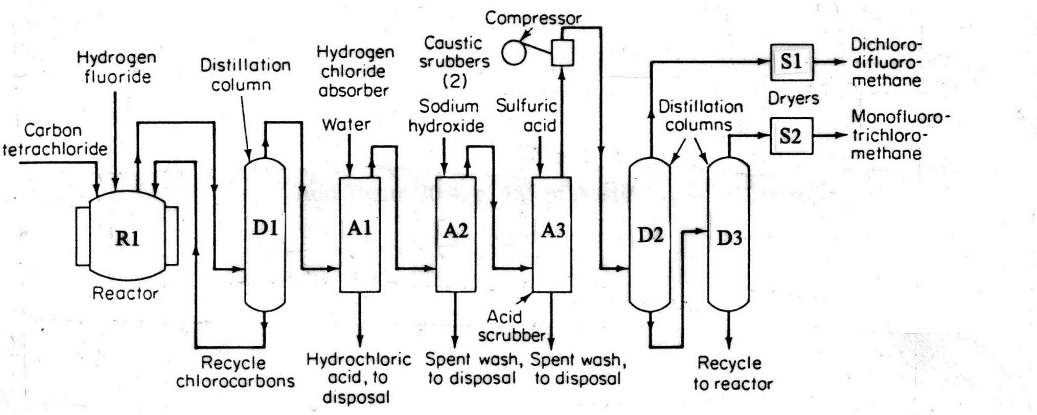
Exercise 1.1 (i)

Known: Fluorocarbons can be produced from the reaction of carbon tetrachloride and hydrogen fluoride followed by a number of separation steps.

Given: Flow diagram and a brief description of a fluorocarbons production process in "Chemical Process Industries" , 4th edition, by Shreve and Brink and also in "Shreve's Chemical Process Industries", 5th edition, by G. T. Austin, pages 353-355 (Fig. 20.4).

Find: Draw a process flow diagram and describe the process.



Description of Process: Two main reactions occur:

$$CCl_4 + HF \rightarrow CCl_3F + HCl$$
$$CCl_3F + HF \rightarrow CCl_2F_2 + HCl$$

Excess carbon tetrachloride is reacted in R1 with HF in the presence of antimony pentoxide catalyst and a small amount of chlorine to maintain catalyst activity. The HF contains a small amount of water as an impurity. The effluent from the R1 is HCl, CCl_3F, CCl_2F_2, unreacted CCl_4, and small amounts of water and chlorine. The normal boiling points in ^oC of these components in the order of decreasing volatility are:

HCl	-84.8
Cl_2	-33.8
CCl_2F_2	-29.8
CCl_3F	23.7
CCl_4	76.7
H_2O	100

Exercise 1.1 (i) (continued)

The reactor effluent is distilled in D1 to remove the CCl_4 as bottoms, which is recycled to R1. The distillate enters absorber A1, where HCl is absorbed by water to produce a byproduct of aqueous HCl. The gas from A1 contains residual HCl, which is neutralized, and chlorine, which is absorbed, by aqueous NaOH, in A2. The effluent liquid from A2 is waste. Moisture is removed from the gas leaving A2 by absorption with H_2SO_4 in A3. The exit liquid from A3 is also waste. The gas leaving A3 is distilled in D2 to obtain CCl_2F_2 as a distillate, which is then dried in S1 by adsorption with activated alumina. Bottoms from D2 is distilled in D3 to recover a distillate of CCl_3F, which is dried with activated alumina in S2. Bottoms from D3, containing residual CCl_4, is recycled to reactor R1.

Exercise 1.2

Subject: Mixing is spontaneous, but separation is not.

Given: Thermodynamic principles.

Find: Explanation for why mixing and separation are different.

Analysis: Mixing is a natural, spontaneous process. It may take time, but concentrations of components in a single fluid phase will tend to become uniform, with an increase in entropy. By the second law of thermodynamics, a natural process tends to randomness. The separation of a mixture does not occur naturally or spontaneously. Energy is required to separate the different molecular species.

Exercise 1.3

Subject: Separation of a mixture requires a transfer of energy to it or the degradation of its energy.

Given: The first and second laws of thermodynamics.

Find: Explain why the separation of a mixture requires energy.

Analysis: As an example, consider the isothermal minimum (reversible) work of separation of an ideal binary gas mixture. Therefore, the change in enthalpy is zero. However, there is a change in entropy, determined as follows. From a chemical engineering thermodynamics textbook or Table 2.1, Eq. (4):

$$W_{\min} = \sum_{out} n(h - T_0 s) - \sum_{in} n(h - T_0 s)$$

$$= RT_0 \left\{ \sum_{out} n_k \left[\sum y_{i,k} \ln\left(y_{i,k}\right) \right] - \sum_{in} n_j \left[\sum y_{i,j} \ln\left(y_{i,j}\right) \right] \right\}$$

It can be shown that regardless of values of y between 0 and 1, that $W_{\min}$ is always positive. This minimum work is independent of the process.

Exercise 1.4

Subject : Use of an ESA or an MSA to make a separations.

Given: Differences between an ESA and an MSA.

Find: State the advantages and disadvantages of ESA and MSA.

Analysis: With an MSA, an additional separator is needed to recover the MSA. Also, some MSA will be lost, necessitating the need for MSA makeup. If the MSA is incompletely recovered, a small amount of contamination may result. The use of an MSA can make possible a separation that can not be carried out with an ESA. An ESA separation is easier to design.

Exercise 1.5(b)

Subject: Producing ethers from olefins and alcohols.

Given: Process flow diagram and for production of methyl tert-butyl ether (MTBE).

Find: List the separation operations.

Analysis: The reactor effluent contains 1-butene, isobutane, n-butane, methanol, and MTBE. The separation steps are as follows:

Separation Step	**Products**
Distillation	Distillate: all C_4s, methanol Bottoms: 99 wt% MTBE
L/L Extraction with water	Extract: methanol, water Raffinate: C_4s
Distillation	Distillate: methanol to recycle Bottoms: water for recycle

Exercise 1.6(c)

Subject: Conversion of propylene to butene-2s.

Given: Process flow diagram and for production of butene-2s.

Find: List the separation operations.

Analysis: The reactor effluent contains ethylene, propylene, propane, butene-2s, and C_5+. The separation steps are as follows:

Separation Step	**Products**
Distillation	Distillate: ethylene Sidestream: propylene, propane Bottoms: butene-2s, C_5+
Distillation	Distillate: propylene Bottoms: propane
Distillation	Distillate: butene-2s Bottoms: C_5+

Exercise 1.7

Subject: Use of osmosis for separating a chemical mixture.

Given: The definition of osmosis.
Find: Explain why osmosis can not be used for separating a mixture.

Analysis: Osmosis is the transfer of a solvent through a membrane into a mixture of solvent and solute. Thus, it is a mixing process, not a separation process.

Exercise 1.8

Subject: Osmotic pressure for the separation of water from sea water by reverse osmosis with a membrane.

Given: Sea water containing 0.035 g of salt/cm^3 of sea water on one side of a membrane
Molecular weight of the salt = 31.5
Temperature = 298 K
Pure water on the other side of a membrane

Find: Minimum required pressure difference in kPa across the membrane

Analysis: The minimum pressure difference across the membrane is equal to the osmotic pressure of the sea water, since the osmotic pressure of pure water on the other side is zero. The equation given for osmotic pressure is $\pi = RTc/M$.

R = 8.314 kPa-m^3/kmol-K
T = 298 K
c = 0.035 g/cm^3 = 35 kg/m^3
M = 31.5 kg/kmol

Minimum pressure difference across a membrane =

$$\pi = \frac{(8.314)(298)(35)}{31.5} = 2,750 \text{ kPa}$$

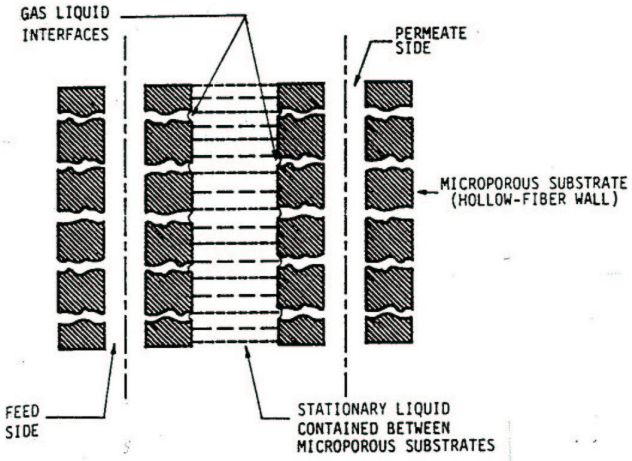
Exercise 1.9

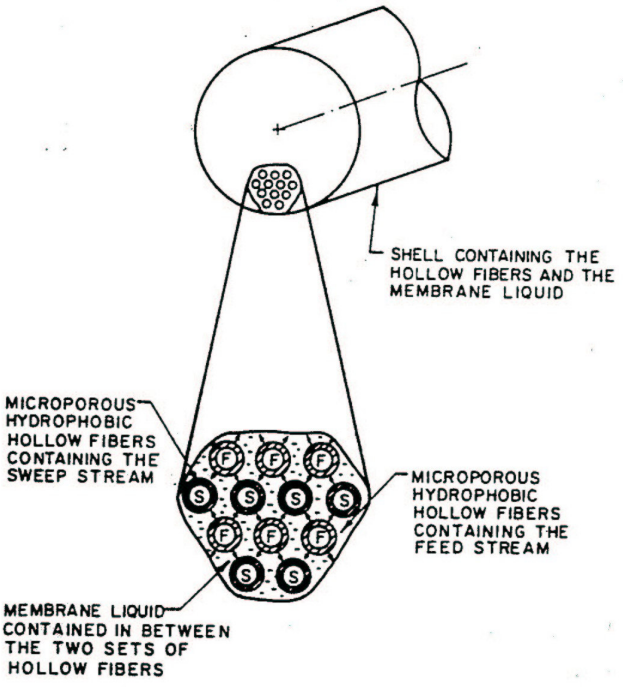
Subject: Use of a liquid membrane to separate the components of a gas mixture

Given: A liquid membrane of ethylenediaminetetraacetic acid, maintained between two sets of microporous, hydrophobic hollow fibers, packed into a cell, for removing sulfur dioxide and nitrogen oxides from flue gas.

Required: A sketch of the membrane device.

Analysis: A sweep fluid is generally required. In some cases, a vacuum could be pulled on the permeate side. The membrane device is shown below.





Exercise 1.10

Wanted: The differences, if any, between adsorption and gas-solid chromatography.

Analysis: Adsorption can be conducted by many techniques including fixed bed, moving bed, slurry, and chromatography. In chromatography, unlike the other adsorption techniques, an eluant is used to carry the mixture through the tube containing the sorbent. Multiple pure products are obtained because of differences in the extent and rate of adsorption, resulting in different residence times in the tube. The tube is made long enough that the residences do not overlap.

Exercise 1.11

Wanted: Is it essential in gas-liquid chromatography that the gas flows through the packed tube in plug flow?

Analysis: Plug flow is not essential, but it can provide sharper fronts and, therefore, the chromatographic columns can be shorter.

Exercise 1.12

Wanted: The reason why most small particles have a negative charge.

Analysis: Small particles can pick up a negative charge from collisions in glass ware. In an aqueous solution, inorganic and polar organic particles develop a charge that depends on the pH of the solution. The charge will be negative at high pH values.

Exercise 1.13

Wanted: Can a turbulent-flow field be used in field-flow fractionation?

Analysis: Field-flow fractionation requires a residence-time distribution of the molecules flowing down the tube. This is provided best by laminar flow. The residence-time distribution with turbulent flow is not nearly as favorable. Turbulent flow would not be practical.

Exercise 1.14

Subject: Sequence of three distillation columns in Fig. 1.9 for separating light hydrocarbons.

Given: Feed to column C3 is stream 5 in Table 1.5. Alter the separation to produce a distillate containing 95 mol% iC_4 at a recovery of 96%.

Find: (a) Component flow rates in the distillate and bottoms from column C3.
(b) Percent purity of nC_4 in the bottoms.
(c) Percent recovery of iC_4, for 95 mol% iC_4 in the distillate, that will maximize the percent purity of nC_4 in the bottoms.

Assumptions: Because of the relatively sharp separation in column C3 between iC_4 and nC_4, assume that all propane in the feed appears in the distillate and all C_5s appear in the bottoms.

Analysis: (a) Isobutane to the distillate = (0.96)(171.1) = 164.3 lbmol/h
Total distillate rate = 164.3/0.95 = 172.9 lbmol/h
Normal butane to the distillate = 172.9 - 2.2 - 164.3 = 6.4

Material balance around column C3, in lbmol/h:

Component	Feed	Distillate	Bottoms
Propane	2.2	2.2	0.0
Isobutane	171.1	164.3	6.8
Normal butane	226.6	6.4	220.2
Isopentane	28.1	0.0	28.1
Normal pentane	17.5	0.0	17.5
Total	445.5	172.9	272.6

(b) % Purity of nC_4 in bottoms = (220.2/272.6) x 100% = 80.8%

(c) Let x = lbmol/h of nC_4 in the distillate
y = lbmol/h of iC_4 in the distillate
P = mole fraction purity of nC_4 in the bottoms

$$P = \frac{226.6 - x}{(171.1 - y) + (226.6 - x) + 28.1 + 17.5} = \frac{226.6 - x}{443.3 - y - x} \qquad (1)$$

$$\text{Fractional purity of } iC_4 \text{ in the distillate} = \frac{y}{2.2 + y + x} = 0.95 \qquad (2)$$

Combining (1) and (2) to eliminate x, and optimization of P with respect to y gives:
P = 0.828 or 82.8 mol% nC_4 in the bottoms, x = 6.8 lbmol/h, y = 171.1 lbmol/h
Therefore, 100% recovery of iC_4 in the distillate maximizes the purity of nC_4 in the bottoms.

Exercise 1.15

Subject: Sequence of two distillation columns, C1- C2, for the separation of alcohols.

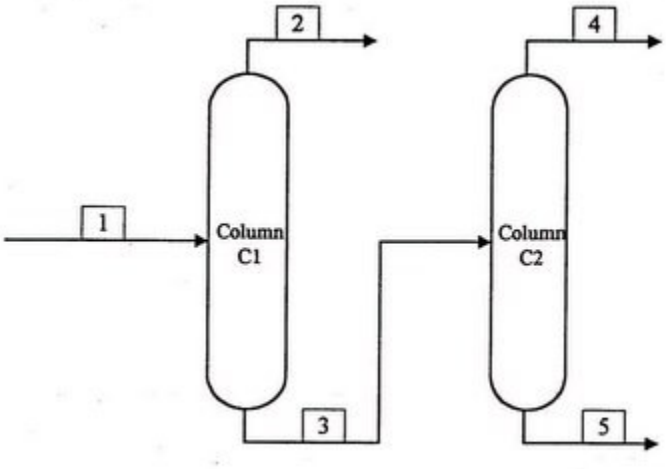
Given: 500 kmol/h feed of 40% methanol (M), 35% ethanol (E), 15% isopropanol (IP), and 10% normal propanol (NP), all in mol%. Distillate from column C1 is 98 mol% M, with a 96% recovery. Distillate from column C2 is 92 mol% E, with a recovery of 95% based on the feed to column C1.

Find: (a) Component flow rates in the feed, distillates and bottoms.
(b) Mol% purity of combined IP and NP in the bottoms from column C2.
(c) Maximum achievable purity of E in the distillate from column C2 for 95% recovery of E from the feed to column C1.
(d) Maximum recovery of E from the feed to column C1 for a 92 mol% purity of E in the distillate from column C2.

Assumptions: Because of the sharp separation in column C1, neglect the presence of propanols in the distillate from column C1. Neglect the presence of M in the bottoms from column C2. The distillate from C2 does not contain normal propanol.

Analysis: (a) M in distillate from C1 = (0.96)(500)(0.40) = 192 kmol/h
Total distillate from C1 = 192/0.98 = 195.92 kmol/h
E in distillate from C1 = 195.92 - 192 = 3.92 kmol/h
E in feed to C2 = (500)(0.35) - 3.92 = 171.08 kmol/h
M in feed to C2 = M in distillate from C2 = (500)(0.40) - 192 = 8 kmol/h
E in distillate from C2 = (500)(0.35)(0.95) = 166.25 kmol/h
Total distillate from C2 = 166.25/0.92 = 180.71 kmol/h
IP in distillate from C2 = 180.71 - 166.25 - 8 = 6.46 kmol/h

Block flow diagram:



Exercise 1.15 (continued)

Analysis: (a) continued

Material balance table (all flow rates in kmol/h):

Component	Stream 1	2	3	4	5
M	200	192.00	8.00	8.00	0.00
E	175	3.92	171.08	166.25	4.83
IP	75	0.00	75.00	6.46	68.54
NP	50	0.00	50.00	0.00	50.00
Total	500	195.92	304.08	180.71	123.37

The assumption of negligible NP in stream 4 is questionable and should be corrected when designing the column.

