is contained in a tank at 800 atm and -70°C. Estimate the specific volume of the mixture in L/mol using Kay's Law.

Solution



Critical Constants: From Table B.1:

$$\begin{aligned} H_2: \quad T_c &= 33\ \text{K} \\ T_c^a &= (33+8)\ \text{K} = 41\ \text{K}\ (\text{Newton's correction : Equation } 5.4-4) \\ P_c &= 12.8\ \text{atm} \\ P_c^a &= (12.8+8)\ \text{atm} = 20.8\ \text{atm}\ (\text{Newton's correction : Equation } 5.4-5) \\ N_2: \quad T_c &= 126.2\ \text{K} \\ P_c &= 33.5\ \text{atm} \end{aligned}$$

Pseudocritical Constants: From Equations 5.4-9 and 5.4-10:

$$T_c' = y_{H_2}(T_c^a)_{H_2} + y_{N_2}(T_c)_{N_2} = 0.75 \times 41\ \text{K} + 0.25 \times 126.2\ \text{K} = 62.3\ \text{K}$$

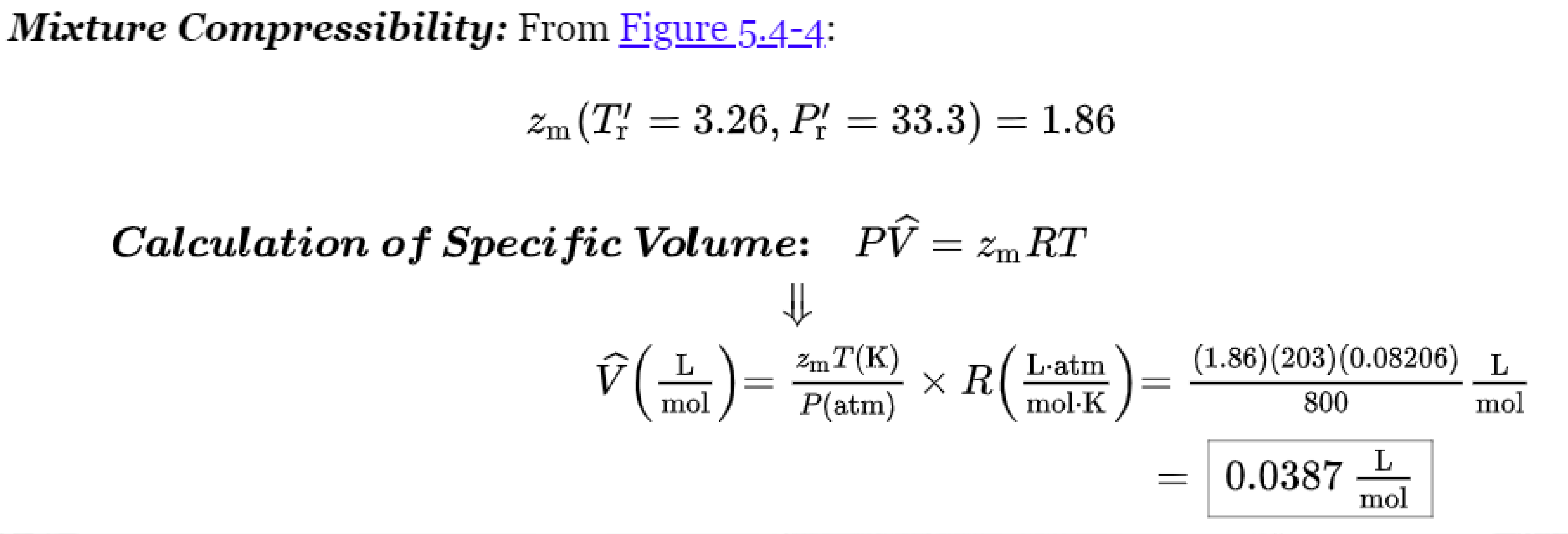
$$P_c' = y_{H_2}(P_c^a)_{H_2} + y_{N_2}(P_c)_{N_2} = 0.75 \times 20.8\ \text{atm} + 0.25 \times 33.5\ \text{atm} = 24.0\ \text{atm}$$

Reduced Conditions:

$$T = (-70+273)\ \text{K} = 203\ \text{K}, P = 800\ \text{atm}$$

$$\begin{aligned} T_r' &= \frac{T}{T_c'} = \frac{203\ \text{K}}{62.3\ \text{K}} = 3.26 \\ P_r' &= \frac{P}{P_c'} = \frac{800\ \text{atm}}{24.0\ \text{atm}} = 33.3 \end{aligned}$$

Solution cont'd



Mixture Compressibility: From Figure 5.4-4:

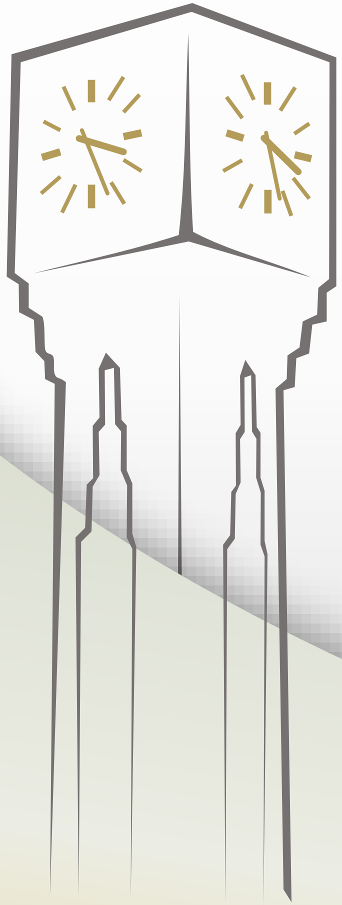
$$z_{\mathrm{m}}(T_{\mathrm{r}}' = 3.26, P_{\mathrm{r}}' = 33.3) = 1.86$$

Calculation of Specific Volume: $P\widehat{V} = z_{\mathrm{m}}RT$

$$\Downarrow$$

$$\widehat{V}\left(\frac{\mathrm{L}}{\mathrm{mol}}\right) = \frac{z_{\mathrm{m}}T(\mathrm{K})}{P(\mathrm{atm})} \times R\left(\frac{\mathrm{L{\cdot}atm}}{\mathrm{mol{\cdot}K}}\right) = \frac{(1.86)(203)(0.08206)}{800}\,\frac{\mathrm{L}}{\mathrm{mol}}$$

$$= \boxed{0.0387\,\frac{\mathrm{L}}{\mathrm{mol}}}$$



Problem Solving

Exercises on Sections 5.2 and 5.4

Exercise 1 – unsolved

Problem 5.34. An ideal-gas mixture contains 35% helium, 20% methane, and 45% nitrogen by volume at 2.00 atm absolute and 90°C.

Calculate:

(a) the partial pressure of each component,

(b) the mass fraction of methane,

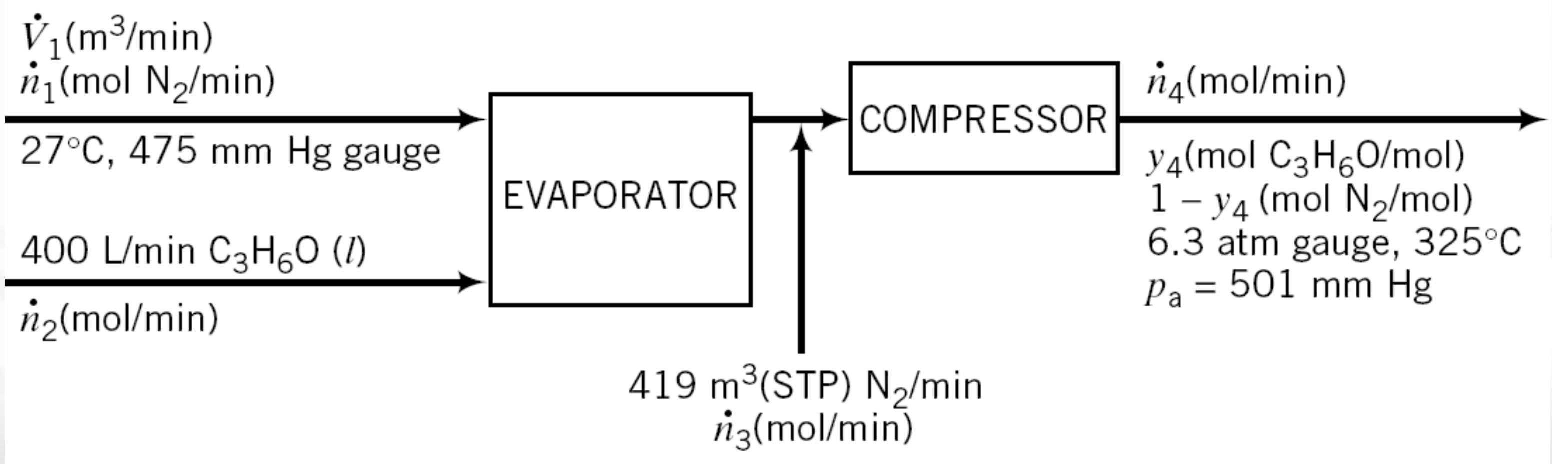
(c) the average molecular weight of the gas, and

(d) the density of the gas in kg/m^3.

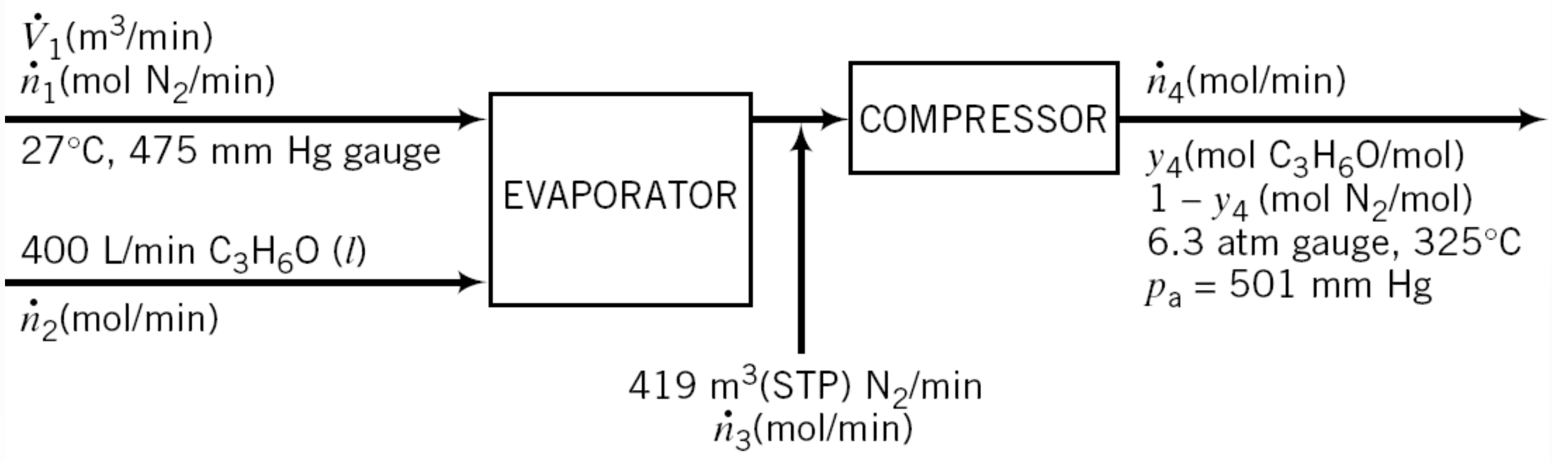
Exercise 2

Example 5.2-5. Liquid acetone (C_3H_6O) is fed at a rate of 400 L/min into a heated chamber, where it evaporates into a nitrogen stream. The gas leaving the heater is diluted by another nitrogen stream flowing at a measured rate of 419 m^3 (STP)/min. the combined gases are then compressed to a total pressure P=6.3 atm gauge at a temperature of 325C. The partial pressure of acetone in this stream is P_a=501 mm Hg. Atmospheric pressure is 763 mm Hg.

1. What is the molar composition of the stream leaving the compressor?
2. What is the volumetric flow rate of the nitrogen entering the evaporator if the temperature and pressure of this stream is 27˚C and 475 mm Hg gauge?



Solution



$\dot{V}_1$ (m^3/min)
$\dot{n}_1$ (mol N_2/min)
27°C, 475 mm Hg gauge

400 L/min C_3H_6O (*l*)
$\dot{n}_2$ (mol/min)

EVAPORATOR

419 m^3(STP) N_2/min
$\dot{n}_3$ (mol/min)

COMPRESSOR

$\dot{n}_4$ (mol/min)
y_4 (mol C_3H_6O/mol)
$1 - y_4$ (mol N_2/mol)
6.3 atm gauge, 325°C
p_a = 501 mm Hg

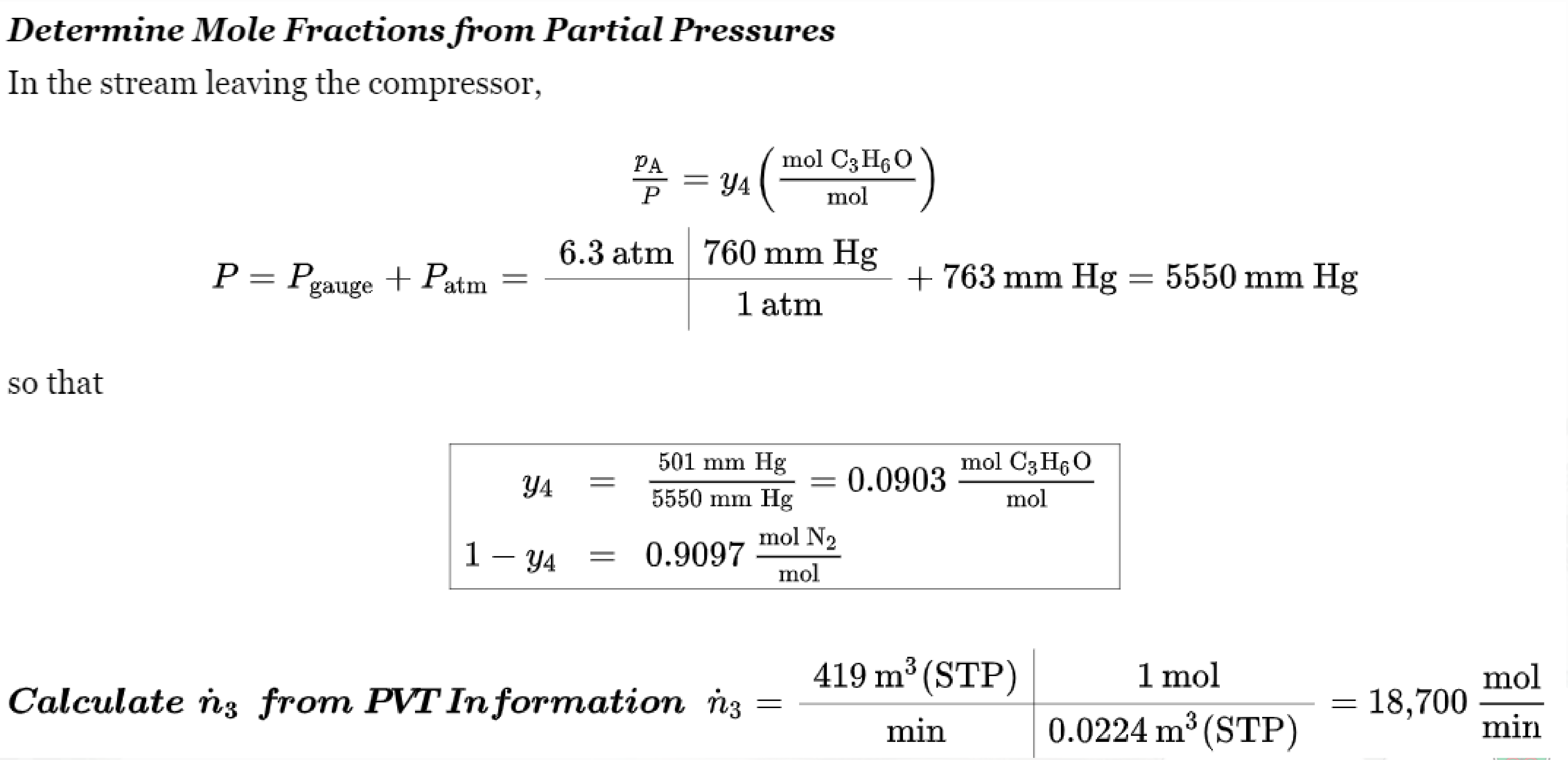
You should be able to examine the flowchart and see exactly how the solution will proceed.

1. Perform a degree-of-freedom analysis for the system and verify that the problem can be solved.
2. Calculate $\dot{n}_2$ (from the given volumetric flow rate and a tabulated density of liquid acetone), $\dot{n}_3$ (from the ideal-gas equation of state), and y_4 $(= p_A/P)$.
3. Calculate $\dot{n}_4$ (overall acetone balance), $\dot{n}_1$ (overall mass balance), and $\dot{V}_1$ (ideal-gas equation of state).

Degree-of-Freedom Analysis

$$
\begin{array}{l}
\ \ 6 \text{ unknowns } (\dot{V}_1, \dot{n}_1, \dot{n}_2, \dot{n}_3, \dot{n}_4, y_4) \\
-1 \text{ specific gravity relationship } (\dot{n}_2) \\
-2 \text{ molecular balances (overall, } C_3H_6O) \\
-1 \text{ ideal} - \text{gas equation of state } (\dot{V}_1) \\
-1 \text{ partial pressure relationship } (y_4) \\
-1 \text{ ideal} - \text{gas equation of state } (\dot{n}_3) \\
\hline
\ \ 0 \text{ degrees of freedom}
\end{array}
$$

Solution cont’d



Determine Mole Fractions from Partial Pressures

In the stream leaving the compressor,

$$\frac{p_A}{P} = y_4\left(\frac{\text{mol C}_3\text{H}_6\text{O}}{\text{mol}}\right)$$

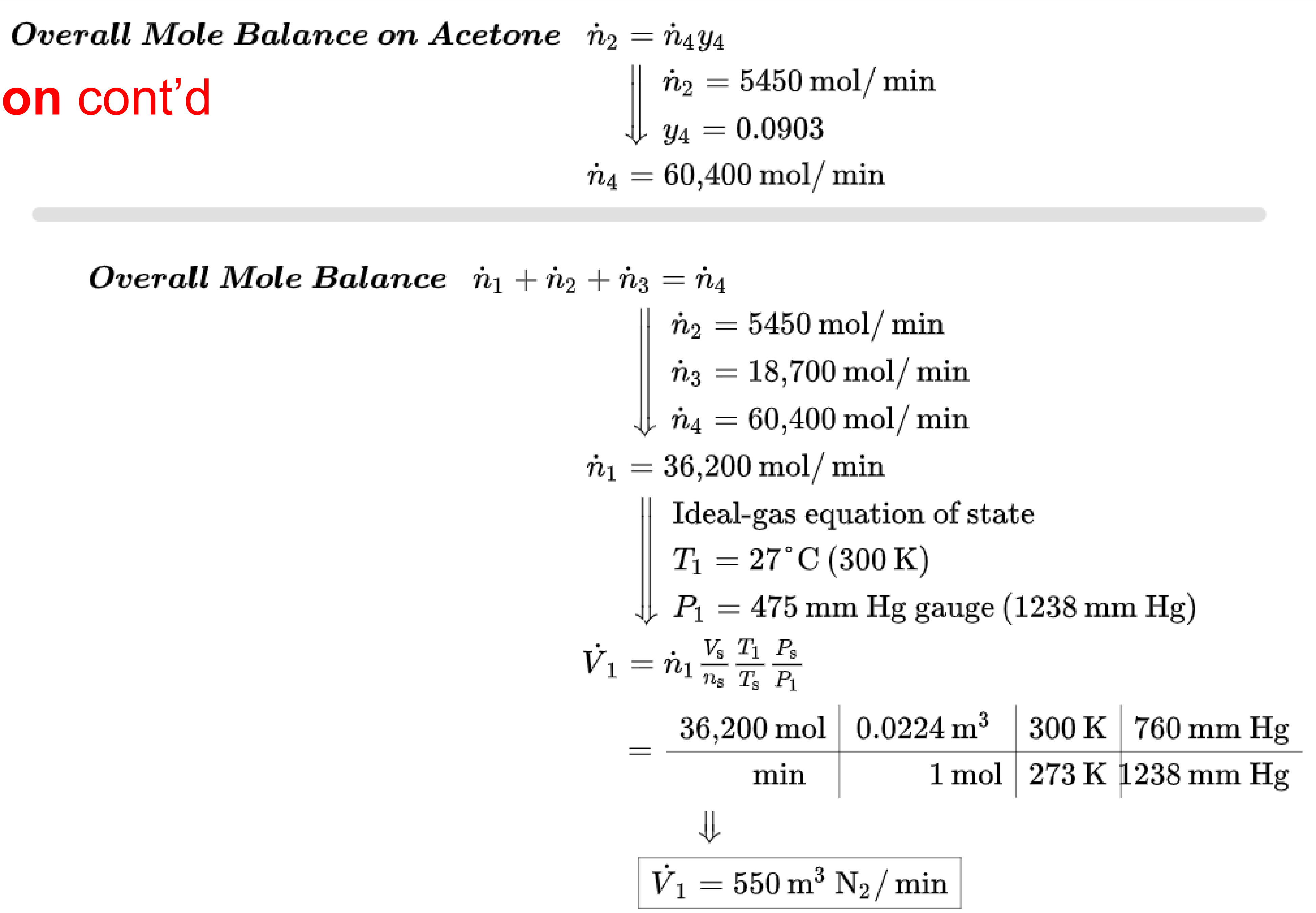
$$P = P_{\text{gauge}} + P_{\text{atm}} = \frac{6.3\ \text{atm}}{}\left|\frac{760\ \text{mm Hg}}{1\ \text{atm}}\right. + 763\ \text{mm Hg} = 5550\ \text{mm Hg}$$

so that

$$\boxed{\begin{aligned} y_4 &= \frac{501\ \text{mm Hg}}{5550\ \text{mm Hg}} = 0.0903\ \frac{\text{mol C}_3\text{H}_6\text{O}}{\text{mol}} \\ 1 - y_4 &= 0.9097\ \frac{\text{mol N}_2}{\text{mol}} \end{aligned}}$$

Calculate $\dot{n}_3$ from PVT Information $\dot{n}_3 = \frac{419\ \text{m}^3(\text{STP})}{\text{min}}\left|\frac{1\ \text{mol}}{0.0224\ \text{m}^3(\text{STP})}\right. = 18{,}700\ \frac{\text{mol}}{\text{min}}$

Solution cont’d



Overall Mole Balance on Acetone $\dot{n}_2 = \dot{n}_4 y_4$

$$\Big\Downarrow \quad \begin{aligned} \dot{n}_2 &= 5450 \text{ mol/ min} \\ y_4 &= 0.0903 \end{aligned}$$

$$\dot{n}_4 = 60{,}400 \text{ mol/ min}$$

Overall Mole Balance $\dot{n}_1 + \dot{n}_2 + \dot{n}_3 = \dot{n}_4$

$$\Big\Downarrow \quad \begin{aligned} \dot{n}_2 &= 5450 \text{ mol/ min} \\ \dot{n}_3 &= 18{,}700 \text{ mol/ min} \\ \dot{n}_4 &= 60{,}400 \text{ mol/ min} \end{aligned}$$

$$\dot{n}_1 = 36{,}200 \text{ mol/ min}$$

$$\Big\Downarrow \quad \begin{aligned} &\text{Ideal-gas equation of state} \\ T_1 &= 27^\circ\text{C (300 K)} \\ P_1 &= 475 \text{ mm Hg gauge (1238 mm Hg)} \end{aligned}$$

$$\dot{V}_1 = \dot{n}_1 \frac{V_s}{n_s} \frac{T_1}{T_s} \frac{P_s}{P_1}$$

$$= \frac{36{,}200 \text{ mol}}{\text{min}} \left| \frac{0.0224 \text{ m}^3}{1 \text{ mol}} \right| \frac{300 \text{ K}}{273 \text{ K}} \left| \frac{760 \text{ mm Hg}}{1238 \text{ mm Hg}} \right.$$

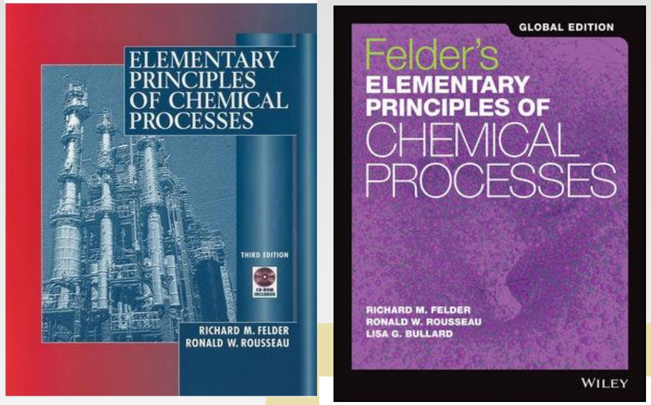
$$\Downarrow$$

$$\boxed{\dot{V}_1 = 550 \text{ m}^3 \text{ N}_2 / \text{min}}$$

Exercise 3 – unsolved

Problem 5.97. A 30-liter cylinder is evacuated and filled with 5.00 kg of a gas containing 10.0 mole% N_2O and the balance N_2. The gas temperature is 24°C. Use the compressibility chart to solve the following problems.

- What is the gauge pressure (atm) of the cylinder gas after the tank is filled?
- A fire breaks out in the plant where the cylinder is kept, and the cylinder valve ruptures when the gas gauge pressure reaches 273 atm. What was the gas temperature (°C) at the moment before the rupture occurred?


ELEMENTARY PRINCIPLES OF CHEMICAL PROCESSES
THIRD EDITION
RICHARD M. FELDER
RONALD W. ROUSSEAU

GLOBAL EDITION
Felder's
ELEMENTARY PRINCIPLES OF CHEMICAL PROCESSES
RICHARD M. FELDER
RONALD W. ROUSSEAU
LISA G. BULLARD
WILEY

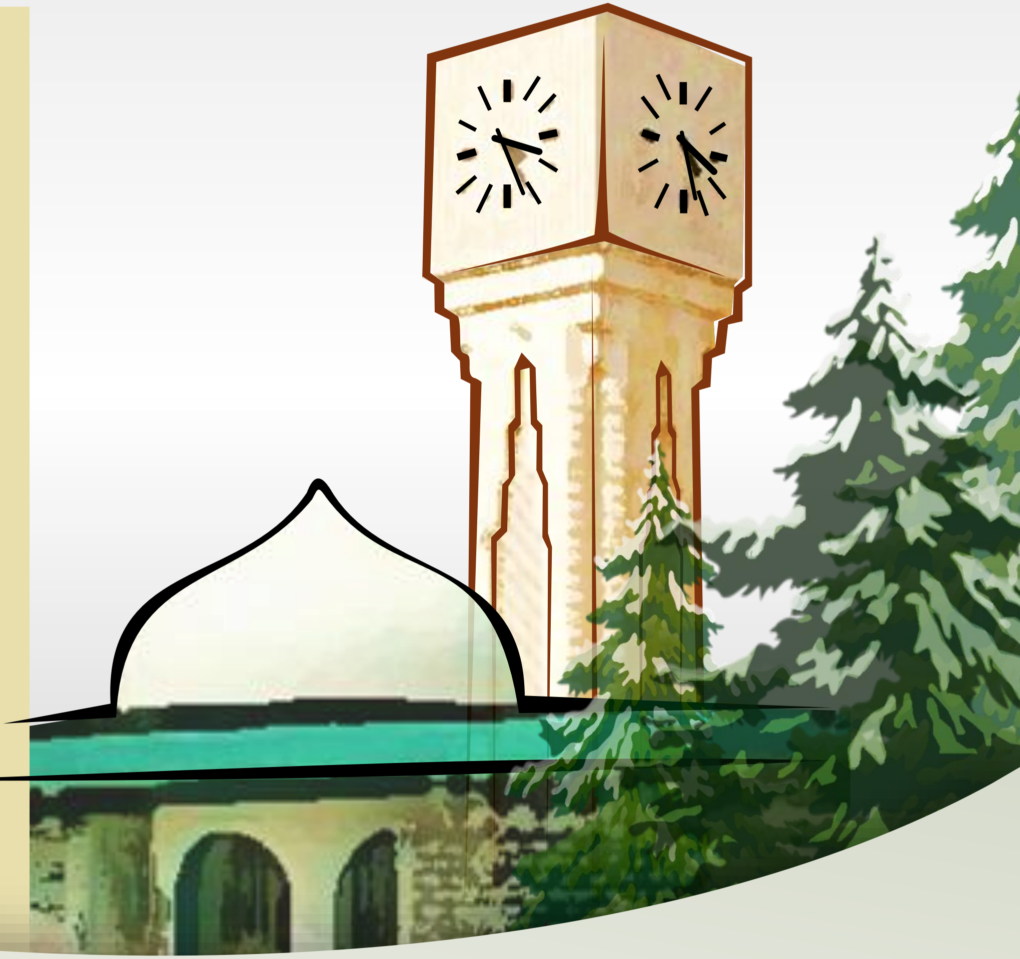
Elementary Principles of Chemical Processes,
3rd or 4th edition,
Wiley & Sons, Inc.
Richard M. Felder, Ronald W. Rousseau, & Lisa G. Bullard.

CHE 0905211

Chemical Engineering Principles 1

Fall 2025

Dr. Hatem Alsyouri	Chapter 6



The University of Jordan
Chemical Engineering Department

Chapter 6

Chapter 6 : Single-Phase Systems

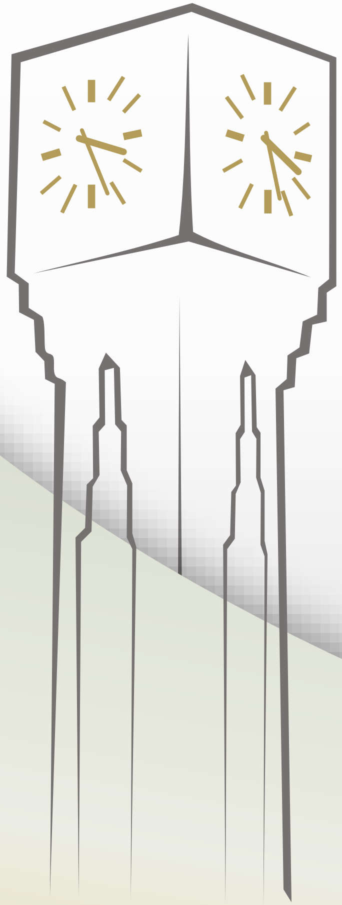
Topics		**6.1 Single component phase equilibrium** 6.1a. Phase diagrams 6.1b. Estimation of vapor pressures **6.2 The The Gibbs Phase Rule** **6.3 Gas-Liquid Systems: One condensable component** **6.4 Multicomponent Gas-Liquid Systems** a. Vapor-liquid equilibrium data b. Raoult's law and Henry's law c. Vapor-liquid equilibrium calculations for solutions that obey Raoult's law	Section 6.1: 2, 3, 6*, 7, 8 Sections 6.2 and 6.3: 9, 10, 12, 18, 19, 22, 25, 26, 29, 33, 35, 39, 41 Section 6.4 a: 43 b: 45, 46, 49, 50
		Problem Solving	
Learning Outcomes			

Notes

This is only a sample material that does not cover the entire topics of the chapter.

Please refer to the textbook for full study, and solve the assigned exercises and suggested problems.

Refer to weekly lesson plan for details of covered topics



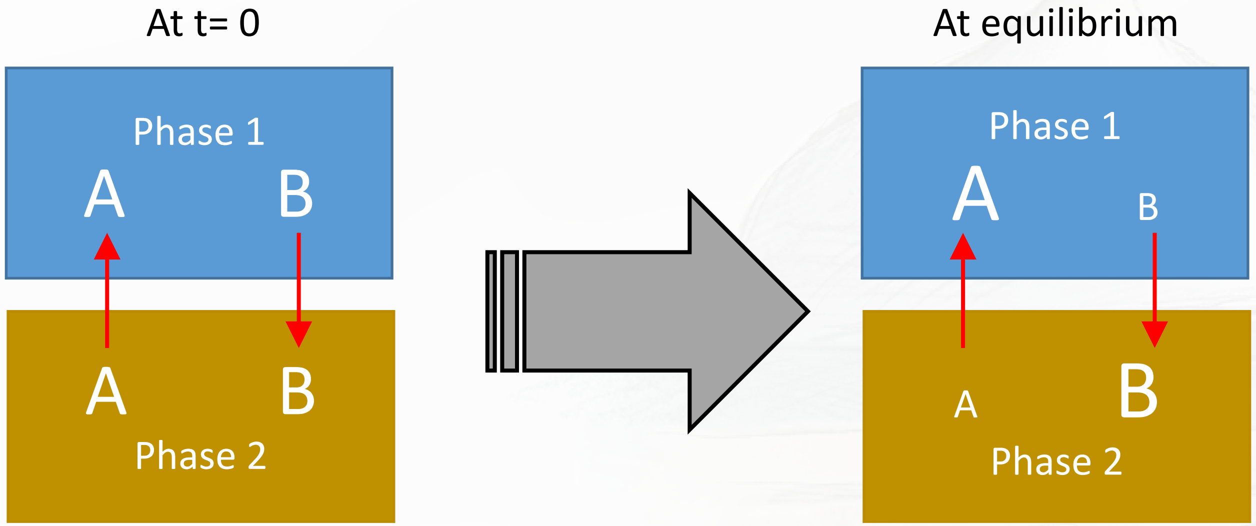
6.1 Single component phase equilibrium

This section outlines the densities of liquid and gases along with the sources of these physical properties.

Introduction

- ***Separation processes*** requires two phases in equilibrium. Components will distribute between the phases. The phases are then separated.
- ***Two-phase systems*** include Vapor-Liquid (V-L), Liquid-Liquid (L-L), Liquid-Solid (L-S), and Vapor-Solid (V-S).
- Two-phases in contact are in ***equilibrium*** when the Temperature (T), Pressure (P), composition, and other variables do not change with time.