(b) Mol% purity of (IP + NP) in bottoms of C2 = (68.54 + 50.00)/123.37 or 96.08%

(c) If the overall recovery of E in the distillate from C2 is fixed at 95%, the maximum purity of E in that distillate occurs when no propanols appear in that distillate. Then,

mol% purity of E = 100% x 166.25/(166.25 + 8.0) = 95.41%

(d) The maximum recovery of E in the distillate from C2 occurs when E does not appear in the bottoms from C2. Thus, that maximum is 100% x (171.08/175) = 97.76%

Exercise 1.16

Subject: Pervaporation for the partial separation of ethanol and benzene

Given: 8,000 kg/h of 23 wt% ethanol and 77 wt% benzene. Polymer membrane is selective for ethanol. Permeate is 60 wt% ethanol. Retentate is 90 wt% benzene.

Find: (a) and (b) Component flow rates in feed, permeate, and retentate on a diagram.
(c) Method to further separate the permeate.

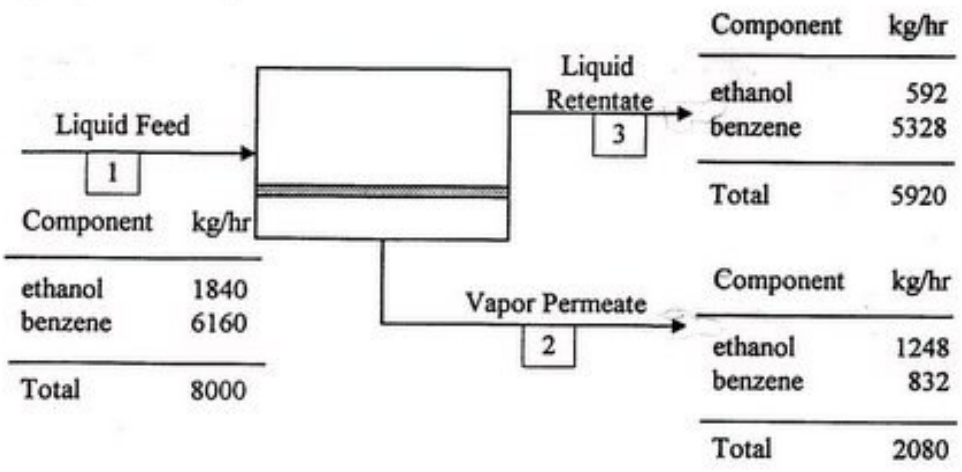
Analysis: (a) and (b) Let: P = permeate flow rate
R = retentate flow rate

Total material balance: $8{,}000 = P + R$ (1)

Ethanol material balance: $8{,}000(0.23) = (0.60)\,P + (0.10)\,R$ (2)

Solving (1) and (2) simultaneously, P = 2,080 kg/h and R = 5,920 kg/h

The resulting material balance and flow diagram is:



(c) Gas adsorption, gas permeation, or distillation to obtain ethanol and the azeotrope, which can be recycled.

Exercise 1.17

Subject: Separation of hydrogen from light gases by gas permeation with hollow fibers.

Given: Feed gas of 42.4 kmol/h of H_2, 7.0 kmol/h of CH_4, and 0.5 kmol/h of N_2 at 40°C and 16.7 MPa. Retentate exits at 16.2 kPa and permeate exits at 4.56 kPa. Gas heat capacity ratio = $\gamma = 1.4$.

Assumptions: Membrane is not permeable to nitrogen. Reversible gas expansion with no heat transfer between the retentate and permeate. Separation index is based on mole fractions.

Find: (a) Component flows in the retentate and permeate if the separation index, SP, for hydrogen relative to methane is 34.13, and the split fraction (recovery), SF, for hydrogen from the feed to the permeate is 0.6038.

(b) Percent purity of hydrogen in the permeate.

(c) Exit temperatures of the retentate and permeate.

(d) Process flow diagram with complete material balance

Analysis: (a) and (d)

Hydrogen in permeate = (0.6038)(42.4) = 25.6 kmol/h

Hydrogen in retentate = 42.4 - 25.6 = 16.8 kmol/h

Let: x = kmol/h of methane in permeate

Then, 7.0 - x = kmol/h of methane in retentate

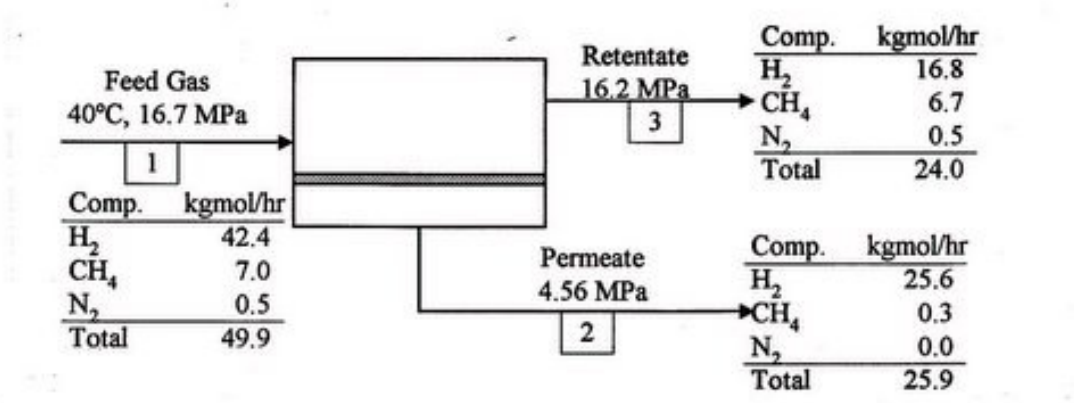
From Eq. (1-4),

$$SP = 34.13 = \frac{25.6/16.8}{x/(7-x)} \qquad (1)$$

Solving (1), x = 0.3 kmol/h of methane in the permeate

Methane in the retentate = 7.0 - 0.3 = 6.7 kmol/h

The resulting material balance and flow diagram is:



Exercise 1.17 (continued)

Analysis: (continued)

(b) Percent purity of hydrogen in permeate = 100% x 25.6/25.9 = 98.8%

(c) For reversible adiabatic (isentropic) expansion, assuming an ideal gas, the final temperature is given from thermodynamics by:

$$T_{out} = T_1\left(\frac{P_{out}}{P_1}\right)^{\frac{\gamma-1}{\gamma}} \qquad (2)$$

where subscript 1 refers to upstream side, subscript out refers to downstream side, both temperature and pressure are absolute, and γ is the gas heat capacity ratio.
For both the retentate and the permeate, T_1 = 40°C = 313 K and P_1 =16.7 MPa.

For the retentate, $P_{out} = P_3$ = 16.2 MPa. From (2),

$$T_{out} = T_3 = 313\left(\frac{16.2}{16.7}\right)^{\frac{1.4-1}{1.4}} = 310 \text{ K} = 37^{\circ}\text{C}$$

For the permeate, P_2 = 4.56 MPa. From (2),

$$T_2 = 313\left(\frac{4.56}{16.7}\right)^{\frac{1.4-1}{1.4}} = 216 \text{ K} = -57^{\circ}\text{C}$$

Exercise 1.18

Subject: Natural gas is produced when injecting nitrogen into oil wells. The nitrogen is then recovered from the gas for recycle.

Given: 170,000 SCFH (60°F and 14.7 psia) of gas containing, in mol%, 18% N_2, 75% CH_4, and 7% C_2H_6 at 100°F and 800 psia. Recover the N_2 by gas permeation followed by adsorption.
The membrane is selective for nitrogen. The adsorbent is selective for methane. The adsorber operates at 100°F, and 275 psia during adsorption and 15 psia during regeneration. Permeate exits the membrane unit at 20°F and a low pressure. Two stages of compression with cooling are needed to deliver the permeate gas to the adsorber. The regenerated gas from the adsorber is compressed in three stages with cooling, and is combined with the retentate to give the natural gas product.

Assumptions: The membrane is not permeable to ethane. The separation index, SP, defined by Eq. (1-4), is applied to the exiting retentate and permeate.

Find: (a) Draw a labeled process flow diagram.
(b) Compute the component material balance, based on the following data:
Separation index, SP, for the membrane = 16 for nitrogen relative to methane. The adsorption step gives 97 mol% methane in the adsorbate with an 85% recovery based on the feed to the adsorber. The pressure drop across the membrane is 760 psi. The retentate exits at 800 psia.
The combined natural gas product contains 3 mol% nitrogen. Place the results of the material balance in a table.

Analysis: (b) Refer to the process flow diagram on next page for stream numbers.
Let: ai = molar flow rate of N_2 in lbmol/h in stream i.
bi = molar flow rate of CH_4 in lbmol/h in stream i
ci = molar flow rate of ethane in lbmol/h in stream i
Feed flow rate = 170,000 SCFM / 379 SCF/lbmole at SC = 448.5 lbmol/h
a1 = 0.18(448.5) = 80.7, b1 = 0.75(448.5) = 336.4, c1 = 0.07(448.5) = 31.4
Because ethane does not permeate through the membrane, c3 = c6 = 31.4
and c2 = c4 = c5 = 0
Solve for a2, a3, a4, a5, a6, and b2, b3, b4, b5, b6 from 10 equations in 10 unknowns.
Membrane selectivity:

$$SP = 16 = \frac{a2 / a3}{b2 / b3} \qquad (1)$$

Component balances around the membrane unit:
a2 + a3 = 80.7 b2 + b3 = 336.4
Component balances around the adsorber:
a2 = a4 + a5 b2 = b4 + b5

Exercise 1.18 (continued)

Component balances around the line mixer that mixes retentate with adsorbate gas:

a6 = a3 + a5 b6 = b3 + b5

Methane purity in the adsorbate:

b5 = 0.97(b5 + a5)

Find: (b) (continued)

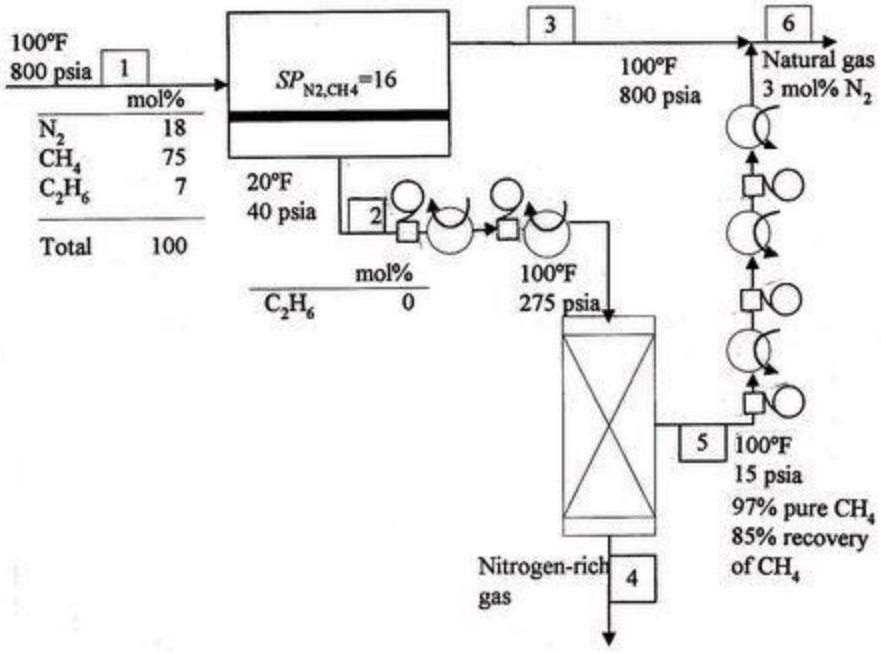
Methane recovery: b5 = 0.85 b2

Mol% nitrogen in the final natural gas: a6 = 0.03(a6 + b6 + 31.4)

All equations are linear except (1). Solving these 10 equations with a nonlinear equation solver, such as in the Polymath program, results in the following material balance table:

			Flow rate, lbmol/h			
Component	Stream 1	2	3	4	5	6
Nitrogen	80.7	73.3	7.4	69.9	3.4	10.8
Methane	336.4	128.7	207.7	19.3	109.4	317.1
Ethane	31.4	0.0	31.4	0.0	0.0	31.4
Total	448.5	202.0	246.5	89.2	112.8	359.3

(a) Labeled process flow diagram



Exercise 1.19

Subject: Separation of a mixture of ethylbenzene, o-xylene, m-xylene, and p-xylene

Find: (a) Reason why distillation is not favorable for the separation of m-xylene from p-xylene.
(b) Properties of m-xylene and p-xylene for determining a means of separation.
(c) Why melt crystallization and adsorption can be used to separate m-xylene from p-xylene.

Analysis: (a) In the order of increasing normal boiling point:

Component	nbp, ^{o}R	Relative volatility
Ethylbenzene	737.3	
		1.08
Paraxylene	741.2	
		1.02
Metaxylene	742.7	
		1.16
Orthoxylene	751.1	

From the values of relative volatility, the separation of p-xylene from m-xylene by distillation is not practical. The other two separations are practical by distillation, but require large numbers of stages.

(b) From Reference 10, the following properties are obtained:

Property	m-xylene	p-xylene
Molecular weight	106.167	106.167
van der Waals volume, m^3/kmol	0.07066	0.07066
van der Waals area, m^2/kmol x 10^{-8}	8.84	8.84
Acentric factor	0.3265	0.3218
Dipole moment, debye	0.30	0.00
Radius of gyration, m x 10^{10}	3.937	3.831
Normal melting point, K	225.3	286.4
Normal boiling point, K	412.3	411.5
Critical temperature, K	617	616.2
Critical pressure, MPa	3.541	3.511

From the table, the difference of 61.1 K in melting points is very significant and can be exploited in melt crystallization. The difference in dipole moments of 0.30, while not large, makes possible the use of adsorption or distillation with a solvent

(c) Explanations are cited in Part (b).

Exercise 1.20

Subject: Separation of a near-azeotropic mixture of ethyl alcohol and water.

Given: A list of possible methods to break the azeotrope.

Find: Reasons why the following separation operations might be used:

(a) Extractive distillation
(b) Azeotropic distillation
(c) Liquid-liquid extreaction
(d) Crystallization
(e) Pervaporation membrane
(f) Adsorption

Analysis:

Pertinent Properties:

Property	Ethanol	Water
Melting point, ^{o}C	-112	0
Dipole moment, debye	1.69	1.85

(a) Extractive distillation is a proven process using ethylene glycol.
(b) Heterogeneous azeotropic distillation is possible with benzene, carbon tetrachloride, trichloroethylene, and ethyl acetate.
(c) Liquid-liquid extraction is possible with n-butanol.
(d) Crystallization is possible because of the large difference in the melting points.
(e) Pervaporation is possible using a polyvinylalcohol membrane.
(f) Adsorption is possible using silica gel or activated alumina to adsorb the water.

Exercise 1.21

Subject: Removal of ammonia from water.

Given: 7,000 kmol/h of water containing 3,000 ppm by weight of ammonia at 350 K and 1 bar.

Find: A method to remove the ammonia.

Analysis: From Perry's Handbook, 7th edition, page 2-87, the volatility of ammonia is much higher than that of water. Therefore, could use distillation or air stripping. Also, could adsorb the ammonia on a carbon molecular sieve or use a liquid organic membrane containing an acidic complexing agent to form an ion-pair with the ammonia ion, NH_4+.

Exercise 1.22

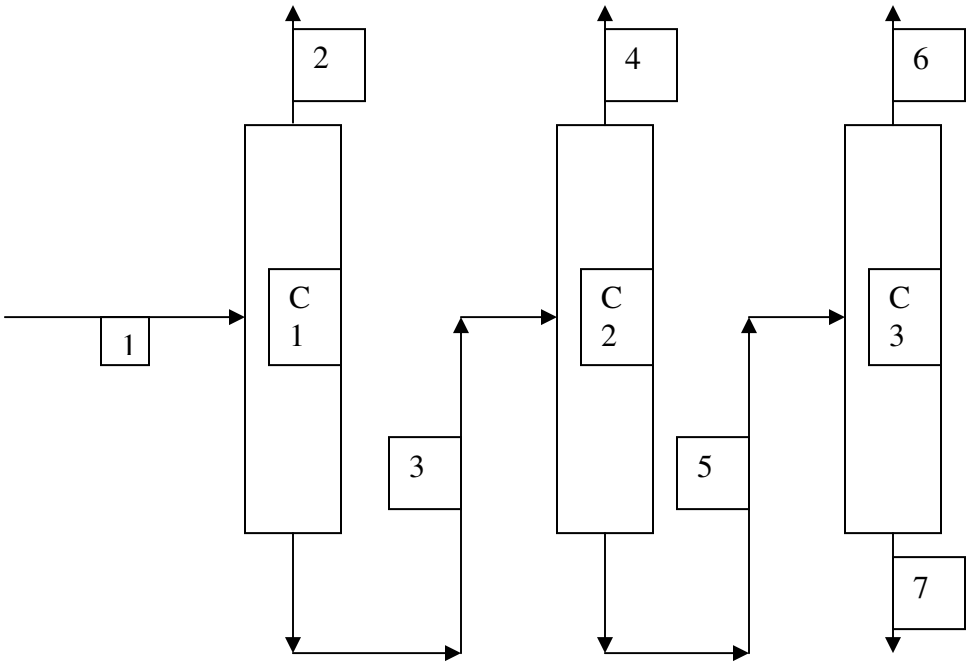
Subject: Separation of a mixture of distillation by a sequence of distillation columns.

Given: Feed stream containing in kmol/h: 45.4 C3, 136.1 iC4, 226.8 nC4, 181.4 iC5, and 317.4 nC5. Three columns in series, C1, C2, and C3. Distillate from C1 is C3-rich with a 98% recovery. Distillate from C2 is iC4-rich with a 98% recovery. Distillate from C3 is nC4-rich with a 98% recovery. Bottoms from C3 is C5s-rich with a 98% recovery.

Find: (a) Process-flow diagram like Figure 1.9.
(b) Material-balance table like Table 1.5.
(c) Mole % purities in a table like Table 1.7

Assumptions: Reasonable values for splits of iC4 to streams where they are not the main component.

Analysis:
(a) Process-flow diagram:



Exercise 1.22 (continued)

(b) Using given recoveries:

Propane in Stream 2 = 0.98(45.4) = 44.5 kmol/h
i-Butane in Stream 4 = 0.98(136.1) = 133.4 kmol/h
n-Butane in Stream 6 = 0.98(226.8) = 222.3 kmol/h
C5s in Stream 7 = 0.98(181.4 + 317.5) = 488.9 kmol/h

Material-balance table in kmol/h:

Comp	1	2	3	4	5	6	7
C3	45.4	44.5	0.9	0.9	0.0	0.0	0.0
iC4	136.1	1.3	134.8	133.4	1.4	1.4	0.0
nC4	226.8	0.5	226.3	2.5	223.8	222.3	1.5
iC5	181.4	0.0	181.4	0.0	181.4	7.0	174.4
nC5	317.5	0.0	317.5	0.0	317.5	3.0	314.5
Total	907.2	46.3	860.9	136.8	724.1	233.7	490.4

(c) Mol% purity of propane-rich product = 45.4/46.3 = 0.961 = 96.1%
Mol% purity of i-butane-rich product = 133.4/136.8 = 0.975 = 97.5%
Mol% purity of n-butane-rich product = 222.3/233.7 = 0.951 = 95.1%
Mol% purity of C5s-rich product = (174.4 + 314.5)/490.4 = 0.997 = 99.7%

Exercise 1.23

Subject: Methods for removing organic pollutants from wastewater.

Given: Available industrial processes:

(1) adsorption
(2) distillation
(3) liquid-liquid extraction
(4) membrane separation
(5) stripping with air
(6) stripping with steam

Find: Advantages and disadvantages of each process.

Analysis:

Some advantages and disadvantages are given in the following table:

Method	**Advantages**	**Disadvantages**
Adsorption	Adsorbents are available.	Difficult to recover pollutant. Best to incinerate it.
Distillation	May be practical if pollutant is more volatile.	Impractical is water is more volatile.
L-L extraction	Solvent are available.	Water will be contaminated with solvent.
Membrane	May be practical if a membrane can be found that is highly selective for pollutant.	May need a large membrane area if water is the permeate.
Air stripping	May be practical if pollutant is more volatile.	Danger of producing a flammable gas mixture.
Steam stripping	May be practical if pollutant is more volatile.	Must be able to selectively condense pollutant from overhead.

With adsorption, can incinerate pollutant, but with a loss of adsorbent.
With distillation, may be able to obtain a pollutant product.
With L-L extraction, will have to separate pollutant from solvent.
With a membrane, may be able to obtain a pollutant product.
With air stripping, may be able to incinerate pollutant.
With steam stripping may be able to obtain a pollutant product.

Exercise 1.24

Subject: Removal of VOCs from a waste gas stream.

Given: Waste gas containing VOCs that must be removed by any of the following methods:

(1) absorption
(2) adsorption
(3) condensation
(4) freezing
(5) membrane separation

Find: Advantages and disadvantages of each method.

Analysis:

Some advantages and disadvantages are given in the following table:

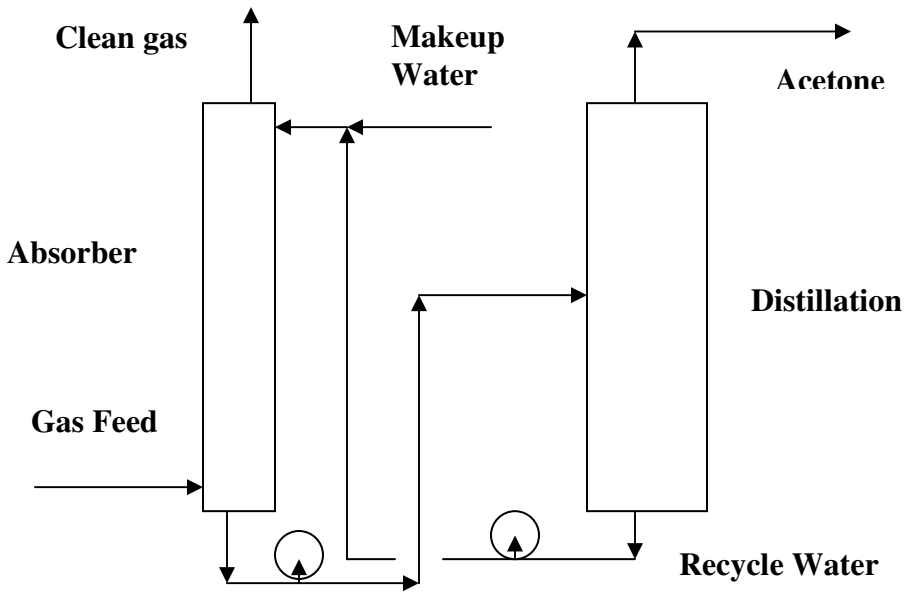
Method	Advantages	Disadvantages
Absorption	Good absorbents probably exist.	Absorbent may stripped into the waste gas.
Adsorption	Good adsorbents probably exist.	May have to incinerate the spent adsorbent.
Condensation	May be able to recover the VOC as a product.	May require high pressure and/or low temperature.
Freezing	May be able to recover the VOC as a product.	May require a low temperature.
Membrane	May be able to recover the VOC as a product.	May be difficult to obtain high selectivity. May require a very high pressure.

With absorption, may be able to distil the VOC from the absorbent.
With adsorption, may be able to incinerate the VOC or recover it.
With condensation, can recover the VOC as a product.
With freezing, can recover the VOC as a product.
With a membrane, can recover the VOC as a product.

The process shown on the following page shows a process for recovering acetone from air. In the first step, the acetone is absorbed with water. Although water is far from being the most ideal solvent because of the high volatility of acetone in water, the air will not be contaminated with an organic solvent. The acetone-water mixture is then easily separated by distillation, with recycle of the water.

Exercise 1.24 (continued)

One possible process-flow diagram:



Exercise 1.25

Subject: Separation of air into nitrogen and oxygen.

Given: Air to be separated.

Find: Three methods for achieving the separation.

Analysis: Three methods are used commercially for separating air into oxygen and nitrogen:

1. Gas permeation mainly for low capacities
2. Pressure-swing gas adsorption for moderate capacities.
3. Low-temperature distillation for high capacities.

Exercise 1.26

Subject: Separation of an azeotropic mixture of water and an organic compound.

Given: An azeotropic mixture of water and an organic compound such as ethanol.

Find: Suitable separation methods.

Analysis:

Several suitable methods are:

- Pervaporation
- Heterogeneous azeotropic distillation
- Liquid-Liquid extraction.

Exercise 1.27

Subject: Production of magnesium sulfate from an aqueous stream.

Given: An aqueous stream containing 5 wt% magnesium sulfate.

Find: Suitable process for producing nearly pure magnesium sulfate.

Analysis: Use evaporation to a near-saturated solution, followed by crystallization to produce a slurry of magnesium sulfate heptahydrate crystals. Use a centrifuge or filter to remove most of the mother liquor from the crystals, followed by drying. A detailed flow sheet of the process is shown and discussed near the beginning of Chapter 17.

Exercise 1.28

Subject: Separation of a mixture of acetic acid and water.

Given: A 10 wt% stream of acetic acid in water

Find: A process that may be more economical than distillation.

Analysis: The solution contains mostly water. Because water is more volatile than acetic acid, distillation will involve the evaporation of large amounts of water with its very high enthalpy of vaporization. Therefore, it is important to consider an alternative method such as liquid-liquid extraction. Such a process is shown and discussed near the beginning of Chapter 8.

Exercise 2.1

Subject: Minimum work for separating a hydrocarbon stream.

Given: Component flow rates, n_i , of feed and product 1, in kmol/h. Phase condition; temperature in K; enthalpy, h, in kJ/kmol; and entropy, s, in kJ/kmol-K for feed, product 1, and product 2. Infinite heat sink temperature = T_0 = 298.15 K.

Find: Minimum work of separation, W_{min} , in kJ/h

Analysis: From Eq. (4), Table 2.1,

$$W_{min} = \sum_{out} nb - \sum_{in} nb$$

From Eq. 2-1,

$$b = h - T_0 s$$

For the feed stream (in), n = 30 + 200 + 370 + 350 + 50 = 1,000 kmol/h
b = 19,480 - (298.15)(36.64) = 8,556 kJ/kmol
For product 1 (out), n = 30 + 192 + 4 + 0 + 0 = 226 kmol/h
b = 25,040 - (298.15)(33.13) = 15,162 kJ/kmol
For product 2 (out), $n = n_{feed} - n_{product\ 1}$ = 1,000 - 226 = 774 kmol/h
b = 25,640 - (298.15)(54.84) = 9,289 kJ/kmol

From Eq. (4), Table 2.1,

$$W_{min} = 226(15{,}162) + 774(9{,}289) - 1{,}000(8{,}556) = 2{,}060 \text{ kJ/h}$$

Exercise 2.2

Subject: Minimum work for separating a mixture of ethylbenzene and xylene isomers.

Given: Component flow rates, n_i , of feed ,in lbmol/h. Component split fractions for three products, Phase condition; temperature in ^oF; enthalpy, h, in Btu/lbmol; and entropy, s, in Btu/lbmol-^oR for feed and three products. Infinite heat sink temperature = $T_0 = 560^oR$.

Find: Minimum work of separation, W_{min} , in kJ/h

Analysis: From Eq. (4), Table 2.1,

$$W_{min} = \sum_{out} nb - \sum_{in} nb$$

From Eq. 2-1,

$$b = h - T_0 s$$

For the feed stream (in), n = 150 +190 + 430 + 230 = 1,000 lbmol/h

b = 29,290 - (560)(15.32) = 20,710 Btu/lbmol

For product 1 (out), using Eq. (1-2),

n = 150(0.96) + 190 (0.005) + 430(0.004) = 146.7 lbmol/h

b = 29,750 - (560)(12.47) = 22,767 Btu/lbmol

For product 2 (out), using Eq. (1-2),

n = 150(0.04) + 190(0.99) + 430(0.99) + 230(0.015) = 623.3 lbmol/h

b = 29,550 - (560)(13.60) = 21,934 Btu/lbmol

For product 3 (out), by total material balance,

n = 1,000 - 146.7 - 623.3 = 230 lbmol/h

b = 28,320 - (560)(14.68) = 20,099 Btu/lbmol

From Eq. (4), Table 2.1,

W_{min} = 146.7(22,767) + 623.3(21,934) + 230(20,099) - 1,000(20,710) = 924,200 Btu/h

Exercise 2.3

Subject: Second-law analysis of a distillation column

Given: Component flow rates, n_i , from Table 1.5 for feed, distillate, and bottoms in kmol/h for column C3 in Figure 1.9. Condenser duty, Q_C , = 27,300,00 kJ/h. Phase condition; temperature in K; enthalpy, h, in kJ/kmol; and entropy, s, in kJ/kmol-K for feed, distillate and bottoms. Infinite heat sink temperature = T_0 = 298.15 K. Condenser cooling water at 25°C = 298.15 K and reboiler steam at 100°C = 373.15 K.

Assumptions: Neglect shaft work associated with column reflux pump.

Find: (a) Reboiler duty, Q_R , kJ/h
(b) Production of entropy, ΔS_{irr} , kJ/h-K
(c) Lost work, LW, kJ/h
(d) Minimum work of separation, W_{min} , kJ/h
(e) Second-law efficiency, η

Analysis: (a) From Eq. (1), the energy balance for column C3,

$$Q_R = Q_C - \sum_{in} nh + \sum_{out} nh$$

$$= 27{,}300{,}000 - 445.5(17{,}000) + 175.5(13{,}420) + 270(15{,}840)$$

$$= 26{,}360{,}000 \text{ kJ/h}$$

(b) From Eq. (2), the entropy balance for column C3,

$$\Delta S_{irr} = \sum_{out}\left(ns + \frac{Q}{T_s}\right) - \sum_{in}\left(ns + \frac{Q}{T_s}\right)$$

$$= 175.5(5.87) + 270(21.22) + \frac{27{,}300{,}000}{298.15} - 445.5(25.05) - \frac{26{,}360{,}000}{373.15}$$

$$= 16{,}520 \text{ kJ/h-K}$$

(c) From Eq. (2-2), LW = $T_0 \Delta S_{irr}$ = 298.15(16,520) = 4,925,000 kJ/h

(d) Combining Eqs. (3) and (4) of Table 2.1,

$$W_{min} = Q_R\left(1 - \frac{T_0}{T_{steam}}\right) - Q_C\left(1 - \frac{T_0}{T_{cw}}\right) - \text{LW}$$

$$= 26{,}360{,}000\left(1 - \frac{298.15}{373.15}\right) - 27{,}300{,}000\left(1 - \frac{298.15}{298.15}\right) - 4{,}925{,}000$$

$$= 373{,}000 \text{ kJ/h}$$

(e) From Eq. (5), Table 2.1, η = 373,000/(4,925,000 + 373,000) = 0.0704
= 7.04%

Exercise 2.4

Subject: Second-law analysis for a membrane separation of a gas mixture

Given: Component flow rates in lbmol/h for the feed. Permeate of 95 mol% H_2 and 5 mol% CH_4. Separation factor, SP, for H_2 relative to CH_4, of 47. Phase condition; temperature in ^oF; enthalpy, h, in Btu/lbmol; and entropy, s, in Btu/lbmol-^oR for the feed, permeate, and retentate. Infinite heat sink temperature = $T_0 = 539.7^oR$.

Assumptions: Neglect heat transfer to or from the membrane.

Find: (a) Production of entropy, ΔS_{irr} ,Btu/h-^oR
(b) Lost work, LW, Btu/h
(c) Minimum work of separation, W_{min} , Btu/h
(d) Second-law efficiency, η
Suggest other separation methods.

Analysis: First compute the material balance to obtain the flow rates of the retentate and permeate. From Eq. (1-4), for the separation factor, SP, using the subscript P for permeate and R for retentate,

$$47 = \frac{\left(n_{H_2}\right)_P / \left(n_{H_2}\right)_R}{\left(n_{CH_4}\right)_P / \left(n_{CH_4}\right)_R} \qquad (1)$$

For 95 mol% H_2 and 5 mol% CH_4 in the permeate,

$$0.95 = \frac{\left(n_{H_2}\right)_P}{\left(n_{H_2}\right)_P + \left(n_{CH_4}\right)_P} \qquad (2)$$

By component material balances for H_2 and CH_4 around the membrane separator.

$$\left(n_{H_2}\right)_F = 3{,}000 = \left(n_{H_2}\right)_P + \left(n_{H_2}\right)_R$$
$$\left(n_{CH_4}\right)_F = 884 = \left(n_{CH_4}\right)_P + \left(n_{CH_4}\right)_R \qquad (3) \text{ and } (4)$$

Solving Eqs. (1), (2), (3), and (4) for the 4 unknowns,
$\left(n_{H_2}\right)_P = 2{,}699.9$ lbmol / h, $\left(n_{H_2}\right)_R = 300.1$ lbmol / h, $\left(n_{CH_4}\right)_P = 142.1$ lbmol / h, $\left(n_{CH_4}\right)_R = 741.9$ lbmol / h

Therefore, $n_P = 2{,}699.9 + 142.1 + 0 = 2{,}842$ lbmol/h
$n_R = 300.1 + 741.9 + 120 = 1{,}162$ lbmol/h
Also, $n_F = 2{,}842 + 1{,}162 = 4{,}004$ lbmol/h

Exercise 2.4 (continued)

Analysis: (continued)

(a) From Eq. (2), the entropy balance for the membrane

$$\Delta S_{irr} = \sum_{out}(ns) - \sum_{in}(ns)$$
$$= 1{,}162(2.742) + 2{,}842(4.222) - 4{,}004(1.520)$$
$$= 9{,}099 \text{ Btu/h-}^{\circ}\text{R}$$

(c) From Eq. (2-2), LW = $T_0 \Delta S_{irr}$ = 536.7(9,099) = 4,883,000 Btu/h

(d) Combining Eqs. (3) and (4) of Table 2.1,

$$W_{min} = -\text{LW}$$
$$= -4{,}883{,}000 \text{ Btu/h}$$

Note the negative value. The energy of separation is supplied from the high pressure of the feed.