Equilibrium concept

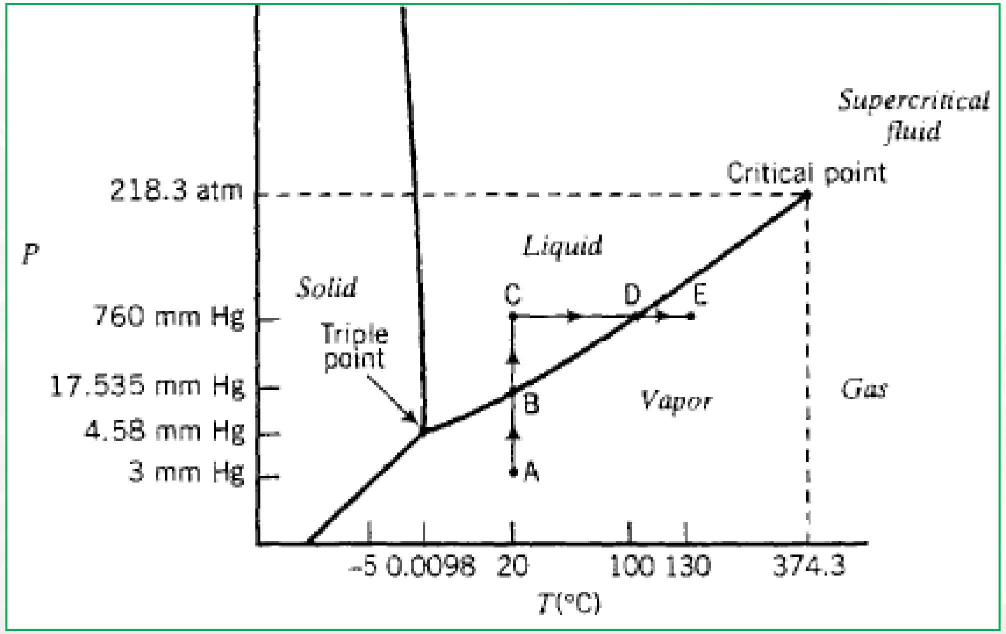


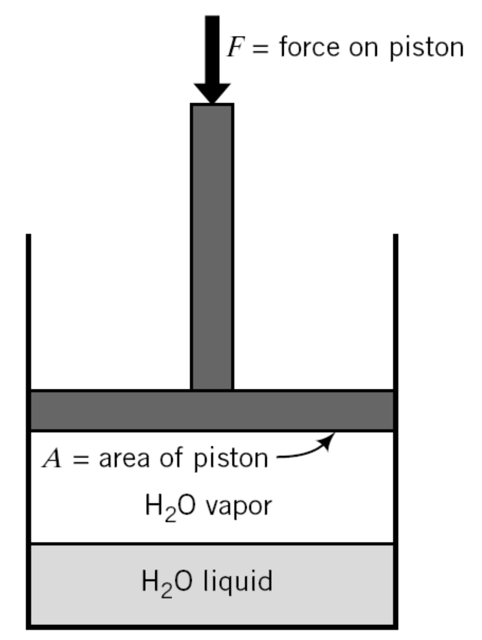
Volatility
Solubility
Miscibility

6.1 Single-Component Phase Equilibrium

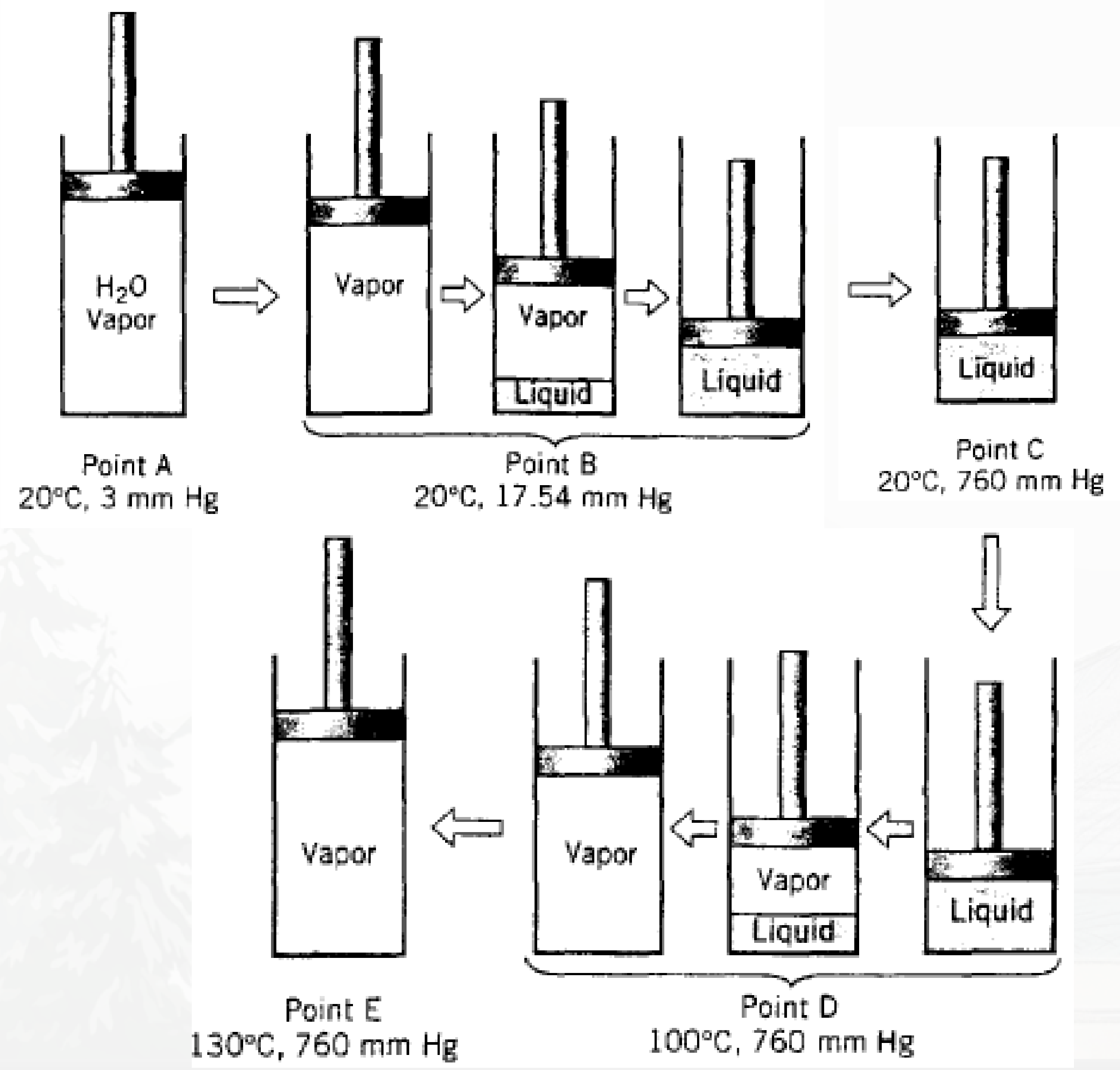
Refer to book to for details and examples of this section

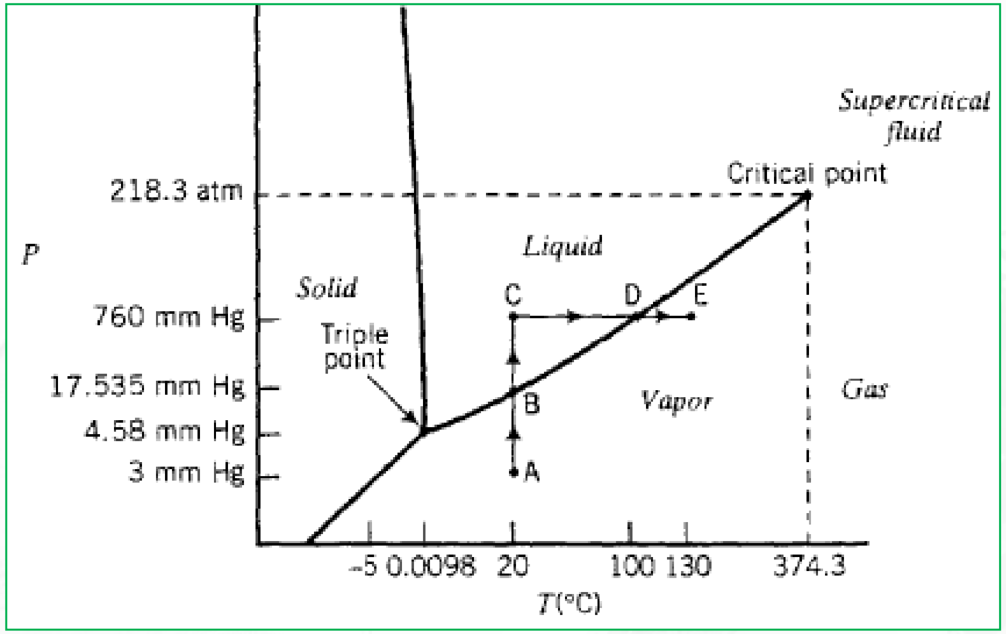
Phase diagram of Water





Brief discussion





Vapor-liquid equilibrium

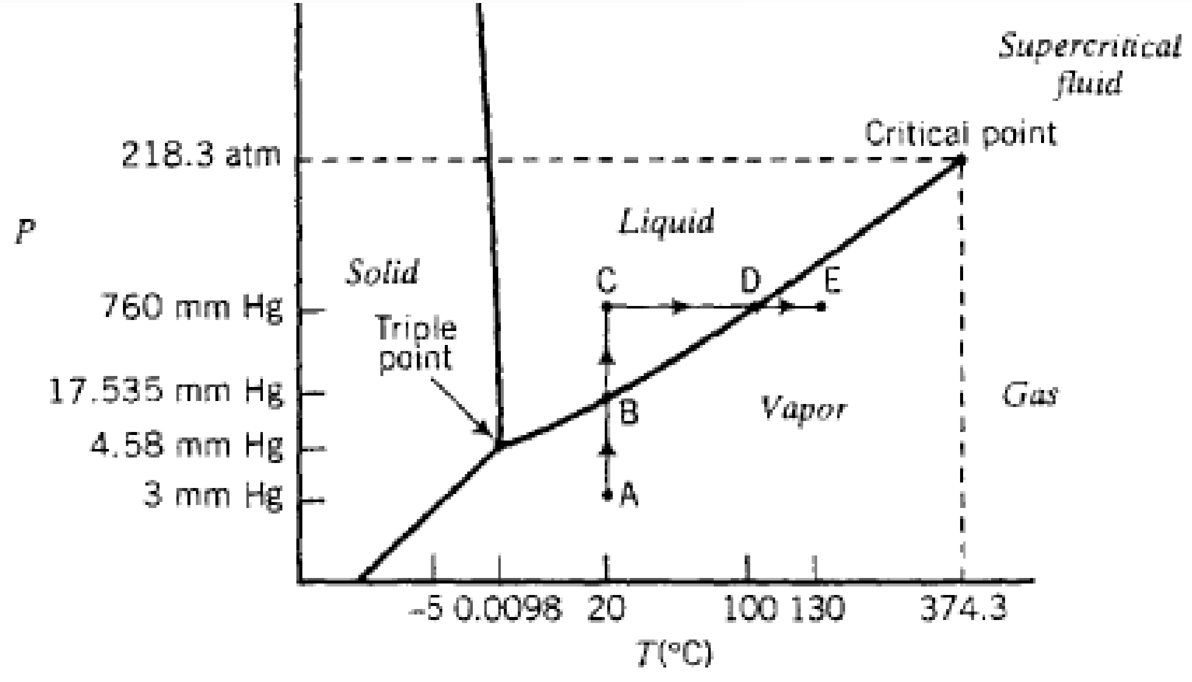
Vapor pressure

Boiling point

Melting/Freezing point

Sublimation/desublimation point

Triple/critical point



Normal boiling point (T_b) and ***melting points (T_m)*** for many substances are given in Table B.1 of Appendix B and for many more substances on pp. 2-7 through 2-47 of Perry's Chemical Engineers' Handbook, and vapor pressures are tabulated on pp. 2-48 through 2-75 of the Handbook.

Refer to book to for details and examples of this section

From Textbook: Table B.1 Physical Property Data

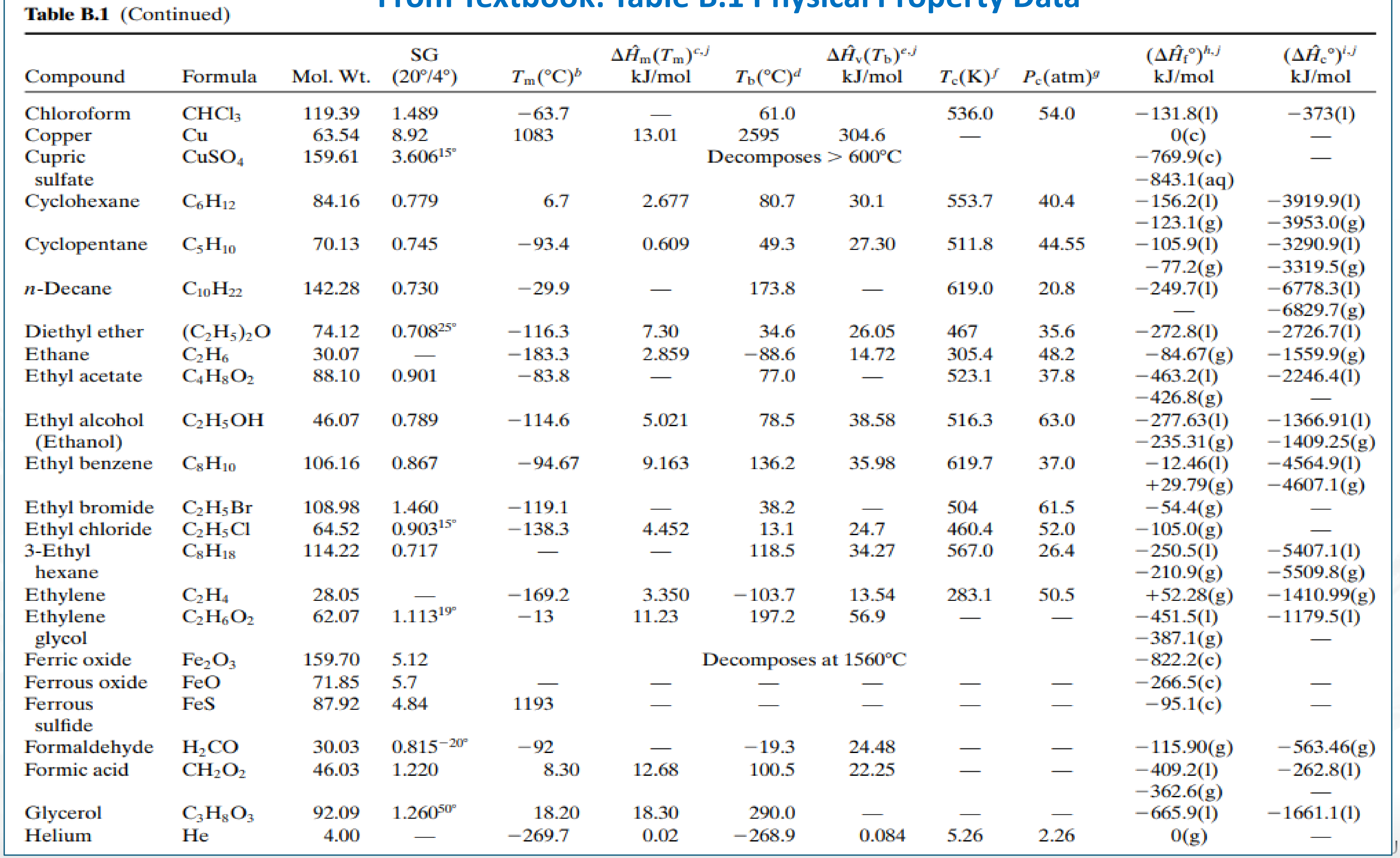


Table B.1 (Continued)

Compound	Formula	Mol. Wt.	SG (20°/4°)	$T_m(°C)^b$	$\Delta\hat{H}_m(T_m)^{c,j}$ kJ/mol	$T_b(°C)^d$	$\Delta\hat{H}_v(T_b)^{e,j}$ kJ/mol	$T_c(K)^f$	$P_c(atm)^g$	$(\Delta\hat{H}_f^\circ)^{h,j}$ kJ/mol	$(\Delta\hat{H}_c^\circ)^{i,j}$ kJ/mol
Chloroform	$CHCl_3$	119.39	1.489	−63.7	—	61.0		536.0	54.0	−131.8(l)	−373(l)
Copper	Cu	63.54	8.92	1083	13.01	2595	304.6	—		0(c)	—
Cupric sulfate	$CuSO_4$	159.61	$3.606^{15°}$			Decomposes > 600°C				−769.9(c) −843.1(aq)	—
Cyclohexane	C_6H_{12}	84.16	0.779	6.7	2.677	80.7	30.1	553.7	40.4	−156.2(l) −123.1(g)	−3919.9(l) −3953.0(g)
Cyclopentane	C_5H_{10}	70.13	0.745	−93.4	0.609	49.3	27.30	511.8	44.55	−105.9(l) −77.2(g)	−3290.9(l) −3319.5(g)
n-Decane	$C_{10}H_{22}$	142.28	0.730	−29.9	—	173.8	—	619.0	20.8	−249.7(l) —	−6778.3(l) −6829.7(g)
Diethyl ether	$(C_2H_5)_2O$	74.12	$0.708^{25°}$	−116.3	7.30	34.6	26.05	467	35.6	−272.8(l)	−2726.7(l)
Ethane	C_2H_6	30.07	—	−183.3	2.859	−88.6	14.72	305.4	48.2	−84.67(g)	−1559.9(g)
Ethyl acetate	$C_4H_8O_2$	88.10	0.901	−83.8	—	77.0	—	523.1	37.8	−463.2(l) −426.8(g)	−2246.4(l) —
Ethyl alcohol (Ethanol)	C_2H_5OH	46.07	0.789	−114.6	5.021	78.5	38.58	516.3	63.0	−277.63(l) −235.31(g)	−1366.91(l) −1409.25(g)
Ethyl benzene	C_8H_{10}	106.16	0.867	−94.67	9.163	136.2	35.98	619.7	37.0	−12.46(l) +29.79(g)	−4564.9(l) −4607.1(g)
Ethyl bromide	C_2H_5Br	108.98	1.460	−119.1	—	38.2	—	504	61.5	−54.4(g)	—
Ethyl chloride	C_2H_5Cl	64.52	$0.903^{15°}$	−138.3	4.452	13.1	24.7	460.4	52.0	−105.0(g)	—
3-Ethyl hexane	C_8H_{18}	114.22	0.717	—	—	118.5	34.27	567.0	26.4	−250.5(l) −210.9(g)	−5407.1(l) −5509.8(g)
Ethylene	C_2H_4	28.05	—	−169.2	3.350	−103.7	13.54	283.1	50.5	+52.28(g)	−1410.99(g)
Ethylene glycol	$C_2H_6O_2$	62.07	$1.113^{19°}$	−13	11.23	197.2	56.9	—	—	−451.5(l) −387.1(g)	−1179.5(l) —
Ferric oxide	Fe_2O_3	159.70	5.12			Decomposes at 1560°C				−822.2(c)	
Ferrous oxide	FeO	71.85	5.7	—	—	—	—	—	—	−266.5(c)	—
Ferrous sulfide	FeS	87.92	4.84	1193	—	—	—	—	—	−95.1(c)	—
Formaldehyde	H_2CO	30.03	$0.815^{-20°}$	−92	—	−19.3	24.48	—	—	−115.90(g)	−563.46(g)
Formic acid	CH_2O_2	46.03	1.220	8.30	12.68	100.5	22.25	—	—	−409.2(l) −362.6(g)	−262.8(l) —
Glycerol	$C_3H_8O_3$	92.09	$1.260^{50°}$	18.20	18.30	290.0	—	—	—	−665.9(l)	−1661.1(l)
Helium	He	4.00	—	−269.7	0.02	−268.9	0.084	5.26	2.26	0(g)	—

6.1b. Estimation of Vapor Pressures (p^*)

Brief discussion

i. **Look It Up**

- Perry's Chemical Engineers' Handbook, nth Edition, R. H. Perry and D. W. Green, Eds.McGraw-Hill, New York, 1997.
- CRC Handbook of Chemistry and Physics, 79th Edition, D. Lide, Ed., Chemical Rubber Company, Boca Raton, FL, 1998

CHARTS
TABLES

ii. **Estimate It**

- Interpolation or extrapolation
- Using Correlations, e.g.,

Bruce E. Poling, John M. Prausnitz, John P. O'Connell, The Properties of Gases and Liquids, 5th Edition, McGraw-Hill, New York, 2004

EQUATIONS

iii. **Measure It**

EXPERIMENTS

(1) Vapor pressure of pure water (p*): Table B.3

Can be used to find:

- Vapor pressure (p*) of pure water at a given temperature (T), or
- Boiling point of water (T_b) at a given pressure (P)

Vapor Pressures from Charts / tables

From our Textbook: Table B.3 Vapor pressure of pure water

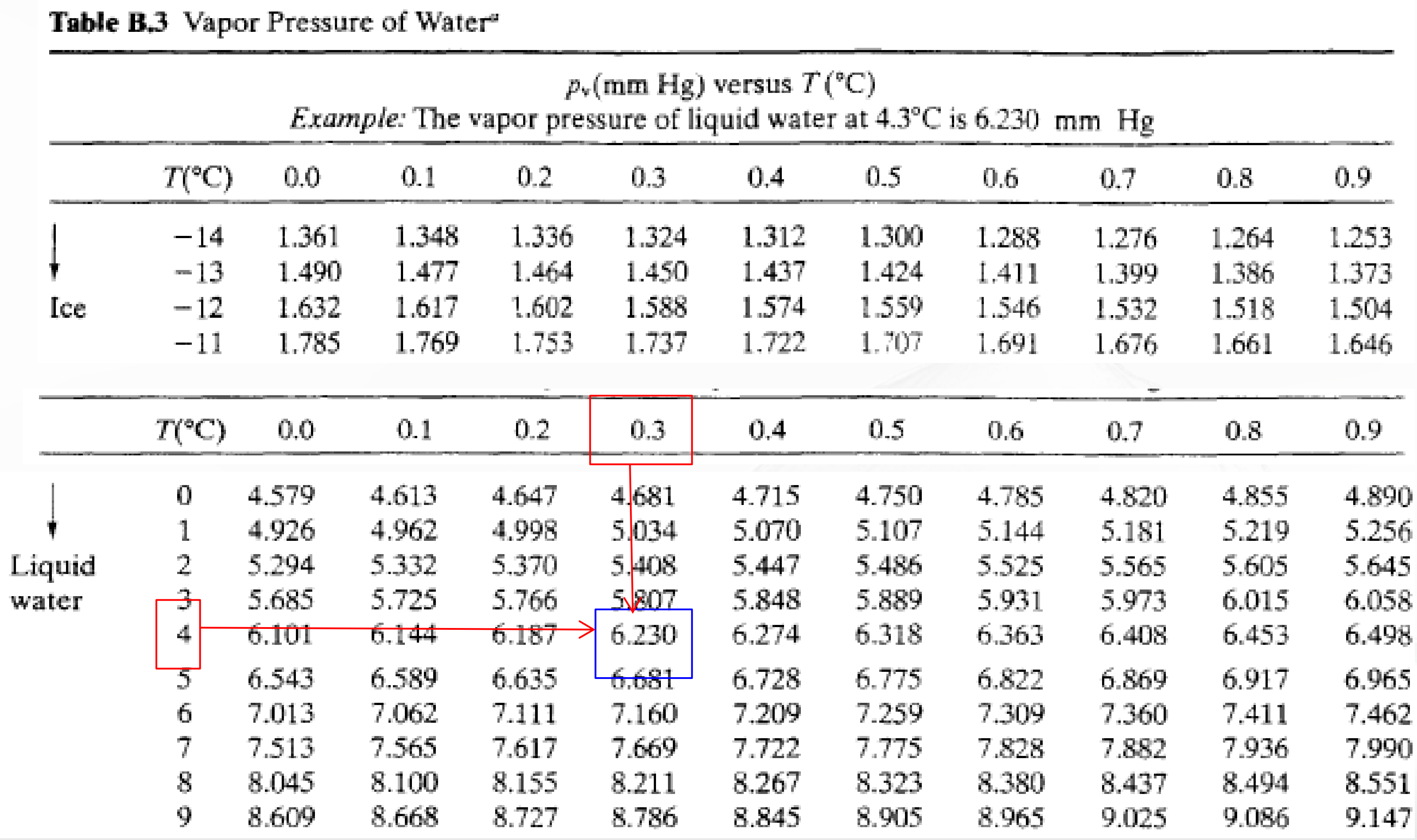


Table B.3 Vapor Pressure of Water[a]

p_v(mm Hg) versus T(°C)

Example: The vapor pressure of liquid water at 4.3°C is 6.230 mm Hg

	T(°C)	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
Ice	−14	1.361	1.348	1.336	1.324	1.312	1.300	1.288	1.276	1.264	1.253
	−13	1.490	1.477	1.464	1.450	1.437	1.424	1.411	1.399	1.386	1.373
	−12	1.632	1.617	1.602	1.588	1.574	1.559	1.546	1.532	1.518	1.504
	−11	1.785	1.769	1.753	1.737	1.722	1.707	1.691	1.676	1.661	1.646

	T(°C)	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
Liquid water	0	4.579	4.613	4.647	4.681	4.715	4.750	4.785	4.820	4.855	4.890
	1	4.926	4.962	4.998	5.034	5.070	5.107	5.144	5.181	5.219	5.256
	2	5.294	5.332	5.370	5.408	5.447	5.486	5.525	5.565	5.605	5.645
	3	5.685	5.725	5.766	5.807	5.848	5.889	5.931	5.973	6.015	6.058
	4	6.101	6.144	6.187	6.230	6.274	6.318	6.363	6.408	6.453	6.498
	5	6.543	6.589	6.635	6.681	6.728	6.775	6.822	6.869	6.917	6.965
	6	7.013	7.062	7.111	7.160	7.209	7.259	7.309	7.360	7.411	7.462
	7	7.513	7.565	7.617	7.669	7.722	7.775	7.828	7.882	7.936	7.990
	8	8.045	8.100	8.155	8.211	8.267	8.323	8.380	8.437	8.494	8.551
	9	8.609	8.668	8.727	8.786	8.845	8.905	8.965	9.025	9.086	9.147

Background learning

A **Background learning** means it’s for your knowledge and will not be part of any assessment/exam

Steam Tables

Background knowledge. Not required in exams. You will see them in details in Principles 2 and Thermodynamics

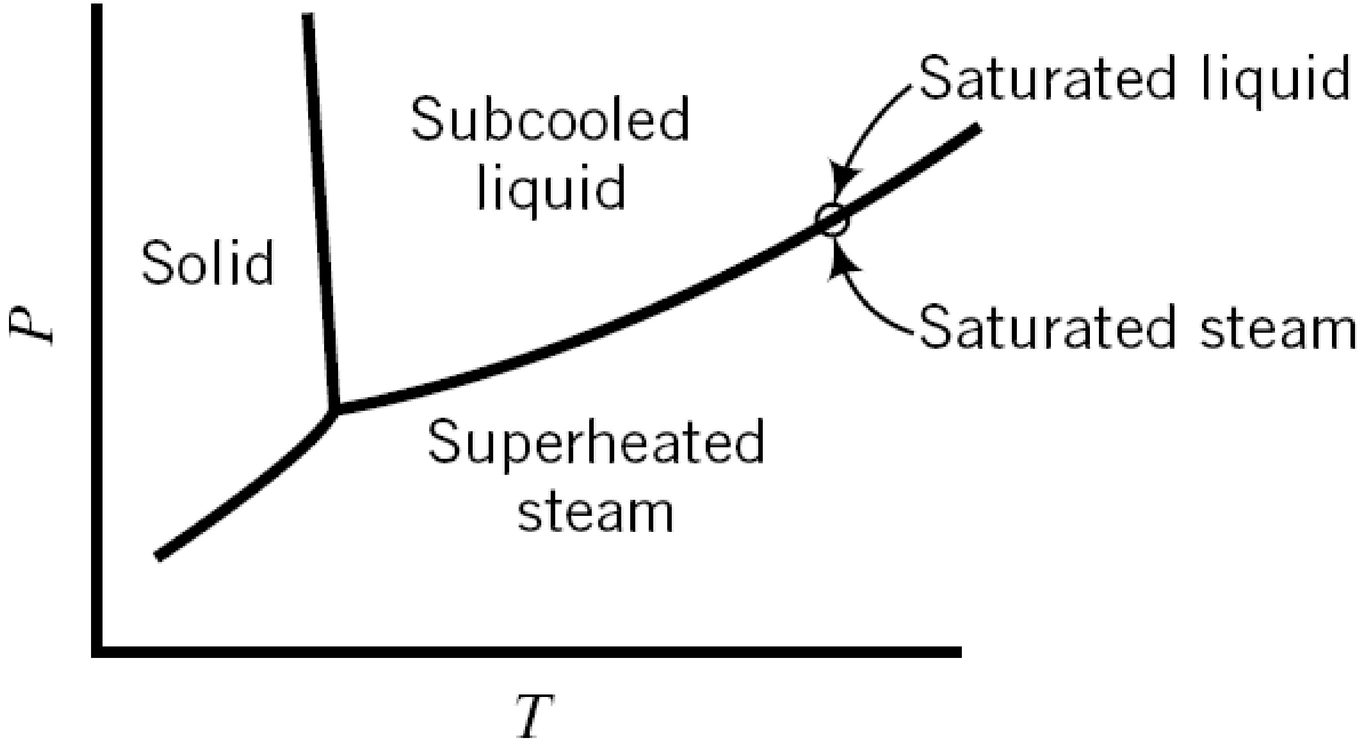
7.5b Steam Tables

Tables that contains the compilations of physical properties of liquid water, saturated steam, and superheated steam.

The ***reference point*** for the tabulated values is ***liquid water at the triple point***

$$[H_2O\ (l, 0.01℃, 0.00611\ bar)]$$

Phase diagram of water



Tabulated Steam Tables

Background learning

Table B.5 Temperature Table

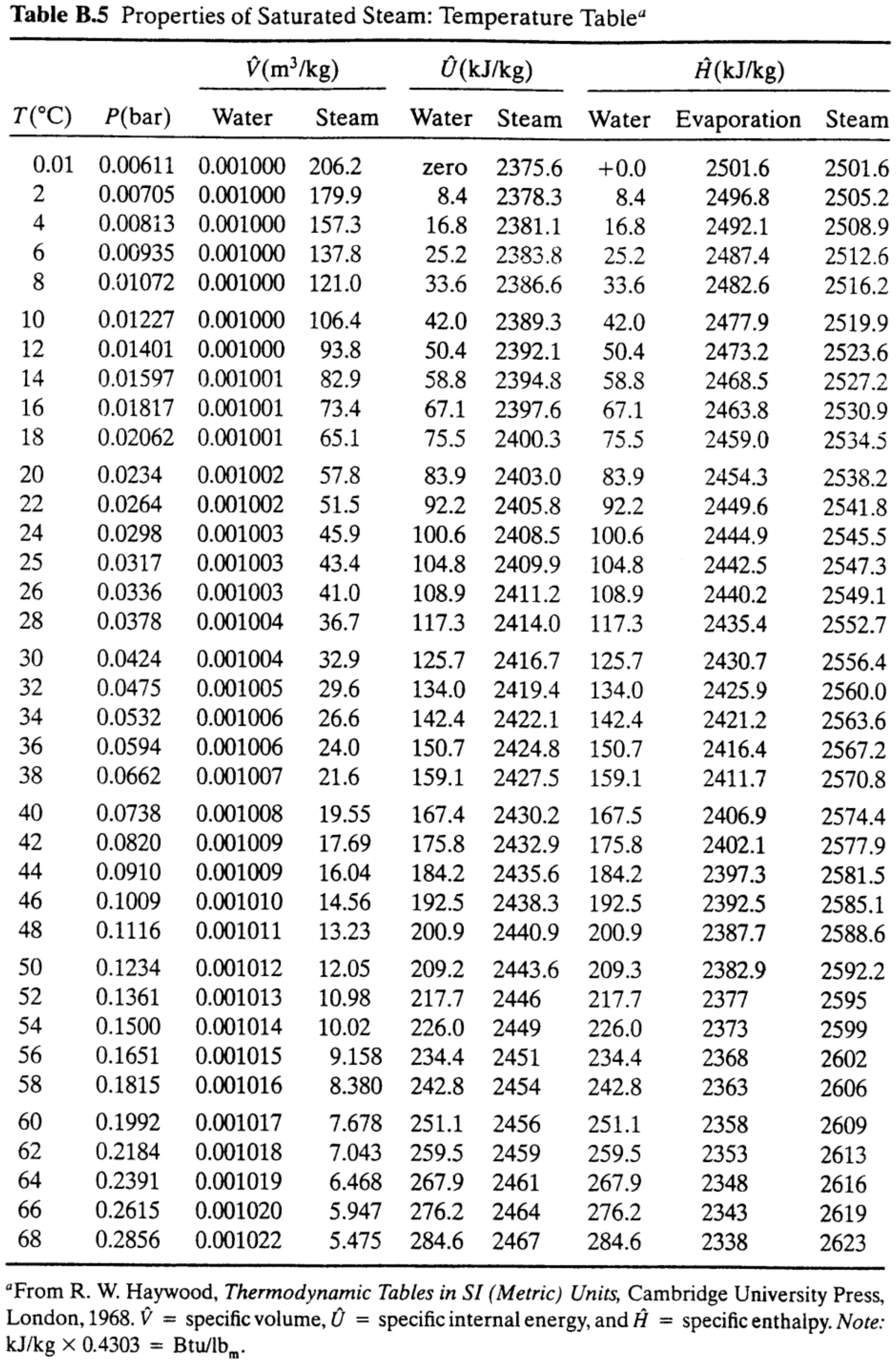


Table B.5 Properties of Saturated Steam: Temperature Table[a]

		$\hat{V}(m^3/kg)$		$\hat{U}$(kJ/kg)		$\hat{H}$(kJ/kg)		
T(°C)	P(bar)	Water	Steam	Water	Steam	Water	Evaporation	Steam
0.01	0.00611	0.001000	206.2	zero	2375.6	+0.0	2501.6	2501.6
2	0.00705	0.001000	179.9	8.4	2378.3	8.4	2496.8	2505.2
4	0.00813	0.001000	157.3	16.8	2381.1	16.8	2492.1	2508.9
6	0.00935	0.001000	137.8	25.2	2383.8	25.2	2487.4	2512.6
8	0.01072	0.001000	121.0	33.6	2386.6	33.6	2482.6	2516.2
10	0.01227	0.001000	106.4	42.0	2389.3	42.0	2477.9	2519.9
12	0.01401	0.001000	93.8	50.4	2392.1	50.4	2473.2	2523.6
14	0.01597	0.001001	82.9	58.8	2394.8	58.8	2468.5	2527.2
16	0.01817	0.001001	73.4	67.1	2397.6	67.1	2463.8	2530.9
18	0.02062	0.001001	65.1	75.5	2400.3	75.5	2459.0	2534.5
20	0.0234	0.001002	57.8	83.9	2403.0	83.9	2454.3	2538.2
22	0.0264	0.001002	51.5	92.2	2405.8	92.2	2449.6	2541.8
24	0.0298	0.001003	45.9	100.6	2408.5	100.6	2444.9	2545.5
25	0.0317	0.001003	43.4	104.8	2409.9	104.8	2442.5	2547.3
26	0.0336	0.001003	41.0	108.9	2411.2	108.9	2440.2	2549.1
28	0.0378	0.001004	36.7	117.3	2414.0	117.3	2435.4	2552.7
30	0.0424	0.001004	32.9	125.7	2416.7	125.7	2430.7	2556.4
32	0.0475	0.001005	29.6	134.0	2419.4	134.0	2425.9	2560.0
34	0.0532	0.001006	26.6	142.4	2422.1	142.4	2421.2	2563.6
36	0.0594	0.001006	24.0	150.7	2424.8	150.7	2416.4	2567.2
38	0.0662	0.001007	21.6	159.1	2427.5	159.1	2411.7	2570.8
40	0.0738	0.001008	19.55	167.4	2430.2	167.5	2406.9	2574.4
42	0.0820	0.001009	17.69	175.8	2432.9	175.8	2402.1	2577.9
44	0.0910	0.001009	16.04	184.2	2435.6	184.2	2397.3	2581.5
46	0.1009	0.001010	14.56	192.5	2438.3	192.5	2392.5	2585.1
48	0.1116	0.001011	13.23	200.9	2440.9	200.9	2387.7	2588.6
50	0.1234	0.001012	12.05	209.2	2443.6	209.3	2382.9	2592.2
52	0.1361	0.001013	10.98	217.7	2446	217.7	2377	2595
54	0.1500	0.001014	10.02	226.0	2449	226.0	2373	2599
56	0.1651	0.001015	9.158	234.4	2451	234.4	2368	2602
58	0.1815	0.001016	8.380	242.8	2454	242.8	2363	2606
60	0.1992	0.001017	7.678	251.1	2456	251.1	2358	2609
62	0.2184	0.001018	7.043	259.5	2459	259.5	2353	2613
64	0.2391	0.001019	6.468	267.9	2461	267.9	2348	2616
66	0.2615	0.001020	5.947	276.2	2464	276.2	2343	2619
68	0.2856	0.001022	5.475	284.6	2467	284.6	2338	2623

[a] From R. W. Haywood, *Thermodynamic Tables in SI (Metric) Units,* Cambridge University Press, London, 1968. $\hat{V}$ = specific volume, $\hat{U}$ = specific internal energy, and $\hat{H}$ = specific enthalpy. *Note:* kJ/kg × 0.4303 = Btu/lb_m.