(e) Because the minimum work of separation is equal to the negative of the lost work, Eq. (5), Table 2.1 does not apply. The efficiency can not be computed unless heat transfer is taken into account to give a permeate temperature of 80°F.

Gas adsorption could also be used to make the separation.

Exercise 2.5

Subject: Expressions for computing *K*-values.

Given: Seven common thermodynamic expressions for estimating *K*-values.

Find: Expression assumptions if not rigorous

Analysis:

(a) $K_i = \frac{\overline{\phi_{iL}}}{\overline{\phi_{iV}}}$ is a rigorous expression.

(b) $K_i = \frac{\phi_{iL}}{\phi_{iV}}$ is not rigorous. It assumes ideal solutions so that γ_{iL} and γ_{iV} are 1.0.

(c) $K_i = \phi_{iL}$ is not rigorous. It assumes ideal solutions and an ideal gas, such that ϕ_{iV} , γ_{iL} , and γ_{iV} are 1.0.

(d) $K_i = \frac{\gamma_{iL}\phi_{iL}}{\overline{\phi_{iV}}}$ is a rigorous expression.

(e) $K_i = \frac{P_i^s}{P}$ is not rigorous. It assumes ideal solutions and an ideal gas, such that ϕ_{iV} , γ_{iL} , and γ_{iV} are 1.0. It also assumes a low pressure for the liquid phase, such that ϕ_{iL}=1.0.

(f) $K_i = \frac{\gamma_{iL}\phi_{iL}}{\gamma_{iV}\phi_{iV}}$ is a rigorous expression

(g) $K_i = \frac{\gamma_{iL}P_i^s}{P}$ is not rigorous. It assumes low pressure for the liquid and the ideal gas law, such that $\phi_{iL} = \frac{P_i^s}{P}$ and ϕ_{iV}=1.0.

Exercise 2.6

Subject: Comparison of experimental *K*-values to Raoult's law predictions.

Given: For the propane-isopentane system at 167°F and 147 psia, propane mole fractions of 0.2900 in the liquid phase and 0.6650 in the vapor phase. Vapor pressures at 167°F of 409.6 psia for propane and 58.6 psia for isopentane.

Find: (a) Experimental *K*-values.
(b) Raoult's law *K*-values.

Analysis: (a) Mole fraction of isopentane in the liquid phase = 1 - 0.2900 = 0.7100
Mole fraction of isopentane in the vapor phase = 1 - 0.6650 = 0.3350
From Eq. (2-9), $K_i = y_i / x_i$
= 0.6650/0.2900 = 2.293 for propane
= 0.3350/0.7100 = 0.472 for isopentane

(b) From Eq. (3), Table 2.3, $K_i = P_i^s / P$
= 409.6/147 = 2.786 for propane
= 58.6/147 = 0.399 for isopentane

This is rather poor agreement. Note that the experimental values give a relative volatility of 2.293/0.472 = 4.86, while Raoult's law predicts 2.786/0.399 = 6.98.

A modified Raoult's law should be used to incorporate a liquid-phase activity coefficient. Also a fugacity correction for the gas phase might improve the agreement.

Exercise 2.7

Subject: Liquid-liquid phase equilibrium data.

Given: Experimental solubility data at 25°C for the isooctane (1)-furfural (2) system.
In the furfural-rich liquid phase, I, $x_1 = 0.0431$
In the isooctane-rich liquid phase, II, $x_1 = 0.9461$

Assumptions: The furfural activity coefficient in phase I = 1.0
The isooctane activity coefficient in phase II = 1.0

Find: (a) The distribution coefficients for isooctane and furfural.
(b) The relative selectivity for isooctane relative to furfural.
(c) The activity coefficients.

Analysis: From summation of mole fractions in each liquid phase,
x_2 in phase I = 1 - 0.0431 = 0.9569
x_2 in phase II = 1 - 0.9461 = 0.0.0539

(a) From Eq. (2-20), $K_{D_i} = x_i^{(\mathrm{I})} / x_i^{(\mathrm{II})}$

$$K_{D_1} = \frac{0.0431}{0.9461} = 0.456 \quad \text{and} \quad K_{D_2} = \frac{0.9461}{0.0539} = 17.75$$

(b) From Eq. (2-22), $\beta_{ij} = K_{D_i} / K_{D_j}$

$$\beta_{12} = \frac{K_{D_1}}{K_{D_2}} = \frac{0.0456}{17.75} = 0.00257$$

Note that the I and II designations for the two liquid phases are arbitrary. If they were interchanged, the relative selectivity would be 1/0.00257 = 389.

(c) From rearrangements of Eq. (2-30),

$$\gamma_1^{(\mathrm{I})} = \gamma_1^{(\mathrm{II})} \frac{x_1^{(\mathrm{II})}}{x_1^{(\mathrm{I})}} = 1.0\left(\frac{0.9461}{0.0431}\right) = 21.95$$

$$\gamma_2^{(\mathrm{II})} = \gamma_2^{(\mathrm{I})} \frac{x_2^{(\mathrm{I})}}{x_2^{(\mathrm{II})}} = 1.0\left(\frac{0.9569}{0.0539}\right) = 17.75$$

Exercise 2.8

Subject: Activity coefficients of solids dissolved in solvents.

Given: Solubility at 25°C of naphthalene in 5 solvents. Vapor pressure equations for solid and liquid naphthalene

Find: Activity coefficient of naphthalene in each solvent.

Analysis: From a rearrangement of Eq. (2-34) for solid-liquid phase equilibrium of naphthalene,

$$\gamma_L = \frac{1}{x_L}\left(\frac{P^s_{\text{solid}}}{P^s_{\text{liquid}}}\right) \qquad (1)$$

From the given naphthalene vapor pressure equations at 25°C = 298.15 K,

$$P^s_{\text{solid}} = \exp\left(26.708 - \frac{8{,}712}{298.15}\right) = 0.080 \text{ torr}$$

$$P^s_{\text{liquid}} = \exp\left(16.1426 - \frac{3992.01}{298.15 - 71.29}\right) = 0.234 \text{ torr}$$

From Eq. (1),

$$\gamma_L = \frac{1}{x_L}\left(\frac{0.080}{0.234}\right) = \frac{0.342}{x_L} \qquad (2)$$

Using the solubility data with Eq. (2),

Solvent	Solubility, x_L	γ_L
Benzene	0.2946	1.16
Cyclohexane	0.1487	2.30
Carbon tetrachloride	0.2591	1.32
n-Hexane	0.1168	2.93
Water	0.18×10^{-5}	190,000

Exercise 2.9

Subject: Minimum isothermal work of separation for a binary gas mixture.

Given: A feed gas mixture, F, of A and B to be separated at infinite surroundings temperature, T_0, into two products, P_1 and P_2.

Assumptions: Ideal gas law and ideal gas solution at temperature T_0. Isobaric at P_0.

Find: Derive an equation for the W_{min} in terms of the mole fractions of the feed and products.
Plot W_{min}/RT_0n_F versus the mole fraction of A in the feed for:

(a) A perfect separation.
(b) A separation with $SF_A = 0.98$ and $SF_B = 0.02$.
(c) A separation with $SR_A = 9.0$ and $SR_B = 1/9$.
(d) A separation with $SF_A = 0.95$ and $SR_B = 361$

Determine the sensitivity of W_{min} to product purities.
Does W_{min} depend on the separation method?
Prove that the largest value of W_{min} occurs for an equimolar feed.

Analysis: From Eq. (4), Table 2.1,

$$W_{\min} = \sum_{\text{out}} nb - \sum_{\text{in}} nb \qquad (1)$$

From Eq. 2-1,

$$b = h - T_0 s \qquad (2)$$

Combining Eqs. (1) and (2) for one feed, F, in and two products, P_1 and P_2, out:

$$W_{\min} = n_{P_1} h_{P_1} + n_{P_2} h_{P_2} - T_0\left(n_{P_1} s_{P_1} + n_{P_2} h_{P_2}\right) - n_F h_F + T_0 n_F s_F \qquad (3)$$

However, for isothermal separation of an ideal gas mixture, the change in enthalpy = 0. Therefore, from Eq. (3),

$$W_{\min} = T_0 n_F s_F - T_0\left(n_{P_1} s_{P_1} + n_{P_2} h_{P_2}\right) \qquad (4)$$

From Eq. (3), Table 2.4, for an ideal gas mixture at T_0 and P_0 ,

$$s = -R\sum_i \left(y_i \ln y_i\right) \qquad (5)$$

Exercise 2.9 (continued)

Analysis: (continued)

Substituting Eq. (5) into Eq. (4),

$$\frac{W_{\min}}{RT_0} = -n_F\left[y_{A_F}\ln y_{A_F} + \left(1-y_{A_F}\right)\ln\left(1-y_{A_F}\right)\right] + n_{P_1}\left[y_{A_{P_1}}\ln y_{A_{P_1}} + \left(1-y_{A_{P_1}}\right)\ln\left(1-y_{A_{P_1}}\right)\right] + n_{P_2}\left[y_{A_{P_2}}\ln y_{A_{P_2}} + \left(1-y_{A_{P_2}}\right)\ln\left(1-y_{A_{P_2}}\right)\right]\} \qquad (6)$$

By combining a component material balance for A with a total material balance,

$$n_{P_1} = n_F\frac{\left(y_{A_F} - y_{A_{P_2}}\right)}{\left(y_{A_{P_1}} - y_{A_{P_2}}\right)} \qquad (7)$$

$$n_{P_2} = n_F\frac{\left(y_{A_F} - y_{A_{P_1}}\right)}{\left(y_{A_{P_2}} - y_{A_{P_1}}\right)} \qquad (8)$$

Equations (6), (7), and (8) give a relationship for W_{min}/RT_0 in terms of the molar feed rate and the
mole fractions of A in the feed and two products.

(a) Let product P_1 be pure A and product P_2 be pure B. Then, from Eqs. (7) and (8),

$$n_{P_1} = y_{A_F}n_F \quad \text{and} \quad n_{P_2} = \left(1-y_{A_F}\right)n_F \quad (9) \text{ and } (10)$$

Combining Eqs. (6) through (10), noting that 1x ln(1) = 0 and 0x ln(0) = 0

$$\frac{W_{\min}}{n_F RT_0} = -\left[y_{A_F}\ln y_{A_F} + \left(1-y_{A_F}\right)\ln\left(1-y_{A_F}\right)\right] \qquad (11)$$

(b) From Eq. (1-2), letting 1 be P_1,

$$y_{A_{P_1}}n_{P_1} = 0.98\,y_{A_F}n_F \quad \text{or} \quad y_{A_{P_1}} = 0.98\,y_{A_F}\frac{n_F}{n_{P_1}} \qquad (12)$$

Exercise 2.9 (continued)

Analysis: (b) (continued)

and,

$$y_{B_{P_1}} = 0.02\left(1 - y_{A_F}\right)\left(\frac{n_F}{n_{P_1}}\right) \qquad (13)$$

Combining (12 and (13) to give $y_{A_{P_1}} + y_{B_{P_1}} = 1$, we obtain,

$$n_{P_1} = n_F\left(0.96 y_{A_F} + 0.02\right) \qquad (14)$$

By total material balance,

$$n_{P_2} = n_F - n_{P_1} \quad \text{or} \quad n_{P_2} = n_F\left(0.98 - 0.96 y_{A_F}\right) \qquad (15)$$

Also, from the $SF_A = 0.98$ for the split fraction of A to P_1, we can write for the split fraction of A to P_2,

$$y_{A_{P_2}} n_{P_2} = 0.02\, y_{A_F} n_F \quad \text{or} \quad y_{A_{P_2}} = 0.02\, y_{A_F} \frac{n_F}{n_{P_2}} \qquad (16)$$

The final equations are (6) combined with (12) and (14) through (16).

(c) From Eq. (1-3),

$$\frac{y_{A_{P_1}} n_{P_1}}{y_{A_{P_2}} n_{P_2}} = 9 \qquad (17)$$

and,

$$\frac{y_{B_{P_1}} n_{P_1}}{y_{B_{P_2}} n_{P_2}} = \frac{1}{9} \qquad (18)$$

Combining (17) and (18), with component and total material balances around the separator gives the following equations that can be used with Eq. (6):

$$y_{A_{P_1}} = 0.9\, y_{A_F} \frac{n_F}{n_{P_1}} \qquad (19)$$

Exercise 2.9 (continued)

Analysis: (c) (continued)

$$y_{A_{P_2}} = 0.1 y_{A_F} \frac{n_F}{n_{P_2}} \qquad (20)$$

$$n_{P_1} = n_F\left(0.8 y_{A_F} + 0.1\right) \qquad (21)$$

$$n_{P_2} = n_F\left(0.9 - 0.8 y_{A_F}\right) \qquad (22)$$

(d) From Eq. (1-5),

$$SP_{A,B} = \frac{SF_A / SF_B}{\left(1 - SF_A\right) / \left(1 - SF_B\right)} = 361 \qquad (23)$$

$SF_A = 0.95$ is given. Combining this with Eq. (23), gives $SF_B = 0.05$.

This part then proceeds as in part (b) to give:

$$n_{P_1} = n_F\left(0.90 y_{A_F} + 0.05\right) \qquad (24)$$

$$n_{P_2} = n_F - n_{P_1} \quad \text{or} \quad n_{P_2} = n_F\left(0.95 - 0.90 y_{A_F}\right) \qquad (25)$$

$$y_{A_{P_1}} = 0.95 y_{A_F} \frac{n_F}{n_{P_1}} \qquad (26)$$

$$y_{A_{P_2}} = 0.05 y_{A_F} \frac{n_F}{n_{P_2}} \qquad (27)$$

Equations (24) through (27) are combined with Eq. (6).

A spreadsheet can be used to compute the dimensionless minimum work,

$$\frac{W_{min}}{RT_0 n_F}$$

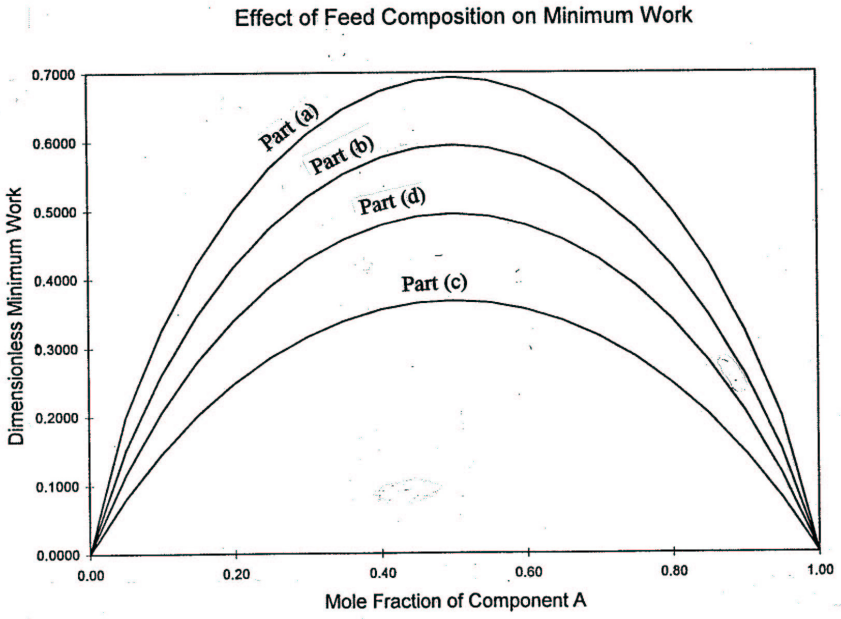
with the following results for Parts (a) through (d):

Exercise 2.9 (continued)

Analysis: Spreadsheet results for Parts (a) through (d)

y_A in Feed	W_{min}/RT_0n_F : Part (a)	Part (b)	Part (c)	Part (d)
0.00	0.0000	0.0000	0.0000	0.0000
0.10	0.3251	0.2608	0.1463	0.2064
0.20	0.5004	0.4186	0.2480	0.3408
0.30	0.6109	0.5195	0.3160	0.4284
0.40	0.6730	0.5766	0.3552	0.4783
0.50	0.6931	0.5951	0.3681	0.4946
0.60	0.6730	0.5766	0.3552	0.4783
0.70	0.6109	0.5195	0.3160	0.4284
0.80	0.5004	0.4186	0.2480	0.3408
0.90	0.3251	0.2608	0.1463	0.2064
1.00	0.0000	0.0000	0.0000	0.0000

These results give the following graph:



Exercise 2.9 (continued)

From the plot on the previous page, it is seen that the dimensionless minimum work is very sensitive to the feed mole fraction and to the product purities.

From the derivation of the minimum work equations, it is seen that they are independent of the separation method and only depend on thermodynamics.

To prove that the largest value of W_{min} occurs for a feed with equimolar quantities of A and B, consider the case of a perfect separation, part (a), as given by Eq. (11).

Let $W = W_{min}/n_F RT_0$ and $y = y_{A_F}$. Then, the derivative of W with respect to y is,

$$\frac{dW}{dy} = -\left[\ln y + \frac{y}{y} - \ln(1-y) + (1-y)\left(\frac{-1}{1-y}\right)\right]$$

$$= -\left[\ln y - \ln(1-y)\right]$$

For min/max, set the derivative to zero and solve for y.

Therefore,

$$\frac{dW}{dy} = 0 = -\left[\ln y - \ln(1-y)\right]$$

Solving, $y = 1-y$ or $y = 0.5$. This is an equimolar feed.

Furthermore, it gives a maximum value of W.

Exercise 2.10

Subject: Relative volatility of the isopentane-normal pentane system

Given: Experimental data for relative volatility 125-250°F. Vapor pressure constants.

Find: Relative volatilities from Raoult's law over the same temperature range and compare them to the experimental values.

Analysis: Combining Eq. (5), Table 2.3, for Raoult's law, with Eq. (2-21) for α.

$$\alpha_{iC_5,nC_5} = \frac{P^s_{iC_5}}{P^s_{nC_5}} \qquad (1)$$

Only the first three constants of the extended Antoine equation are given. (T=K, P= kPa)

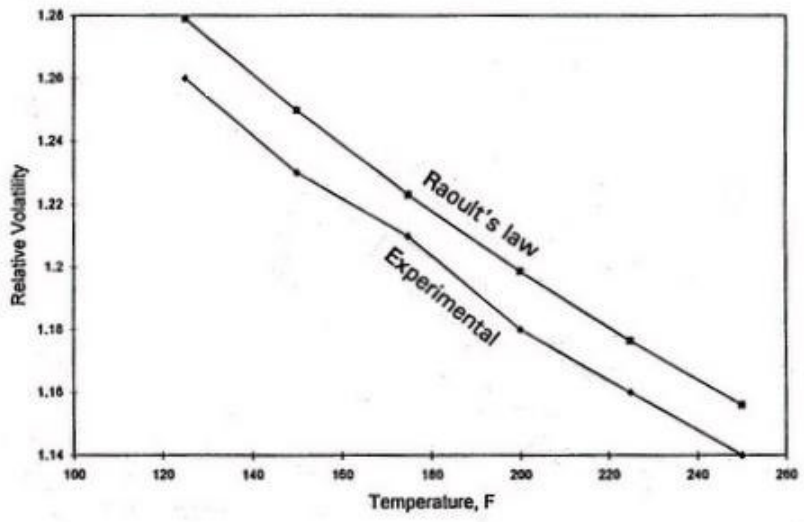
$$P^s_{iC_5} = \exp\left(13.6106 - \frac{2345.09}{T - 40.2128}\right)$$

$$P^s_{nC_5} = \exp\left(13.9778 - \frac{2554.60}{T - 36.2529}\right) \qquad (2), (3)$$

Using a spreadsheet to calculate the relative volatility from Eqs. (1), (2), and (3):

T, F	Expt. α	T, K	$P^s_{iC_5}$, kPa	$P^s_{nC_5}$, kPa	Raoult's law α
125	1.26	325	214	167	1.28
150	1.23	339	314	251	1.25
175	1.21	352	446	364	1.22
200	1.18	366	614	512	1.20
225	1.16	380	823	700	1.18
250	1.14	394	1079	834	1.16

The Raoult's law values are within 2% of the experimental values.



Exercise 2.11

Subject: Condenser duty of a vacuum distillation column separating ethyl benzene (EB) and styrene (S).

Given: Phase condition, temperature, pressure, flow rate, and compositions for streams entering and leaving a condenser, which produces subcooled reflux and distillate. Property constants in Example 2.3.

Assumptions: Ideal gas and ideal gas and liquid solutions.

Find: Condenser duty in kJ/h.

Analysis: For the thermodynamic path, cool the overhead from 331 K to 325 K. Then condense at 325 K. Because this temperature change is small, compute vapor specific heats at the two temperatures and take the arithmetic average. From Eq. (2-35) and the constants in Example 2.3, for vapor heat capacity in J/kmol-K and temperature in K,

$$C^o_{P_{\mathrm{EB}}} = -43098.9 + 707.151T - 0.481063T^2 + 1.30084\times10^{-4}T^3$$
$$C^o_{P_{\mathrm{S}}} = -28248.3 + 615.878T - 0.40231T^2 + 0.993528\times10^{-4}T^3$$

Solving,

				Vapor heat capacity, J/kmol-K		
Comp.	**kg/h**	**MW**	**kmol/h**	**331 K**	**325 K**	**Avg.**
EB	77,500	106.17	729.975	142,980	140,380	141,680
S	2,500	104.15	24.003	132,130	132,830	133,980

The sensible vapor enthalpy change, Q_{sensible} from 331 K to 325 K is,

$$\begin{aligned} Q_{\mathrm{sensible}} &= \sum_i n_i C^o_{P_i}\Delta T = \sum_i n_i C^o_{P_i}(331-325) \\ &= 729.975(141{,}680)(331-325) + 24.003(133{,}980)(331-325) \\ &= 620{,}560{,}000 \text{ J / h} \;=\; 620{,}560 \text{ kJ / h} \end{aligned}$$

For the latent heat of condensation, use Eq. (2-41) to estimate the molar heats of vaporization of at 325 K for the two components, using the vapor pressure constants given in Example 2.3.

Exercise 2.11 (continued)

$$\Delta H_{EB}^{vap} = 8314(325)^2\left[-\frac{-7440.61}{(325)^2} + 0.00623121 + \frac{-9.87052}{325} + 6(4.13065\times10^{-18})(325)^5\right]$$

$$= 40{,}740{,}000 \text{ J / kmol} \;=\; 40{,}740 \text{ kJ / kmol}$$

$$\Delta H_{S}^{vap} = 8314(325)^2\left[-\frac{-9141.07}{(325)^2} + 0.0143369 + \frac{-17.0918}{325} + 6(1.8375\times10^{-18})(325)^5\right]$$

$$= 42{,}440{,}000 \text{ J / kmol} \;=\; 42{,}440 \text{ kJ / kmol}$$

The latent heat of condensation, Q_{latent}, in kJ/kmol is,

$$Q_{latent} = \sum_i n_i \Delta H_i^{vap} = 729.975(40{,}740) + 24.003(42{,}440)$$

$$= 30{,}760{,}000 \text{ kJ / h}$$

The total condenser duty = $Q_{sensible}$ + Q_{latent} = 620,000 + 30,760,000 = 31,380,000 kJ/h

Exercise 2.12

Subject: Thermodynamic properties of a benzene (B) -toluene (T) feed to a distillation column.

Given: Temperature, pressure, and component flow rates for the column feed. Property constants, critical temperature

Assumptions: Phase condition is liquid (needs to be verified). Ideal gas and liquid solution.

Find: Molar volume, density, enthalpy, and entropy of the liquid feed.

Analysis: The feed is at 100°F and 20 psia. From Fig. 2.4, since the vapor pressures of benzene and toluene are 3.3 and 0.95 psia, respectively, the feed is a subcooled liquid. T = 311 K.
From Eqs. (4) , Table 2.4 and (2-38),

$$v_{L_i} = \frac{M_i}{\rho_{L_i}} = \frac{M_i}{AB^{-\left(1-\frac{T}{T_c}\right)^{2/7}}}$$

$$v_{L_B} = \frac{78.11}{304.1(0.269)^{-\left(1-\frac{311}{562}\right)^{2/7}}} = 0.0905 \text{ m}^3/\text{kmol}$$

$$v_{L_T} = \frac{92.14}{290.6(0.265)^{-\left(1-\frac{311}{593.1}\right)^{2/7}}} = 0.1083 \text{ m}^3/\text{kmol}$$

Total flow rate = 415 + 131 = 546 kmol/h
Benzene mole fraction = 415/546 = 0.760 Toluene mole fraction = 1-0.76 = 0.240

From Eq. (4), Table 2.4 for a mixture (additive volumes),
v_L = 0.76(0.0905) + 0.24(0.1083) = 0.0948 m^3/kmol = 1.52 ft^3/lbmol

Mixture molecular weight = M = 0.76(78.11) + 0.24(92.14) = 81.48

From Eq. (4), Table 2.4 for conversion to density,
$\rho_L = M/v_L$ = 81.48/1.52 = 53.6 lb/ft^3

Exercise 2.13

Subject: Liquid density of the bottoms from a distillation column.

Given: Temperature, pressure, component flow rates

Assumptions: Ideal liquid solution so that volume of mixing = 0

Find: Liquid density in various units using Fig. 2.3 for pure component densities.

Analysis: From Eq. (4), Table 2.4,

$$\upsilon_L = \sum_i x_i \upsilon_{iL} = \frac{M}{\rho_L}$$

$$\upsilon_{iL} = \frac{M}{\rho_{iL}}$$

The calculations are summarized as follows using Fig. 2.3 for pure component densities,

Comp.	*MW*	Flow rate, lbmol/h	Mole fraction, x_i	Density, Fig. 2.3, g/cm^3	Molar volume, υ_i cm^3/mol	$x_i \upsilon_i$
C_3	44.09	2.2	0.0049	0.2	220	1.1
iC_4	58.12	171.1	0.3841	0.40	145	55.7
nC_4	58.12	226.6	0.5086	0.43	135	68.7
iC_5	72.15	28.1	0.0631	0.515	140	8.8
nC_5	72.15	17.5	0.0393	0.525	130	5.1

$$\upsilon_L = \sum_i x_i \upsilon_{iL} = 139.4 \text{ cm}^3/\text{mol} \qquad \text{MW} = 59.5$$

$$\rho_L = \frac{\text{MW}}{\upsilon_L} = \frac{59.5}{139.4} = 0.427 \text{ g/cm}^3$$

$$= 427 \text{ kg/m}^3$$
$$= 26.6 \text{ lb/ft}^3$$
$$= 3.56 \text{ lb/gal}$$
$$= 149 \text{ lb/bbl}$$

where 1 bbl = 42 gal

Exercise 2.14

Subject: Condenser duty for a distillation column, where the overhead vapor condenses into two liquid phases.

Given: Temperature, pressure, and component flow rates of overhead vapor and the two liquid phases.

Assumptions: Ideal gas and ideal liquid solution for each liquid phase.

Find: Condenser duty in Btu/h and kJ/h

Analysis: Take a thermodynamic path of vapor from 76°C to 40°C and condensation at 40°C.

For water, use the steam tables. Change in enthalpy from vapor at 76°C to 40°C and 1.4 bar = 1133.8 - 71.96 = 1,062 Btu/lb = 2,467,000 J/kg = 2,467 kJ/kg.

For benzene, using data on p. 2-221 from Perry's 7th edition, change in enthalpy from vapor at 76°C to 40°C and 1.4 bar = 874 - 411 = 463 kJ/kg

For isopropanol, using data on p. 2-179 from Perry's 7th edition,
Average C_P over the temperature range = 1.569 kJ/kg-K
From data of p. 2-157 of Perry's 7th edition,
Heat of vaporization at 40°C = 313 K = 770.4 kJ/kg

Therefore, the enthalpy change of isopropanol = 1.569(76-40) +770.4 = 827 kJ/kg

Condenser duty, Q_C = 2,350(2,467) + 24,600(463) + 6,800(827)

= 22,810,000 kJ/h

= 21,640,000 Btu/h

Exercise 2.15

Subject: *K*-values and vapor tendency of light gases and hydrocarbons

Given: Temperature of 250°F and pressure of 500 psia.

Find: *K*-values in Fig. 2.8 and vapor tendency.

Analysis: If the *K*-value is < 1.0, tendency is for liquid phase. If the *K*-value > 1.0, tendency is for vapor phase. Using Fig. 2.8,

Component	*K*-value	Tendency
N_2	17	vapor
H_2S	3.1	vapor
CO_2	5.5	vapor
C_1	8	vapor
C_2	3	vapor
C_3	1.5	vapor
iC_4	0.71	liquid
nC_4	0.35	liquid
iC_5	0.38	liquid
nC_5	0.10	liquid

Exercise 2.16

Subject: Recovery of acetone from air by absorption in water.

Given: Temperature, pressure, phase condition, and component flow rates of feeds to and products from the absorber, except for exiting liquid temperature.

Assumptions: Ideal gas and zero heat of mixing.

Find: Temperature of exiting liquid phase. Potential for explosion hazard.

Analysis: From the given component flow rates, water evaporates at the rate of 22 lbmol/h, and 14.9 lbmol/h of acetone is condensed. Take a thermodynamic path that evaporates water at 90°F and condenses acetone at 78°F.

Energy to heat air from 78°F to 80°F = $nC_P\Delta T$ = 687(7)(80-78)=9,620 Btu/h
Energy to heat unabsorbed acetone from 78°F to 80°F is negligible.
Energy to vaporize water at 90°F = $n\Delta H^{vap}$ = 22(1,043)(18) = 413,000 Btu/h
Total required energy = 9,620 + 413,000 = 423,000 Btu/h

Energy available from condensation of acetone with ΔH^{vap} = 237 Btu/lb and a molecular weight of 58.08 = 14.9(58.08)(237) = 205,000 Btu/h
Energy available from the cooling of evaporated water from 90°F to 80°F = 22(18)(0.44)(90-80) = 2,000 Btu/h
Total available energy = 205,000 + 2,000 = 207,000 Btu/h
Energy required - Energy available = 423,000 - 207,000 = 216,000 Btu/h
This energy must come from cooling of the water absorbent from 90°F to T , and condensed acetone from 78°F to T.

Therefore, using a C_P of 0.53 for liquid acetone,

$$216{,}000 = 14.9(58.08)(78-T) + 1{,}722(18)(1.0)(90-T)$$

Solving, T = temperature of exiting liquid = 83°F.

The mol% acetone in the entering gas = 15/702 x 100% = 2.14 %.
This is outside of the explosive limits range of 2.5 to 13 mol%.

Exercise 2.17

Subject: Volumetric flow rates of entering and exiting streams of an adsorber for removing nitrogen from subquality natural gas.

Given: Temperature and pressure of feed gas and two product gases. Composition of the feed gas. Specification of 90% removal of nitrogen and a 97% methane natural gas product.

Assumptions: Applicability of the Redlich-Kwong equation of state.

Find: Volumetric flow rates of the entering and exiting gas streams in actual ft^3/h.

Analysis: Removal of nitrogen = 0.9(176) = 158.4 lbmol/h

Nitrogen left in natural gas = 176 - 158.4 = 17.6 lbmol/h

Methane in natural gas product = 17.6(97/3) = 569.1 lbmol/h

Material balance summary:

	lbmol/h:		
Component	**Feed gas**	**Waste gas**	**Natural gas**
Nitrogen	176	158.4	17.6
Methane	704	134.9	569.1
Totals	880	293.3	586.7
Temperature, ^oF	70	70	100
Pressure, psia	800	280	790

Using the ChemCAD simulation program, the following volumetric flow rates are computed using the Redlich-Kwong equation of state:

Stream	**Actual volumetric flow rate, ft^3/h**
Feed gas	5,844
Waste gas	5,876
Natural gas	4,162

Exercise 2.18

Subject: Estimation of partial fugacity coefficients of propane and benzene using the R-K equation of state.

Given: From Example 2.5, a vapor mixture of 39.49 mol% propane and 60.51 mol% benzene at 400°F and 410.3 psia.

Assumptions: Applicability of the Redlich-Kwong equation of state.

Find: Partial fugacity coefficients

Analysis: From Example 2.5, the following conditions and constants apply, where the Redlich-Kwong constants, A and B, for each component are computed from Eqs. (2-47) and (2-48) respectively.