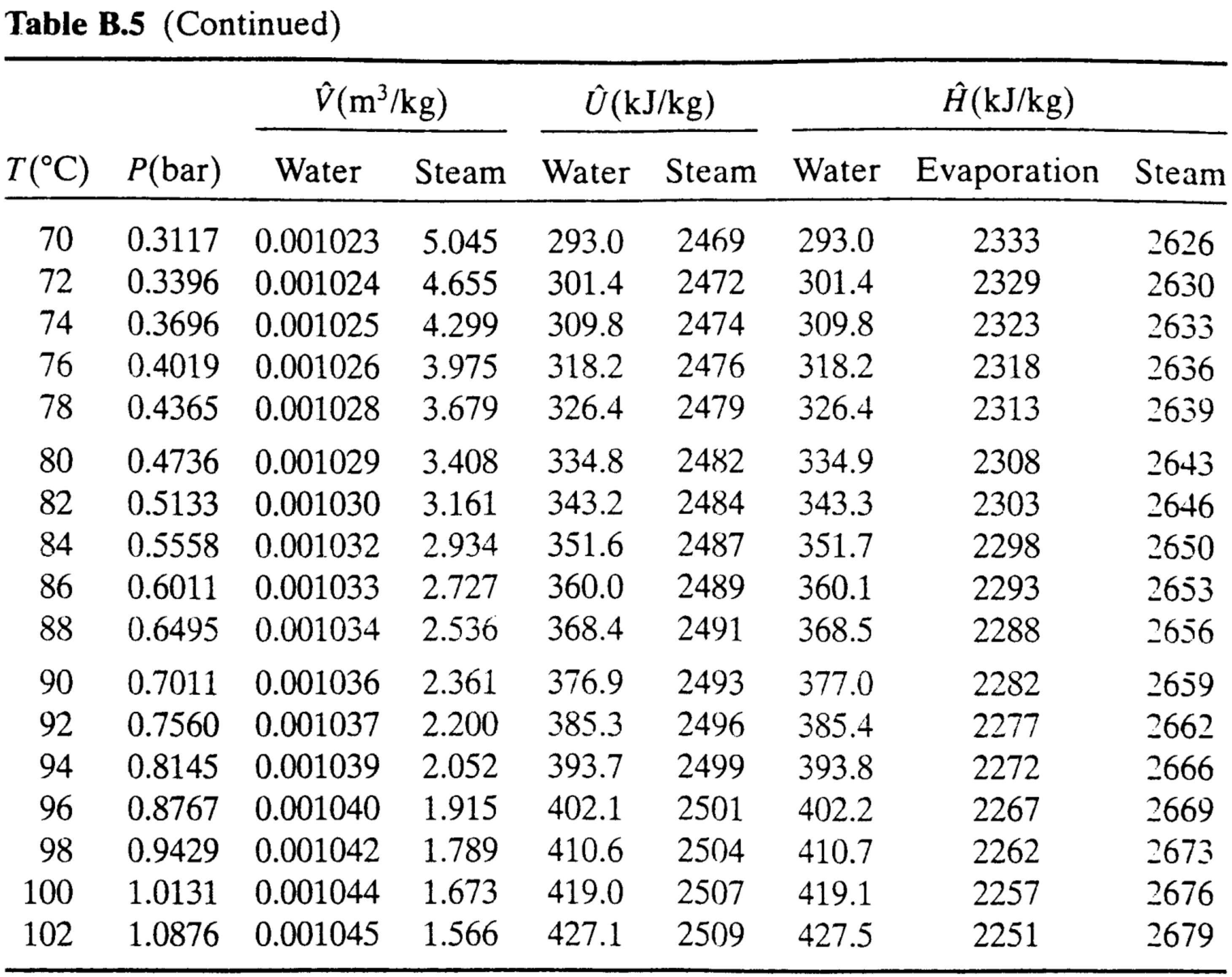


Table B.5 (Continued)

		$\hat{V}(\text{m}^3/\text{kg})$		$\hat{U}(\text{kJ/kg})$		$\hat{H}(\text{kJ/kg})$		
T(°C)	P(bar)	Water	Steam	Water	Steam	Water	Evaporation	Steam
70	0.3117	0.001023	5.045	293.0	2469	293.0	2333	2626
72	0.3396	0.001024	4.655	301.4	2472	301.4	2329	2630
74	0.3696	0.001025	4.299	309.8	2474	309.8	2323	2633
76	0.4019	0.001026	3.975	318.2	2476	318.2	2318	2636
78	0.4365	0.001028	3.679	326.4	2479	326.4	2313	2639
80	0.4736	0.001029	3.408	334.8	2482	334.9	2308	2643
82	0.5133	0.001030	3.161	343.2	2484	343.3	2303	2646
84	0.5558	0.001032	2.934	351.6	2487	351.7	2298	2650
86	0.6011	0.001033	2.727	360.0	2489	360.1	2293	2653
88	0.6495	0.001034	2.536	368.4	2491	368.5	2288	2656
90	0.7011	0.001036	2.361	376.9	2493	377.0	2282	2659
92	0.7560	0.001037	2.200	385.3	2496	385.4	2277	2662
94	0.8145	0.001039	2.052	393.7	2499	393.8	2272	2666
96	0.8767	0.001040	1.915	402.1	2501	402.2	2267	2669
98	0.9429	0.001042	1.789	410.6	2504	410.7	2262	2673
100	1.0131	0.001044	1.673	419.0	2507	419.1	2257	2676
102	1.0876	0.001045	1.566	427.1	2509	427.5	2251	2679

Tabulated Steam Tables

Table B.6 Pressure Table

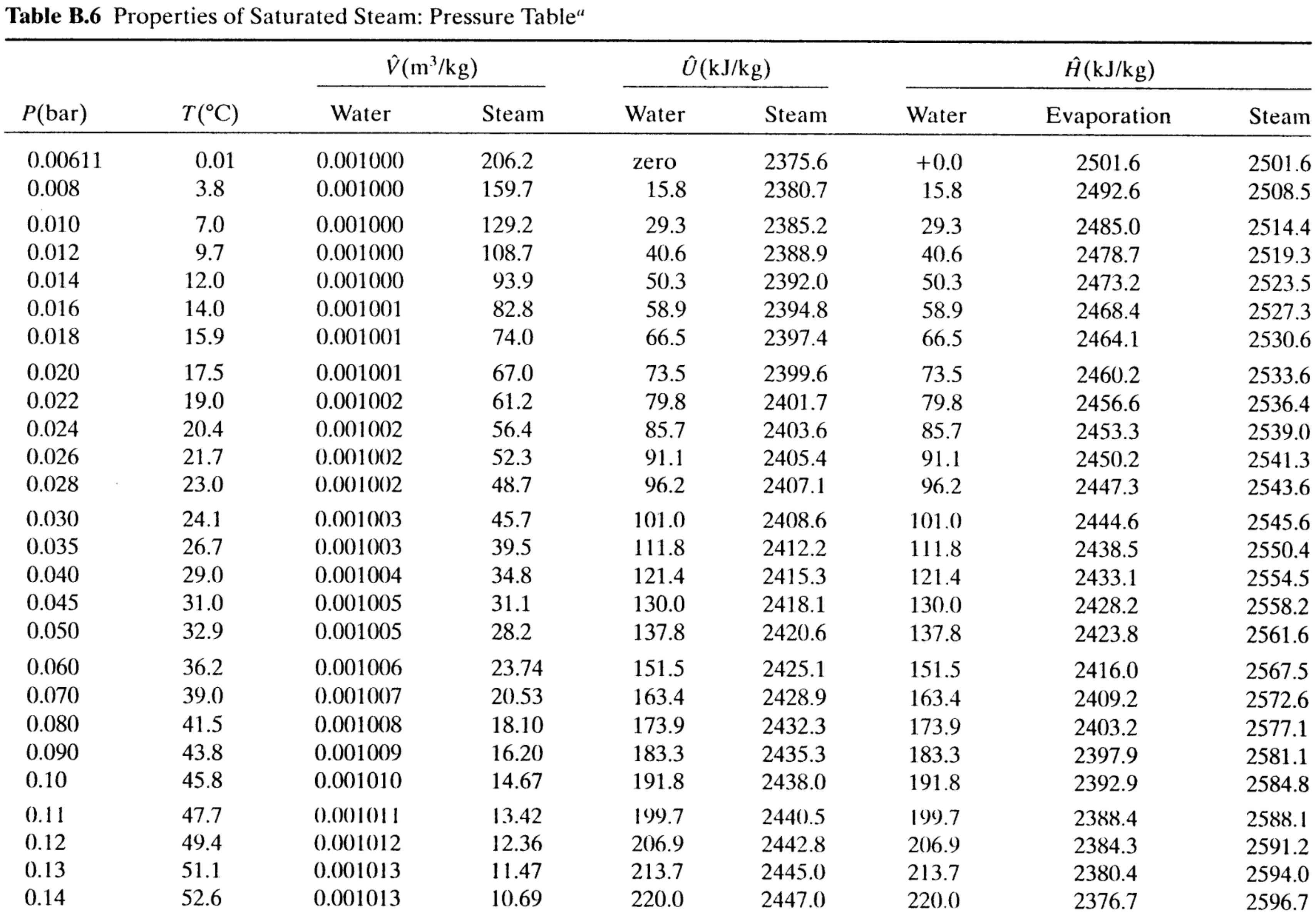


Table B.6 Properties of Saturated Steam: Pressure Table[a]

		$\hat{V}$(m^3/kg)		$\hat{U}$(kJ/kg)		$\hat{H}$(kJ/kg)		
P(bar)	T(°C)	Water	Steam	Water	Steam	Water	Evaporation	Steam
0.00611	0.01	0.001000	206.2	zero	2375.6	+0.0	2501.6	2501.6
0.008	3.8	0.001000	159.7	15.8	2380.7	15.8	2492.6	2508.5
0.010	7.0	0.001000	129.2	29.3	2385.2	29.3	2485.0	2514.4
0.012	9.7	0.001000	108.7	40.6	2388.9	40.6	2478.7	2519.3
0.014	12.0	0.001000	93.9	50.3	2392.0	50.3	2473.2	2523.5
0.016	14.0	0.001001	82.8	58.9	2394.8	58.9	2468.4	2527.3
0.018	15.9	0.001001	74.0	66.5	2397.4	66.5	2464.1	2530.6
0.020	17.5	0.001001	67.0	73.5	2399.6	73.5	2460.2	2533.6
0.022	19.0	0.001002	61.2	79.8	2401.7	79.8	2456.6	2536.4
0.024	20.4	0.001002	56.4	85.7	2403.6	85.7	2453.3	2539.0
0.026	21.7	0.001002	52.3	91.1	2405.4	91.1	2450.2	2541.3
0.028	23.0	0.001002	48.7	96.2	2407.1	96.2	2447.3	2543.6
0.030	24.1	0.001003	45.7	101.0	2408.6	101.0	2444.6	2545.6
0.035	26.7	0.001003	39.5	111.8	2412.2	111.8	2438.5	2550.4
0.040	29.0	0.001004	34.8	121.4	2415.3	121.4	2433.1	2554.5
0.045	31.0	0.001005	31.1	130.0	2418.1	130.0	2428.2	2558.2
0.050	32.9	0.001005	28.2	137.8	2420.6	137.8	2423.8	2561.6
0.060	36.2	0.001006	23.74	151.5	2425.1	151.5	2416.0	2567.5
0.070	39.0	0.001007	20.53	163.4	2428.9	163.4	2409.2	2572.6
0.080	41.5	0.001008	18.10	173.9	2432.3	173.9	2403.2	2577.1
0.090	43.8	0.001009	16.20	183.3	2435.3	183.3	2397.9	2581.1
0.10	45.8	0.001010	14.67	191.8	2438.0	191.8	2392.9	2584.8
0.11	47.7	0.001011	13.42	199.7	2440.5	199.7	2388.4	2588.1
0.12	49.4	0.001012	12.36	206.9	2442.8	206.9	2384.3	2591.2
0.13	51.1	0.001013	11.47	213.7	2445.0	213.7	2380.4	2594.0
0.14	52.6	0.001013	10.69	220.0	2447.0	220.0	2376.7	2596.7

Tabulated Steam Tables

Table B.6 Pressure Table

Background learning

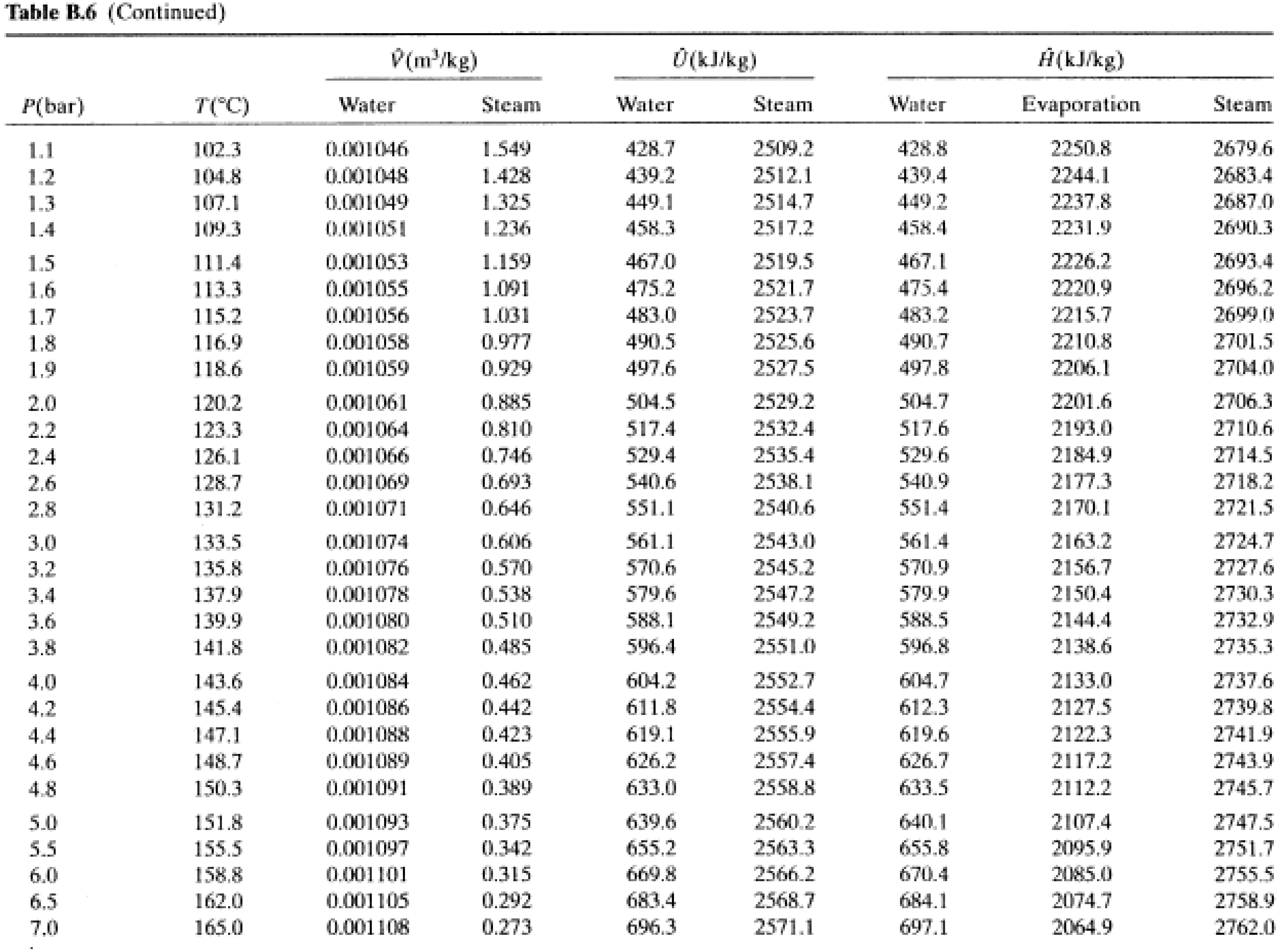


Table B.6 (Continued)

		$\hat{V}$(m^3/kg)		$\hat{U}$(kJ/kg)		$\hat{H}$(kJ/kg)		
P(bar)	T(°C)	Water	Steam	Water	Steam	Water	Evaporation	Steam
1.1	102.3	0.001046	1.549	428.7	2509.2	428.8	2250.8	2679.6
1.2	104.8	0.001048	1.428	439.2	2512.1	439.4	2244.1	2683.4
1.3	107.1	0.001049	1.325	449.1	2514.7	449.2	2237.8	2687.0
1.4	109.3	0.001051	1.236	458.3	2517.2	458.4	2231.9	2690.3
1.5	111.4	0.001053	1.159	467.0	2519.5	467.1	2226.2	2693.4
1.6	113.3	0.001055	1.091	475.2	2521.7	475.4	2220.9	2696.2
1.7	115.2	0.001056	1.031	483.0	2523.7	483.2	2215.7	2699.0
1.8	116.9	0.001058	0.977	490.5	2525.6	490.7	2210.8	2701.5
1.9	118.6	0.001059	0.929	497.6	2527.5	497.8	2206.1	2704.0
2.0	120.2	0.001061	0.885	504.5	2529.2	504.7	2201.6	2706.3
2.2	123.3	0.001064	0.810	517.4	2532.4	517.6	2193.0	2710.6
2.4	126.1	0.001066	0.746	529.4	2535.4	529.6	2184.9	2714.5
2.6	128.7	0.001069	0.693	540.6	2538.1	540.9	2177.3	2718.2
2.8	131.2	0.001071	0.646	551.1	2540.6	551.4	2170.1	2721.5
3.0	133.5	0.001074	0.606	561.1	2543.0	561.4	2163.2	2724.7
3.2	135.8	0.001076	0.570	570.6	2545.2	570.9	2156.7	2727.6
3.4	137.9	0.001078	0.538	579.6	2547.2	579.9	2150.4	2730.3
3.6	139.9	0.001080	0.510	588.1	2549.2	588.5	2144.4	2732.9
3.8	141.8	0.001082	0.485	596.4	2551.0	596.8	2138.6	2735.3
4.0	143.6	0.001084	0.462	604.2	2552.7	604.7	2133.0	2737.6
4.2	145.4	0.001086	0.442	611.8	2554.4	612.3	2127.5	2739.8
4.4	147.1	0.001088	0.423	619.1	2555.9	619.6	2122.3	2741.9
4.6	148.7	0.001089	0.405	626.2	2557.4	626.7	2117.2	2743.9
4.8	150.3	0.001091	0.389	633.0	2558.8	633.5	2112.2	2745.7
5.0	151.8	0.001093	0.375	639.6	2560.2	640.1	2107.4	2747.5
5.5	155.5	0.001097	0.342	655.2	2563.3	655.8	2095.9	2751.7
6.0	158.8	0.001101	0.315	669.8	2566.2	670.4	2085.0	2755.5
6.5	162.0	0.001105	0.292	683.4	2568.7	684.1	2074.7	2758.9
7.0	165.0	0.001108	0.273	696.3	2571.1	697.1	2064.9	2762.0

Tabulated Steam Tables

Table B.7 Superheated Steam

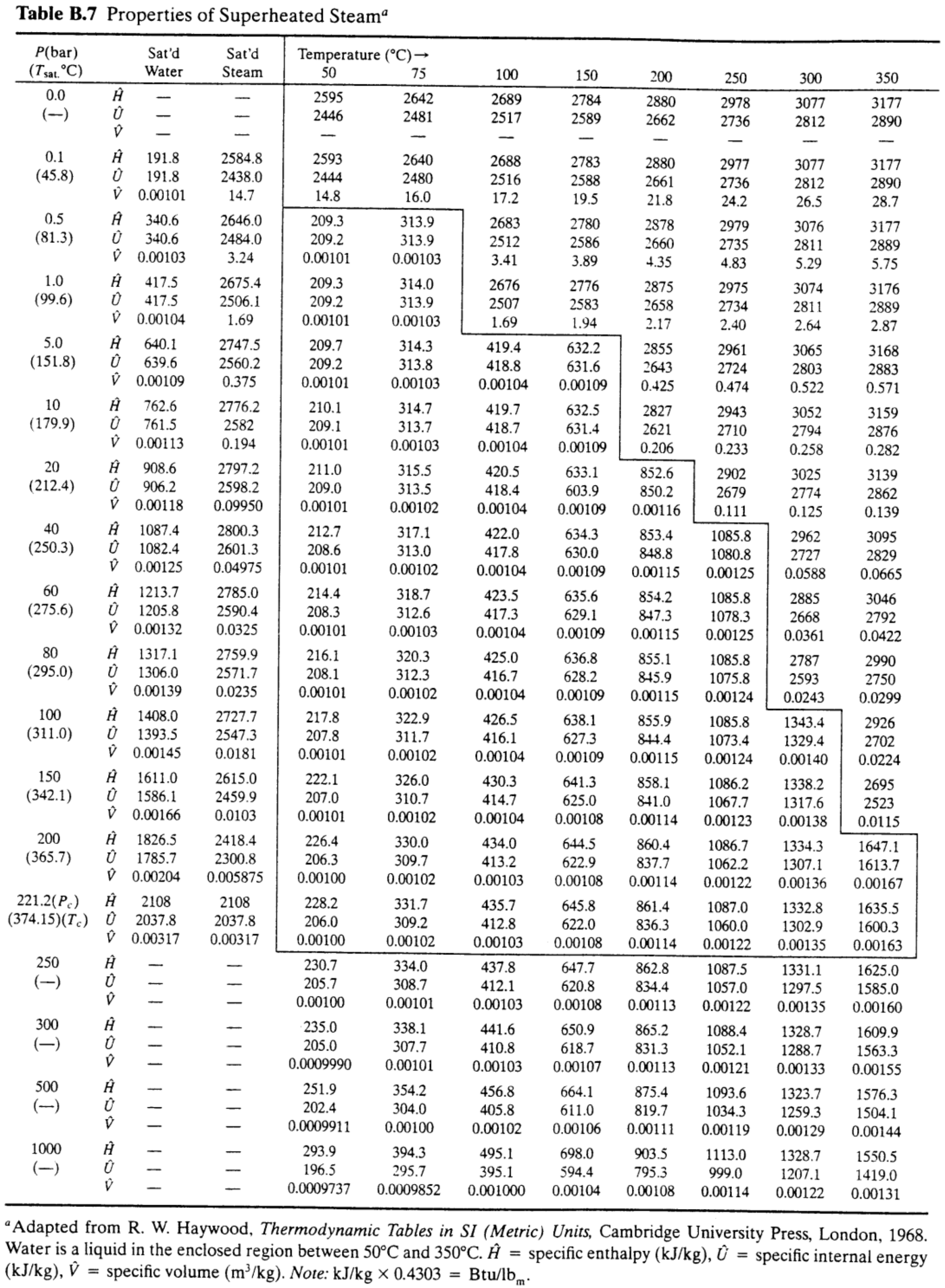


Table B.7 Properties of Superheated Steam[a]

P(bar) ($T_{sat.}$ °C)		Sat'd Water	Sat'd Steam	Temperature (°C)→ 50	75	100	150	200	250	300	350
0.0 (—)	$\hat{H}$	—	—	2595	2642	2689	2784	2880	2978	3077	3177
	$\hat{U}$	—	—	2446	2481	2517	2589	2662	2736	2812	2890
	$\hat{V}$	—	—	—	—	—	—	—	—	—	—
0.1 (45.8)	$\hat{H}$	191.8	2584.8	2593	2640	2688	2783	2880	2977	3077	3177
	$\hat{U}$	191.8	2438.0	2444	2480	2516	2588	2661	2736	2812	2890
	$\hat{V}$	0.00101	14.7	14.8	16.0	17.2	19.5	21.8	24.2	26.5	28.7
0.5 (81.3)	$\hat{H}$	340.6	2646.0	209.3	313.9	2683	2780	2878	2979	3076	3177
	$\hat{U}$	340.6	2484.0	209.2	313.9	2512	2586	2660	2735	2811	2889
	$\hat{V}$	0.00103	3.24	0.00101	0.00103	3.41	3.89	4.35	4.83	5.29	5.75
1.0 (99.6)	$\hat{H}$	417.5	2675.4	209.3	314.0	2676	2776	2875	2975	3074	3176
	$\hat{U}$	417.5	2506.1	209.2	313.9	2507	2583	2658	2734	2811	2889
	$\hat{V}$	0.00104	1.69	0.00101	0.00103	1.69	1.94	2.17	2.40	2.64	2.87
5.0 (151.8)	$\hat{H}$	640.1	2747.5	209.7	314.3	419.4	632.2	2855	2961	3065	3168
	$\hat{U}$	639.6	2560.2	209.2	313.8	418.8	631.6	2643	2724	2803	2883
	$\hat{V}$	0.00109	0.375	0.00101	0.00103	0.00104	0.00109	0.425	0.474	0.522	0.571
10 (179.9)	$\hat{H}$	762.6	2776.2	210.1	314.7	419.7	632.5	2827	2943	3052	3159
	$\hat{U}$	761.5	2582	209.1	313.7	418.7	631.4	2621	2710	2794	2876
	$\hat{V}$	0.00113	0.194	0.00101	0.00103	0.00104	0.00109	0.206	0.233	0.258	0.282
20 (212.4)	$\hat{H}$	908.6	2797.2	211.0	315.5	420.5	633.1	852.6	2902	3025	3139
	$\hat{U}$	906.2	2598.2	209.0	313.5	418.4	603.9	850.2	2679	2774	2862
	$\hat{V}$	0.00118	0.09950	0.00101	0.00102	0.00104	0.00109	0.00116	0.111	0.125	0.139
40 (250.3)	$\hat{H}$	1087.4	2800.3	212.7	317.1	422.0	634.3	853.4	1085.8	2962	3095
	$\hat{U}$	1082.4	2601.3	208.6	313.0	417.8	630.0	848.8	1080.8	2727	2829
	$\hat{V}$	0.00125	0.04975	0.00101	0.00102	0.00104	0.00109	0.00115	0.00125	0.0588	0.0665
60 (275.6)	$\hat{H}$	1213.7	2785.0	214.4	318.7	423.5	635.6	854.2	1085.8	2885	3046
	$\hat{U}$	1205.8	2590.4	208.3	312.6	417.3	629.1	847.3	1078.3	2668	2792
	$\hat{V}$	0.00132	0.0325	0.00101	0.00103	0.00104	0.00109	0.00115	0.00125	0.0361	0.0422
80 (295.0)	$\hat{H}$	1317.1	2759.9	216.1	320.3	425.0	636.8	855.1	1085.8	2787	2990
	$\hat{U}$	1306.0	2571.7	208.1	312.3	416.7	628.2	845.9	1075.8	2593	2750
	$\hat{V}$	0.00139	0.0235	0.00101	0.00102	0.00104	0.00109	0.00115	0.00124	0.0243	0.0299
100 (311.0)	$\hat{H}$	1408.0	2727.7	217.8	322.9	426.5	638.1	855.9	1085.8	1343.4	2926
	$\hat{U}$	1393.5	2547.3	207.8	311.7	416.1	627.3	844.4	1073.4	1329.4	2702
	$\hat{V}$	0.00145	0.0181	0.00101	0.00102	0.00104	0.00109	0.00115	0.00124	0.00140	0.0224
150 (342.1)	$\hat{H}$	1611.0	2615.0	222.1	326.0	430.3	641.3	858.1	1086.2	1338.2	2695
	$\hat{U}$	1586.1	2459.9	207.0	310.7	414.7	625.0	841.0	1067.7	1317.6	2523
	$\hat{V}$	0.00166	0.0103	0.00101	0.00102	0.00104	0.00108	0.00114	0.00123	0.00138	0.0115
200 (365.7)	$\hat{H}$	1826.5	2418.4	226.4	330.0	434.0	644.5	860.4	1086.7	1334.3	1647.1
	$\hat{U}$	1785.7	2300.8	206.3	309.7	413.2	622.9	837.7	1062.2	1307.1	1613.7
	$\hat{V}$	0.00204	0.005875	0.00100	0.00102	0.00103	0.00108	0.00114	0.00122	0.00136	0.00167
221.2(P_c) (374.15)(T_c)	$\hat{H}$	2108	2108	228.2	331.7	435.7	645.8	861.4	1087.0	1332.8	1635.5
	$\hat{U}$	2037.8	2037.8	206.0	309.2	412.8	622.0	836.3	1060.0	1302.9	1600.3
	$\hat{V}$	0.00317	0.00317	0.00100	0.00102	0.00103	0.00108	0.00114	0.00122	0.00135	0.00163
250 (—)	$\hat{H}$	—	—	230.7	334.0	437.8	647.7	862.8	1087.5	1331.1	1625.0
	$\hat{U}$	—	—	205.7	308.7	412.1	620.8	834.4	1057.0	1297.5	1585.0
	$\hat{V}$	—	—	0.00100	0.00101	0.00103	0.00108	0.00113	0.00122	0.00135	0.00160
300 (—)	$\hat{H}$	—	—	235.0	338.1	441.6	650.9	865.2	1088.4	1328.7	1609.9
	$\hat{U}$	—	—	205.0	307.7	410.8	618.7	831.3	1052.1	1288.7	1563.3
	$\hat{V}$	—	—	0.0009990	0.00101	0.00103	0.00107	0.00113	0.00121	0.00133	0.00155
500 (—)	$\hat{H}$	—	—	251.9	354.2	456.8	664.1	875.4	1093.6	1323.7	1576.3
	$\hat{U}$	—	—	202.4	304.0	405.8	611.0	819.7	1034.3	1259.3	1504.1
	$\hat{V}$	—	—	0.0009911	0.00100	0.00102	0.00106	0.00111	0.00119	0.00129	0.00144
1000 (—)	$\hat{H}$	—	—	293.9	394.3	495.1	698.0	903.5	1113.0	1328.7	1550.5
	$\hat{U}$	—	—	196.5	295.7	395.1	594.4	795.3	999.0	1207.1	1419.0
	$\hat{V}$	—	—	0.0009737	0.0009852	0.001000	0.00104	0.00108	0.00114	0.00122	0.00131

---

[a] Adapted from R. W. Haywood, *Thermodynamic Tables in SI (Metric) Units,* Cambridge University Press, London, 1968. Water is a liquid in the enclosed region between 50°C and 350°C. $\hat{H}$ = specific enthalpy (kJ/kg), $\hat{U}$ = specific internal energy (kJ/kg), $\hat{V}$ = specific volume (m^3/kg). *Note:* kJ/kg × 0.4303 = Btu/lb_m.

Table B.7 Superheated Steam

Background learning

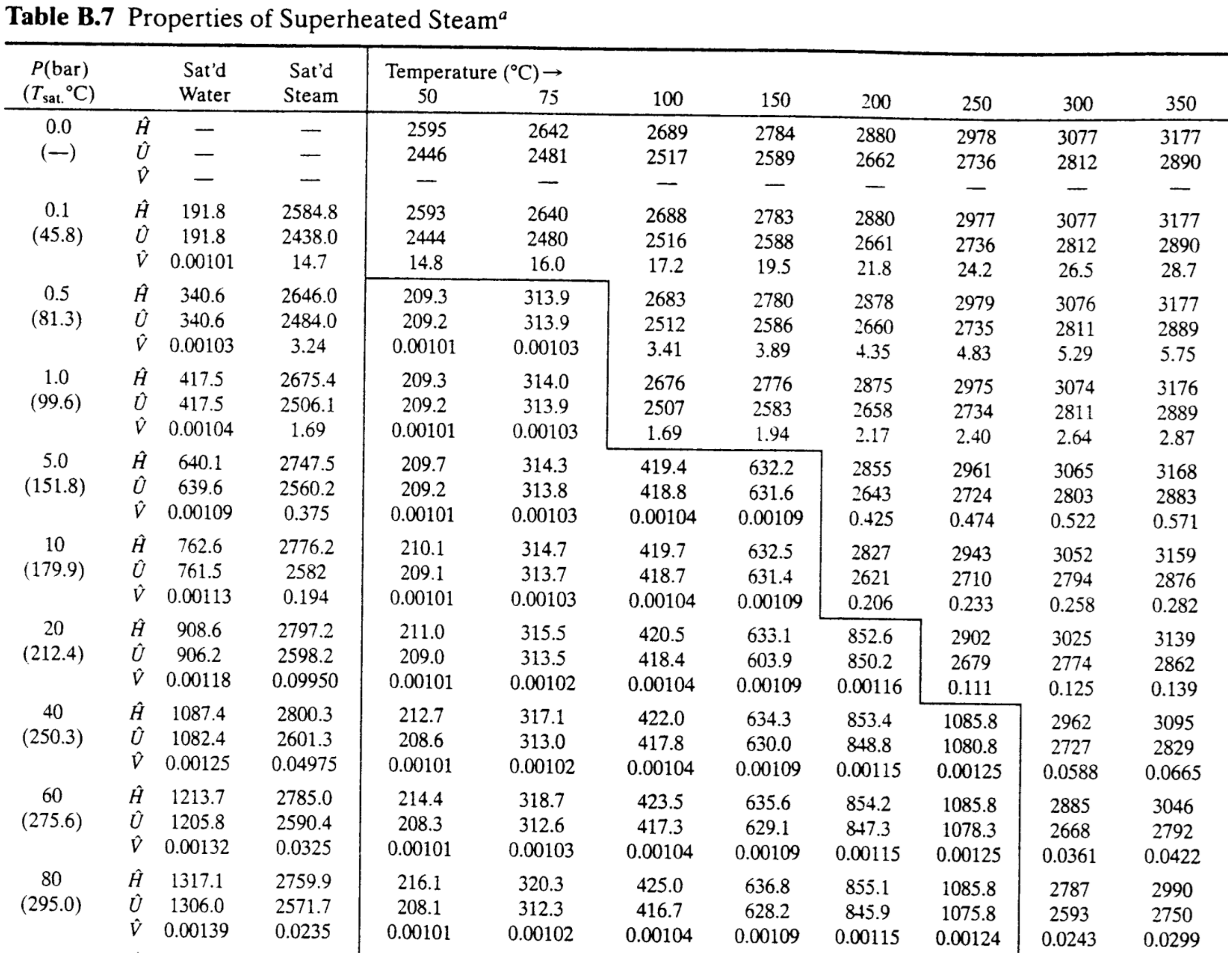


Table B.7 Properties of Superheated Steam[a]

P(bar) ($T_{\text{sat.}}$°C)		Sat'd Water	Sat'd Steam	Temperature (°C)→ 50	75	100	150	200	250	300	350
0.0	$\hat{H}$	—	—	2595	2642	2689	2784	2880	2978	3077	3177
(—)	$\hat{U}$	—	—	2446	2481	2517	2589	2662	2736	2812	2890
	$\hat{V}$	—	—	—	—	—	—	—	—	—	—
0.1	$\hat{H}$	191.8	2584.8	2593	2640	2688	2783	2880	2977	3077	3177
(45.8)	$\hat{U}$	191.8	2438.0	2444	2480	2516	2588	2661	2736	2812	2890
	$\hat{V}$	0.00101	14.7	14.8	16.0	17.2	19.5	21.8	24.2	26.5	28.7
0.5	$\hat{H}$	340.6	2646.0	209.3	313.9	2683	2780	2878	2979	3076	3177
(81.3)	$\hat{U}$	340.6	2484.0	209.2	313.9	2512	2586	2660	2735	2811	2889
	$\hat{V}$	0.00103	3.24	0.00101	0.00103	3.41	3.89	4.35	4.83	5.29	5.75
1.0	$\hat{H}$	417.5	2675.4	209.3	314.0	2676	2776	2875	2975	3074	3176
(99.6)	$\hat{U}$	417.5	2506.1	209.2	313.9	2507	2583	2658	2734	2811	2889
	$\hat{V}$	0.00104	1.69	0.00101	0.00103	1.69	1.94	2.17	2.40	2.64	2.87
5.0	$\hat{H}$	640.1	2747.5	209.7	314.3	419.4	632.2	2855	2961	3065	3168
(151.8)	$\hat{U}$	639.6	2560.2	209.2	313.8	418.8	631.6	2643	2724	2803	2883
	$\hat{V}$	0.00109	0.375	0.00101	0.00103	0.00104	0.00109	0.425	0.474	0.522	0.571
10	$\hat{H}$	762.6	2776.2	210.1	314.7	419.7	632.5	2827	2943	3052	3159
(179.9)	$\hat{U}$	761.5	2582	209.1	313.7	418.7	631.4	2621	2710	2794	2876
	$\hat{V}$	0.00113	0.194	0.00101	0.00103	0.00104	0.00109	0.206	0.233	0.258	0.282
20	$\hat{H}$	908.6	2797.2	211.0	315.5	420.5	633.1	852.6	2902	3025	3139
(212.4)	$\hat{U}$	906.2	2598.2	209.0	313.5	418.4	603.9	850.2	2679	2774	2862
	$\hat{V}$	0.00118	0.09950	0.00101	0.00102	0.00104	0.00109	0.00116	0.111	0.125	0.139
40	$\hat{H}$	1087.4	2800.3	212.7	317.1	422.0	634.3	853.4	1085.8	2962	3095
(250.3)	$\hat{U}$	1082.4	2601.3	208.6	313.0	417.8	630.0	848.8	1080.8	2727	2829
	$\hat{V}$	0.00125	0.04975	0.00101	0.00102	0.00104	0.00109	0.00115	0.00125	0.0588	0.0665
60	$\hat{H}$	1213.7	2785.0	214.4	318.7	423.5	635.6	854.2	1085.8	2885	3046
(275.6)	$\hat{U}$	1205.8	2590.4	208.3	312.6	417.3	629.1	847.3	1078.3	2668	2792
	$\hat{V}$	0.00132	0.0325	0.00101	0.00103	0.00104	0.00109	0.00115	0.00125	0.0361	0.0422
80	$\hat{H}$	1317.1	2759.9	216.1	320.3	425.0	636.8	855.1	1085.8	2787	2990
(295.0)	$\hat{U}$	1306.0	2571.7	208.1	312.3	416.7	628.2	845.9	1075.8	2593	2750
	$\hat{V}$	0.00139	0.0235	0.00101	0.00102	0.00104	0.00109	0.00115	0.00124	0.0243	0.0299

Table B.7 Superheated Steam

Background learning

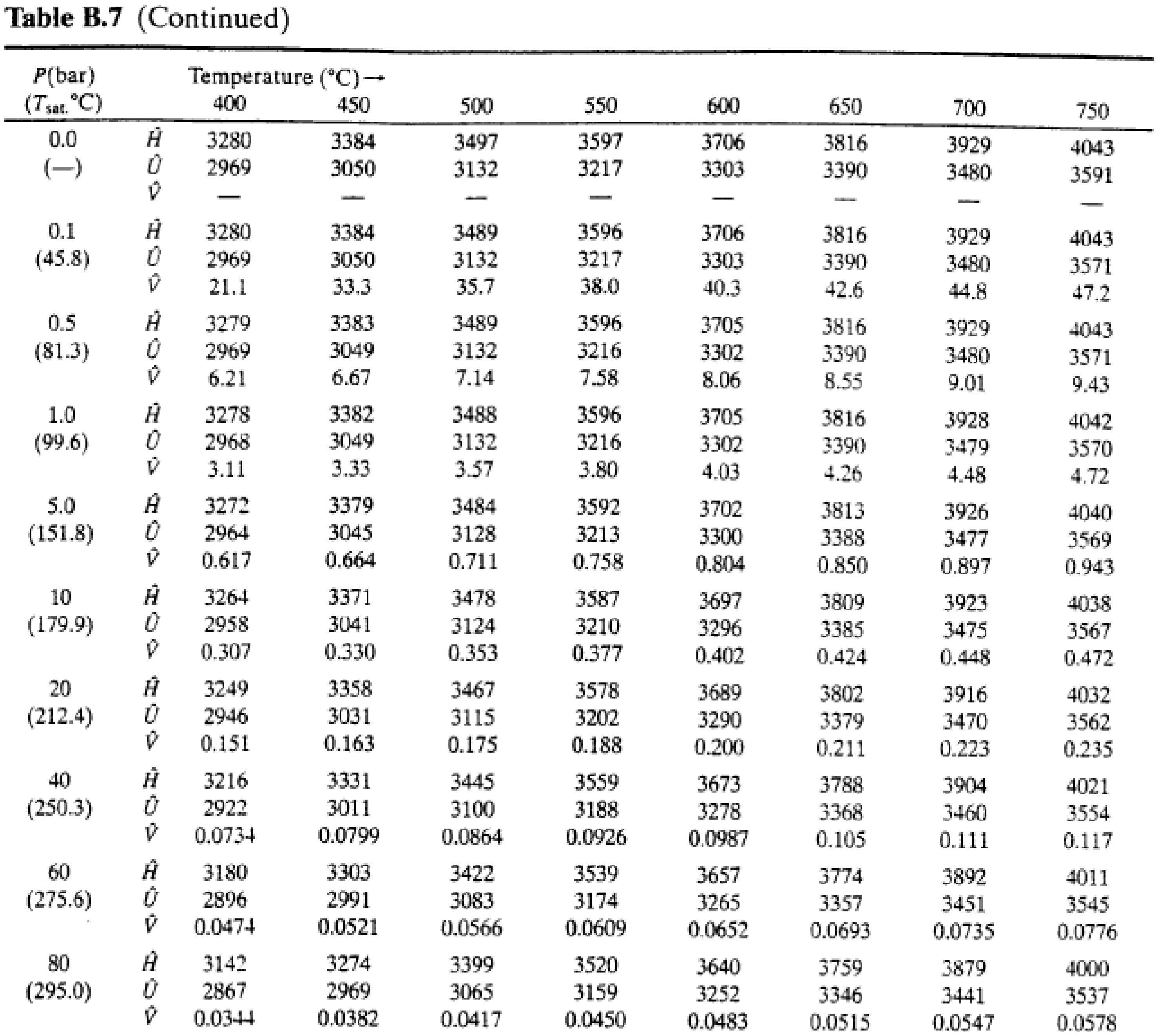


Table B.7 (Continued)

P(bar) ($T_{sat.}$°C)		Temperature (°C)→ 400	450	500	550	600	650	700	750
0.0	$\hat{H}$	3280	3384	3497	3597	3706	3816	3929	4043
(—)	$\hat{U}$	2969	3050	3132	3217	3303	3390	3480	3591
	$\hat{V}$	—	—	—	—	—	—	—	—
0.1	$\hat{H}$	3280	3384	3489	3596	3706	3816	3929	4043
(45.8)	$\hat{U}$	2969	3050	3132	3217	3303	3390	3480	3571
	$\hat{V}$	21.1	33.3	35.7	38.0	40.3	42.6	44.8	47.2
0.5	$\hat{H}$	3279	3383	3489	3596	3705	3816	3929	4043
(81.3)	$\hat{U}$	2969	3049	3132	3216	3302	3390	3480	3571
	$\hat{V}$	6.21	6.67	7.14	7.58	8.06	8.55	9.01	9.43
1.0	$\hat{H}$	3278	3382	3488	3596	3705	3816	3928	4042
(99.6)	$\hat{U}$	2968	3049	3132	3216	3302	3390	3479	3570
	$\hat{V}$	3.11	3.33	3.57	3.80	4.03	4.26	4.48	4.72
5.0	$\hat{H}$	3272	3379	3484	3592	3702	3813	3926	4040
(151.8)	$\hat{U}$	2964	3045	3128	3213	3300	3388	3477	3569
	$\hat{V}$	0.617	0.664	0.711	0.758	0.804	0.850	0.897	0.943
10	$\hat{H}$	3264	3371	3478	3587	3697	3809	3923	4038
(179.9)	$\hat{U}$	2958	3041	3124	3210	3296	3385	3475	3567
	$\hat{V}$	0.307	0.330	0.353	0.377	0.402	0.424	0.448	0.472
20	$\hat{H}$	3249	3358	3467	3578	3689	3802	3916	4032
(212.4)	$\hat{U}$	2946	3031	3115	3202	3290	3379	3470	3562
	$\hat{V}$	0.151	0.163	0.175	0.188	0.200	0.211	0.223	0.235
40	$\hat{H}$	3216	3331	3445	3559	3673	3788	3904	4021
(250.3)	$\hat{U}$	2922	3011	3100	3188	3278	3368	3460	3554
	$\hat{V}$	0.0734	0.0799	0.0864	0.0926	0.0987	0.105	0.111	0.117
60	$\hat{H}$	3180	3303	3422	3539	3657	3774	3892	4011
(275.6)	$\hat{U}$	2896	2991	3083	3174	3265	3357	3451	3545
	$\hat{V}$	0.0474	0.0521	0.0566	0.0609	0.0652	0.0693	0.0735	0.0776
80	$\hat{H}$	3142	3274	3399	3520	3640	3759	3879	4000
(295.0)	$\hat{U}$	2867	2969	3065	3159	3252	3346	3441	3537
	$\hat{V}$	0.0344	0.0382	0.0417	0.0450	0.0483	0.0515	0.0547	0.0578

(3a) Fit a function to the data

Vapor Pressures from Equations

Antoine Equation

Antoine equation for estimating vapor pressure

A relatively simple empirical equation that correlates vapor pressure-temperature data extremely well is the **Antoine equation.**

$$\log_{10} p^* = A - \frac{B}{T + C}$$

Values of A, B and C for several compounds are listed in Table B.4. **Observe the units** of $p^*$and T (mmHg and °C respectively for the constants in Table B.4) and the logarithm base (10 in the case of Equation 6.1-4 and Table B.4).

Refer to book to for details and examples of this section

Table B.4 Antoine Equation Constants

$$\log_{10} p^* = A - \frac{B}{T + C}$$

p^* in mmHg

T in °C

Example: The vapor pressure of *acetaldehyde* at 25°C is determined as follows:

$$\log_{10} p^*_{C_2H_4O}(25°\text{C}) = 8.00552 - \frac{1600.017}{25 + 291.809} = 2.9551 \quad \Rightarrow p^*_{C_2H_4O}(25°\text{C}) = 10^{2.9551} = 902\ mmHg$$

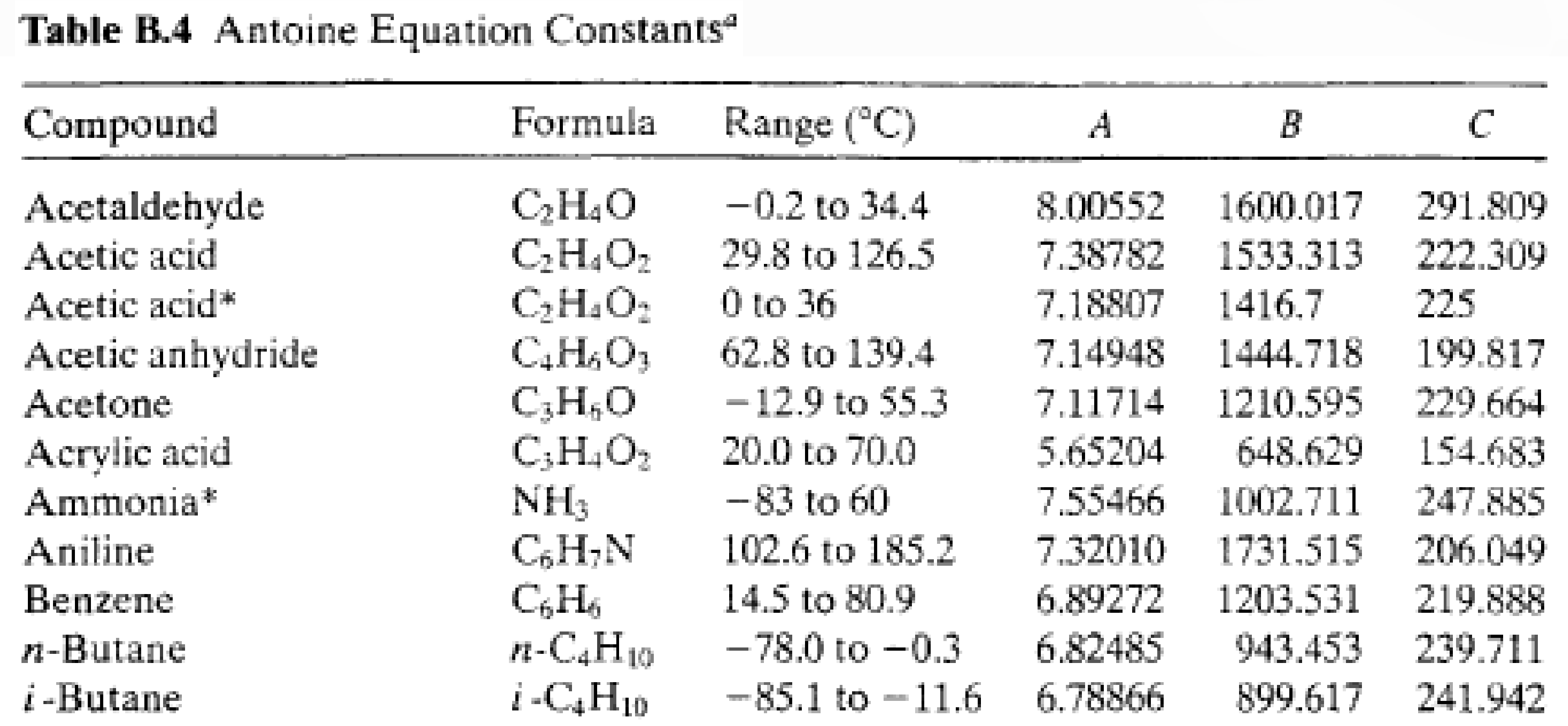


Table B.4 Antoine Equation Constants[a]

Compound	Formula	Range (°C)	*A*	*B*	*C*
Acetaldehyde	C_2H_4O	−0.2 to 34.4	8.00552	1600.017	291.809
Acetic acid	$C_2H_4O_2$	29.8 to 126.5	7.38782	1533.313	222.309
Acetic acid*	$C_2H_4O_2$	0 to 36	7.18807	1416.7	225
Acetic anhydride	$C_4H_6O_3$	62.8 to 139.4	7.14948	1444.718	199.817
Acetone	C_3H_6O	−12.9 to 55.3	7.11714	1210.595	229.664
Acrylic acid	$C_3H_4O_2$	20.0 to 70.0	5.65204	648.629	154.683
Ammonia*	NH_3	−83 to 60	7.55466	1002.711	247.885
Aniline	C_6H_7N	102.6 to 185.2	7.32010	1731.515	206.049
Benzene	C_6H_6	14.5 to 80.9	6.89272	1203.531	219.888
n-Butane	$n\text{-}C_4H_{10}$	−78.0 to −0.3	6.82485	943.453	239.711
i-Butane	$i\text{-}C_4H_{10}$	−85.1 to −11.6	6.78866	899.617	241.942

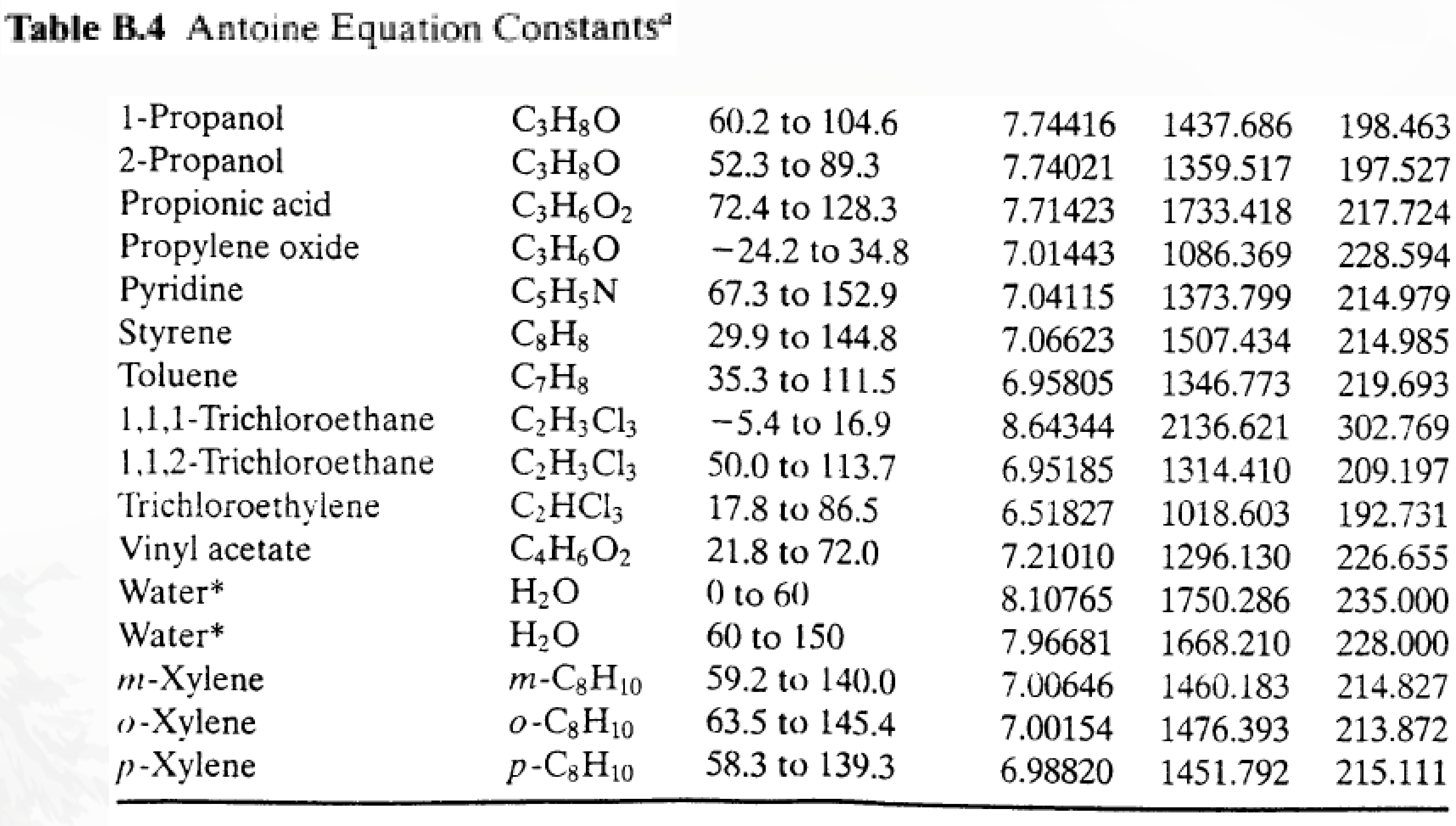


Table B.4 Antoine Equation Constants[a]

1-Propanol	C_3H_8O	60.2 to 104.6	7.74416	1437.686	198.463
2-Propanol	C_3H_8O	52.3 to 89.3	7.74021	1359.517	197.527
Propionic acid	$C_3H_6O_2$	72.4 to 128.3	7.71423	1733.418	217.724
Propylene oxide	C_3H_6O	−24.2 to 34.8	7.01443	1086.369	228.594
Pyridine	C_5H_5N	67.3 to 152.9	7.04115	1373.799	214.979
Styrene	C_8H_8	29.9 to 144.8	7.06623	1507.434	214.985
Toluene	C_7H_8	35.3 to 111.5	6.95805	1346.773	219.693
1,1,1-Trichloroethane	$C_2H_3Cl_3$	−5.4 to 16.9	8.64344	2136.621	302.769
1,1,2-Trichloroethane	$C_2H_3Cl_3$	50.0 to 113.7	6.95185	1314.410	209.197
Trichloroethylene	C_2HCl_3	17.8 to 86.5	6.51827	1018.603	192.731
Vinyl acetate	$C_4H_6O_2$	21.8 to 72.0	7.21010	1296.130	226.655
Water*	H_2O	0 to 60	8.10765	1750.286	235.000
Water*	H_2O	60 to 150	7.96681	1668.210	228.000
m-Xylene	m-C_8H_{10}	59.2 to 140.0	7.00646	1460.183	214.827
o-Xylene	o-C_8H_{10}	63.5 to 145.4	7.00154	1476.393	213.872
p-Xylene	p-C_8H_{10}	58.3 to 139.3	6.98820	1451.792	215.111

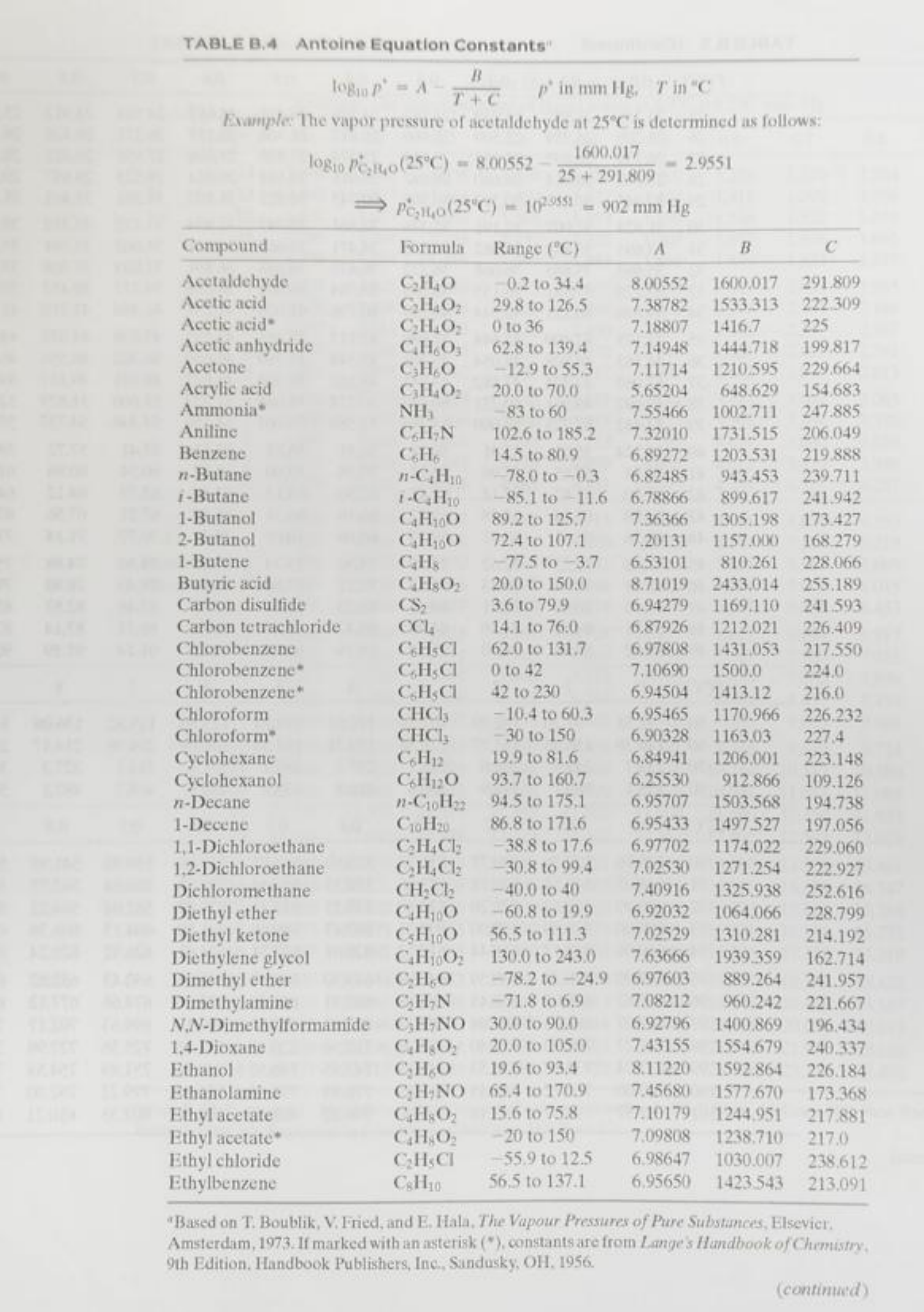


TABLE B.4 Antoine Equation Constants[a]

$$\log_{10} p^* = A - \frac{B}{T + C} \qquad p^* \text{ in mm Hg}, \quad T \text{ in °C}$$

Example: The vapor pressure of acetaldehyde at 25°C is determined as follows:

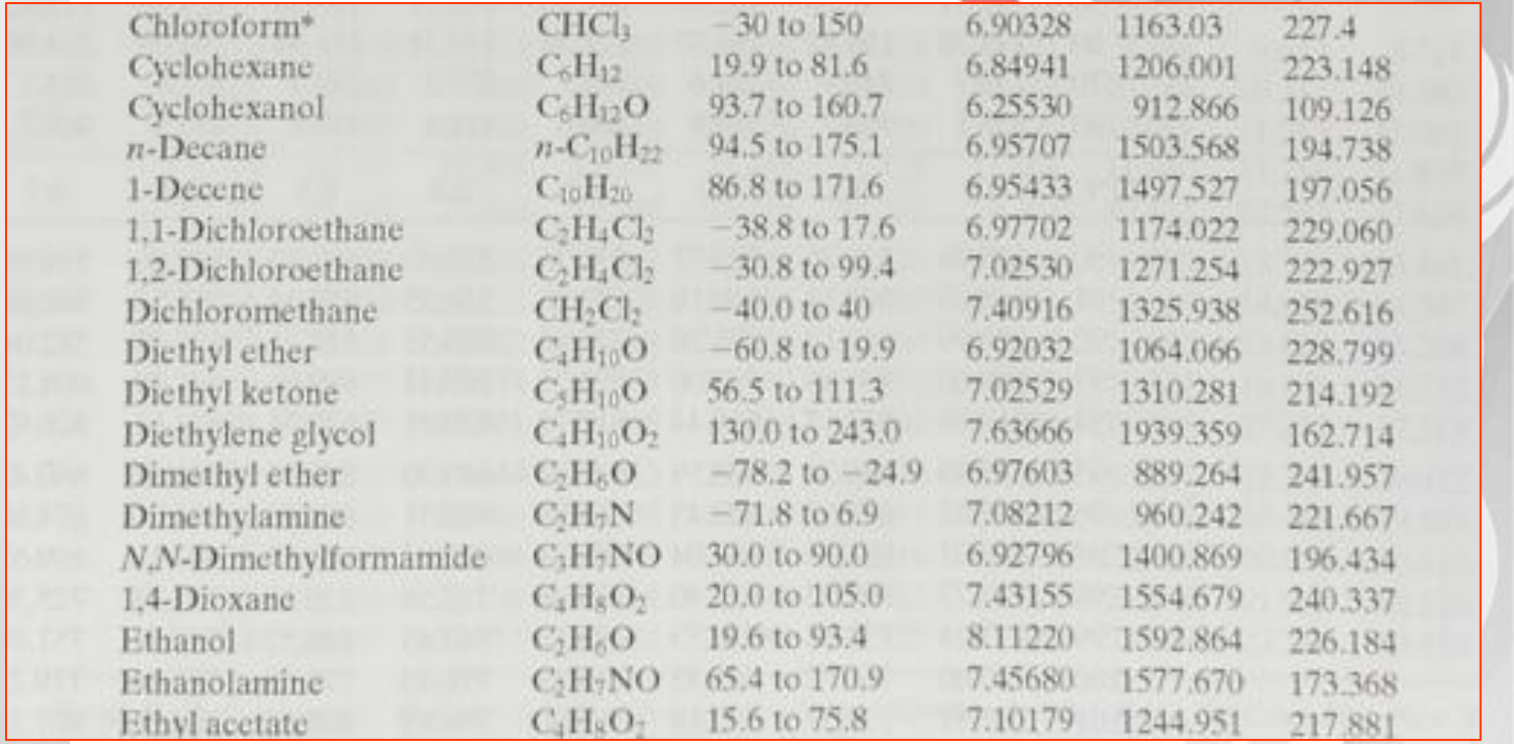
$$\log_{10} p^*_{C_2H_4O}(25°C) = 8.00552 - \frac{1600.017}{25 + 291.809} = 2.9551$$

$$\Longrightarrow p^*_{C_2H_4O}(25°C) = 10^{2.9551} = 902 \text{ mm Hg}$$

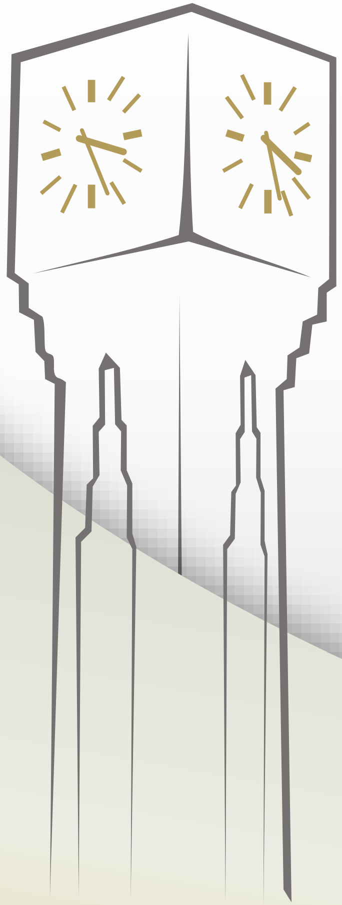
Compound	Formula	Range (°C)	*A*	*B*	*C*
Acetaldehyde	C_2H_4O	−0.2 to 34.4	8.00552	1600.017	291.809
Acetic acid	$C_2H_4O_2$	29.8 to 126.5	7.38782	1533.313	222.309
Acetic acid*	$C_2H_4O_2$	0 to 36	7.18807	1416.7	225
Acetic anhydride	$C_4H_6O_3$	62.8 to 139.4	7.14948	1444.718	199.817
Acetone	C_3H_6O	−12.9 to 55.3	7.11714	1210.595	229.664
Acrylic acid	$C_3H_4O_2$	20.0 to 70.0	5.65204	648.629	154.683
Ammonia*	NH_3	−83 to 60	7.55466	1002.711	247.885
Aniline	C_6H_7N	102.6 to 185.2	7.32010	1731.515	206.049
Benzene	C_6H_6	14.5 to 80.9	6.89272	1203.531	219.888
n-Butane	$n\text{-}C_4H_{10}$	−78.0 to −0.3	6.82485	943.453	239.711
i-Butane	$i\text{-}C_4H_{10}$	−85.1 to −11.6	6.78866	899.617	241.942
1-Butanol	$C_4H_{10}O$	89.2 to 125.7	7.36366	1305.198	173.427
2-Butanol	$C_4H_{10}O$	72.4 to 107.1	7.20131	1157.000	168.279
1-Butene	C_4H_8	−77.5 to −3.7	6.53101	810.261	228.066
Butyric acid	$C_4H_8O_2$	20.0 to 150.0	8.71019	2433.014	255.189
Carbon disulfide	CS_2	3.6 to 79.9	6.94279	1169.110	241.593
Carbon tetrachloride	CCl_4	14.1 to 76.0	6.87926	1212.021	226.409
Chlorobenzene	C_6H_5Cl	62.0 to 131.7	6.97808	1431.053	217.550
Chlorobenzene*	C_6H_5Cl	0 to 42	7.10690	1500.0	224.0
Chlorobenzene*	C_6H_5Cl	42 to 230	6.94504	1413.12	216.0
Chloroform	$CHCl_3$	−10.4 to 60.3	6.95465	1170.966	226.232
Chloroform*	$CHCl_3$	−30 to 150	6.90328	1163.03	227.4
Cyclohexane	C_6H_{12}	19.9 to 81.6	6.84941	1206.001	223.148
Cyclohexanol	$C_6H_{12}O$	93.7 to 160.7	6.25530	912.866	109.126
n-Decane	$n\text{-}C_{10}H_{22}$	94.5 to 175.1	6.95707	1503.568	194.738
1-Decene	$C_{10}H_{20}$	86.8 to 171.6	6.95433	1497.527	197.056
1,1-Dichloroethane	$C_2H_4Cl_2$	−38.8 to 17.6	6.97702	1174.022	229.060
1,2-Dichloroethane	$C_2H_4Cl_2$	−30.8 to 99.4	7.02530	1271.254	222.927
Dichloromethane	CH_2Cl_2	−40.0 to 40	7.40916	1325.938	252.616
Diethyl ether	$C_4H_{10}O$	−60.8 to 19.9	6.92032	1064.066	228.799
Diethyl ketone	$C_5H_{10}O$	56.5 to 111.3	7.02529	1310.281	214.192
Diethylene glycol	$C_4H_{10}O_2$	130.0 to 243.0	7.63666	1939.359	162.714
Dimethyl ether	C_2H_6O	−78.2 to −24.9	6.97603	889.264	241.957
Dimethylamine	C_2H_7N	−71.8 to 6.9	7.08212	960.242	221.667
N,N-Dimethylformamide	C_3H_7NO	30.0 to 90.0	6.92796	1400.869	196.434
1,4-Dioxane	$C_4H_8O_2$	20.0 to 105.0	7.43155	1554.679	240.337
Ethanol	C_2H_6O	19.6 to 93.4	8.11220	1592.864	226.184
Ethanolamine	C_2H_7NO	65.4 to 170.9	7.45680	1577.670	173.368
Ethyl acetate	$C_4H_8O_2$	15.6 to 75.8	7.10179	1244.951	217.881
Ethyl acetate*	$C_4H_8O_2$	−20 to 150	7.09808	1238.710	217.0
Ethyl chloride	C_2H_5Cl	−55.9 to 12.5	6.98647	1030.007	238.612
Ethylbenzene	C_8H_{10}	56.5 to 137.1	6.95650	1423.543	213.091

[a] Based on T. Boublik, V. Fried, and E. Hala, *The Vapour Pressures of Pure Substances*, Elsevier, Amsterdam, 1973. If marked with an asterisk (*), constants are from *Lange's Handbook of Chemistry*, 9th Edition, Handbook Publishers, Inc., Sandusky, OH, 1956.

(*continued*)



Chloroform*	$CHCl_3$	−30 to 150	6.90328	1163.03	227.4
Cyclohexane	C_6H_{12}	19.9 to 81.6	6.84941	1206.001	223.148
Cyclohexanol	$C_6H_{12}O$	93.7 to 160.7	6.25530	912.866	109.126
n-Decane	$n\text{-}C_{10}H_{22}$	94.5 to 175.1	6.95707	1503.568	194.738
1-Decene	$C_{10}H_{20}$	86.8 to 171.6	6.95433	1497.527	197.056
1,1-Dichloroethane	$C_2H_4Cl_2$	−38.8 to 17.6	6.97702	1174.022	229.060
1,2-Dichloroethane	$C_2H_4Cl_2$	−30.8 to 99.4	7.02530	1271.254	222.927
Dichloromethane	CH_2Cl_2	−40.0 to 40	7.40916	1325.938	252.616
Diethyl ether	$C_4H_{10}O$	−60.8 to 19.9	6.92032	1064.066	228.799
Diethyl ketone	$C_5H_{10}O$	56.5 to 111.3	7.02529	1310.281	214.192
Diethylene glycol	$C_4H_{10}O_2$	130.0 to 243.0	7.63666	1939.359	162.714
Dimethyl ether	C_2H_6O	−78.2 to −24.9	6.97603	889.264	241.957
Dimethylamine	C_2H_7N	−71.8 to 6.9	7.08212	960.242	221.667
N,N-Dimethylformamide	C_3H_7NO	30.0 to 90.0	6.92796	1400.869	196.434
1,4-Dioxane	$C_4H_8O_2$	20.0 to 105.0	7.43155	1554.679	240.337
Ethanol	C_2H_6O	19.6 to 93.4	8.11220	1592.864	226.184
Ethanolamine	C_2H_7NO	65.4 to 170.9	7.45680	1577.670	173.368
Ethyl acetate	$C_4H_8O_2$	15.6 to 75.8	7.10179	1244.951	217.881



6.2 The Gibbs Phase Rule

This section outlines

6.2 The Gibbs Phase Rule

The variables that describe the condition of a process system fall into two categories:

Extensive variables: which depend on the size of the system.
Example: mass and volume

Intensive variables: which do not depend on the size of the system.
Example: temperature, pressure, density, specific volume, mass and mole fractions

Degrees of freedom of the system is
The number of intensive variables that can be specified independently for a system at equilibrium to completely define the system.

$$\boxed{DF = 2 + C - \pi - r}$$

The relationship among DF, π, c, r is called **The Gibbs Phase Rule**

where

- c = number of independent chemical species
- π = number of phases in a system at equilibrium
- r = number of independent equilibrated chemical reactions among the species
- DF = degrees of freedom

Degrees of freedom
Process system vs. Gibbs phase rule

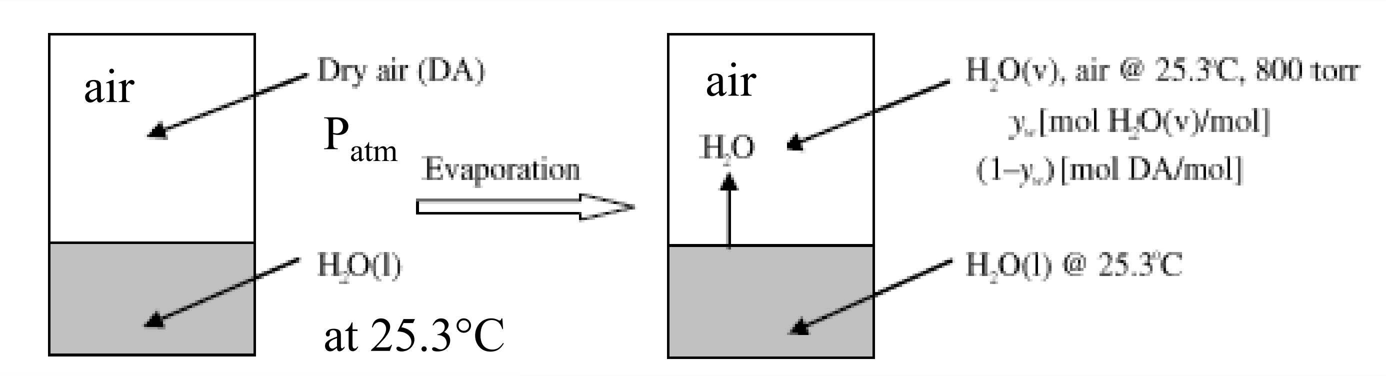
DOF
Arbitrary process system

DOF tells you how many process variable (extensive & intensive) must be specified to calculate the rest

DOF
Using Gibbs phase rule

DOF tells you the number of intensive variables that must be specified for a system at equilibrium to calculate all the other intensive variables

Example - Application of Gibbs Phase Rule

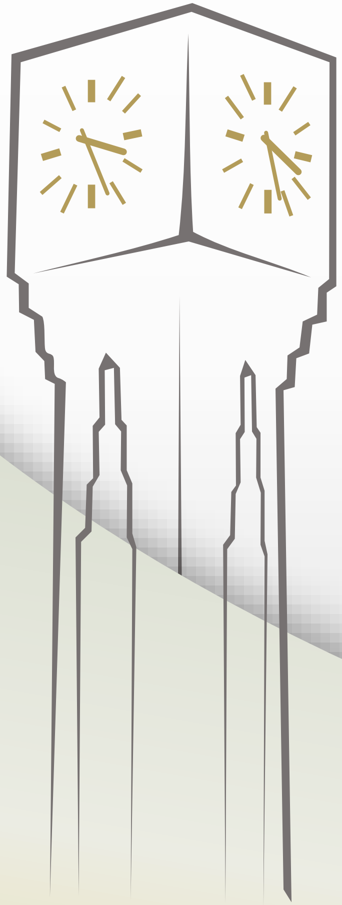


Q. Can you calculate the vapor-phase composition at equilibrium from the data given?

Using the Gibbs Phase Rule:

$$DF = 2 + c - \pi - r = 2 + \underset{H_2O,\,air}{2} - \underset{L,V}{2} - 0 = 2$$

Since we know ***(T = 25.3 ℃)*** and ***(P_{atm} = 800 torr)***, then all other set (e.g., ρ_w and y) can be calculated from the Equation of state or another relation; e.g., Raoult's law (to be introduced next section)



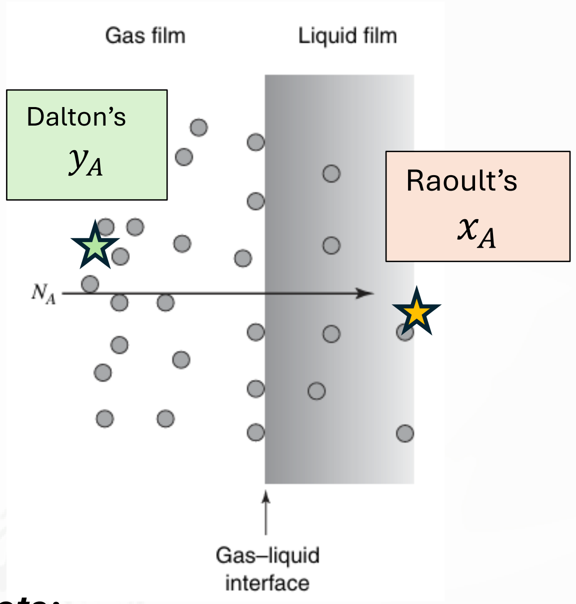
Important Equilibrium Relations

This section outlines

Volatility

- ***Volatility*** of a species is the tendency to go from liquid (or solid) to vapor.
- *The vapor pressure (p*) of a species is a measure of its volatility*:
  - High vapor pressure ⇒ high volatility
  - Low boiling point ⇒ high volatility
- At a given temperature and pressure, a highly volatile substance is much more likely to be found as a vapor than is a substance with low volatility, which is more likely to be found in a condensed phase (liquid or solid).
- Separation processes such as distillation are used to separate more volatile species from less volatile species by partially vaporizing liquid mixtures.
- The vapor product is relatively rich in the more volatile feed components and the residual liquid is rich in the components with lower volatility.
- Engineers who design and analyze separation processes therefore need to know the vapor pressures of process species as functions of temperature.