$T = 477.6$ K	$Z_V = 0.7314$	$A = 0.2724$
$P = 2829$ kPa	$R = 8.314$ kPa-m^3/kmol-K	$B = 0.05326$

From Eqs. (2-47) and (2-48),

$$A_i = \frac{a_i P}{R^2 T^2} = \frac{a_i (2819)}{(8.314)^2 (477.6)^2} = \frac{a_i}{5593}$$

$$B_i = \frac{b_i P}{RT} = \frac{b_i (2819)}{(8.314)(477.6)} = 0.7099 b_i$$

Component, *i*	***a*, kPa-m^6/kmol^2**	***b*, m^3/kmol**	A_i	B_i
Propane	836.7	0.06268	0.1496	0.04450
Benzene	2,072	0.08263	0.3705	0.05866

The Redlich-Kwong equation for partial vapor fugacity coefficients is given by Eq. (2-56). Applying it to propane (P) and benzene (B), using the above values for constants and conditions,

$$\bar{\phi}_{P_V} = \exp\left[(0.7314-1)\frac{0.04450}{0.05326} - \ln(0.7314-0.05326) - \frac{0.2724}{0.05326}\left(2\sqrt{\frac{0.1496}{0.2724}} - \frac{0.04450}{0.05326}\right)\ln\left(1+\frac{0.05326}{0.7314}\right)\right]$$

$$= 0.934$$

$$\bar{\phi}_{B_V} = \exp\left[(0.7314-1)\frac{0.05866}{0.05326} - \ln(0.7314-0.05326) - \frac{0.2724}{0.05326}\left(2\sqrt{\frac{0.3705}{0.2724}} - \frac{0.05866}{0.05326}\right)\ln\left(1+\frac{0.05326}{0.7314}\right)\right]$$

$$= 0.705$$

Exercise 2.19

Subject: Estimation of *K*-values by the P-R and S-R-K equations of state for a butanes-butenes stream.

Given: Experimental *K*-values for an equimolar mixture of isobutane, isobutene, n-butane, 1-butene, trans-2-butene, and cis-2-butene at 220°F and 276.5 psia.

Find: *K*-values by the P-R and S-R-K equations of state using a process simulator.

Analysis: Using the ChemCAD process simulation program, the following values are obtained and compared to the experimental values:

Component	Experimental *K*-value	P-R *K*-value	S-R-K *K*-value
Isobutane	1.067	1.088	1.095
Isobutene	1.024	1.029	1.036
n-butane	0.922	0.923	0.929
1-butene	1.024	1.015	1.022
Trans-2-butene	0.952	0.909	0.916
Cis-2-butene	0.876	0.882	0.889

The experimental and estimated *K*-values agree to within 3% for all components except trans-2-butene. For that component, the P-R and S-R-K values are in close agreement, but deviate from the experimental value by from 4 to 5%.

Exercise 2.20

Subject: Cooling and partial condensation of the reactor effluent in a toluene disproportionation process.

Given: Reactor effluent component flow rates, and temperature and pressure before and after a cooling-water heat exchanger.

Find: Using the S-R-K and P-R equations of state with a process simulation program, compute the component *K*-values, and flow rates in the vapor and liquid streams leaving the cooling-water heat exchanger, and the rate of heat transfer in the cooling-water heat exchanger.

Analysis: Using the ChemCAD simulation program, the following phase equilibrium results are obtained for 100°F and 485 psia.

S-R-K Equation of State:

		lbmol/h:		
Component	***K*-value**	**Reactor effluent**	**Equilib. Vapor**	**Equilib. liquid**
Hydrogen	85.2	1900	1873.79	26.21
Methane	10.12	215	192.35	22.65
Ethane	1.715	17	10.03	6.97
Benzene	0.00827	577	3.98	573.02
Toluene	0.00264	1349	2.98	1346.02
Paraxylene	0.000881	508	0.37	507.63
Total		4566	2083.51	2482.49

P-R Equation of State:

		lbmol/h:		
Component	***K*-value**	**Reactor effluent**	**Equilib. Vapor**	**Equilib. liquid**
Hydrogen	34.4	1900	1834.46	65.54
Methane	11.27	215	193.85	21.15
Ethane	1.890	17	10.30	6.70
Benzene	0.0110	577	4.95	572.05
Toluene	0.00359	1349	3.93	1345.07
Paraxylene	0.001008	508	0.42	507.58
Total		4566	2047.91	2518.09

Except for hydrogen, the results are in good agreement.

The rate of heat transfer is computed by an energy balance, using an exchanger inlet condition of 235°F and 490 psia. Stream enthalpies are obtained from the ChemCAD program.

For S-R-K, Q_C = 25,452,000 - (-6,018,000) - 15,059,000 = 16,411,000 Btu/h

For P-R, Q_C = 26,001,000 - (-6,057,000) - 15,928,000 = 16,130,000 Btu/h

Exercise 2.21

Subject: Minimum work for the separation of a nonideal liquid mixture.

Given: A 35 mol% acetone (1) and 65 mol% water (2) liquid mixture at 298 K and 101.3 kPa, to be separated into 99 mol% acetone and 98 mol% water. Van Laar constants for the system.

Find: Minimum work for the separation in kJ/kmol of feed.

Analysis: Material balance for 1 kmol of feed.

Let the two products be R and S, where the former is acetone-rich.

Total mole balance: $1 = n_R + n_S$

Acetone balance: $0.35 = 0.99\, n_R + 0.02\, n_S$

Solving, $n_R = 0.3469$ kmol and $n_S = 0.6531$ kmol

From the problem statement,

$$\frac{W_{\min}}{RT_0} = n_R\left[\sum_{i\text{R}} x_i \ln(\gamma_i x_i)\right] + n_S\left[\sum_{i\text{S}} x_i \ln(\gamma_i x_i)\right] - n_F\left[\sum_{i\text{S}} x_i \ln(\gamma_i x_i)\right] \qquad (1)$$

The activity coefficients are given by the van Laar equations, (3) in Table 2.9, which with the given constants, $A_{12} = 2.0$ and $A_{21} = 1.7$, become,

$$\ln\gamma_1 = \frac{2.0}{\left[1+\dfrac{2.0x_1}{1.7x_2}\right]^2} \qquad (2) \qquad\qquad \ln\gamma_2 = \frac{1.7}{\left[1+\dfrac{1.7x_2}{2.0x_1}\right]^2} \qquad (3)$$

Applying Eqs. (2) and (3) to the given mole-fraction compositions,

	Feed		Product R		Product S	
Component	x	γ	x	γ	x	γ
Acetone (1)	0.35	2.116	0.99	1.000	0.02	6.735
Water (2)	0.65	1.291	0.01	5.318	0.98	1.000

Substituting the above values into Eq. (1),

Exercise 2.21 (continued)

Analysis: (continued)

$$\frac{W_{\min}}{RT_0} = 0.3469\{0.99\ln[(0.99)(1.00)] + 0.01\ln[(0.01)(5.318)]\}$$
$$+0.6531\{0.02\ln[(0.02)(6.735)] + 0.98\ln[(0.98)(1.00)]\}$$
$$-1.0000\{0.35\ln[(0.35)(2.116)] + 0.65\ln[(0.65)(1.291)]\}$$
$$= 0.1664 \text{ kmol}$$
$$W_{\min} = 0.1664RT_0 = 0.1664(8.314)(298) = 412 \text{ kJ/kmol feed}$$

For ideal liquid solutions, all values of γ are equal to 1.0. Therefore,

$$\frac{W_{\min}}{RT_0} = 0.3469\{0.99\ln[(0.99)(1.00)] + 0.01\ln[(0.01)(1.00]\}$$
$$+0.6531\{0.02\ln[(0.02)(1.00)] + 0.98\ln[(0.98)(1.00)]\}$$
$$-1.0000\{0.35\ln[(0.35)(1.00)] + 0.65\ln[(0.65)(1.00)]\}$$
$$= 0.5639 \text{ kmol}$$
$$W_{\min} = 0.5639RT_0 = 0.5639(8.314)(298) = 1,397 \text{ kJ/kmol feed}$$

Thus, the minimum work of separation for the ideal solution is 3.4 times that of the nonideal solution.

Exercise 2.22

Subject: Relative volatility and activity coefficients of the benzene (B) - cyclohexane (CH) azeotropic system at 1 atm

Given: Experimental vapor-liquid equilibrium data, including liquid-phase activity coefficients, and Antoine vapor pressure constants.

Assumptions: Ideal gas and gas solutions

Find: (a) Relative volatility of benzene with respect to cyclohexane as a function of benzene mole fraction in the liquid phase.

(b) Van Laar constants from the azeotropic point and comparison of van Laar predictions with experimental data.

Analysis: (a) From Eqs. (2-21), (2-19), and (3) in Table 2.3,

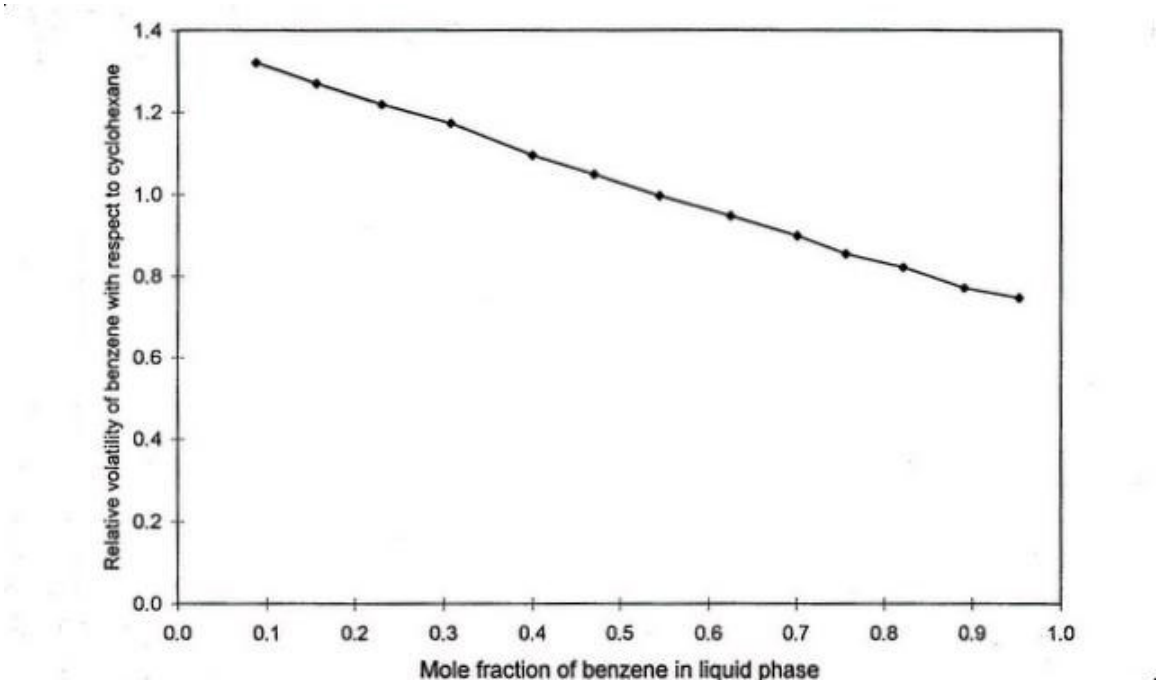
$$\alpha_{B,CH} = \frac{K_B}{K_{CH}} = \frac{y_B / x_B}{y_{CH} / x_{CH}} = \frac{y_B / x_B}{(1-y_B)/(1-x_B)} = \frac{\gamma_B P_B^s}{\gamma_{CH} P_{CH}^s} \qquad (1)$$

Using the *y*-*x* data for benzene, the following values of relative volatility are computed from (1):

Temperature, °C	x_B	y_B	$\alpha_{B,CH}$
79.7	0.088	0.113	1.317
79.1	0.156	0.190	1.269
78.5	0.231	0.268	1.218
78.0	0.308	0.343	1.173
77.7	0.400	0.422	1.095
77.6	0.470	0.482	1.049
77.6	0.545	0.544	0.996
77.6	0.625	0.612	0.946
77.8	0.701	0.678	0.898
78.0	0.757	0.727	0.854
78.3	0.822	0.791	0.821
78.9	0.891	0.863	0.771
79.5	0.953	0.938	0.746

Exercise 2.22 (continued)

Analysis: (a) (continued)



(b) From the data, take the azeotrope at $x_B = y_B = 0.545$ and $x_{CH} = y_{CH} = 1 - 0.545 = 0.455$, and with $\gamma_B = 1.079$ and $\gamma_{CH} = 1.102$.

To determine the van Laar constants, use Eqs. (2-73) and (2-74) with 1= benzene and 2 = cyclohexane:

$$A_{B,CH} = \ln 1.079\left[1-\frac{0.455\ln 1.102}{0.545\ln 1.079}\right]^2 = 0.3247$$

$$A_{CH,B} = \ln 1.102\left[1-\frac{0.545\ln 1.079}{0.455\ln 1.102}\right]^2 = 0.3247$$

Compute with a spreadsheet values of activity coefficients, using these values for the binary interaction parameters with the van Laar equations, (3), Table 2.9:

$$\ln\gamma_B = \frac{1}{\left[1+\left(0.3247x_B\right)/\left(0.3647x_{CH}\right)\right]^2}$$

$$\ln\gamma_{CH} = \frac{1}{\left[1+\left(0.3647x_{CH}\right)/\left(0.3247x_B\right)\right]^2}$$

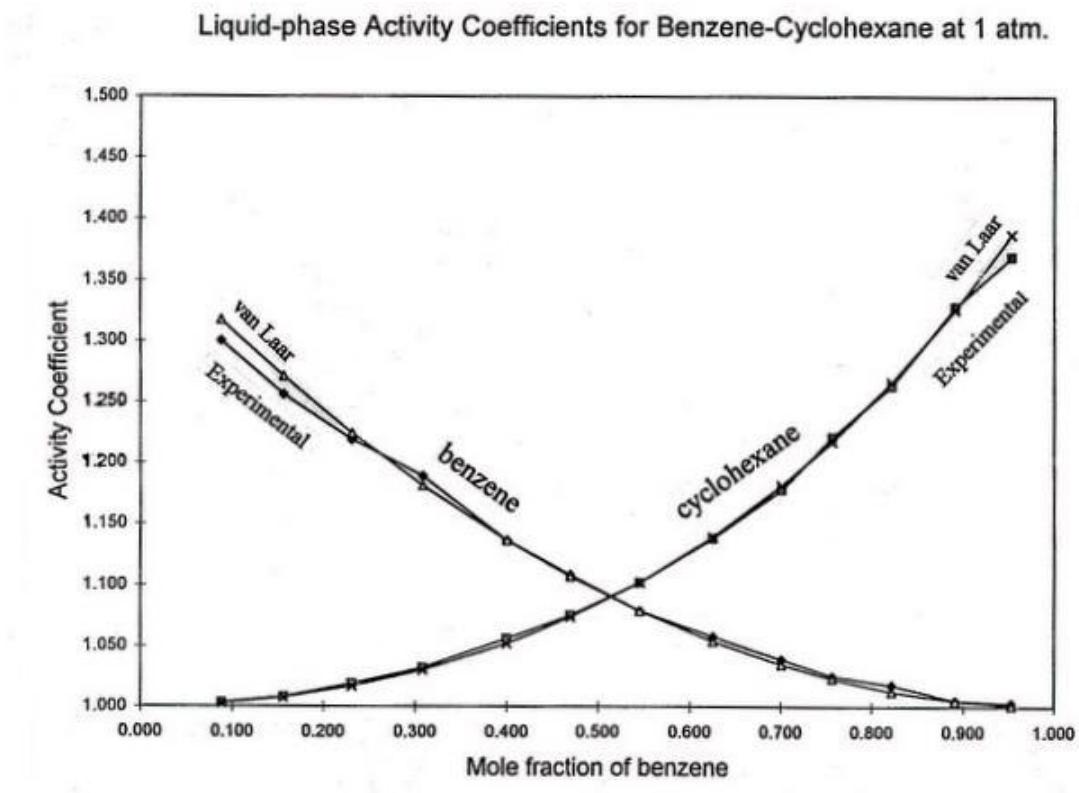
Note that because the activity coefficients are provided, the vapor pressure data are not needed.

Exercise 2.22

Analysis: (b) (continued)

	Experimental			van Laar	
Temp., °C	x_B	γ_B	γ_{CH}	γ_B	γ_{CH}
79.7	0.088	1.300	1.003	1.317	1.002
79.1	0.156	1.256	1.008	1.271	1.007
78.5	0.231	1.219	1.019	1.224	1.016
78.0	0.308	1.189	1.032	1.181	1.030
77.7	0.400	1.136	1.056	1.136	1.052
77.6	0.470	1.108	1.075	1.107	1.074
77.6	0.545	1.079	1.102	1.079	1.102
77.6	0.625	1.058	1.138	1.054	1.139
77.8	0.701	1.039	1.178	1.035	1.181
78.0	0.757	1.025	1.221	1.023	1.218
78.3	0.822	1.018	1.263	1.013	1.266
78.9	0.891	1.005	1.328	1.005	1.326
79.5	0.953	1.003	1.369	1.001	1.387

It is seen that the van Laar equation fits the experimental data quite well.



Exercise 2.23

Subject: Activity coefficients from the Wilson equation for the ethanol-benzene system at 45°C.

Given: Wilson constants and experimental activity coefficient data.

Find: Wilson activity coefficients and comparison with experimental data.

Analysis: Let: 1 = ethanol and 2 = benzene

The Wilson constants are $\Lambda_{12} = 0.124$ and $\Lambda_{21} = 0.523$

From Eqs. (4), Table 2.9,

$$\ln \gamma_1 = -\ln\left(x_1 + 0.124x_2\right) + x_2\left[\frac{0.124}{x_1 + 0.124x_2} - \frac{0.523}{x_2 + 0.523x_1}\right]$$

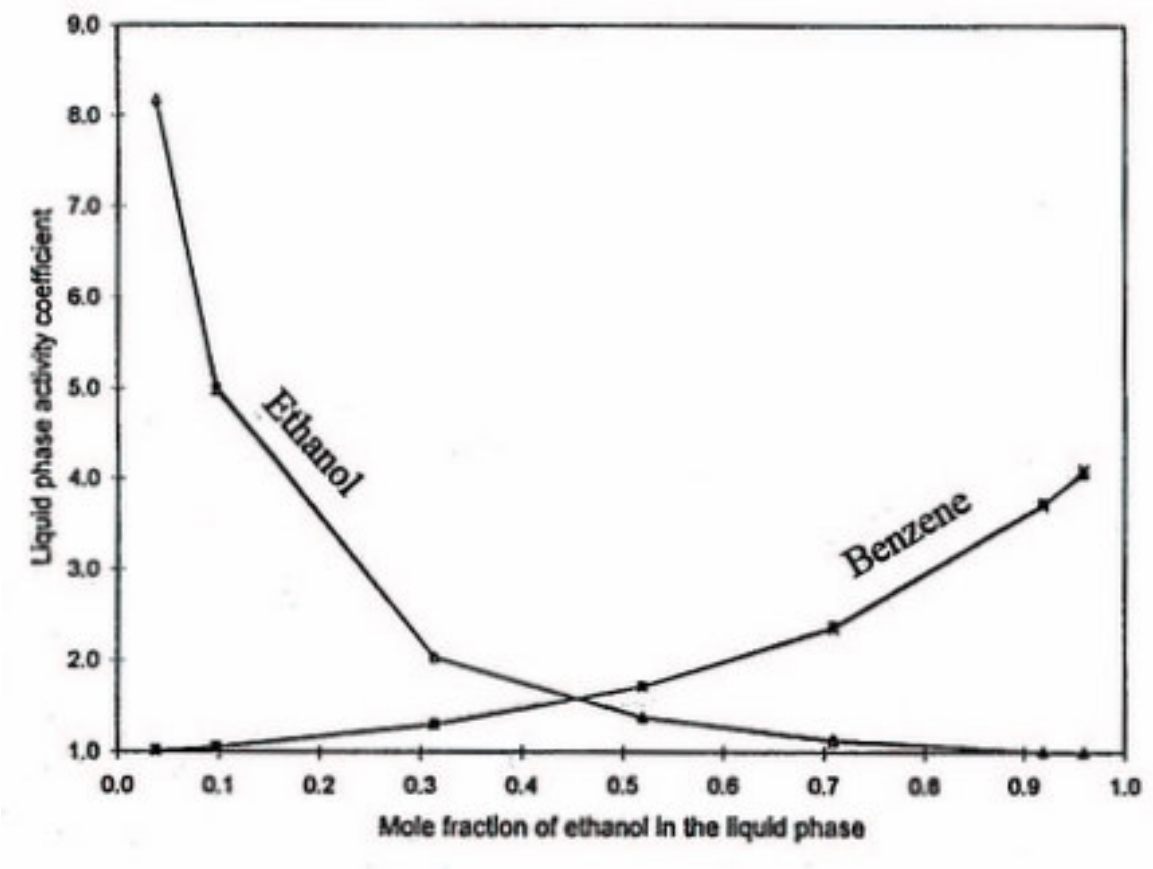
$$\ln \gamma_2 = -\ln\left(x_2 + 0.523x_1\right) - x_1\left[\frac{0.124}{x_1 + 0.124x_2} - \frac{0.523}{x_2 + 0.523x_1}\right]$$

Using a spreadsheet and noting that $\gamma = \exp(\ln \gamma)$, the following values are obtained,

	Experimental		Wilson	
x_1	γ_1	γ_2	γ_1	γ_2
0.0374	8.142	1.022	8.182	1.008
0.0972	5.029	1.053	4.977	1.044
0.3141	2.032	1.297	2.033	1.294
0.5199	1.368	1.715	1.370	1.708
0.7087	1.140	2.374	1.120	2.350
0.9193	1.000	3.735	1.009	3.709
0.9591	0.992	4.055	1.002	4.108

It is seen that the Wilson equation fits the data very well.

Exercise 2.23 (continued)



Exercise 2.24

Subject: Activity coefficients for the ethanol (1) - isooctane (2) system at 50°C.

Given: Infinite-dilution activity coefficients for the liquid phase.

Find: (a) van Laar constants
(b) Wilson constants
(c) Activity coefficients from van Laar and Wilson equations
(d) Comparison to azeotropic point
(e) *y-x* curve from van Laar equation to show erroneous prediction of phase splitting

Analysis: (a) From van Laar Eqs. (2-72) for infinite dilution,

$$A_{12} = \ln \gamma_1^\infty = \ln(21.17) = 3.053$$
$$A_{21} = \ln \gamma_2^\infty = \ln(9.84) = 2.286$$

(b) From Wilson Eqs. (2-80) and (2-81) for infinite dilution,

$$\ln \gamma_1^\infty = 3.053 = 1 - \ln \Lambda_{12} - \Lambda_{21} \qquad (1)$$
$$\ln \gamma_2^\infty = 2.286 = 1 - \ln \Lambda_{21} - \Lambda_{12} \qquad (2)$$

Solving simultaneous, nonlinear Eqs. (1) and (2) using Newton's method,

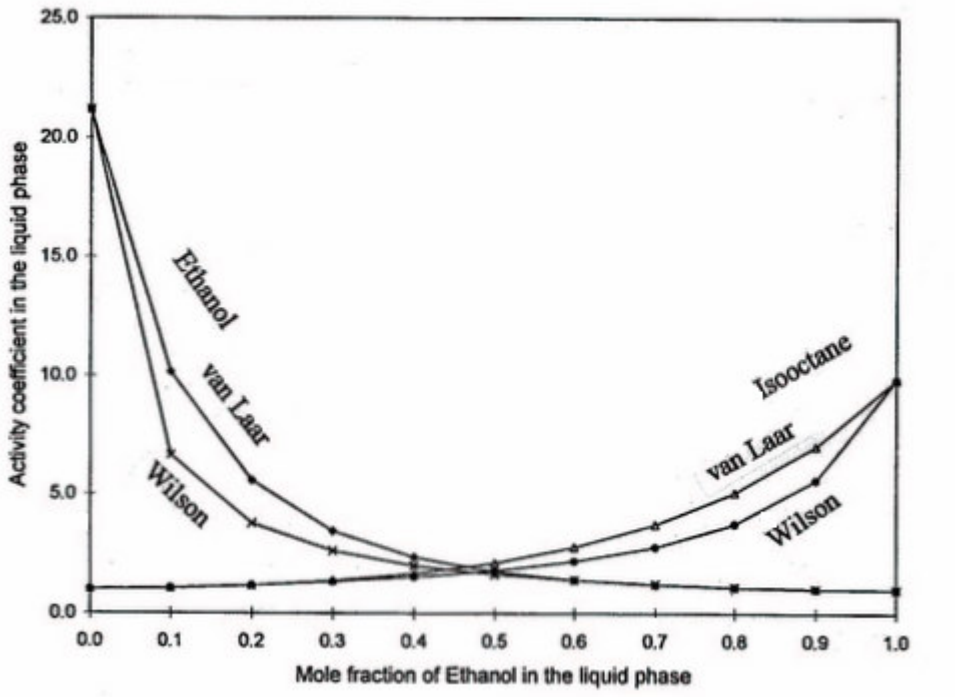
$\Lambda_{12} = 0.1004$ and $\Lambda_{21} = 0.2493$

(c) Activity coefficients can be calculated with the above constants, using Eqs. (3), Table 2.9 for the van Laar equations and Eqs. (4), Table 2.9 for the Wilson equations. Results from a spreadsheet are as follows:

	van Laar		Wilson	
x_1	γ_1	γ_2	γ_1	γ_2
0.0	21.17	1.000	21.17	1.000
0.1	10.13	1.039	6.63	1.054
0.2	5.56	1.154	3.76	1.162
0.3	3.44	1.354	2.61	1.310
0.4	2.35	1.661	2.00	1.510
0.5	1.75	2.11	1.631	1.784
0.6	1.40	2.77	1.387	2.174
0.7	1.198	3.71	1.219	2.77
0.8	1.079	5.06	1.103	3.74
0.9	1.018	7.02	1.029	5.58
1.0	1.000	9.84	1.000	9.84

Exercise 2.24 (continued)

Analysis: (c) (continued)



Note that the Wilson activity coefficients vary more steeply at the infinite-dilution ends.

(d) At the azeotropic point, $x_1 = 0.5941$ and $x_2 = 0.4059$. Using the van Laar constants from part (a) with Eqs. (3), Table 2.9,

van Laar gives $\gamma_1 = 1.419$, compared to 1.44 experimental

van Laar gives $\gamma_2 = 2.72$, compared to 2.18 experimental

Using the Wilson constants from part (b) with Eqs. (4), Table 2.9,

Wilson gives $\gamma_1 = 1.400$, compared to 1.44 experimental

Wilson gives $\gamma_2 = 2.147$, compared to 2.18 experimental

The Wilson equation is acceptable for both components. The van Laar equation gives poor agreement for isooctane.

(e) At 50°C, the vapor pressures are 221 torr for ethanol and 146 torr for isooctane. Thus, system pressure will be low over the entire range of composition. Therefore, the modified Raoult's law *K*-value expression, given by Eq. (4), Table 2.3 applies. When combined with Eq. (2-19), we obtain the following expression for predicting the *y* - *x* curve:

$$y_1 = \frac{x_1 \gamma_1 P_1^s}{P} \qquad (3)$$

Exercise 2.24 (continued)

Analysis: (e) (continued)

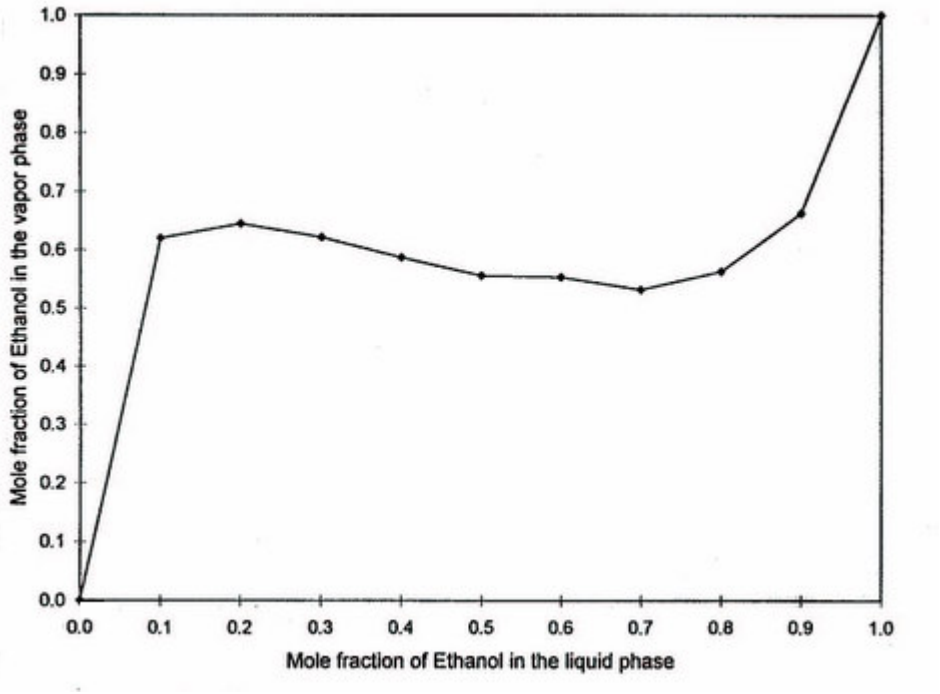
By Raoult's law, partial pressure is given by $p_i = x_i P_i^s$
Therefore, the modified Raoult's law gives $p_i = x_i\ \gamma_i P_i^s$
By Dalton's law, the sum of the partial pressures equals total pressure. Thus,

$$P = \sum_i p_i = \sum_i x_i \gamma_i P_i^s \qquad (4)$$

Using a spreadsheet with Eqs. (3) and (4) and the van Laar activity coefficients from the table above in part (c), values of y_1 are computed for values of x_1:

x_1	P, torr	y_1
0.0	146	0.000
0.1	361	0.620
0.2	381	0.645
0.3	367	0.622
0.4	356	0.587
0.5	348	0.556
0.6	349	0.553
0.7	348	0.532
0.8	339	0.563
0.9	305	0.663
1.0	221	1.000

The *y*-*x* plot exhibits the same characteristics as the system in Fig. 2.20. Therefore, the van Laar equation erroneously predicts phase splitting.



Exercise 3.1

Subject: Evaporation of a mixture of ethanol (AL) and ethyl acetate (AC) from a beaker into still air within the beaker.

Given: Initial equimolar mixture of AL and AC, evaporating into still air at 0°C and 1 atm. Vapor pressures and diffusivities in air of AL and AC at 0°C.

Assumptions: Well-mixed liquid and Raoult's law. Negligible bulk flow effect. Air sweeps across the top of the beaker at a rate such the mole fractions of AL and AC in the air at the top of the beaker are zero.

Find: Composition of the remaining liquid when 50% of the initial AL has evaporated.

Analysis: All of the mass-transfer resistance is in the still air layer in the beaker, which increases in height, z, as evaporation takes place. Apply Fick's law to both AL and AC with negligible bulk flow effect. Thus, from Eq. (3-16), the molar flux for ethanol through the gas layer in the beaker is as follows, where D_i is the diffusivity of component i in air.

$$N_{AL} = -D_{AL}\frac{dc_{AL}}{dz} = -D_{AL}c\frac{dy_{AL}}{dz}$$

$$\text{Rearranging,} \quad N_{AL}\int dz = -D_{AL}c\int_{y_{AL}}^{0} dy_{AL} \qquad (1)$$

$$\text{Similarly,} \quad N_{AC}\int dz = -D_{AC}c\int_{y_{AC}}^{0} dy_{AC} \qquad (2)$$

Dividing Eq. (1) by (2),

$$\frac{N_{AL}}{N_{AC}} = \frac{D_{AL}y_{AL}}{D_{AC}y_{AC}} = \frac{6.45\times10^{-6}\,y_{AL}}{9.29\times10^{-6}\,y_{AC}} \qquad (3)$$

where y_{AL} and y_{AC} are mole fractions in the vapor at the vapor-liquid interface.
By material balance, the molar flux of component i is equal to the rate of decrease in moles, n_i, of component i in the well-mixed liquid in the beaker per unit of mass-transfer area. Thus,

$$N_{AL} = -\frac{dn_{AL}}{Adt} \qquad (4)$$

$$N_{AC} = -\frac{dn_{AC}}{Adt} \qquad (5)$$

By Raoult's law, at the gas-liquid interface, using Eqs. (2-19) and (3) in Table 2.3,

$$y_{AL} = \frac{P^s_{AL}}{P}x_{AL} = \frac{P^s_{AL}}{P}\left(\frac{n_{AL}}{n_{AL}+n_{AC}}\right) = \frac{1.62}{101}\left(\frac{n_{AL}}{n_{AL}+n_{AC}}\right) \qquad (6)$$

$$y_{AC} = \frac{P^s_{AC}}{P}x_{AC} = \frac{P^s_{AC}}{P}\left(\frac{n_{AC}}{n_{AL}+n_{AC}}\right) = \frac{3.23}{101}\left(\frac{n_{AC}}{n_{AL}+n_{AC}}\right) \qquad (7)$$

Exercise 3.1 (continued)

Analysis: (continued)

Substituting Eqs. (4) to (7) into (3), and rearranging,

$$\frac{dn_{AL}}{dn_{AC}} = \left(\frac{1.62}{3.23}\right)\left(\frac{9.29}{6.45}\right)\left(\frac{n_{AL}}{n_{AC}}\right) \qquad (8)$$

Integrating Eq. (8) from the start of the evaporation, letting n_{i_0} be the initial values,

$$\ln\left(\frac{n_{AL}}{n_{AL_0}}\right) = 0.722 \ln\left(\frac{n_{AC}}{n_{AC_0}}\right) \qquad (9)$$

As a basis, assume 100 moles of original mixture. Thus,

$n_{AL_0} = 50$ mol and $n_{AC_0} = 50$ mol

When $n_{AL_0} = 25$ mol, i.e. half of the original, Eq. (9) gives $n_{AC} = 19.2$ mol

Therefore, the mole fractions in the well-mixed liquid when 50% of the AL has evaporated are,

$$x_{AL} = \frac{25}{25+19.2} = 0.566$$

$$x_{AC} = \frac{19.2}{25+19.2} = 0.434$$

Exercise 3.2

Subject: Evaporation of benzene (B) at 25°C and 1 atm from an open tank through a stagnant air layer of constant thickness.