Ideal Gas–Liquid Equilibrium Relations (*Raoult's Law*)



Note:

The same equilibrium relation may be written using concentration c_A instead of mole fraction x_A. The value and unit of H are adjusted accordingly.

When the gas phase is ideal, **Dalton's law (ideal gas)** applies:

$$p_A = y_A P \qquad \textbf{(1)}$$

- where y_A is the gas-phase mole fraction and P is the total pressure.

When the liquid phase is ideal, **Raoult's law (idea liquid)** applies:

$$p_A = x_A P^*_A \qquad \textbf{(2)}$$

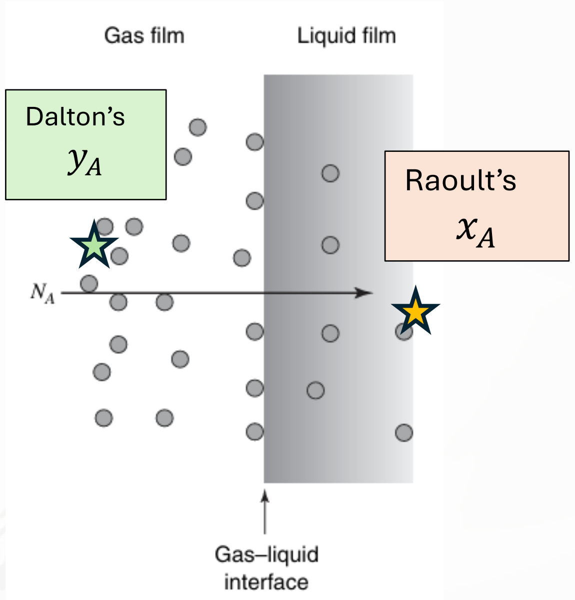
- where p_A is the equilibrium partial pressure of A
- x_A is the liquid-phase mole fraction, and
- P^*_A is the **vapor pressure of pure A at the systems temperature**, usually termed as $P^*_A\ (T)$ ← important

When both phases are ideal, Raoult's and Dalton's laws combine (equate Equations 1 = Equation 2) to give the **Raoult–Dalton equilibrium relation**:

$$\boxed{y_A P = x_A P^*_A}$$

Raoult's Law

Ideal Gas–Liquid Equilibrium Relations (*Henry's Law*)



For gas–liquid systems involving **dilute solutions**, equilibrium is described by Henry's law:

$$\boldsymbol{p_A = H \cdot x_A}$$

- where $\boldsymbol{x_A}$is the liquid-phase mole fraction
- $\boldsymbol{H}$ is Henry's law constant at the system's temperature = $H_A\ (T)$
- In the same manner as Raoult's Law, the patrial pressure $\boldsymbol{p_A}$ can be substituted using Dalton's, $p_A = y_A P$

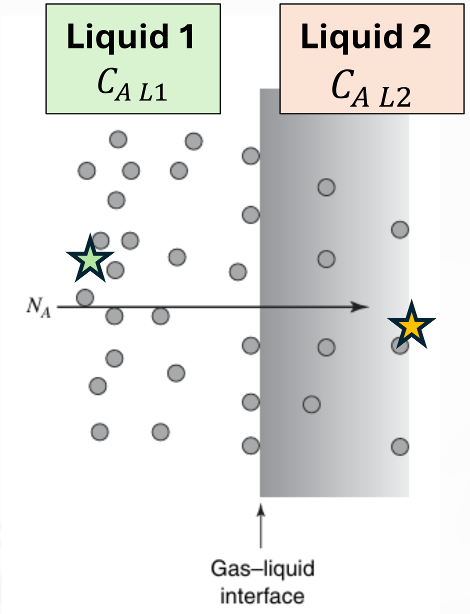
$$\boxed{\boldsymbol{y_A P = x_A \cdot H_A}}$$

Henry's Law

Note:

The same equilibrium relation may be written using concentration $\boldsymbol{c_A}$ instead of mole fraction $\boldsymbol{x_A}$. The value and unit of $\boldsymbol{H}$ are adjusted accordingly.

Liquid–Liquid Equilibrium (*Distribution Law*)



A similar relation applies to solute partitioning between **two immiscible liquids**, known as the distribution law:

$$\boxed{c_{A,\ Liq\ 1} = K \cdot c_{A,\ Liq\ 2}}$$

Distribution Law

- $c_{A,}$ is the concentration of solute A in the specified liquid phase
- K is the partition or distribution coefficient.

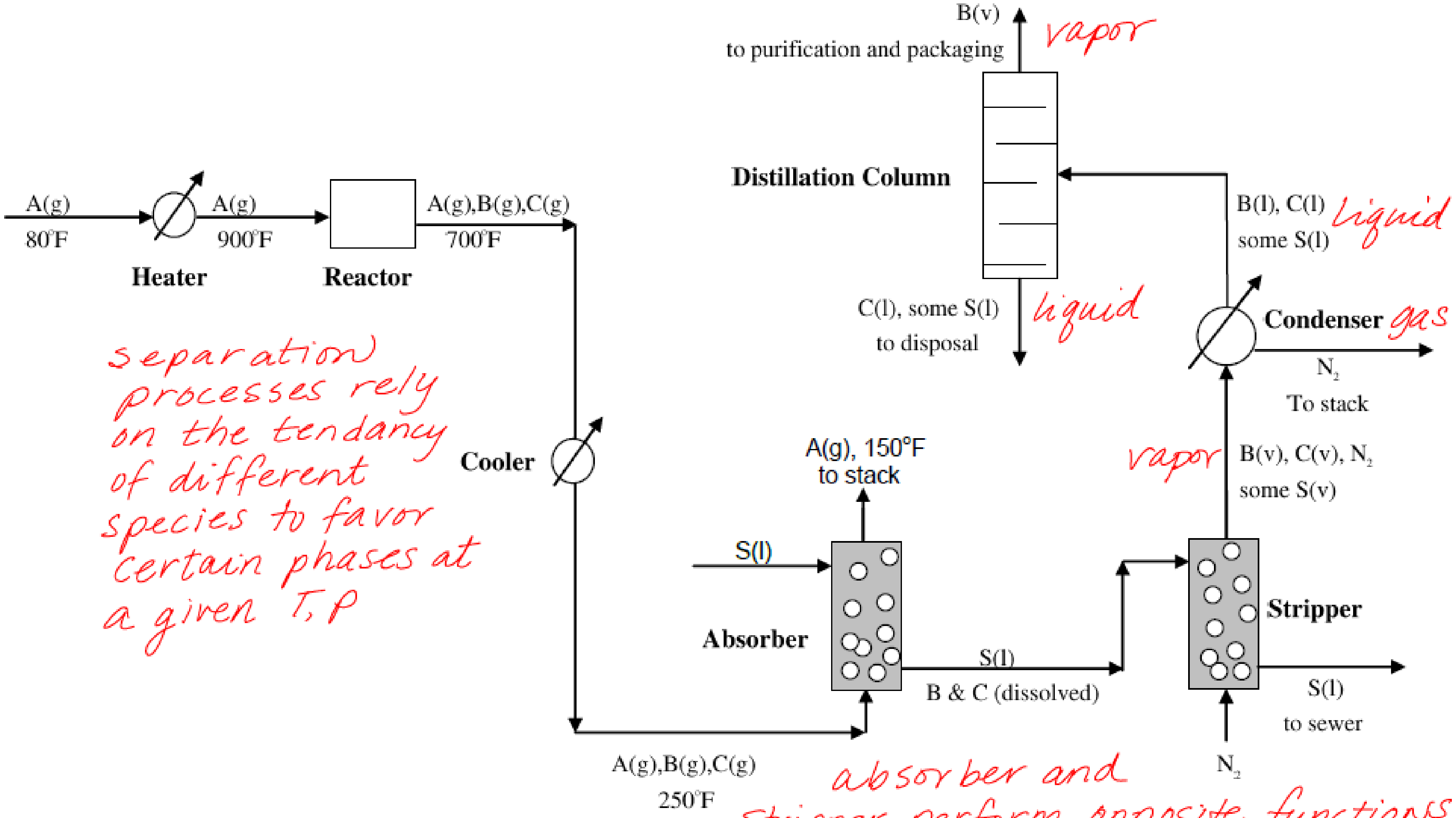
This relation governs liquid–liquid extraction processes and serves the same equilibrium-linking role as Henry's law in gas–liquid systems

A comparison point:

- Raoult's law ($y_A P = x_A\ \boldsymbol{P^*}_{\boldsymbol{A}}$) can be written in a way similar to the Distribution Law in the form: $y_A = K\ x_A$, where the constant is called K-value and it is a thermodynamic value used in the design

Balances on Multiphase Systems

A → B, B → C   A– feedstock, B – desired product, C – byproduct (waste)

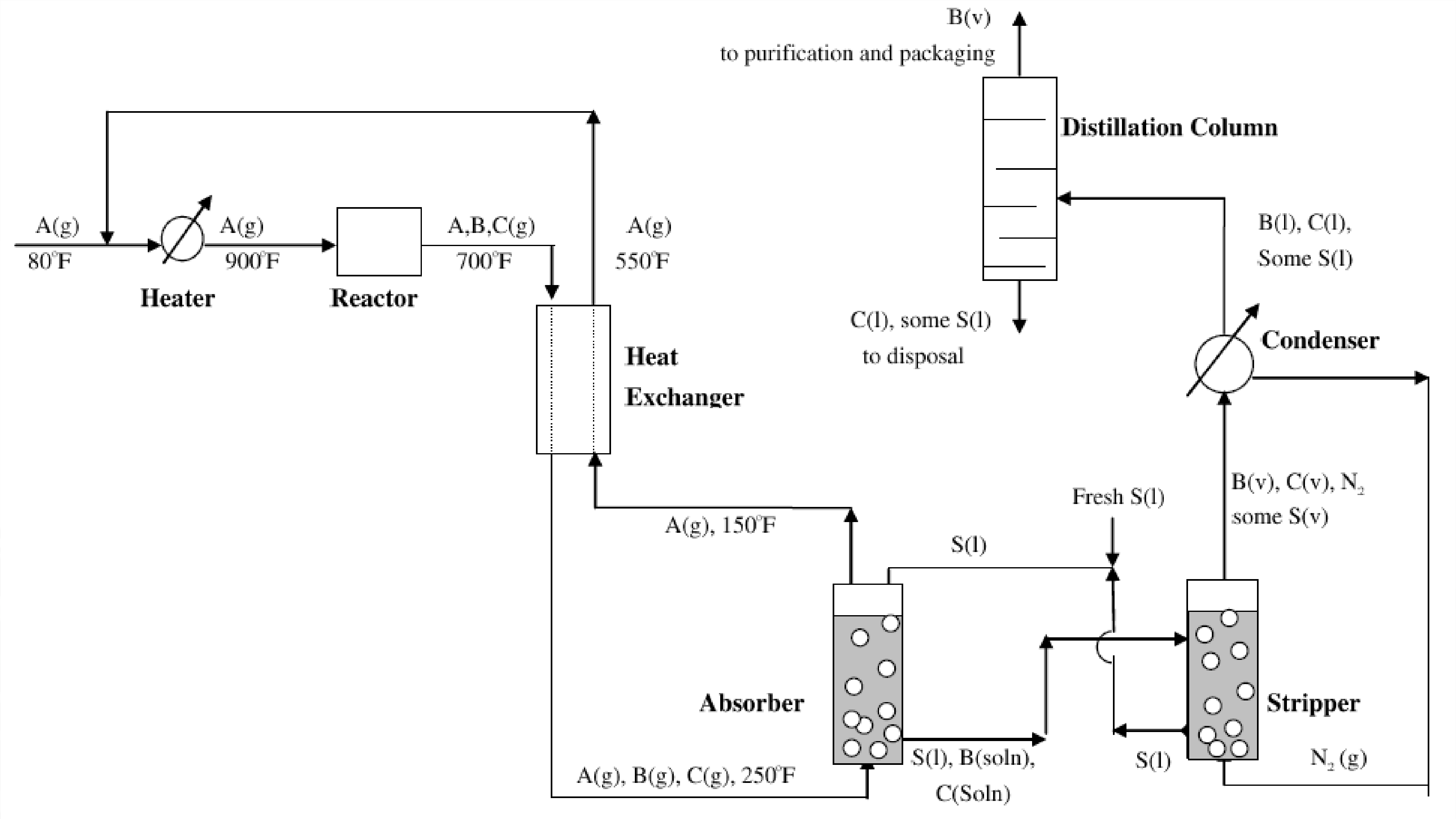


separation processes rely on the tendancy of different species to favor certain phases at a given T, P

absorber and stripper perform opposite functions

This process is expensive, wasteful, & inefficient — how would you modify it?

A → B, B → C A–feedstock, B–desired product, C–byproduct (waste)



The function of most chemical process units is to separate mixtures into their components, as in the process just shown.

Q: What types of information do we need to know to design this system?

A: solubilities of A,B,C in solvent S (want A to be insoluble, B&C soluble)
volatilities of B and C (want B to be more volatile)

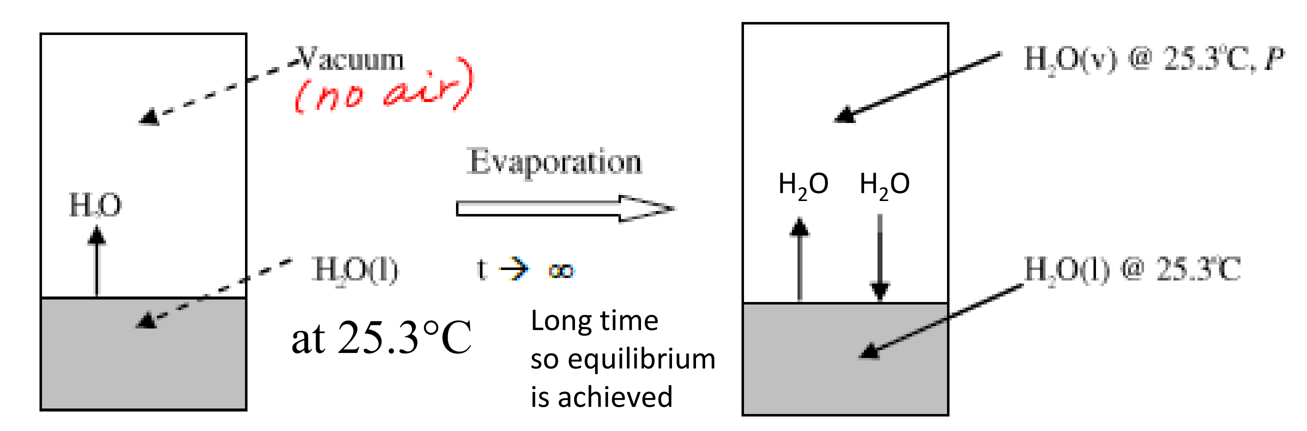
6.3 Gas-Liquid Systems: One condensable component

This section outlines

6.3 Gas-Liquid systems: One condensable component

- Gas-liquid systems
- Saturation and Humidity

Evacuate a beaker, charge it with water at 23.5 °C, let it reach equilibrium.



Important

$p_i^*\ (T)$ *means*
p_i^* *at* (T)
not $p_i^* \times (T)$

Q. What is ***P*** in the gas in the container at equilibrium?
(Hint: liquid and vapor are coexisting at the same temperature. Think about the phase diagram)

P = $p_{H_2O}^*\ (T = 25.3°C)$

$p_{H_2O}^*\ (T = 25.3°C)$ = 24.182 mmHg

$p^*_{H_2O}\ (T = 25.3°C)$

Unit of p* in this able is mmHg

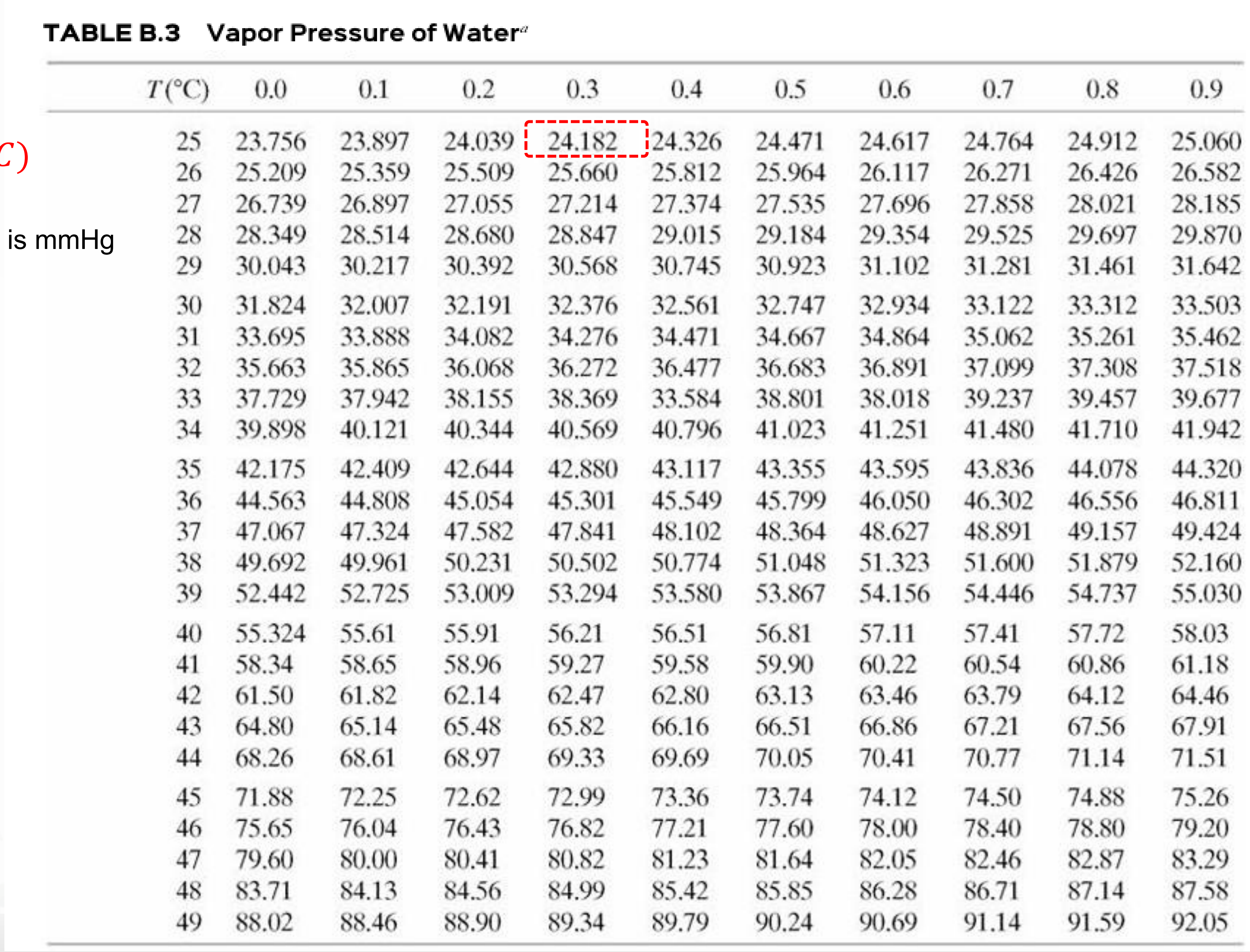


TABLE B.3 Vapor Pressure of Water[a]

T(°C)	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
25	23.756	23.897	24.039	24.182	24.326	24.471	24.617	24.764	24.912	25.060
26	25.209	25.359	25.509	25.660	25.812	25.964	26.117	26.271	26.426	26.582
27	26.739	26.897	27.055	27.214	27.374	27.535	27.696	27.858	28.021	28.185
28	28.349	28.514	28.680	28.847	29.015	29.184	29.354	29.525	29.697	29.870
29	30.043	30.217	30.392	30.568	30.745	30.923	31.102	31.281	31.461	31.642
30	31.824	32.007	32.191	32.376	32.561	32.747	32.934	33.122	33.312	33.503
31	33.695	33.888	34.082	34.276	34.471	34.667	34.864	35.062	35.261	35.462
32	35.663	35.865	36.068	36.272	36.477	36.683	36.891	37.099	37.308	37.518
33	37.729	37.942	38.155	38.369	33.584	38.801	38.018	39.237	39.457	39.677
34	39.898	40.121	40.344	40.569	40.796	41.023	41.251	41.480	41.710	41.942
35	42.175	42.409	42.644	42.880	43.117	43.355	43.595	43.836	44.078	44.320
36	44.563	44.808	45.054	45.301	45.549	45.799	46.050	46.302	46.556	46.811
37	47.067	47.324	47.582	47.841	48.102	48.364	48.627	48.891	49.157	49.424
38	49.692	49.961	50.231	50.502	50.774	51.048	51.323	51.600	51.879	52.160
39	52.442	52.725	53.009	53.294	53.580	53.867	54.156	54.446	54.737	55.030
40	55.324	55.61	55.91	56.21	56.51	56.81	57.11	57.41	57.72	58.03
41	58.34	58.65	58.96	59.27	59.58	59.90	60.22	60.54	60.86	61.18
42	61.50	61.82	62.14	62.47	62.80	63.13	63.46	63.79	64.12	64.46
43	64.80	65.14	65.48	65.82	66.16	66.51	66.86	67.21	67.56	67.91
44	68.26	68.61	68.97	69.33	69.69	70.05	70.41	70.77	71.14	71.51
45	71.88	72.25	72.62	72.99	73.36	73.74	74.12	74.50	74.88	75.26
46	75.65	76.04	76.43	76.82	77.21	77.60	78.00	78.40	78.80	79.20
47	79.60	80.00	80.41	80.82	81.23	81.64	82.05	82.46	82.87	83.29
48	83.71	84.13	84.56	84.99	85.42	85.85	86.28	86.71	87.14	87.58
49	88.02	88.46	88.90	89.34	89.79	90.24	90.69	91.14	91.59	92.05

Table B.5 Temperature Table

Or by using the Steam Tables with interpolation

$p^*_{H_2O}\ (T = 25.3°C)$

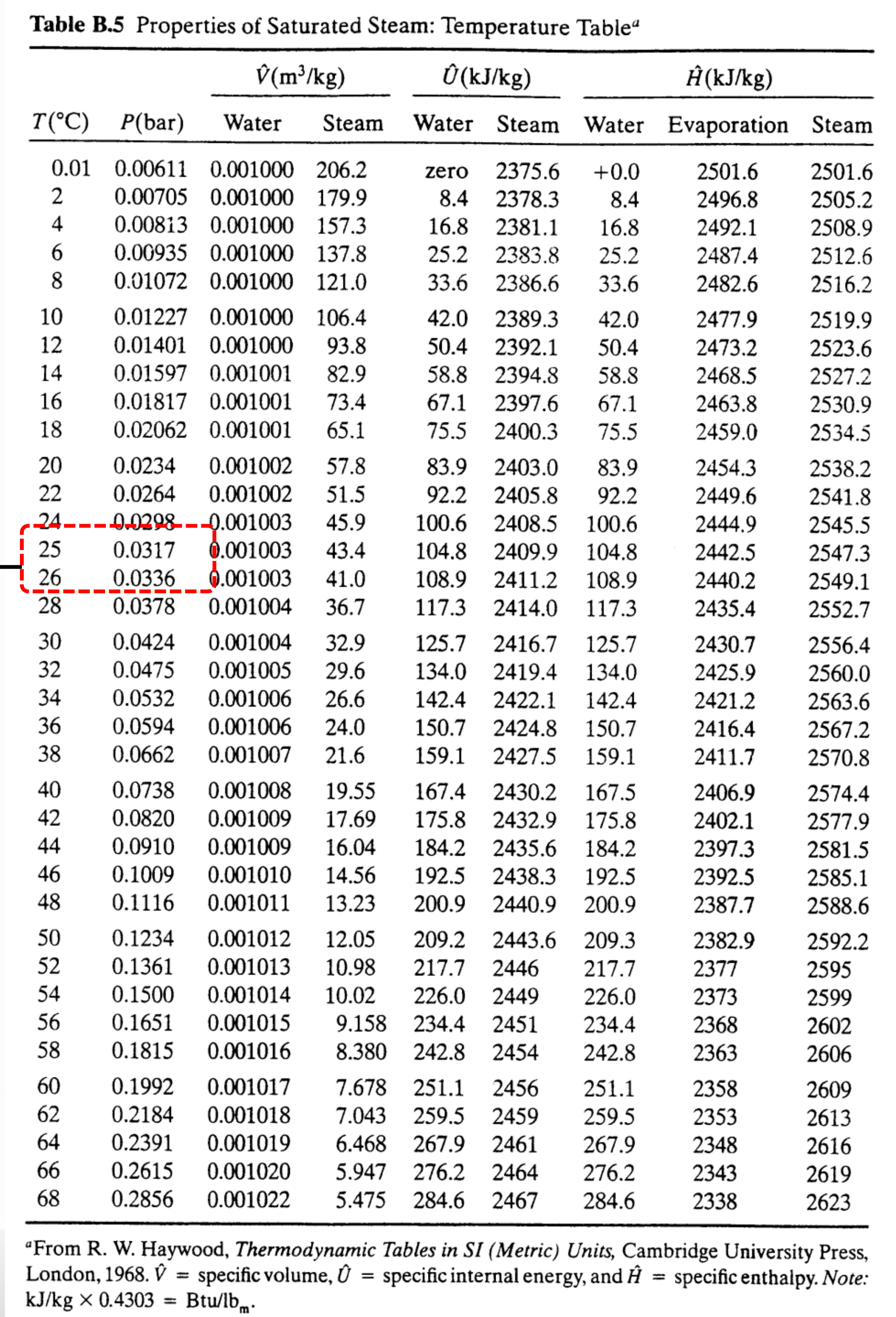


Table B.5 Properties of Saturated Steam: Temperature Table[a]

		$\hat{V}$(m³/kg)		$\hat{U}$(kJ/kg)		$\hat{H}$(kJ/kg)		
T(°C)	P(bar)	Water	Steam	Water	Steam	Water	Evaporation	Steam
0.01	0.00611	0.001000	206.2	zero	2375.6	+0.0	2501.6	2501.6
2	0.00705	0.001000	179.9	8.4	2378.3	8.4	2496.8	2505.2
4	0.00813	0.001000	157.3	16.8	2381.1	16.8	2492.1	2508.9
6	0.00935	0.001000	137.8	25.2	2383.8	25.2	2487.4	2512.6
8	0.01072	0.001000	121.0	33.6	2386.6	33.6	2482.6	2516.2
10	0.01227	0.001000	106.4	42.0	2389.3	42.0	2477.9	2519.9
12	0.01401	0.001000	93.8	50.4	2392.1	50.4	2473.2	2523.6
14	0.01597	0.001001	82.9	58.8	2394.8	58.8	2468.5	2527.2
16	0.01817	0.001001	73.4	67.1	2397.6	67.1	2463.8	2530.9
18	0.02062	0.001001	65.1	75.5	2400.3	75.5	2459.0	2534.5
20	0.0234	0.001002	57.8	83.9	2403.0	83.9	2454.3	2538.2
22	0.0264	0.001002	51.5	92.2	2405.8	92.2	2449.6	2541.8
24	0.0298	0.001003	45.9	100.6	2408.5	100.6	2444.9	2545.5
25	0.0317	0.001003	43.4	104.8	2409.9	104.8	2442.5	2547.3
26	0.0336	0.001003	41.0	108.9	2411.2	108.9	2440.2	2549.1
28	0.0378	0.001004	36.7	117.3	2414.0	117.3	2435.4	2552.7
30	0.0424	0.001004	32.9	125.7	2416.7	125.7	2430.7	2556.4
32	0.0475	0.001005	29.6	134.0	2419.4	134.0	2425.9	2560.0
34	0.0532	0.001006	26.6	142.4	2422.1	142.4	2421.2	2563.6
36	0.0594	0.001006	24.0	150.7	2424.8	150.7	2416.4	2567.2
38	0.0662	0.001007	21.6	159.1	2427.5	159.1	2411.7	2570.8
40	0.0738	0.001008	19.55	167.4	2430.2	167.5	2406.9	2574.4
42	0.0820	0.001009	17.69	175.8	2432.9	175.8	2402.1	2577.9
44	0.0910	0.001009	16.04	184.2	2435.6	184.2	2397.3	2581.5
46	0.1009	0.001010	14.56	192.5	2438.3	192.5	2392.5	2585.1
48	0.1116	0.001011	13.23	200.9	2440.9	200.9	2387.7	2588.6
50	0.1234	0.001012	12.05	209.2	2443.6	209.3	2382.9	2592.2
52	0.1361	0.001013	10.98	217.7	2446	217.7	2377	2595
54	0.1500	0.001014	10.02	226.0	2449	226.0	2373	2599
56	0.1651	0.001015	9.158	234.4	2451	234.4	2368	2602
58	0.1815	0.001016	8.380	242.8	2454	242.8	2363	2606
60	0.1992	0.001017	7.678	251.1	2456	251.1	2358	2609
62	0.2184	0.001018	7.043	259.5	2459	259.5	2353	2613
64	0.2391	0.001019	6.468	267.9	2461	267.9	2348	2616
66	0.2615	0.001020	5.947	276.2	2464	276.2	2343	2619
68	0.2856	0.001022	5.475	284.6	2467	284.6	2338	2623

[a] From R. W. Haywood, *Thermodynamic Tables in SI (Metric) Units*, Cambridge University Press, London, 1968. $\hat{V}$ = specific volume, $\hat{U}$ = specific internal energy, and $\hat{H}$ = specific enthalpy. *Note:* kJ/kg × 0.4303 = Btu/lb$_m$.

Example of interpolation

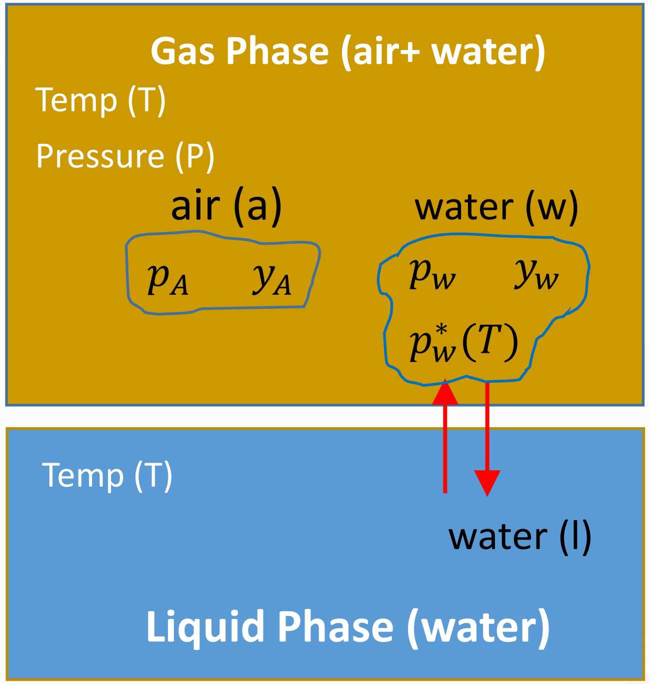
How much is $p^*_{H_2O}$ at $T = 25.3°C$?

$$\frac{26-25}{25.3-25} = \frac{0.0336-0.0317}{p^*_{25.3C}-0.0317}$$

$$p^*_{25.3C} = 0.0323\ bar \times \frac{100{,}000\ Pa}{1\ bar} \times \frac{760\ mmHg}{101{,}325\ Pa}$$

$$p^*_{25.3C} = 24.23\ mmHg$$

Vapor-liquid equilibrium for a multicomponent gas with a single condensable species



Refer to book to for details and examples of this section

RAOULT'S LAW, Single Condensable Species

System total pressure

system temperature

$$\boxed{p_i = y_i\,P = p_i^*(T)}$$

Partial pressure of condensable species

composition of condensable species

vapor pressure of condensable species

- L/V at equilibrium
- Saturated vapor
- p_i^* *at* (T), *not* $p_i^* \times (T)$

Raoult's Law $y_A P = x_A\,\boldsymbol{P^*}_{\boldsymbol{A}}$

Single condensable liquid → $x_A = 1$

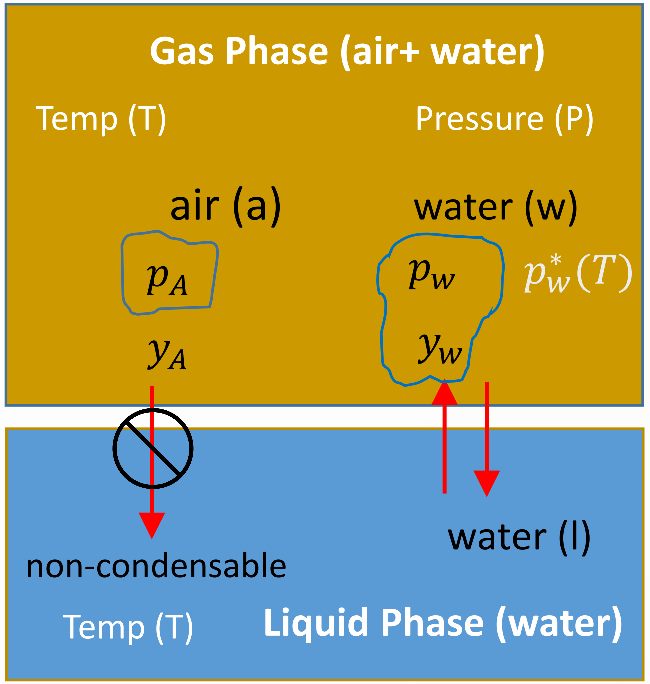
$$y_A P = (1)\,\boldsymbol{P^*}_{\boldsymbol{A}}$$

$$\Rightarrow \qquad y_A P = \boldsymbol{P^*}_{\boldsymbol{A}}$$

Examples of Liquid –Vapor units:

- Distillation, absorption, stripping
- Evaporation, drying, and humidification (transfer of species from liquid into gas)
- Condensation, dehumidification (transfer of species from the gas to liquid)

at equilibrium



$$p_w = y_w\,P = p_w^*(T)$$ **Raoult's law**

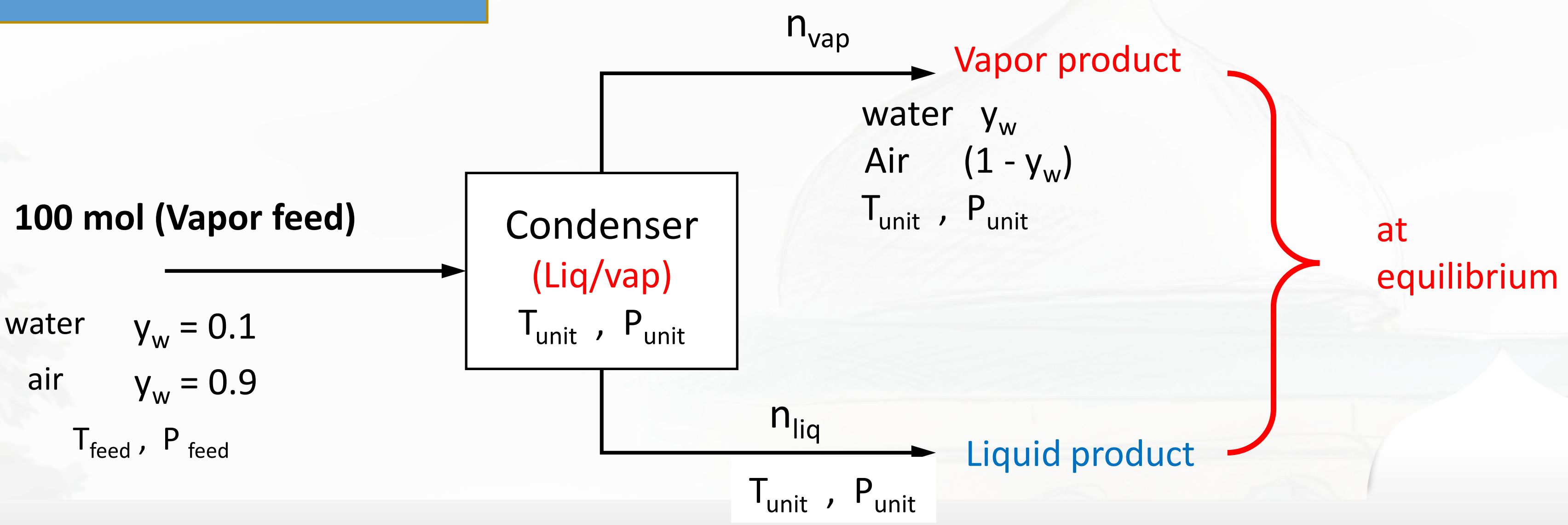
applies only to condensable species (H_2O not air)

$$p_A = y_A\,P$$

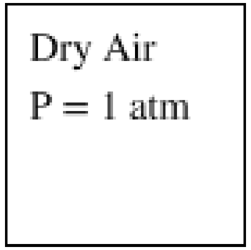
$$P = p_w + p_A$$ **Dalton's law**

$$y_w = \frac{p_w}{P} = \frac{p_w^*(T)}{P} = \frac{n_w}{n}$$

$$y_A = \frac{p_A}{P} = \frac{n_A}{n}$$

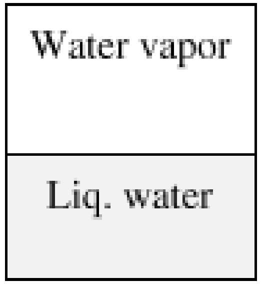


Example - Partial pressure and Vapor pressure



What is p_{N_2} (the partial pressure of nitrogen)?

$$p_{N_2} = y_{N_2}P = (0.79)(1\ atm) = 0.79\ atm$$

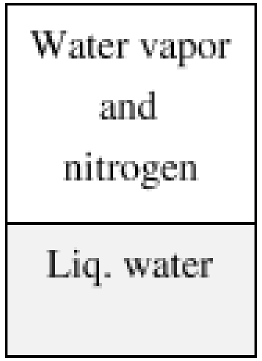


T = 25°C

At equilibrium, what is the pressure of the vapor in the container?

Pure gas phase and liquid phase (no mixtures)

$$p_{H_2O} = P = p^*_{H_2O}\ (T = 25°C) = 23.756\ mmHg$$ (Table B.3 or Steam table)



T = 25°C

At equilibrium, what is p_{H_2O} (the partial pressure of water)?

Single condensable material (x_w= 1)

$$P = p_{H_2O} + p_{N_2}\ \ (p_{H_2O} < P)$$

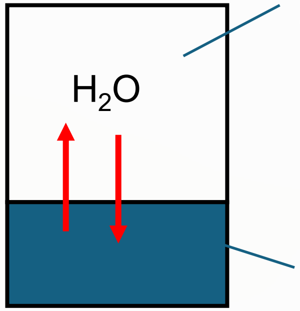
$$p_{H_2O} = p^*_{H_2O}\ (25°C) = 23.756\ mmHg$$

Total pressure (P) is higher than $p^*_{H_2O}$ due to presence of N_2

Example 6.3-1

Composition of a Saturated Gas–Vapor System

Air and liquid water are contained at equilibrium in a closed chamber at 75°C and 760 mm Hg. Calculate the molar composition of the gas phase.



H_2O (v) + air

75°C, P= 760 mmHg

y_w

$(1-y_w)$

H_2O (*l*) at 75°C

$x_w = 1$

The gas and liquid are in equilibrium, the air must be saturated with water vapor

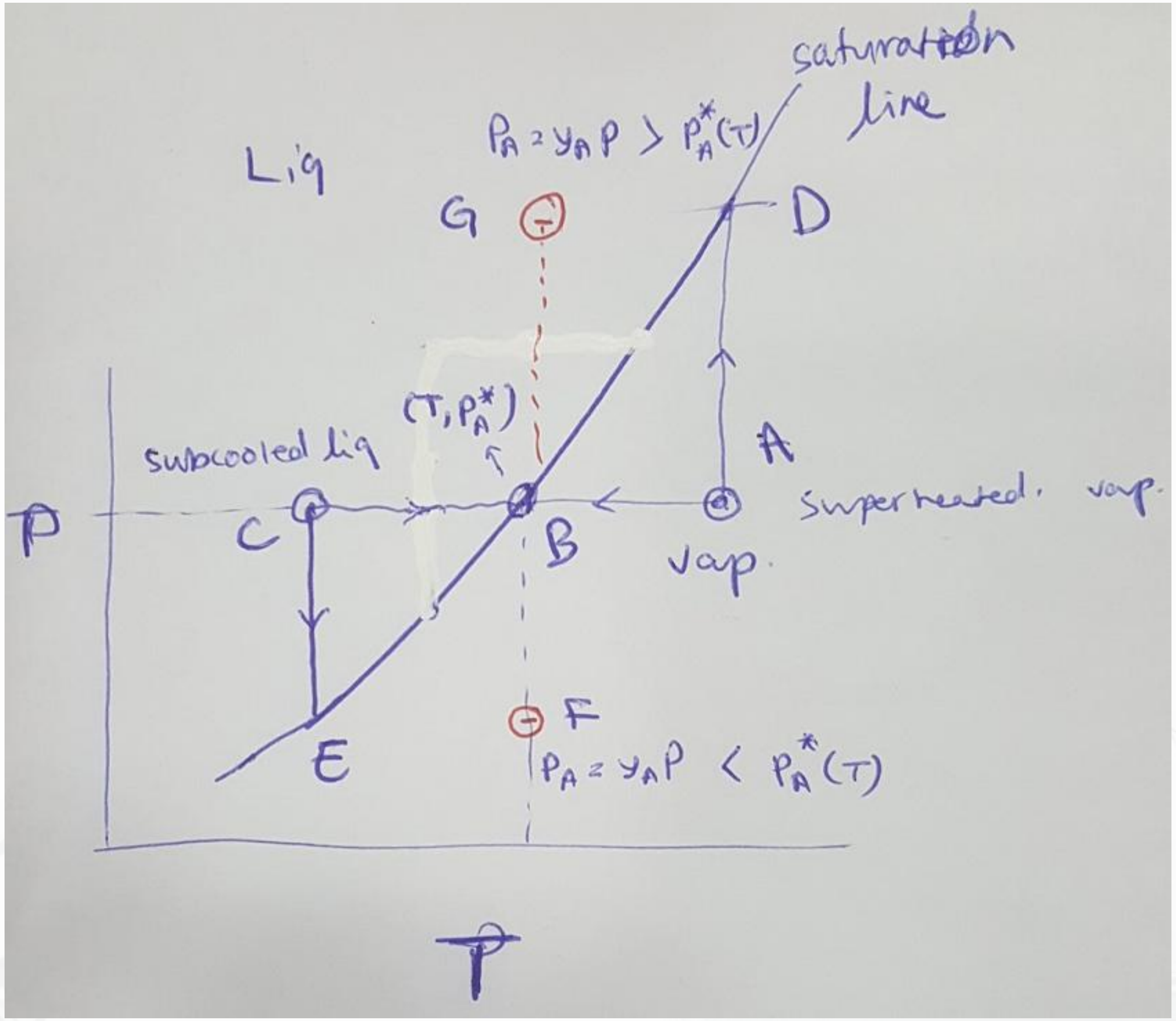
Raoult's Law

$$p_w = y_w\,P = p_w^*(T) \quad \Rightarrow y_w = \frac{p_w^*(75°C)}{P}$$

From Table B.3 in Appendix B, $p^*_{H_2O}(75°C) = 289$ mm Hg.

$$y_{H_2O} = \frac{289 \text{ mm Hg}}{760 \text{ mm Hg}} = \boxed{0.380 \ \frac{\text{mol } H_2O}{\text{mol}}}$$

$$y_{\text{dry air}} = 1 - y_{H_2O} = \boxed{0.620 \ \frac{\text{mol dry air}}{\text{mol}}}$$



$$p_i > p_i^*(T)$$
$$\Rightarrow subcooled\ liquid$$

$$p_i = p_i^*(T)$$
$$\Rightarrow saturated\ liq$$
$$or\ saturated\ vapor$$

$$p_i < p_i^*(T)$$
$$\Rightarrow superheated\ vap$$

RAOULT'S LAW, Single Condensable Species

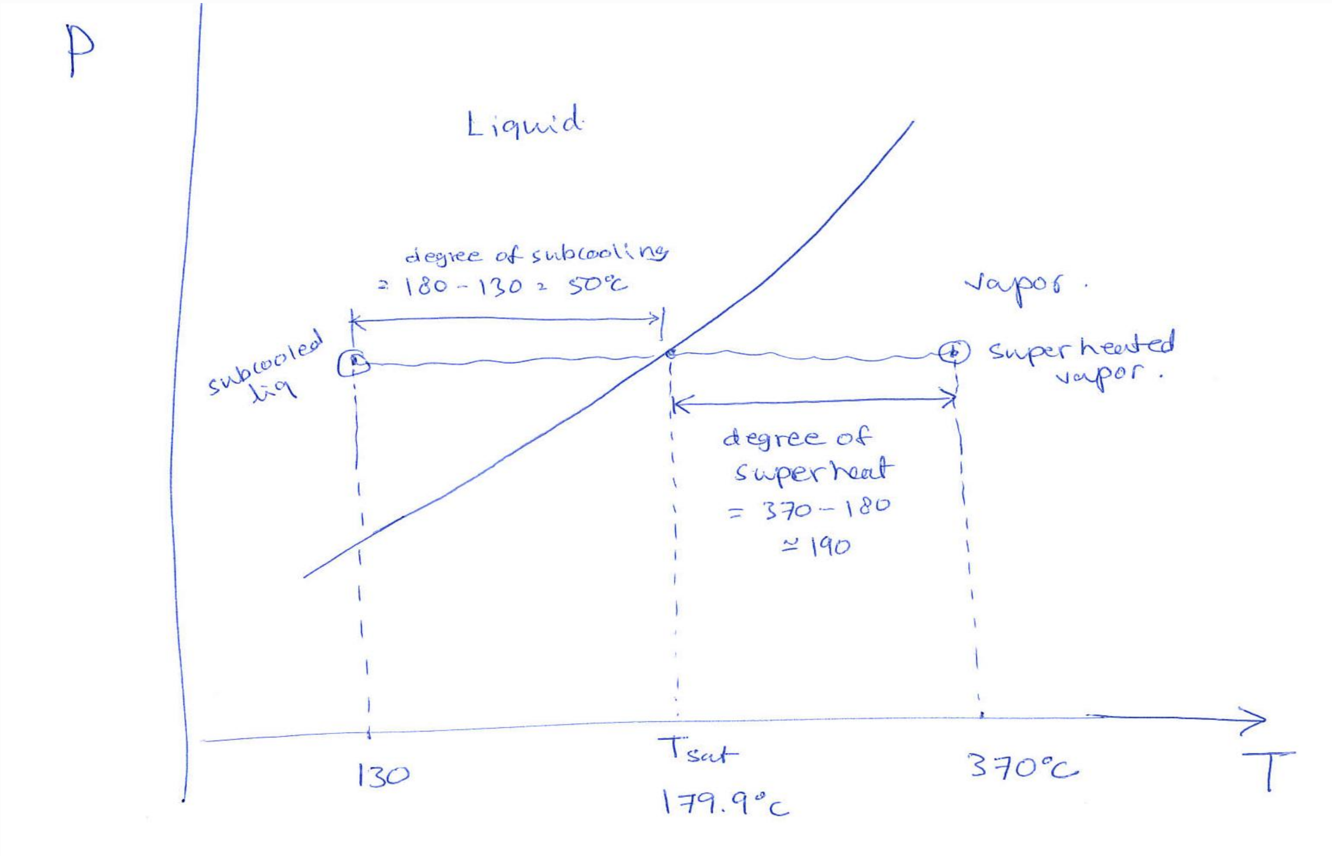
$$\boxed{p_i = y_i P = p_i^*(T)}$$

- L/V at equilibrium
- Saturated vapor

For gas-liquid systems

Refer to book to for details and examples of this section

Degree of subcooling / Degrees of superheat



Degrees of subcooling: The difference *between the actual temperature of the subcooled liquid and the* saturation temperature (dew point of a gas) for the same pressure

Degrees of superheat: The difference *between the actual temperature of the superheated vapor and the* saturation temperature (dew point of a gas) for the same pressure

Important Concept – Boiling Point of a Pure material and a Mixture

1) Boiling point of a pure material

A pure liquid boils when its vapor pressure equals the external (system) pressure:

$$\boxed{p^*(T_b) = P}$$

- $p^*(T)$ = vapor (or saturation) pressure of the pure liquid (an equilibrium property)
- P= external pressure
- T_b =boiling temperature at pressure P (an equilibrium property)

Physical meaning:

At this condition, vapor bubbles can form inside the liquid without collapsing.

2) Boiling point of a binary mixture (A + B)

A liquid mixture boils when the sum of the partial pressures of all volatile components equals the external pressure:

$$\boxed{p_A + p_B = P}$$

For an **ideal liquid mixture** (Raoult's law applies):

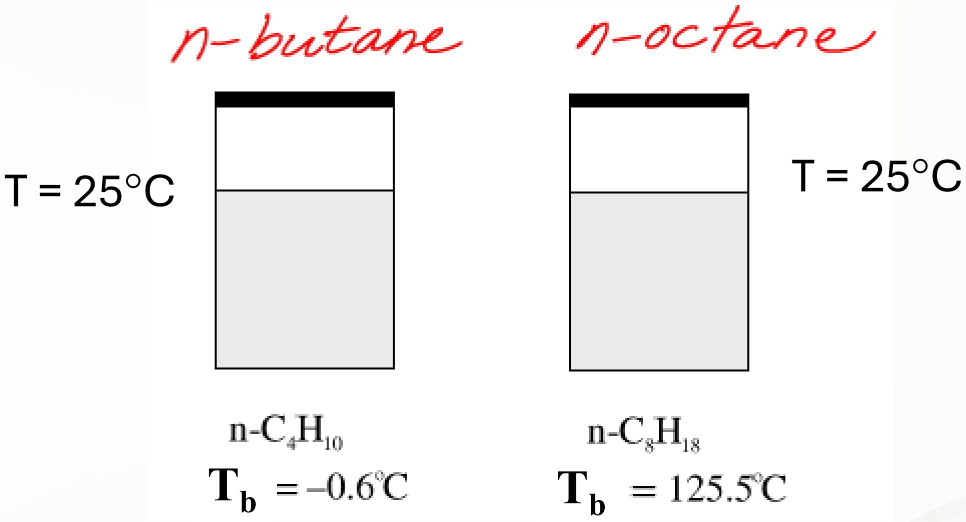
$$\boxed{x_A\, p_A^*(T_b) + x_B\, p_B^*(T_b) = P}$$

- p_i =partial pressure of component $i$in the vapor
- x_i =mole fraction of component $i$in the liquid
- $p_i^*(T)$ =vapor pressure of pure component i
- T_b = bubble-point (boiling) temperature of the mixture

Important

Exercise on Volatility

Consider two beakers, once containing n-butane, the other n-octane, at room temperature (T= °25C)



What would happen if the lids (covers) were removed?

The butane would *boil immediately*

The octane would *evaporate slowly*

Additional Quantities that describe the composition of a gas containing a single condensable vapor.

These definitions are related to partial pressure and vapor pressures

In the definitions to be given, the term «saturation» refers to any gas-vapor combination, while «humidity» refers specifically to an air-water system.

Suppose a gas at temperature T and pressure P contains a vapor whose partial pressure is p_i and whose vapor pressure is $p_i^*(T)$.

Relative Saturation (Relative Humidity):

$$s_r(h_r) = \frac{p_i}{p_i^*(T)} \times 100\%$$

Example: Relative humidity of 40% the partial pressure of water vapor equals 4/10 of the vapor pressure of water at the system temperature.

Molal Saturation (Molal Humidity):

$$s_m(h_m) = \frac{p_i}{P - p_i} = \frac{moles\ of\ vapor}{moles\ of\ vapor - free\ gas\ (or\ dry\ gas)}$$

Absolute Saturation (Absolute Humidity):

$$s_a(h_a) = \frac{p_i \times M_i}{(P - p_i) \times M_{dry}} = \frac{mass\ of\ vapor}{mass\ of\ vapor - free\ (dry) gas}$$

M_i: molecular weight of the vapor

M_{dry}: average molecular weight of the dry gas

Percentage Saturation (Percentage Humidity):

$$s_p(h_p) = \frac{s_m}{s_m^*} \times 100\% = \frac{p_i/(P - p_i)}{p_i^*/(P - p_i^*)} \times 100\%$$

Exercises on Humidity (Problem 6.13, 3rd ed)

The latest weather report includes the following statement: “***The temperature is 78°F, barometric pressure is 29.9 inches mercury, and the relative humidity is 87%.***”
From this information, estimate:

1. The **mole fraction of water** in the air
2. The **dew point (°F)**
3. The **molal humidity** of the air
4. The **absolute humidity** of the air
5. The **percentage humidity** of the air

Solution (Problem 6.13 - 3rd ed.)

$\boldsymbol{T = 78°\mathrm{F}} \qquad \boldsymbol{P_{bar} = 29.9\ in\ Hg} \qquad \boldsymbol{h_r = 87\%}$

1. Estimate the **mole fraction of water** in the air

$T = 78°\mathrm{F} = 25.56°\mathrm{C} \qquad P_{bar} = 29.9\ in\ Hg = 759.5\ mm\ Hg \qquad h_r = 87\%$

The humid air is a gas containing single condensable vapor which is water vapor.
Use the relation of relative humidity

$$h_r = \frac{p_w}{p_w^*(T)} \rightarrow p_w = h_r \times p_w^*(T) \rightarrow y_w P = h_r \times p_w^*(25.56°\mathrm{C})$$

Table B.3

$p_w^*(25.56°\mathrm{C}) = 24.56\ mmHg$

See next slide

$$y_w \times 759.5\ mmHg = 0.87 \times 24.56\ mmHg$$

$$\boxed{\boldsymbol{y_w = 0.0281}}$$

$p_w^*(25.56°C)$

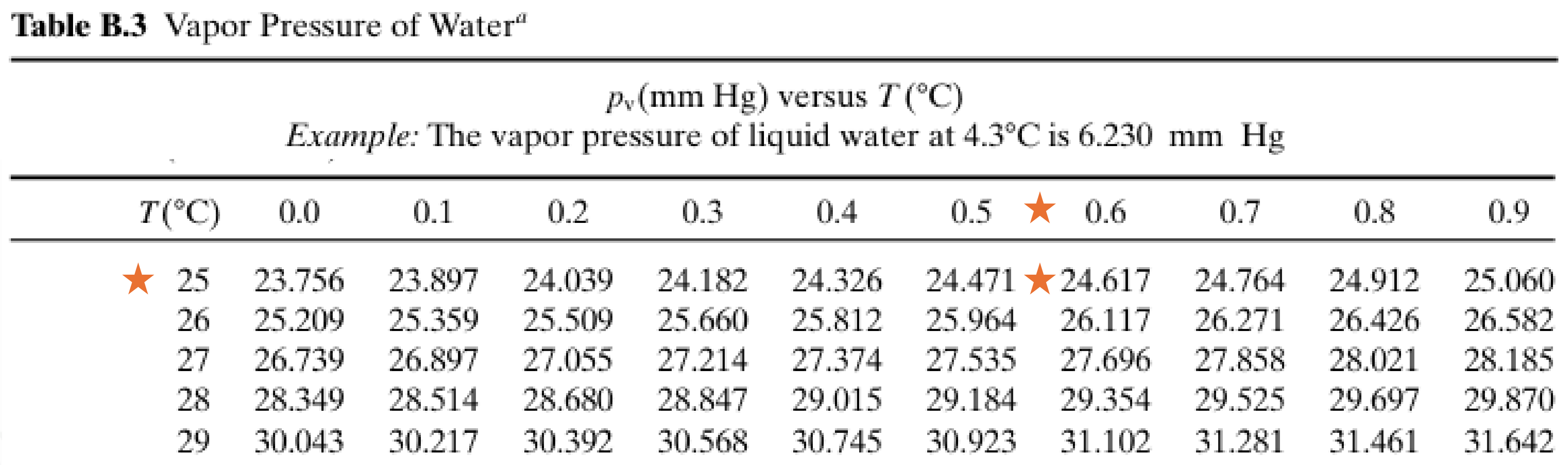


Table B.3 Vapor Pressure of Water[a]

p_v(mm Hg) versus T(°C)

Example: The vapor pressure of liquid water at 4.3°C is 6.230 mm Hg

T(°C)	0.0	0.1	0.2	0.3	0.4	0.5	★ 0.6	0.7	0.8	0.9
★ 25	23.756	23.897	24.039	24.182	24.326	24.471	★ 24.617	24.764	24.912	25.060
26	25.209	25.359	25.509	25.660	25.812	25.964	26.117	26.271	26.426	26.582
27	26.739	26.897	27.055	27.214	27.374	27.535	27.696	27.858	28.021	28.185
28	28.349	28.514	28.680	28.847	29.015	29.184	29.354	29.525	29.697	29.870
29	30.043	30.217	30.392	30.568	30.745	30.923	31.102	31.281	31.461	31.642

By interpolation,

$$\frac{25.6-25.5}{25.56-25.5}=\frac{24.617-24.471}{p^*_{25.56C}-24.471}$$

Important
Example on interpolation

$$\boxed{p_w^*(25.56°C) = 24.56\ mmHg}$$

Solution (Problem 6.13 - 3rd ed.) cont'd

$T = 78°\text{F} = 25.56°\text{C}$ $P_{bar} = 29.9 \text{ in Hg} = 759.5 \text{ mm Hg}$ $h_r = 87\%$

2. Calculate the **dew point (°F)**

Dew point (T_{dp}) is the saturation (or equilibrium) value. At this point $p_w^*(T_{dp}) = p_w$
In other words; $h_r = 1 \text{ or } 100\%$

Important
Mathematical definition of the Dew Point

$$p_w^*(T_{dp}) = p_w = y_w P = 0.0281 \times 759.5\, mmHg = 21.34\, mmHg$$

From Table B.3, find the Temperature at which **p* = 21.34 mmHg**.
This is done by interpolation. This corresponds to **T= 23.21°C**

$$\boxed{T_{dp} = 23.21°\text{C}}$$

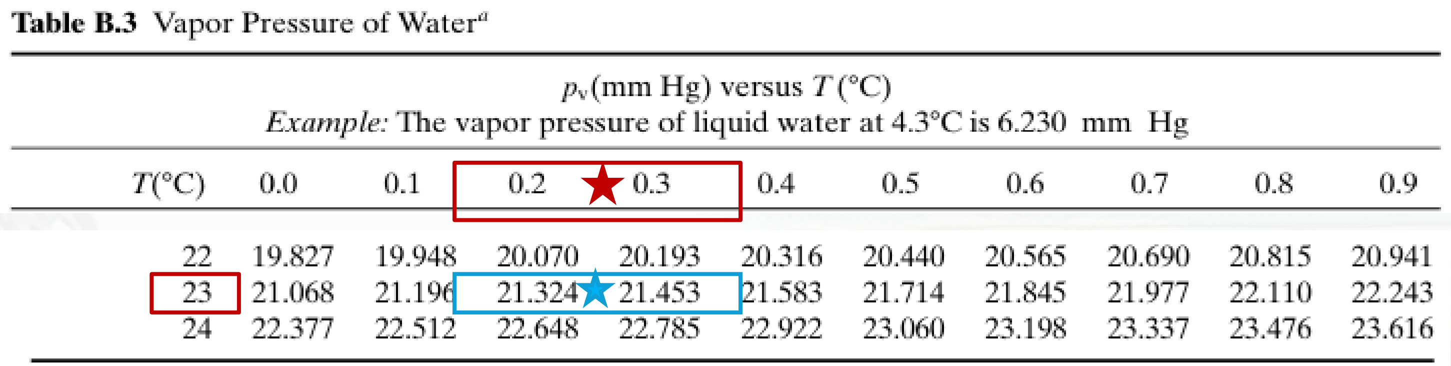


Table B.3 Vapor Pressure of Water[a]

p_v(mm Hg) versus T(°C)
Example: The vapor pressure of liquid water at 4.3°C is 6.230 mm Hg

T(°C)	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
22	19.827	19.948	20.070	20.193	20.316	20.440	20.565	20.690	20.815	20.941
23	21.068	21.196	21.324	21.453	21.583	21.714	21.845	21.977	22.110	22.243
24	22.377	22.512	22.648	22.785	22.922	23.060	23.198	23.337	23.476	23.616

Solution (Problem 6.13 - 3rd ed.) cont'd

$\boldsymbol{T = 78°\text{F} = 25.56°\text{C}}$ $\boldsymbol{P_{bar} = 29.9\ in\ Hg = 759.5\ mm\ Hg}$ $\boldsymbol{h_r = 87\%}$

3. Calculate the **molal humidity** of the air

Refer to part 2 to see calculation of $p_w = 21.34\ \text{mmHg}$

Molal Humidity:

$$\boldsymbol{h_m} = \frac{p_i}{P - p_i} = \frac{p_w}{P - p_w} = \frac{21.34}{759.5 - 21.34}$$

$$\boxed{\boldsymbol{h_m = 0.0289}\ \textbf{mole } \mathbf{H_2O}\textbf{/mol dry air}}$$

4. Calculate the **absolute humidity** of the air

$$\boldsymbol{h_a} = \frac{p_i \times M_i}{(P - p_i) \times M_{dry}} = h_m \frac{M_w}{M_{dry\ air}} = 0.0289 \times \frac{18}{29}$$

$$\boxed{\boldsymbol{h_a = 0.0179}\ \ \textbf{g } \mathbf{H_2O}\textbf{/g dry air}}$$

Solution (Problem 6.13 - 3rd ed.) cont'd

$\boldsymbol{T = 78°\text{F} = 25.56°\text{C}}$ $\boldsymbol{P_{bar} = 29.9\ in\ Hg = 759.5\ mm\ Hg}$ $\boldsymbol{h_r = 87\%}$

5. Calculate the **percentage humidity** of the air

We obtained these values from previous parts:

$h_m = 0.0289$; $p_w = 21.4$ mmHg; $p_w^* = 24.56\ mmHg$

Percentage Humidity: $$h_p = \frac{h_m}{h_m^*} \times 100\% = \frac{p_i/(P - p_i)}{p_i^*/(P - p_i^*)} \times 100\%$$

$$\boldsymbol{h_P} = \frac{h_m}{h_m^*} = \frac{h_m}{p_w^*/(P - p_w^*)} = \frac{0.0289}{24.56/(759.5 - 24.56)} \times 100\%$$

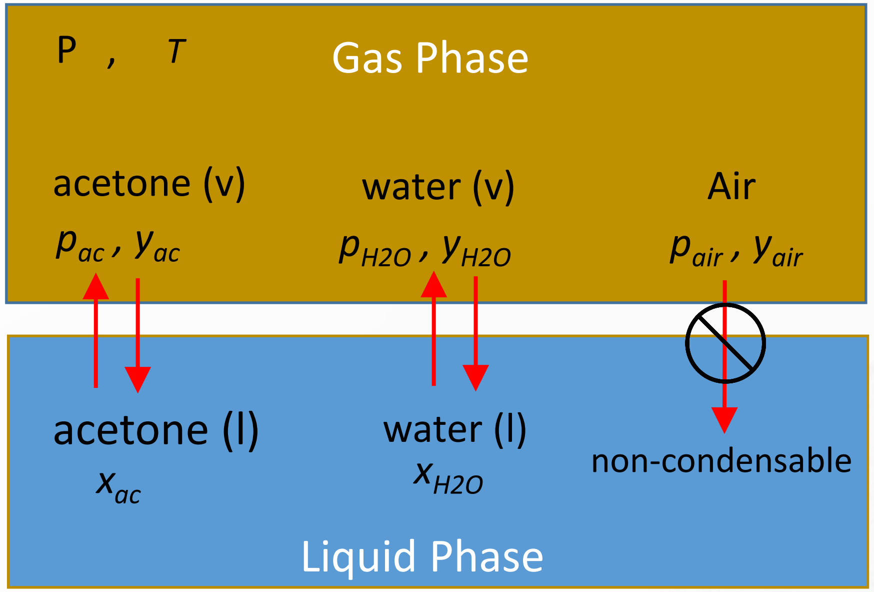
$$\boxed{\boldsymbol{h_P = 86.4\%}}$$

6.4 Multicomponent Gas-Liquid Systems

6.4 Gas-Liquid systems: Multi-component Gas-Liquid Systems

Refer to book to for details and examples of this section

At equilibrium



P , *T* Gas Phase

acetone (v) p_{ac} , y_{ac}

water (v) p_{H2O} , y_{H2O}

Air p_{air} , y_{air}

acetone (l) x_{ac}

water (l) x_{H2O}

non-condensable

Liquid Phase

VLE Data

is about distribution of component (i) between V and L phases

Relation between

$\boldsymbol{y_i}$ *and* $\boldsymbol{x_i}$

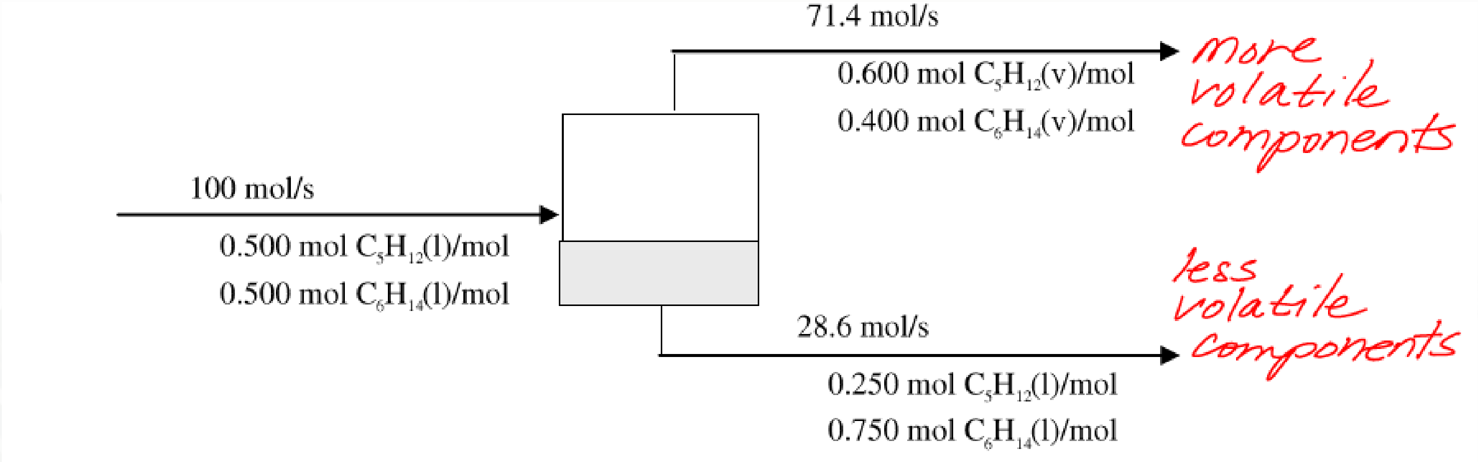
Raoult's Law

Multi-condensable liquids

$$\Rightarrow \quad y_A P = x_A \boldsymbol{P^*}_{\boldsymbol{A}}$$

Common examples of separation processes where Vapor and Liquid Phases co-exist

Vaporization/Condensation: Partially vaporize a liquid mixture of volatile species or partially condense a vapor mixture. The vapor product will be richer in the more volatile species, the liquid product richer in the less volatile species.



71.4 mol/s

0.600 mol $C_5H_{12}(v)$/mol

0.400 mol $C_6H_{14}(v)$/mol

more volatile components

100 mol/s

0.500 mol $C_5H_{12}(l)$/mol

0.500 mol $C_6H_{14}(l)$/mol

less volatile components

28.6 mol/s

0.250 mol $C_5H_{12}(l)$/mol

0.750 mol $C_6H_{14}(l)$/mol

Distillation: Do a series of vaporizations and condensations to improve the separation of components you can get in a single stage operation. The plate is the most widely used type distillation column. The number of trays in the column is dependent on the desired purity and difficulty of separation.

(Copyright Vendome Copper& Brass Works, Inc., Louisville, KY)

Common examples of separation processes where Vapor and Liquid Phases co-exist


(Tri-Mer Corporation, Owosso, MI)

Absorption or (environmental) scrubbing: Bubble a non-condensable gas through a liquid solvent or spray a liquid solvent mist into a stream of gas, generally at low T and high P, getting some or essentially all of the gas into solution. The higher the solubility of the gas at equilibrium, the more concentrated the product solution can be.


(Ducon Technologies, Inc., Farmingdale, NY)

Desorption or stripping: Bring a dissolved species out of solution into the gas phase at high T and/or low P (desorption), possibly by bubbling an insoluble gas through the solution (stripping). Note that absorption and stripping operations may be linked to transfer a species from one gas mixture to another one.

6.4 a. Vapor-Liquid Equilibrium Data

Refer to book to for details and examples of this section

Two-phase vapor-liquid mixtures at equilibrium

Refer to book to for details and examples of this section

6.4 b. Raoult's Law and Henry's Law

Provides relationships between the partial pressure of A in the gas phase (p_A) and the mole fraction of A in the liquid phase (x_A).

Raoult's law

$$\boxed{p_A \equiv y_A P = x_A \cdot p_A^*(T)}$$

where $p_A^*(T)$ is the vapor pressure of pure liquid A at temperature T, y_A is the mole fraction in the gas phase, and x_A is the mole fraction in the liquid phase.

Validity:

Raoult's law is accurate in the following cases:

Mixtures of structurally similar liquids (straight chain alcohols, aromatic hydrocarbons…)

- Pentane, hexane, heptane
- Methanol, ethanol, propanol
- Benzene, toluene, xylene

A component of a liquid mixture for which $x_A \approx 1$ (the liquid is almost pure)
Apply with care to dissimilar liquids, never to immiscible liquids (e.g., hydrocarbons and water).

Henry's law

$$\boxed{p_A \equiv y_A\, P = x_A \cdot H_A(T)}$$

where $H_A(T)$ is the **Henry's law constant** for A in a specific solvent

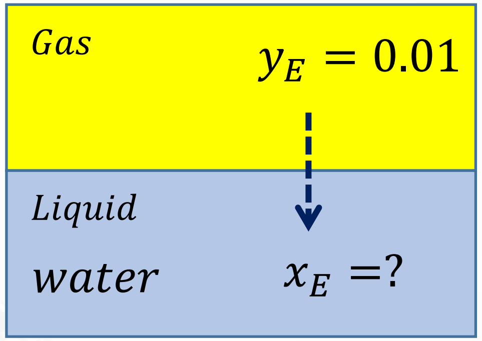
VALIDITY

- Henry's law is used primarily for a component whose mole fraction approaches zero (dilute solutions). Examples:
  - *Dilute gas dissolved in a liquid*
  - *Non-dissociating, non-ionizing, non-reactive component of a liquid mixture for which $x_A \cong 0$.*
  - Solute in a very dilute solution or absorbed gas with a low solubility.
- Lookup H values in **Perry's Chemical Engineers' Handbook.**

Example 6.4-2 Raoult’s Law and Henry’s Law

Use either Raoult’s law or Henry’s law to solve the following problems

1. A gas containing 1.00 mole% ethane is in contact with water at 25.0 °C and 20.0 atm. Estimate the mole fraction of dissolved ethane.



Gas $y_E = 0.01$

Liquid

water $x_E = ?$

$T = 25°C$
$P = 20\ atm$

Hydrocarbons (ethane: C_2H_6) are relatively ***insoluble*** in water, so that the solution of ethane is probably extremely dilute

$\Rightarrow$ **Apply Henry’s Law**

$$p_E = y_E\, P = x_E \cdot H_E(T)$$

$$0.01\ (20\ atm) = x_E \cdot \boldsymbol{H_E(25°C)}$$

Henry’s Law constant for ethane in water at 25 °C: 2.67×10^4 atm/mole fraction

$$0.01 \times 20\ atm = x_E \times 2.67 \times 10^4$$

$$x_E = \frac{y_E P}{H_E} \frac{(0.01)(20\ atm)}{2.67 \times 10^4\ \boldsymbol{atm/mole\ fraction}}$$

$$\boxed{x_E = 7.49 \times 10^{-6} \frac{mol\ ethane}{mol}}$$

Example 6.4-2 Raoult’s Law and Henry’s Law

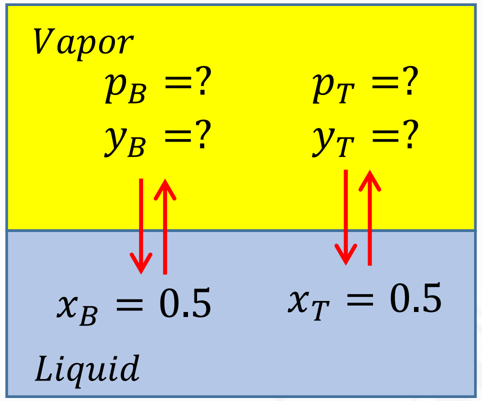
Equimolar means same number of moles

Use either Raoult’s law or Henry’s law to solve the following problems

2. An equimolar liquid mixture of benzene (B) and toluene (T) is in equilibrium with its vapor at 30.0 °C. What is the system pressure and the composition of the vapor?

$T = 30°\text{C}$

$P = ??$



Benzene (B) and Toluene (T) are structurally similar compounds

⇒ **Apply Raoults’s Law**

Benzene

$$p_B = y_B\, P = x_B \cdot p_B^*(T)$$

$$p_B = 0.5 \times p_B^*(30°\text{C})$$

Toluene

$$p_T = y_T\, P = x_T \cdot p_T^*(T)$$

$$p_T = 0.5 \times p_T^*(30°\text{C})$$

Vapor pressures for benzene and toluene using Antoin equation (constants from Table B.4)

$$log_{10}p_B^* = 6.89272 - \frac{1203.531}{T + 219.888} \quad for\ T = 30°\text{C} \ \rightarrow p_B^* = 119.2\ mm\ Hg$$

$$log_{10}p_T^* = 6.95805 - \frac{1346.773}{T + 219.693} \quad for\ T = 30°\text{C} \ \rightarrow p_T^* = 36.7\ mm\ Hg$$

Constants of Antoin equation (Table B.4)

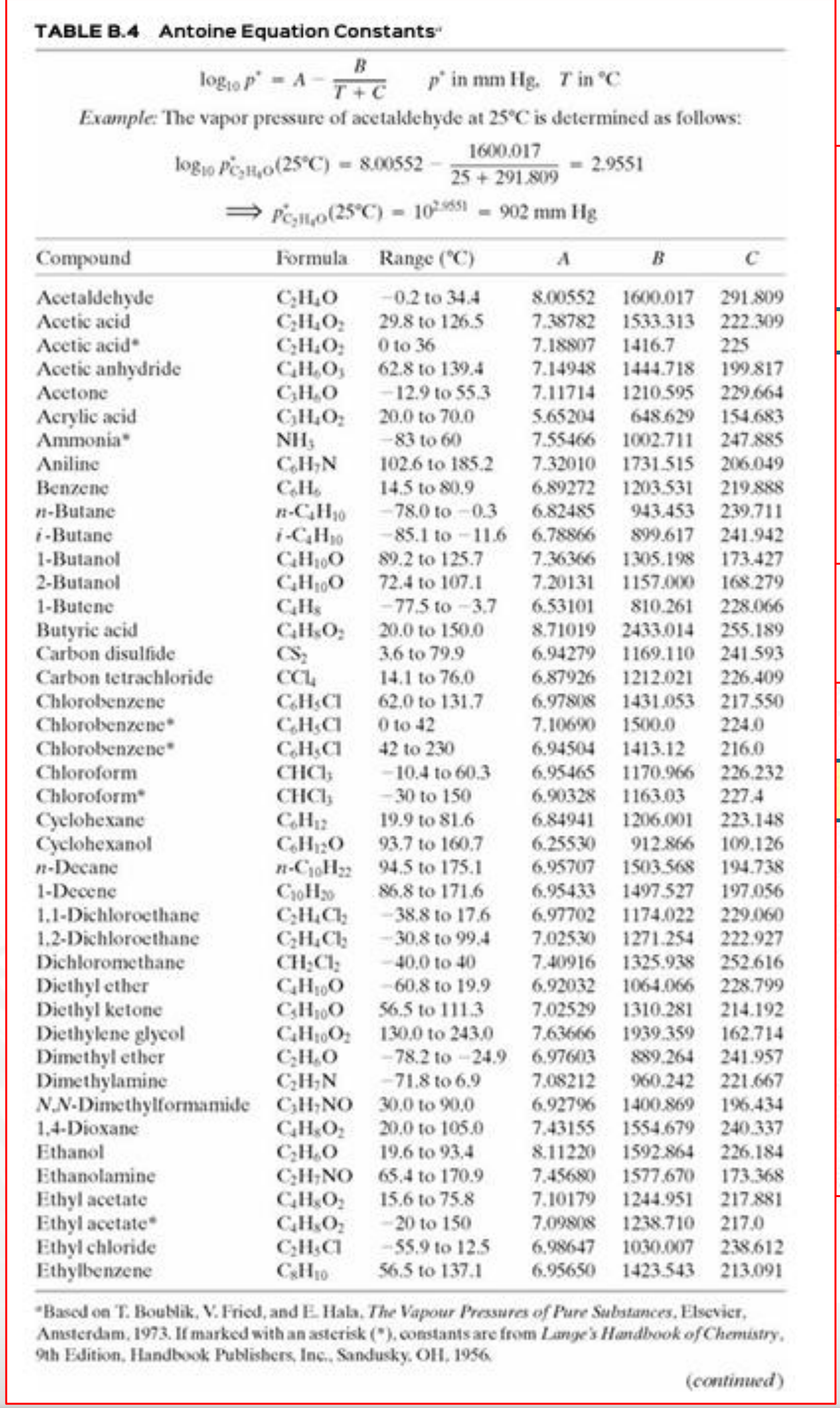


TABLE B.4 Antoine Equation Constants[a]

$$\log_{10} p^* = A - \frac{B}{T + C} \qquad p^* \text{ in mm Hg}, \quad T \text{ in } ^\circ\text{C}$$

Example: The vapor pressure of acetaldehyde at 25°C is determined as follows:

$$\log_{10} p^*_{C_2H_4O}(25^\circ C) = 8.00552 - \frac{1600.017}{25 + 291.809} = 2.9551$$

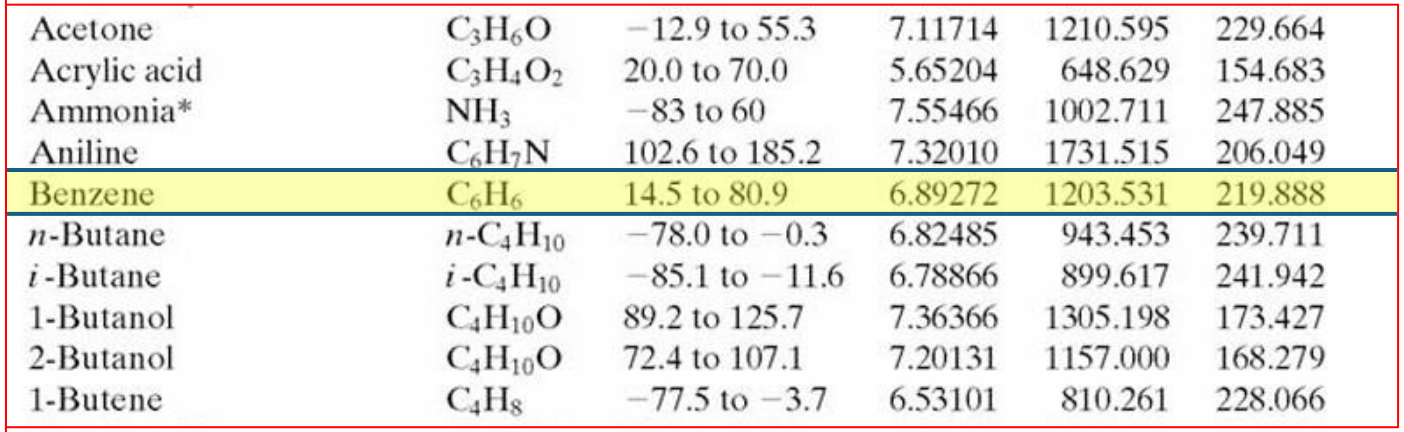
$$\Longrightarrow p^*_{C_2H_4O}(25^\circ C) = 10^{2.9551} = 902 \text{ mm Hg}$$

Compound	Formula	Range (°C)	*A*	*B*	*C*
Acetaldehyde	C_2H_4O	−0.2 to 34.4	8.00552	1600.017	291.809
Acetic acid	$C_2H_4O_2$	29.8 to 126.5	7.38782	1533.313	222.309
Acetic acid*	$C_2H_4O_2$	0 to 36	7.18807	1416.7	225
Acetic anhydride	$C_4H_6O_3$	62.8 to 139.4	7.14948	1444.718	199.817
Acetone	C_3H_6O	−12.9 to 55.3	7.11714	1210.595	229.664
Acrylic acid	$C_3H_4O_2$	20.0 to 70.0	5.65204	648.629	154.683
Ammonia*	NH_3	−83 to 60	7.55466	1002.711	247.885
Aniline	C_6H_7N	102.6 to 185.2	7.32010	1731.515	206.049
Benzene	C_6H_6	14.5 to 80.9	6.89272	1203.531	219.888
n-Butane	$n\text{-}C_4H_{10}$	−78.0 to −0.3	6.82485	943.453	239.711
i-Butane	$i\text{-}C_4H_{10}$	−85.1 to −11.6	6.78866	899.617	241.942
1-Butanol	$C_4H_{10}O$	89.2 to 125.7	7.36366	1305.198	173.427
2-Butanol	$C_4H_{10}O$	72.4 to 107.1	7.20131	1157.000	168.279
1-Butene	C_4H_8	−77.5 to −3.7	6.53101	810.261	228.066
Butyric acid	$C_4H_8O_2$	20.0 to 150.0	8.71019	2433.014	255.189
Carbon disulfide	CS_2	3.6 to 79.9	6.94279	1169.110	241.593
Carbon tetrachloride	CCl_4	14.1 to 76.0	6.87926	1212.021	226.409
Chlorobenzene	C_6H_5Cl	62.0 to 131.7	6.97808	1431.053	217.550
Chlorobenzene*	C_6H_5Cl	0 to 42	7.10690	1500.0	224.0
Chlorobenzene*	C_6H_5Cl	42 to 230	6.94504	1413.12	216.0
Chloroform	$CHCl_3$	−10.4 to 60.3	6.95465	1170.966	226.232
Chloroform*	$CHCl_3$	−30 to 150	6.90328	1163.03	227.4
Cyclohexane	C_6H_{12}	19.9 to 81.6	6.84941	1206.001	223.148
Cyclohexanol	$C_6H_{12}O$	93.7 to 160.7	6.25530	912.866	109.126
n-Decane	$n\text{-}C_{10}H_{22}$	94.5 to 175.1	6.95707	1503.568	194.738
1-Decene	$C_{10}H_{20}$	86.8 to 171.6	6.95433	1497.527	197.056
1,1-Dichloroethane	$C_2H_4Cl_2$	−38.8 to 17.6	6.97702	1174.022	229.060
1,2-Dichloroethane	$C_2H_4Cl_2$	−30.8 to 99.4	7.02530	1271.254	222.927
Dichloromethane	CH_2Cl_2	−40.0 to 40	7.40916	1325.938	252.616
Diethyl ether	$C_4H_{10}O$	−60.8 to 19.9	6.92032	1064.066	228.799
Diethyl ketone	$C_5H_{10}O$	56.5 to 111.3	7.02529	1310.281	214.192
Diethylene glycol	$C_4H_{10}O_2$	130.0 to 243.0	7.63666	1939.359	162.714
Dimethyl ether	C_2H_6O	−78.2 to −24.9	6.97603	889.264	241.957
Dimethylamine	C_2H_7N	−71.8 to 6.9	7.08212	960.242	221.667
N,N-Dimethylformamide	C_3H_7NO	30.0 to 90.0	6.92796	1400.869	196.434
1,4-Dioxane	$C_4H_8O_2$	20.0 to 105.0	7.43155	1554.679	240.337
Ethanol	C_2H_6O	19.6 to 93.4	8.11220	1592.864	226.184
Ethanolamine	C_2H_7NO	65.4 to 170.9	7.45680	1577.670	173.368
Ethyl acetate	$C_4H_8O_2$	15.6 to 75.8	7.10179	1244.951	217.881
Ethyl acetate*	$C_4H_8O_2$	−20 to 150	7.09808	1238.710	217.0
Ethyl chloride	C_2H_5Cl	−55.9 to 12.5	6.98647	1030.007	238.612
Ethylbenzene	C_8H_{10}	56.5 to 137.1	6.95650	1423.543	213.091

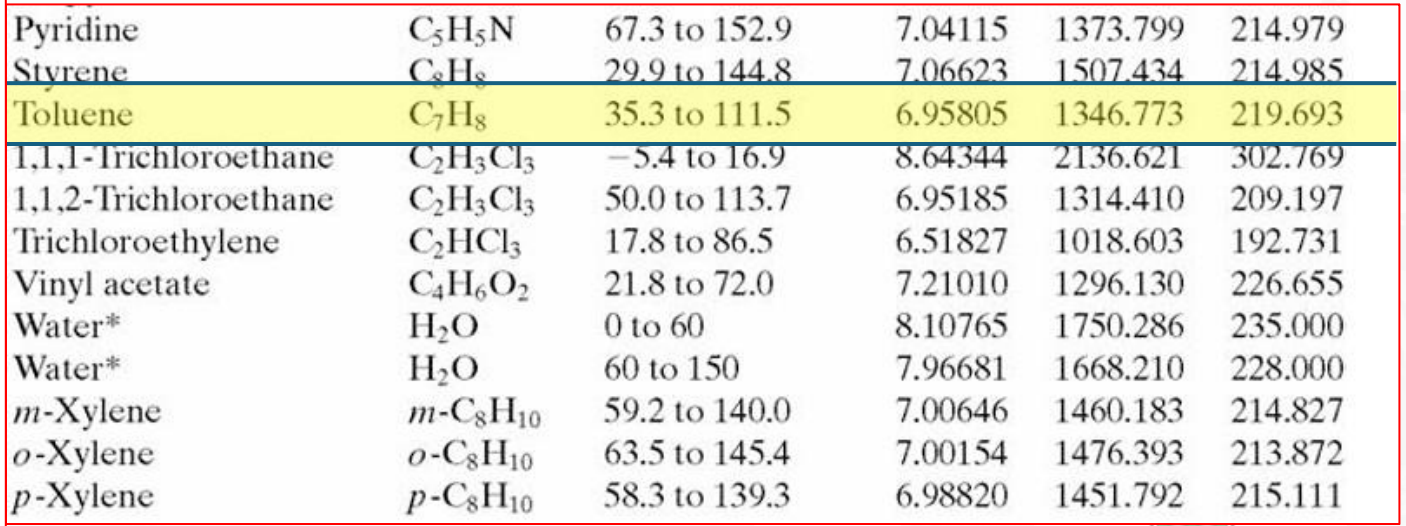
---

[a] Based on T. Boublik, V. Fried, and E. Hala, *The Vapour Pressures of Pure Substances*, Elsevier, Amsterdam, 1973. If marked with an asterisk (*), constants are from *Lange's Handbook of Chemistry*, 9th Edition, Handbook Publishers, Inc., Sandusky, OH, 1956.

(continued)



Acetone	C_3H_6O	−12.9 to 55.3	7.11714	1210.595	229.664
Acrylic acid	$C_3H_4O_2$	20.0 to 70.0	5.65204	648.629	154.683
Ammonia*	NH_3	−83 to 60	7.55466	1002.711	247.885
Aniline	C_6H_7N	102.6 to 185.2	7.32010	1731.515	206.049
Benzene	C_6H_6	14.5 to 80.9	6.89272	1203.531	219.888
n-Butane	$n\text{-}C_4H_{10}$	−78.0 to −0.3	6.82485	943.453	239.711
i-Butane	$i\text{-}C_4H_{10}$	−85.1 to −11.6	6.78866	899.617	241.942
1-Butanol	$C_4H_{10}O$	89.2 to 125.7	7.36366	1305.198	173.427
2-Butanol	$C_4H_{10}O$	72.4 to 107.1	7.20131	1157.000	168.279
1-Butene	C_4H_8	−77.5 to −3.7	6.53101	810.261	228.066



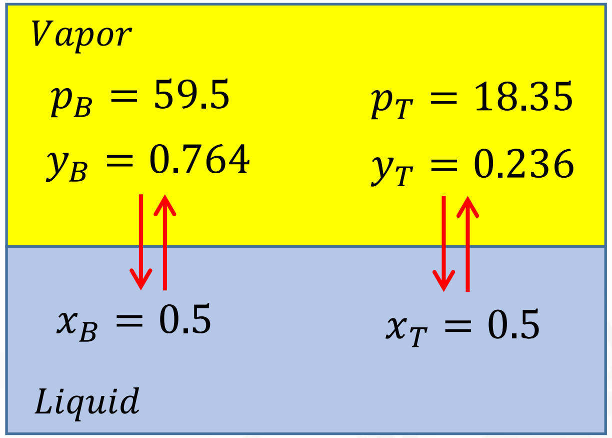
Pyridine	C_5H_5N	67.3 to 152.9	7.04115	1373.799	214.979
Styrene	C_8H_8	29.9 to 144.8	7.06623	1507.434	214.985
Toluene	C_7H_8	35.3 to 111.5	6.95805	1346.773	219.693
1,1,1-Trichloroethane	$C_2H_3Cl_3$	−5.4 to 16.9	8.64344	2136.621	302.769
1,1,2-Trichloroethane	$C_2H_3Cl_3$	50.0 to 113.7	6.95185	1314.410	209.197
Trichloroethylene	C_2HCl_3	17.8 to 86.5	6.51827	1018.603	192.731
Vinyl acetate	$C_4H_6O_2$	21.8 to 72.0	7.21010	1296.130	226.655
Water*	H_2O	0 to 60	8.10765	1750.286	235.000
Water*	H_2O	60 to 150	7.96681	1668.210	228.000
m-Xylene	$m\text{-}C_8H_{10}$	59.2 to 140.0	7.00646	1460.183	214.827
o-Xylene	$o\text{-}C_8H_{10}$	63.5 to 145.4	7.00154	1476.393	213.872
p-Xylene	$p\text{-}C_8H_{10}$	58.3 to 139.3	6.98820	1451.792	215.111

Example 6.4-2 continued

Use either Raoult's law or Henry's law to solve the following problems

2. An equimolar liquid mixture of benzene (B) and toluene (T) is in equilibrium with its vapor at 30.0 °C. What is the system pressure and the composition of the vapor?

$$T = 30°C$$
$$P = 78\ mmHg$$



$Vapor$

$p_B = 59.5$ $\quad p_T = 18.35$

$y_B = 0.764$ $\quad y_T = 0.236$

$x_B = 0.5$ $\quad x_T = 0.5$

$Liquid$

$$p_B = x_B \times p_B^* = (0.500)(119.2\ mm\ Hg) = 59.6\ mm\ Hg$$

$$p_T = x_T \times p_T^* = (0.500)(36.7\ mm\ Hg) = 18.4\ mm\ Hg$$

$$P = p_B + p_T = \boxed{78\ mm\ Hg}$$

$$y_B = p_B/P = \boxed{0.764\ \ mole\ benzene/mole}$$

$$y_T = p_T/P = \boxed{0.236\ \ mole\ toluene/mole}$$

$$\boldsymbol{K_i\ value = \frac{y_i}{x_i}}$$

K_i is the distribution coefficient for component (i) between the two phases

B likes to be in the vapor phase more than the liquid phase $\leftarrow$ $K_B = \frac{y_B}{x_B} = \frac{0.764}{0.50} = 1.5$

T likes to be in the vapor phase more than the liquid phase $\leftarrow$ $K_T = \frac{y_T}{x_T} = \frac{0.236}{0.50} = 0.5$

6.4c. Vapor-Liquid Equilibrium Calculations for Ideal Solutions

Important Theory

Behavior of single species liquid, in a close vessel, upon heating at constant pressure:

- The temperature increases until the boiling point of the liquid is reached, and thereafter
- The liquid vaporizes at a constant temperature.
- Once the vaporization is complete, further addition of heat raises the temperature of the vapor.

Behavior of several component-liquid (mixture) , in a close vessel, upon heating at constant pressure:

- The liquid temperature rises until a temperature is reached at which the first bubble of vapor forms.
- The vapor generated generally will have a composition different from that of the liquid.
- As vaporization proceeds, the composition of the remaining liquid continuously changes, and hence so does its vaporization temperature

Refer to book to for details and examples of this section

A similar phenomenon occurs if a mixture of vapors is subjected to a condensation process at constant pressure:

- At some temperature the first droplet of liquid forms, and thereafter
- The composition of the vapor and the condensation temperature both change.

To design or control an evaporation or condensation process, separation processes such as ***distillation, absorption,*** **and** ***stripping*** requires information on the conditions at which phase transitions occur and on the compositions of the resulting phases.

The **bubble-point temperature** of a **liquid at the given pressure** is the temperature at which the first vapor bubble forms when the liquid is heated slowly at constant pressure.

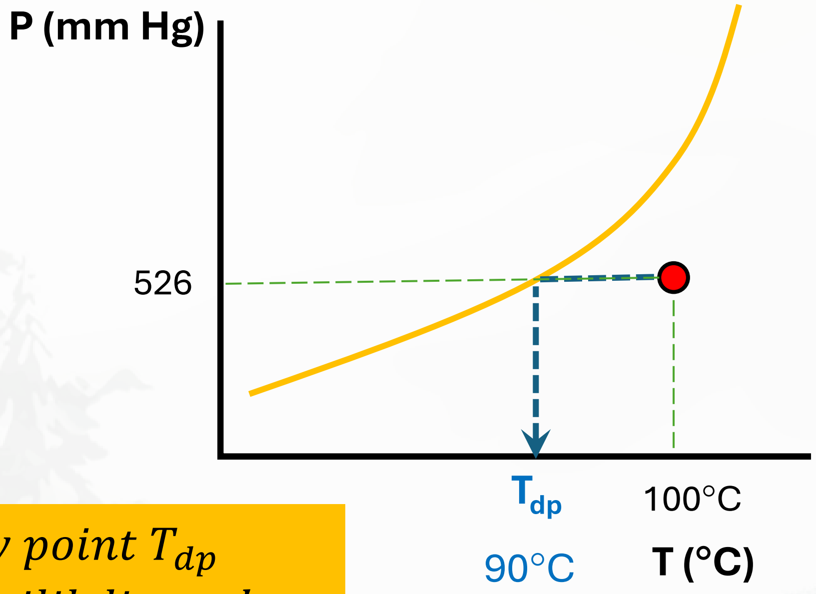
The **dew-point temperature of** a **vapor at the given pressure** is the temperature at which the first liquid droplet forms when a gas (vapor) is cooled slowly at constant pressure.

Important

Exercise (based on Example 6.3-2) –

Calculation of Dew Point (T_{dew})

A stream of air at 100°C and 5260 mm Hg contains 10.0% water by volume. Calculate the dew point and degrees of superheat of the air.



Dew point T_{dp} is on equilib line where

$$p_w = p_w^*(T_{dp})$$

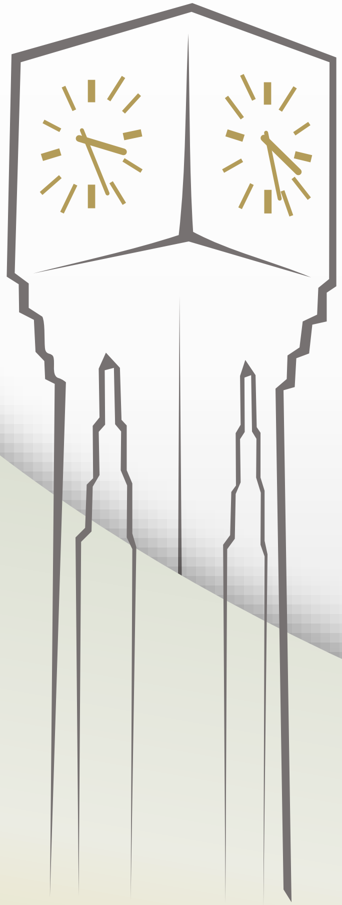
$$p_w = y_w P = 0.1(5260) = 526 \; mm\, Hg$$

At dew point (T_{dp})

$$p_w = p_w^*(T_{dp}) \Rightarrow 526 = p_w^*(T_{dp})$$

From Table B.3 $\quad T_{dp} = 90°C$

Degrees of superheat $= 100°C - 90°C = 10°C$ of superheat



Problem Solving

Exercises on Section 6.2-6.4

Exercise 1 – Vapor pressure

1) Using the Antoine equation, calculate the normal boiling point of diethyl ether.

2) Using the Antoine equation, calculate the vapor pressure of the carbon tetrachloride (CCl_4) at 50°C.

Solution

(1) Normal boiling point is the temperature at which $p^*_{DE}(T_b) = P_{sys} = 1\ atm = 760\ mmHg$

p^*_{DE} vs. T_b can be obtained from Antoine Equation:

$$\log_{10} p^* = A - \frac{B}{T + C}$$

where the units of P and. T are mmHg and °C respectively

Values of A, B, and C can be found from Table A.4. Constants for Diethyl Ether are:

A = 6.92032 B = 1064.070 C = 228.8

$$p^*_{DE}(T_b) = P_{sys} = 760\ mmHg$$

Use Antione equation to find T_b corresponding $p^*_{DE} = 760\ \ mmHg$

$\boxed{T_b = 34.6\ °C}$

Exercise 1 – cont’d

2) Using the Antoine equation, calculate the vapor pressure of the carbon tetrachloride (CCl_4) at 50^0C.

Solution

For carbon tetrachloride:
A = 6.8941
B = 1219.580
C = 227.17

The vapor pressure corresponding to a temperature of 50 °C is **312 mmHg**.

Exercise 2 – Bubble Point Calculation

Suppose that a liquid mixture of 4.0 mol % n-hexane in n-octane is vaporized. What is the composition of the first vapor formed if the total pressure is 1 atm? [**ans. y_{hexane}=0.164; y_{octane}=0.836**].

Solution

The mixture can be treated as an ideal mixture because the components are quite similar.
We can use the Antoine equation to relate p* to T. We have to look up the coefficients of the Antoine equation to obtain the vapor pressures of the two components:

$$\ln(p^*) = A - \frac{B}{C+T}$$

p* is in mm Hg and T is in K

Important
In this exercise and given coefficients, the Antoin equation is based on natural logarithm values (ln) instead of log.

	A	B	C
n-hexane (C_6)	15.8366	2697.55	-48.784
N-octane (C_8)	15.9798	3127.60	-63.633

Basis: 1 kg mol of liquid

We need to solve the following equation to get the bubble point temperature using a nonlinear equation solver:

Note: Definition of Boiling point

A liquid mixture boils when the sum of the partial pressures of all volatile components equals the external pressure: $p_A + p_B = \mathrm{P}$

For an **ideal liquid mixture** (Raoult's law applies):

$$P = x_A\, p_A^*(T_b) + x_B\, p_B^*(T_b)$$

$$760 = exp\left(15.8366 - \frac{2697.55}{-48.784 + T}\right)(0.040) + exp\left(15.9798 - \frac{3127.60}{-63.633 + T}\right)(0.960)$$

Find T by trial and error or by using a mathematical software

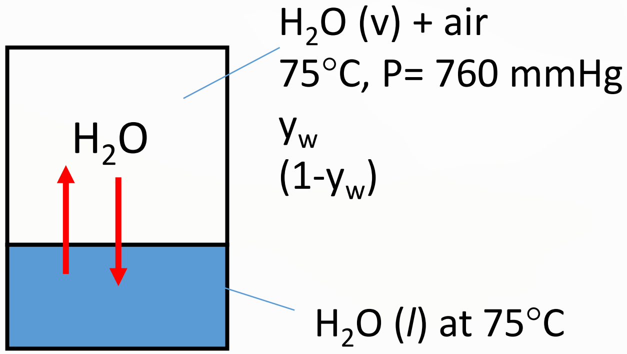
The solution via polymath is $\boldsymbol{T = 393.6\ K}$. At this temperature, the vapor pressure of hexane is 3114 mm Hg, and the vapor pressure of octane is 661 mm Hg. The respective mole fractions in the vapor phase:

$$y_{c6} = \frac{p_{C6}^*}{P_{total}} x_{C6} = \frac{3114}{760}(0.04) = 0.164$$

$$y_{c8} = 1 - 0.164 = 0.836$$

Exercise 3 **(Example 6.3-1)** Composition of a Saturated Gas-Vapor System

Air and liquid water are contained at equilibrium in a closed chamber at 75°C and 760 mm Hg. Calculate the molar composition of the gas phase.



The gas and liquid are in equilibrium, the air must be saturated with water vapor.

Raoult's Law $p_w = y_w P = p_w^*(T) \Rightarrow y_w = \dfrac{p_w^*(75°C)}{P}$

From Table B.3 in Appendix B, $p_{H_2O}^*(75°C) = 289\ mm\ Hg$

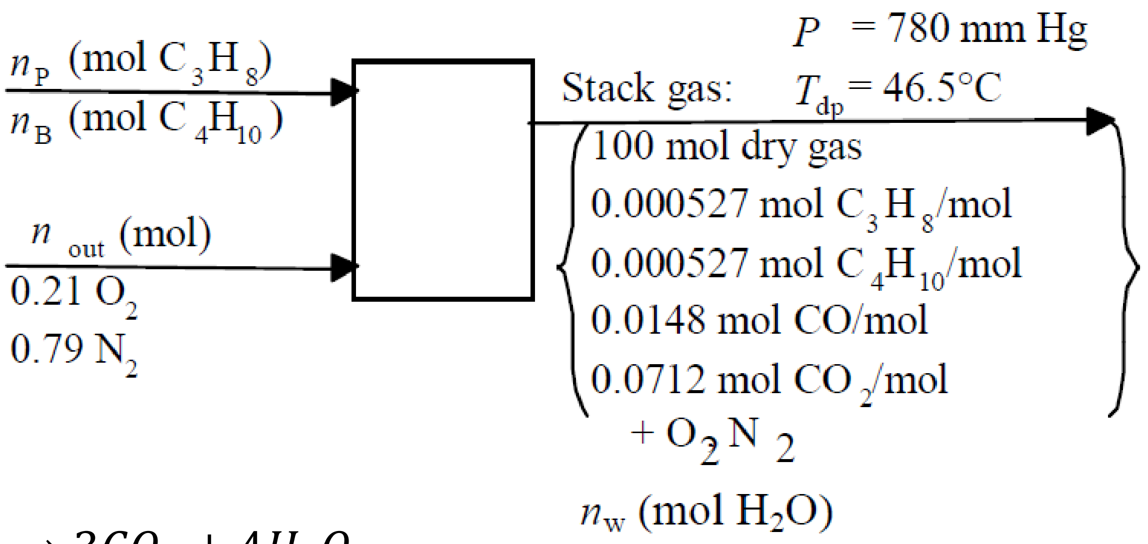
$$y_{H_2O} = \frac{289\ mm\ Hg}{760\ mm\ Hg} = 0.380\ \frac{mol\ H_2O}{mol}$$

$$y_{dry\ air} = 1 - y_{H_2O} = 0.620\ \frac{mol\ dry\ air}{mol}$$

Exercise 4

A mixture of propane and butane is burned with air. A dry-basis analysis of the flue (stack) gas gives the following volume (mole) percentages: 0.00527% C_3H_8, 0.0527% C_4H_{10}, 1.48% CO, and 7.12% CO_2. The stack gas is at an absolute pressure of 780 mmHg, and its dew point is 46.5°C. Calculate the molar (mole-fraction) composition of the fuel.

Basis: 100 mol dry stack gas



n_P (mol C_3H_8)

n_B (mol C_4H_{10})

n_{out} (mol)

0.21 O_2

0.79 N_2

Stack gas: $P = 780$ mm Hg

$T_{dp} = 46.5$°C

100 mol dry gas

0.000527 mol C_3H_8/mol

0.000527 mol C_4H_{10}/mol

0.0148 mol CO/mol

0.0712 mol CO_2/mol

+ O_2 N_2

n_w (mol H_2O)

$$C_3H_8 + 5O_2 \rightarrow 3CO_2 + 4H_2O$$

$$C_4H_{10} + \frac{13}{2}O_2 \rightarrow 4CO_2 + 5H_2O$$

$$\textbf{Dew point} = 46.5\ ℃ \rightarrow y_w P = p_w^*(46.5\ ℃) \rightarrow y_w = \frac{77.6\ mm\ Hg}{780\ mm\ Hg} = 0.0995\ \frac{mol\ H_2O}{mol}$$

$$y_w = \frac{n_w}{100 + n_w} = 0.0995\ \rightarrow n_w = 11.0\ mol\ H_2O$$

$$\textbf{C balance}:\ 3n_P + 4n_B = (100)[(0.000527)(3) + (0.000527)(4) + 0.0148 + 0.0712]$$

$$\rightarrow\ 3n_P + 4n_B = 8.969 \qquad (1)$$

$$\textbf{H balance}:\ 8n_P + 10n_B = (100)[(0.000527)(8) + (0.000527)(10)] + (11.0)(2)$$

$$\rightarrow 8n_P + 10n_B = 23.149 \qquad (2)$$

$$n_P = 1.454\ mol\ C_3H_8 \qquad \rightarrow \qquad 56\%\ C_3H_7$$

$$n_B = 1.152\ mol\ C_4H_{10} \qquad\qquad 44\%\ C_4H_{10}$$

Exercise 5 - Unsolved Gibbs Phase Rule Without Reaction

Calculate the number of degrees of freedom (how many additional intensive variables must be specified to fix the system) from the phase rule for the following materials at equilibrium:

a) Pure liquid benzene [ans. 2]
b) A mixture of ice and water only [ans. 1]
c) A mixture of liquid benzene, benzene vapor and helium gas [ans. 2]
d) A mixture of salt and water designed to achieve a specific vapor pressure [ans. 2]

What variables might be specified in each case?

Exercise 6 - Unsolved Gibbs Phase Rule With Reaction

Calculate the number of degrees of freedom (from the phase rule for the following systems at equilibrium:

a) You have a gas composed of CO, CO_2, H_2, H_2O and CH_4 [ans. 4]
b) Sulfur can be removed from high temperature gas streams by a bed of zinc oxide pellets. The results of the decomposition of zinc oxide with carbon show the presence of the following compounds: ZnO, C, CO, Zn [ans. 1]

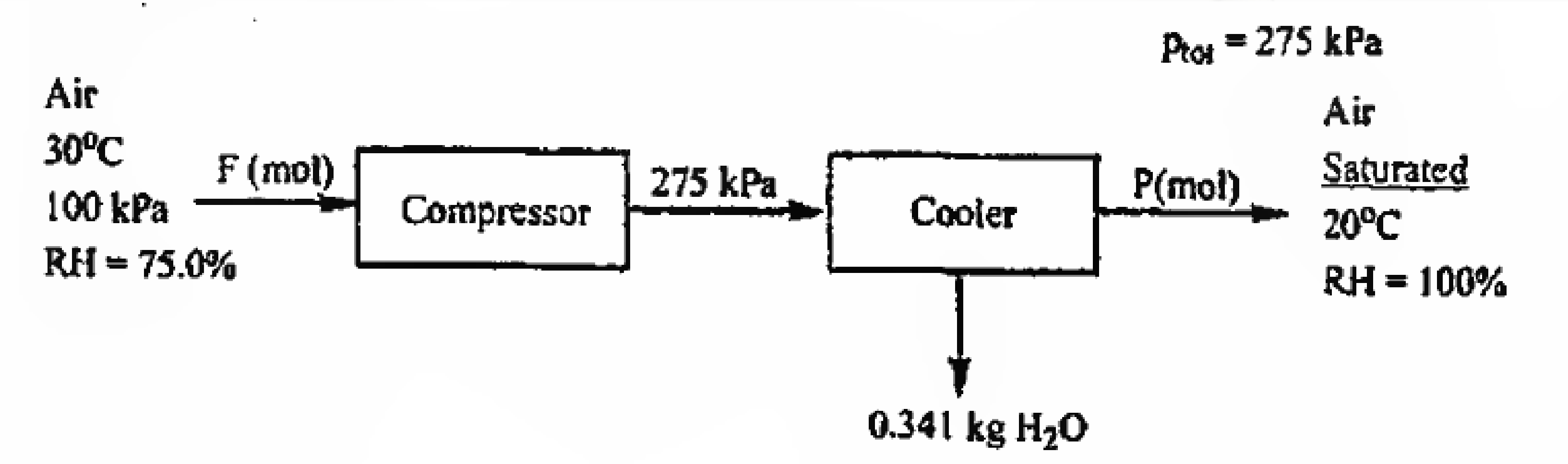
Note

Some of the following exercises are obtained from an external reference, so the terminology may be different. You should achieve the same final answers based on the terminology of our textbook

Exercise 7 - Wet gas & Relative humidity

A wet air gas stream at 30°C and 100 kPa with a relative humidity of 75.0% was compressed to 275 kPa, and then cooled to 20°C.

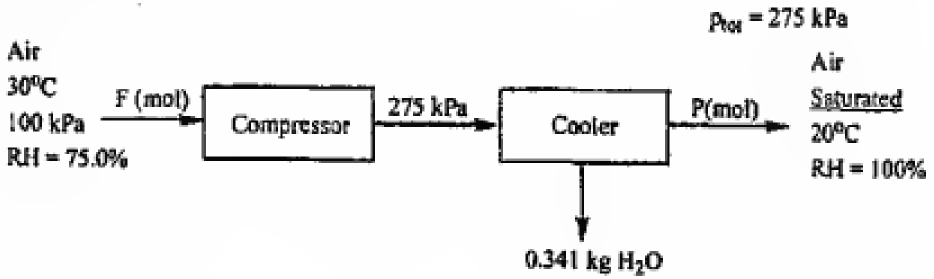
How many m^3 of the original gas was compressed if 0.341 kg of the condensate (water) was removed from the cooler unit? [ans. 20.3 m^3]



Solution

18.13

Steps 1, 2, 3, and 4:



$p^*_{H_2O}$ = 0.6153 psia
= 4.241 kPa

$p^*_{H_2O}$ = 0.3388 psia
= 2.34 kPa

p_{H_2O} = 4.241 (.75) = 3.18 kPa

System: overall

Step 5: Basis: 0.341 kg H2O (0.341/18) kg mol

Step 6 and 7: Unknowns: F, P Balances: air, H_2O

Steps 8 and 9: Balances are in kg mol

$$\left.\begin{aligned} &\text{Total: } F = P + \frac{0.341}{18} \\ &\text{Air: } F\left(\frac{100-3.18}{100}\right) = P\left(\frac{275-2.34}{275}\right) \\ &H_2O\text{: } F\left(\frac{3.18}{100}\right) = \frac{0.341}{18} + P\left(\frac{2.34}{275}\right) \end{aligned}\right\}$$

Solve any two to get

F = 0.804 kg mol

$$V = \frac{0.804 \text{ kg mol} \,|\, 8.314 \,|\, 303}{\quad\quad\quad \,|\, 100 \,|\quad} = \boxed{20.3 \text{ m}^3 \text{ at 301C and 100 kPa}}$$

Exercise 8 VLE single condensable component

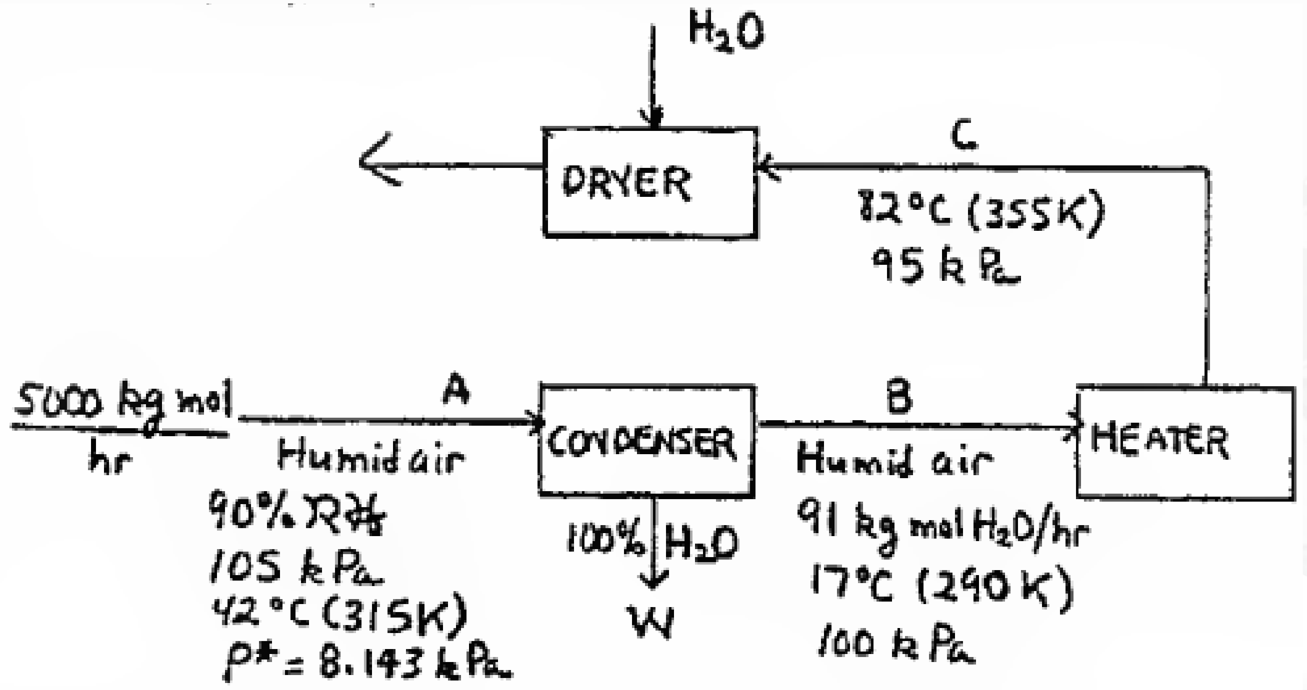
Hot air that is used to dry pharmaceuticals is recycled in a closed loop to prevent the contamination if the moist material from the atmospheric impurities. In the first conditioning step for the air, 5000 kgmol/h at 105 kPa and 42°C with 90% relative humidity are fed to a condenser to remove some of the water picked up previously in the process. The air exits the condenser at 17°C and 100 kPa containing 91 kgmol/h of water vapor. Next, the air enters the dryer, the pressure of the stream has dropped to 95 kPa and the temperature is 82°C.

a) How many moles of water per hour enters the condenser?

b) What is the flow rate of the condenser water in kg/h?

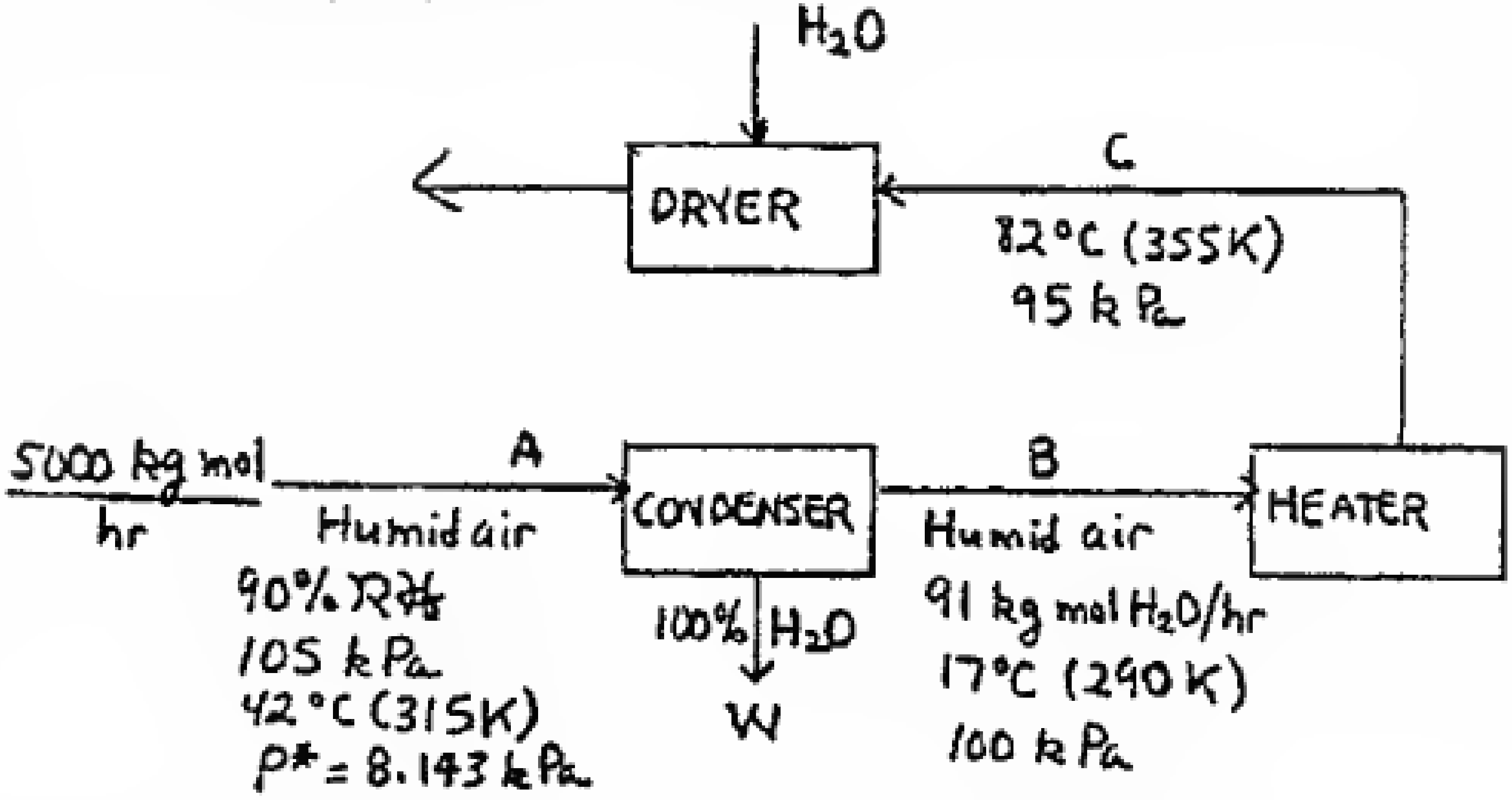
c) What is the dew point of the air in the stream exiting the condenser?

d) What is the dew point of the air in the stream entering the dryer?



Solution

18.21 Note: This problem will give different results depending on the source of the vapor pressure data (steam tables, Antoine Eq., CD, Perry, etc.)

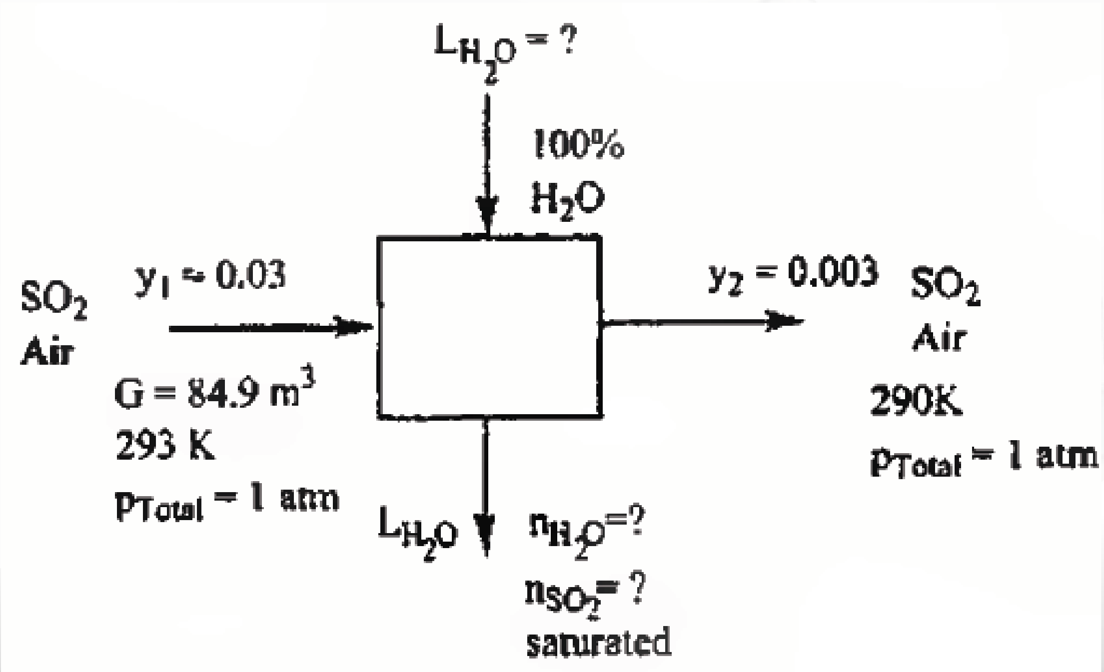


(steam tables p* = 8.214; paper steam tables p* = 8.143; CD p* = 8.181)

Exercise 9 VLE using Henry's law

You are asked to remove 90% of the sulfur dioxide (SO_2) in a gas stream of air and SO_2 that flows at the rate of 85 m^3/min and contains 3% SO_2. The SO_2 is to be removed by a stream of water. The entering water contains no SO_2. The temperature is 290 K and the pressure on the process is 1 atm.

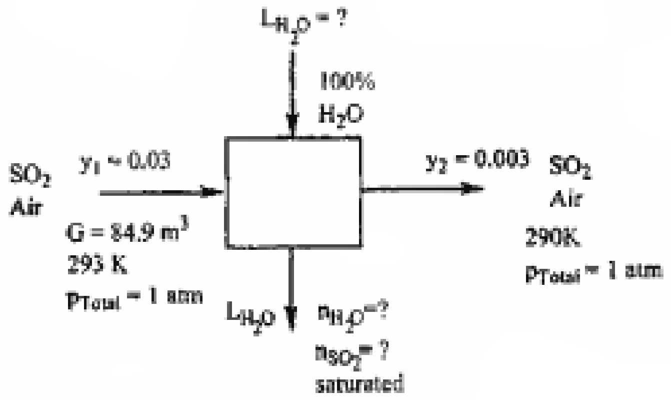
a) Find the kg of water per minute needed to remove the SO_2 assuming that the exit water is in equilibrium with the entering gas.
b) Find the ratio of the water stream to the gas stream. The Henry's law constant for SO_2 at 290 K is 43 atm/mol fraction.



Solution

19.13

Steps 2, 3, and 4:



Step 5: Basis: 1 min (85 m^3 entering gas)

Steps 6 and 7:

Unknowns: $n^L_{H_2O}$, $n^L_{SO_2}$, Air

Equations. Material balances: H_2O, SO_2, Air

$y_i > Hx_i$

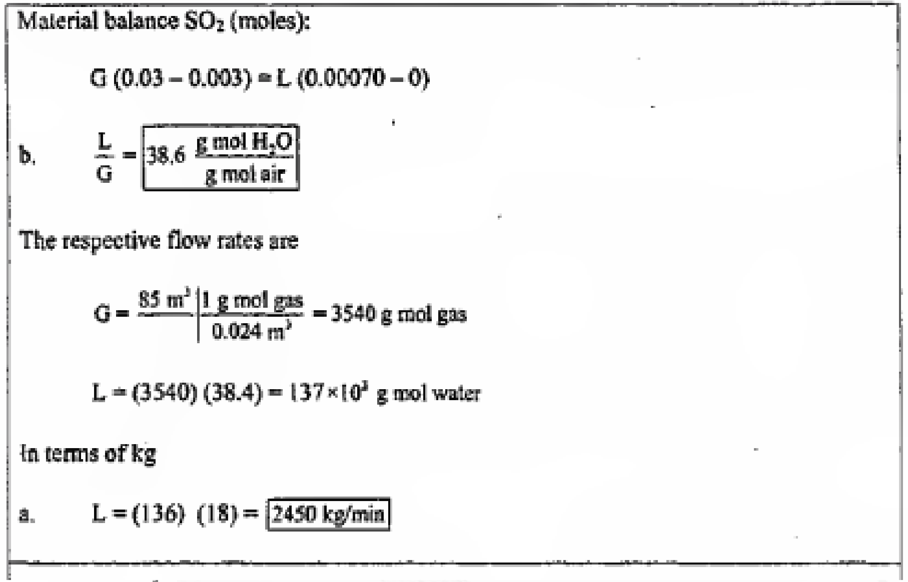
Steps 8 and 9:

The liquid and vapor are assumed to be in equilibrium at the exit, and the water is saturated with SO_2 so that

$$y_i = Hx_i$$

$$0.03 = (43)\ x_{SO_2} = \text{so that}\ \ x_{SO_2} = 0.00070 \text{ mol fraction}$$

(continued)



Material balance SO_2 (moles):

$$G\,(0.03 - 0.003) = L\,(0.00070 - 0)$$

b. $$\frac{L}{G} = \boxed{38.6\ \frac{\text{g mol H}_2\text{O}}{\text{g mol air}}}$$

The respective flow rates are

$$G = \frac{85\ m^3}{}\left|\frac{1\text{ g mol gas}}{0.024\ m^3}\right. = 3540\text{ g mol gas}$$

$$L = (3540)\,(38.4) = 137\times10^3\text{ g mol water}$$

In terms of kg

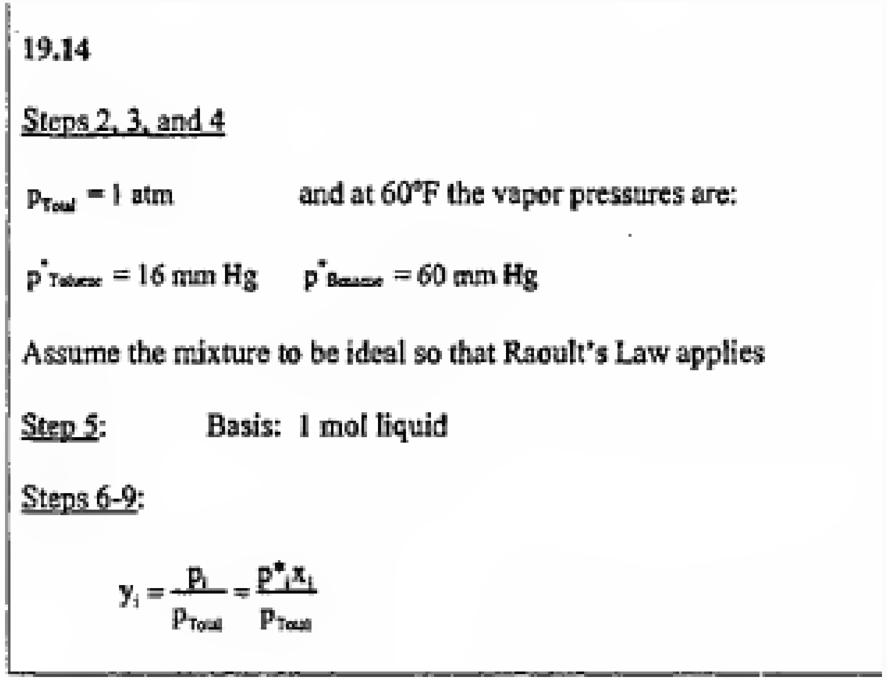
a. $$L = (136)\ (18) = \boxed{2450\text{ kg/min}}$$

Exercise 10 VLE – Raoult’s law - Flammability

A tank contains a liquid composed of 60 mol% toluene and 40 mol% benzene in equilibrium with the vapor phase and air at 1 atm and 60°F.

a) What is the concentration of hydrocarbons in the vapor phase?
b) If the lower flammability limit for toluene in air is 1.27% and benzene is 1.4%, is the vapor phase flammable?

Solution



19.14

Steps 2, 3, and 4

$p_{Total} = 1$ atm and at 60°F the vapor pressures are:

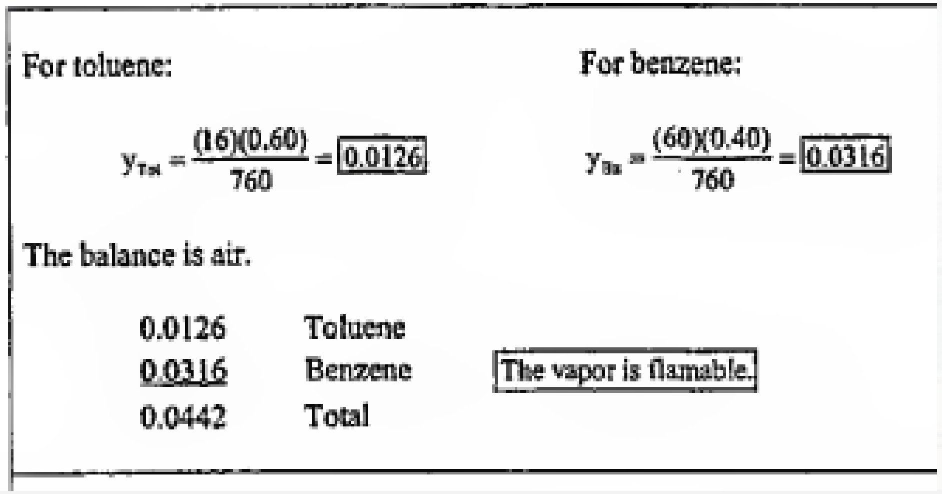
$p^*_{Toluene} = 16$ mm Hg $p^*_{Benzene} = 60$ mm Hg

Assume the mixture to be ideal so that Raoult's Law applies

Step 5: Basis: 1 mol liquid

Steps 6-9:

$$y_i = \frac{p_i}{p_{Total}} = \frac{p^*_i x_i}{p_{Total}}$$



For toluene:

$$y_{Tol} = \frac{(16)(0.60)}{760} = \boxed{0.0126}$$

For benzene:

$$y_{Bz} = \frac{(60)(0.40)}{760} = \boxed{0.0316}$$

The balance is air.

0.0126 Toluene
0.0316 Benzene
0.0442 Total

The vapor is flamable.

Example 11 VLE – Raoult's law

A vapor phase is equilibrium with a liquid mixture of 20% pentane and 80% heptane at 50°F. Assume the mixture is ideal one at equilibrium.

a) What is the pressure in the vapor phase?
b) Calculate the composition of the vapor phase.

Use the Antoine equation or the physical property package on the CD to get the vapor pressure of pentane (P) and heptane (H). Assume ideal liquid and vapor.

Basis: Data given in problem statement

$$\ln p^*_P(\text{mm}) = 15.8333 - \frac{2477.07}{T - 39.94} \qquad p^*_P = 283.6 \text{ mm Hg } (5.48 \text{ psia})$$

$$\ln p^*_H(\text{mm}) = 15.8737 - \frac{2911.32}{T - 56.51} \qquad p^*_H = 20.6 \text{ mm Hg } (0.40 \text{ psia})$$

Convert mass fractions to mole fractions:

Basis: 100 g liquid

	g	MW	g mol	mol. fr.
P	20	72.15	0.28	0.23
H	80	86.17	0.93	0.77
	100		1.21	1.00

Equations to use, i = P and H

$$\Sigma y_i = 1 \qquad y_i = \frac{p^*_i x_i}{p_{Total}}$$

a. $$\frac{p^*_P}{p_{Total}} x_P + \frac{p^*_H}{p_{Total}} x_H = 1 \qquad p_{Total} = (283.6)(0.23) + 20.6(0.77) = \boxed{80.95 \text{ mm Hg}}$$

3.19 in Hg
10.8 kPa
1.57 psia

b. $$y_i = \frac{p^*_i x_i}{p_{Total}}$$

$$y_P = \frac{16}{4.07}(0.23) = \boxed{0.90}$$

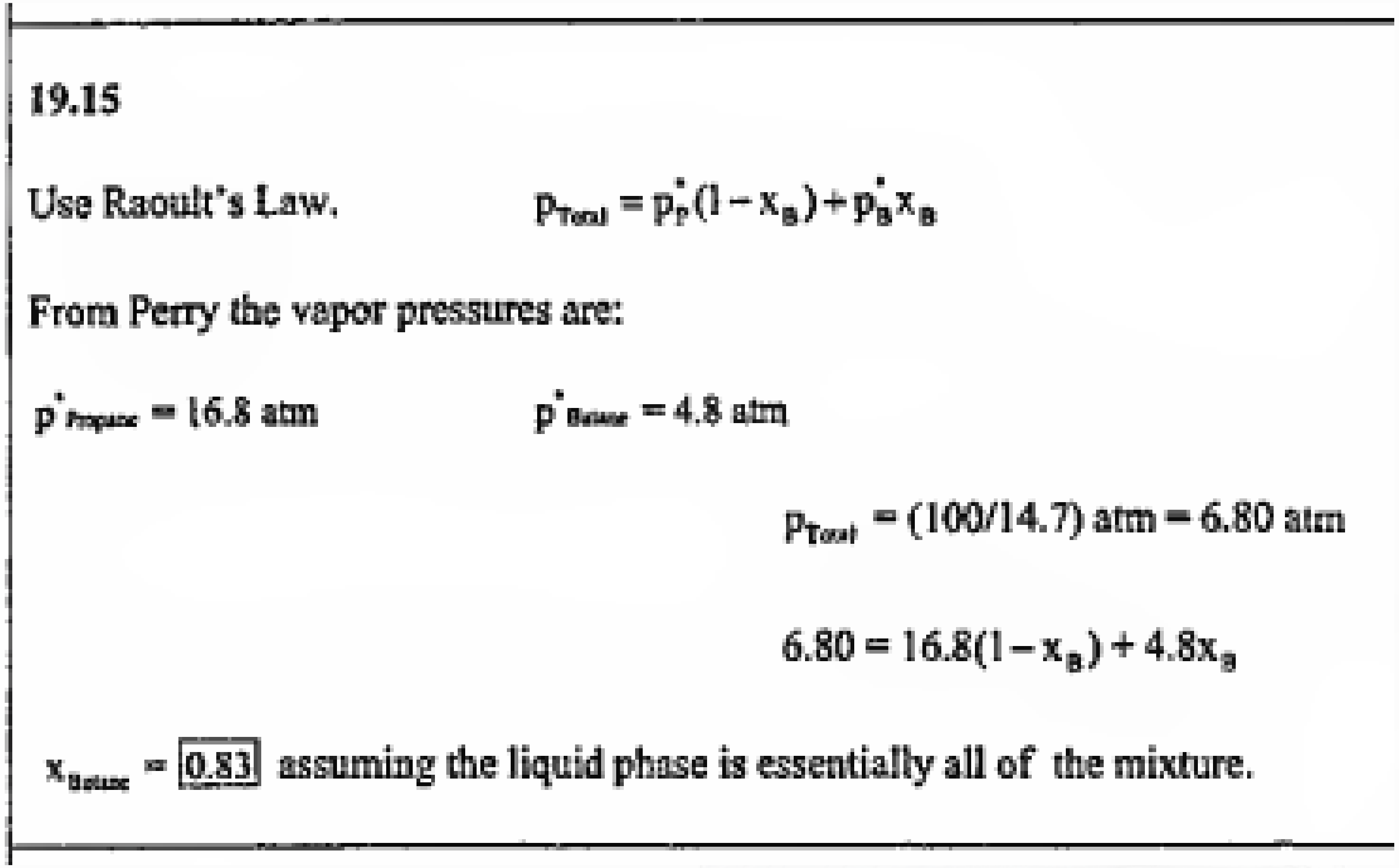
$$y_H = \frac{0.5}{4.07}(0.77) = \boxed{0.10}$$

$$\overline{1.00}$$

Example 12 VLE – Raoult’s law

Fuel tanks for barbeques contain propane and n-butane. At 120°F, if an essentially full tank of liquid that contains liquid and vapor in equilibrium and exhibits a pressure of 100 psia, what is the overall (vapor plus liquid) mole fraction of butane in the tank?

Solution



19.15

Use Raoult's Law. $p_{Total} = p_P^*(1-x_B)+p_B^*x_B$

From Perry the vapor pressures are:

$p^*_{Propane} = 16.8$ atm $p^*_{Butane} = 4.8$ atm

$$p_{Total} = (100/14.7)\text{ atm} = 6.80\text{ atm}$$

$$6.80 = 16.8(1-x_B)+4.8x_B$$

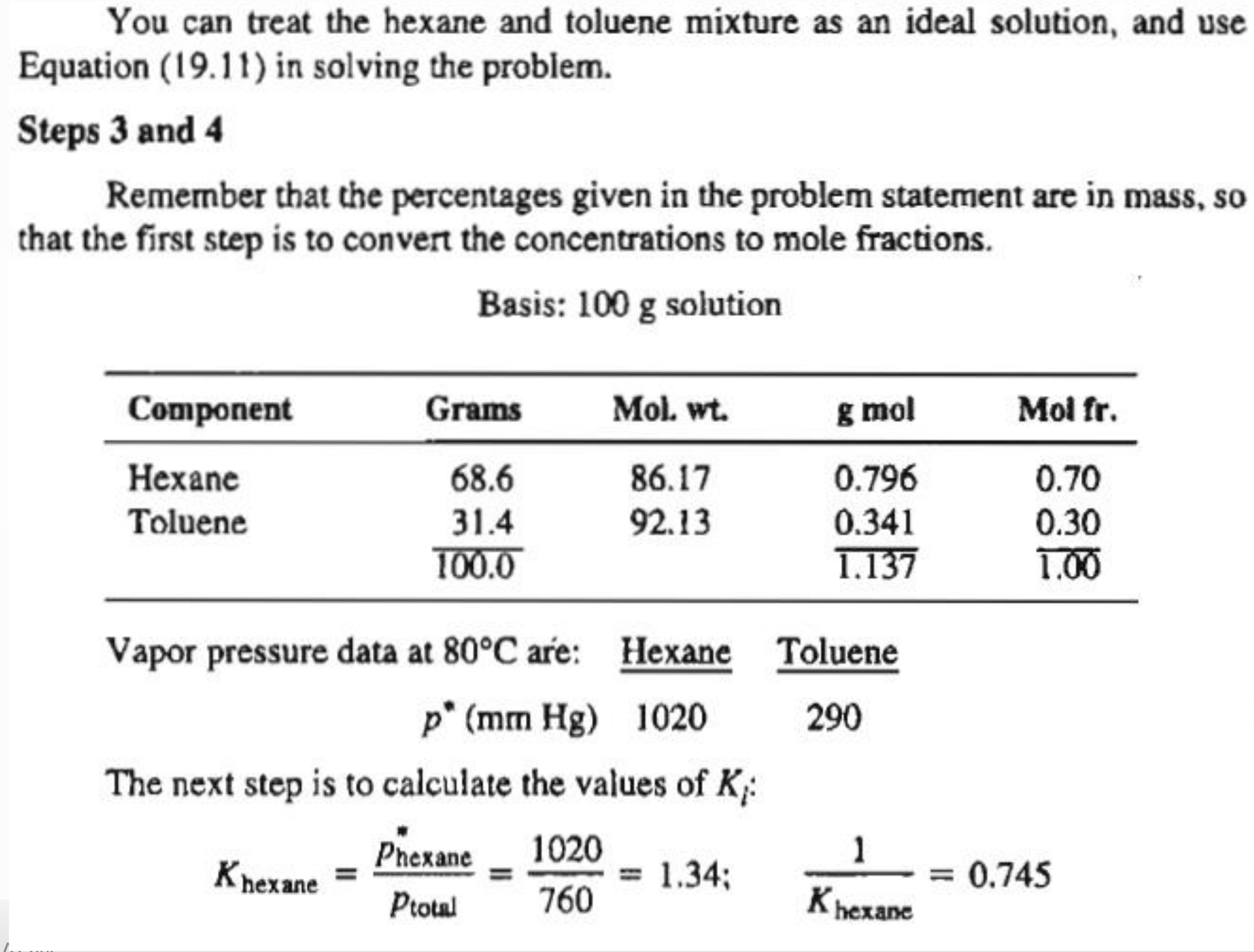
$x_{Butane} = \boxed{0.83}$ assuming the liquid phase is essentially all of the mixture.

Example 13 VLE K value

Calculate the fraction of liquid that will remain at equilibrium when a mixture of 68.6% hexane and 31.4 % of toluene is vaporized at 80°C and 1 atm.[ans. L/F=0.745]

K value = y_i / x_i

Solution



You can treat the hexane and toluene mixture as an ideal solution, and use Equation (19.11) in solving the problem.

Steps 3 and 4

Remember that the percentages given in the problem statement are in mass, so that the first step is to convert the concentrations to mole fractions.

Basis: 100 g solution

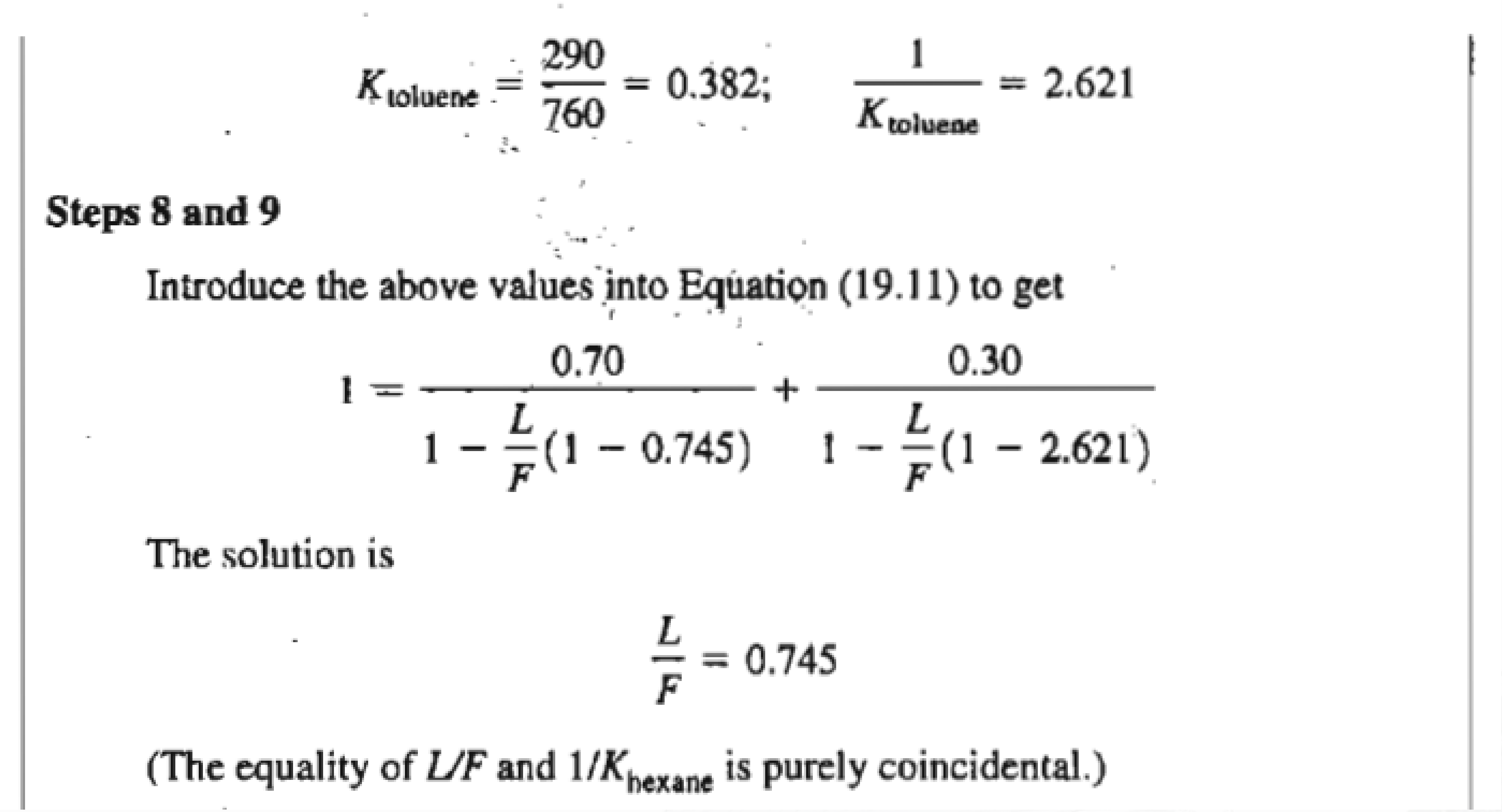
Component	Grams	Mol. wt.	g mol	Mol fr.
Hexane	68.6	86.17	0.796	0.70
Toluene	31.4	92.13	0.341	0.30
	100.0		1.137	1.00

Vapor pressure data at 80°C are:	Hexane	Toluene
p^* (mm Hg)	1020	290

The next step is to calculate the values of K_i:

$$K_{\text{hexane}} = \frac{p^*_{\text{hexane}}}{p_{\text{total}}} = \frac{1020}{760} = 1.34; \qquad \frac{1}{K_{\text{hexane}}} = 0.745$$

Solution



$$K_{\text{toluene}} = \frac{290}{760} = 0.382; \qquad \frac{1}{K_{\text{toluene}}} = 2.621$$

Steps 8 and 9

Introduce the above values into Equation (19.11) to get

$$1 = \frac{0.70}{1 - \frac{L}{F}(1 - 0.745)} + \frac{0.30}{1 - \frac{L}{F}(1 - 2.621)}$$

The solution is

$$\frac{L}{F} = 0.745$$

(The equality of L/F and $1/K_{\text{hexane}}$ is purely coincidental.)

END.