Given: Tank diameter = 10 ft, with a stagnant gas layer above liquid benzene of 0.2-in. thickness. For benzene, liquid density = 0.877 g/cm^3, MW = 78.11, vapor pressure = 100 torr, and the diffusivity in air = 0.08 cm^2/s.

Assumptions: All mass-transfer resistance is in the thin gas layer of constant thickness. Steady-state with a benzene mole fraction in the air adjacent to the liquid given by Raoult's law, and the benzene mole fraction in the air at the other side of the gas layer equal to zero, assuming the evaporated benzene is continuously swept away as in Example 3.2. Ideal gas.

Find: Loss of benzene by evaporation in pounds per day.

Analysis: From Eq. (3-35) for unimolecular diffusion, taking into account bulk flow,

$$N_B = \frac{cD_B\left(y_{B_1} - 0\right)}{\Delta z\left(1 - y_B\right)_{LM}} \qquad (1)$$

where, the total gas concentration, c, is obtained from the ideal gas law,

$c = P/RT = 1/(82.06)(298) = 4.09 \times 10^{-5}$ mol/cm^3

From Eq. (2-44) for Raoult's law, noting that for pure benzene liquid, $x_B = 1$,

y_B at the gas-liquid interface = $P^s/P = 100/760 = 0.132$

The gas film thickness = Δz = 0.2 in. = 0.508 cm

$$\left(1 - y_B\right)_{LM} = \frac{(1-0) - \left(1 - y_{B_1}\right)}{\ln\left(\dfrac{1-0}{1-y_{B_1}}\right)} = \frac{(1-0) - (1-0.132)}{\ln\left(\dfrac{1-0}{1-0.132}\right)} = 0.930$$

Substituting these values into Eq. (1),

$$N_B = \frac{\left(4.09 \times 10^{-5}\right)(0.08)(0.132 - 0)}{0.508(0.930)} = 9.14 \times 10^{-7} \text{ mol benzene / cm}^2\text{ - s}$$

Cross-sectional area of the tank = mass-transfer area = $\pi D^2/4$

$= (3.14)(10)^2/4 = 78.5$ ft^2 = 72,930 cm^3

Benzene loss rate = 9.14×10^{-7} (78.11)(72,930)(3600)(24)/454 = 991 lb/day

Exercise 3.3

Subject: Countercurrent diffusion of toluene (T) and benzene (B) across vapor film at 170°F (630°R) and 1 atm.

Given: Stagnant vapor film of 0.1-inch (0.00833-ft) thickness, containing 30 mol% toluene and 70 mol% benzene, in contact with liquid reflux containing 40 mol% toluene and 60 mol% benzene. Diffusivity of toluene in benzene = 0.2 ft^2/h. Vapor pressure of toluene = 400 torr.

Assumptions: Equal molar heats of vaporization for benzene and toluene, such that diffusion is equimolar, countercurrent. Ideal gas law and Raoult's law apply. All mass transfer resistance is in the vapor phase, i.e. liquid is assumed to be uniform in composition. Given vapor composition is for bulk conditions. Phase equilibrium at the vapor-liquid interface.

Find: Mass transfer rate of toluene in lbmol/h-ft^2.

Analysis: At the vapor-liquid interface, use Raoult's law**,** Eq. (2-44). Then, the mole fraction of toluene at the interface is,

$$y_{T_i} = x_T \frac{P_T^s}{P} = 0.4\left(\frac{400}{760}\right) = 0.211$$

From ideal gas law, total gas concentration, c, is P/RT = 1/(0.7302)(630) = 0.00217 lbmol/ft^3
From the finite-difference form of Fick's law, Eq. (3-16), for the diffusion of toluene from the bulk vapor to the vapor-liquid interface,

$$N_T = \frac{cD_{T,B}\left(y_T - y_{T_i}\right)}{\Delta z} = \frac{(0.00217)(0.2)(0.300-0.211)}{0.00833}$$

$$= 0.00464 \text{ lbmol/h-ft}^2$$

Benzene diffuses at the same rate in the opposite direction.

Exercise 3.4

Subject: Drop in level of water (W) contained in a vertical tube when evaporating into air at 25°C (537°R).

Given: Tube with an inside diameter of 0.83 inch. Initial liquid level of water in tube = 0.5 inch from the top. Air above the tube has a dew point of 0°C. Diffusivity of water vapor in air = 0.256 cm^2/s or 0.992 ft^2/h.

Assumptions: Pressure = 1 atm. Ideal gas. Phase equilibrium at the gas-liquid interface with Raoult's law for mole fraction of water in the vapor adjacent to liquid water.

Find: (a) Time for the liquid level to drop from 0.5 inch to 3.5 inches.
(b) Plot of liquid level as a function of time.

Analysis: (a) The mole fraction of water in the air adjacent to the gas-liquid interface is obtained from Raoult's law, Eq. (2-44), with $x_W = 1$ for pure liquid water, using a vapor pressure of 0.45 psia for water at 25°C.

$$y_{W_I} = \frac{P_W^s}{P} = \frac{0.45}{14.7} = 0.0306$$

In the bulk air, the mole fraction of water is obtained from the dew-point condition. Thus, the partial pressure of water vapor = vapor pressure of water at 0°C = 0.085 psia. Therefore,

$$y_W = \frac{p_W}{P} = \frac{P_W^s}{P} = \frac{0.085}{14.7} = 0.00578$$

The equation for the time, t, for the water level to drop from level $z_1 = 0.5$ inch (0.0417 ft) to level z_2 equal to as large as 3.5 inches (0.2917 ft) is derived in Example 3.2, where the result is given by Eq. (6). Applying that equation here, with $\rho_A = 62.4$ lb/ft^3 for liquid water, total gas concentration, c, by the ideal gas law to give $c=P/RT$ = 1/(0.7302)(537) = 0.00255 lbmol/ft^3, and a bulk flow factor = $(1 - x_W)_{LM}$ = to a good approximation to the arithmetic average = [(1 - 0.0306) + (1 - 0.00578)]/2 = 0.982.

$$t = \frac{\rho_L (1 - x_W)_{LM}}{M_W c D_W (y_{W_I} - y_W)} (z_2^2 - z_1^2) = \frac{(62.4)(0.982)}{(18.02)(0.00255)(0.992)(0.0306 - 0.00578)} (z_2^2 - z_1^2)$$

$$= 54{,}200 \, (z_2^2 - z_1^2) = 54{,}200 (z_2^2 - 0.0417^2) \qquad (1)$$

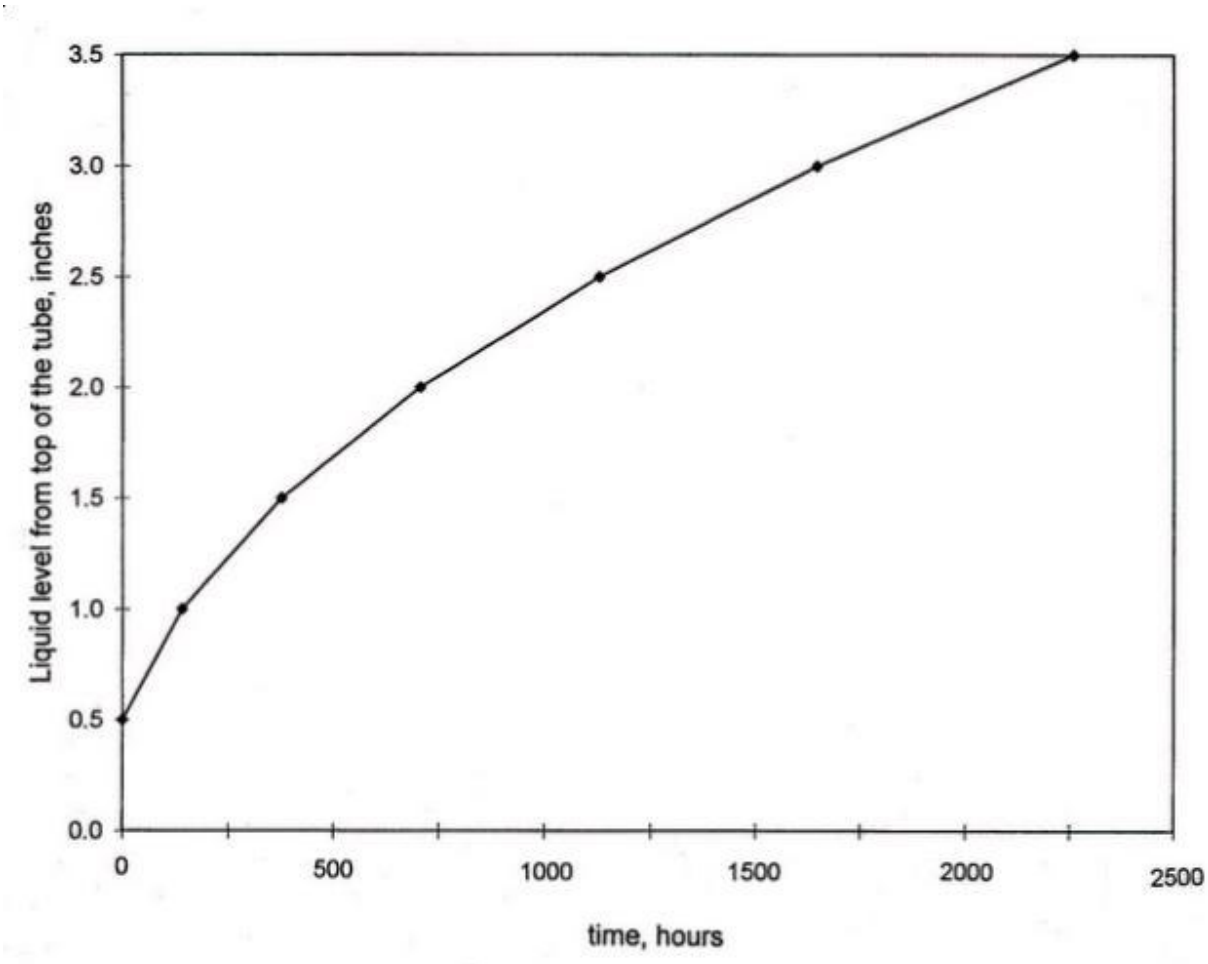
When $z_2 = 3.5$ inches = 0.2917 ft, Eq. (1) gives $t = 4{,}520$ h

Exercise 3.4 (continued)

Analysis: (continued)

(b) For other values of z_2 , the following results are obtained using a spreadsheet with Eq. (1) above:

z_2 , inches	z_2 , feet	time, hours
0.5	0.0417	0
1.0	0.0833	282
1.5	0.1250	753
2.0	0.1667	1,412
2.5	0.2083	2,259
3.0	0.2500	3,294
3.5	0.2917	4,520



Exercise 3.5

Subject: Mixing of argon (A) and xenon (X) by molecular diffusion.

Given: Bulb 1 containing argon. Bulb 2 containing xenon. Bulbs connected by a 0.002 m (0.2 cm) inside diameter by 0.2 m (20 cm) long tube. 105°C (378 K) and 1 atm are maintained. At time, t, equal 0, diffusion is allowed to occur through the connecting tube. Diffusivity = 0.180 cm^2/s.

Assumptions: Gas in each bulb is perfectly mixed. The only mass transfer resistance is in the connecting tube. Ideal gas law. Equimolar, countercurrent diffusion.

Find: At a time when the argon mole fraction = 0.75 in one bulb and 0.20 in the other bulb, determine,

(a) Rates and directions of mass transfer for A and X.
(b) Transport velocities of A and X.
(c) Molar average velocity of the gas mixture.

Analysis: This exercise is similar to Example 3.1.

Area normal to diffusion = $A = 3.14(0.2)^2/4 = 0.0314$ cm^2

From the ideal gas law, total concentration of gas =

$c = P/RT = 1/(82.06)(378) = 0.0000322$ mol/cm^3

(a) From form of Eq. (3-18),

$$n_A = \frac{cD_{A,X}A\left(y_{A_1} - y_{A_2}\right)}{\Delta z} = \frac{(0.0000322)(0.180)(0.0314)(0.75-0.20)}{20}$$

$$= 5\times10^{-9} \text{ mol/s} \quad \text{from bulb 1 to 2}$$

$$n_X = 5\times10^{-9} \text{ mol/s} \quad \text{from bulb 2 to 1}$$

(b) Because of equimolar, countercurrent diffusion, species velocities relative to stationary coordinates are equal to diffusion velocities. From Eq. (3-9), for argon (A),

$$v_A = v_{A_D} = \frac{J_A}{c_A} = \frac{n_A}{Acy_A} = \frac{5\times10^{-9}}{(0.314)(0.0000322)(y_A)} = \frac{0.00495}{y_A} \qquad (1)$$

$$v_X = \frac{0.00495}{y_X} \qquad (2)$$

Thus, the transport velocities depend on the mole fractions.

Exercise 3.5 (continued)

Analysis: (b) (continued)

Using Eqs. (1) and (2) over the range of mole fractions, noting that mole fractions are linear with distance because of equimolar, countercurrent diffusion,

Distance from Bulb 1, cm	y_A	y_X	υ_A, cm/s	υ_Ξ, cm/s
0 (Bulb 1)	0.7500	0.2500	0.0066	0.7500
5	0.6125	0.3875	0.0081	0.6111
10	0.4750	0.5250	0.0104	0.4760
15	0.3375	0.6625	0.0147	0.3367
20 (Bulb 2)	0.2000	0.8000	0.0248	0.1996

(c) Because we have equimolar, countercurrent diffusion, the molar average velocity of the mixture is zero.

Exercise 3.6

Subject: Measurement of diffusivity of toluene (T) in air (A), and comparison with prediction.

Given: Vertical tube, 3 mm in diameter and open at the top, containing toluene at 39.4°C (312.6 K). Initially, the toluene level, z_1, is 1.9 cm below the top. It takes 960,000 s for the level to drop to z_2 equal to 7.9 cm below the top. The toluene vaporizes into 1-atm (760 torr) air, which is stagnant inside the tube. The density of toluene is 0.852 g/cm^2. Its vapor pressure is 57.3 torr.

Assumptions: Isothermal vaporization. Mass transfer resistance only in the air in the tube. Neglect counterdiffusion of air. Molecular diffusion of toluene through the air in the tube. Toluene mole fraction of zero in the air at the top of the tube. Phase equilibrium at the gas-liquid interface, given by Raoult's law. Ideal gas law.

Find: Experimental and predicted values of diffusivity of toluene in air at 39.4°C and 1 atm.

Analysis: Applying Raoult's law, Eq. (2-44), to the gas-liquid interface,

$$y_T = x_T\left(\frac{P_T^s}{P}\right) = 1.0\left(\frac{57.3}{760}\right) = 0.0754$$

Therefore, the driving force for molecular diffusion, $\Delta y_T = 0.0754 - 0.0 = 0.0754$
Total gas concentration from ideal gas law, $c = P/RT = 1/(82.06)(312.6) = 3.9 \times 10^{-5}$ mol/cm^3
Molecular weight of toluene = $M_L = 92.1$
The correction for bulk flow = $(1\text{-}x_A)_{LM}$ = approximately $[(1\text{-}0) + (1\text{-}0.0754)]/2 = 0.962$
Integrating and solving Eq. (6) in Example 3.2 for the experimental gas diffusivity,

$$D_{T,A} = \frac{\rho_L (1-x_A)_{LM}}{tM_L c(\Delta y_T)}\left(\frac{z_2^2 - z_1^2}{2}\right) = \frac{(0.852)(0.962)}{(960,000)(92.1)(3.9\times10^{-5})(0.0754)}\left(\frac{7.9^2 - 1.9^2}{2}\right) = 0.0927 \text{ cm}^2/\text{s}$$

Compute the predicted value from Eq. (3-36) of Fuller, Schettler, and Giddings, with:

$$M_{T,A} = \frac{2}{\frac{1}{92.1} + \frac{1}{29}} = 44.1$$

From Table 3.1, $\left(\sum v\right)_A = 19.7, \quad \left(\sum v\right)_T = 7(15.9) + 8(2.31) - 18.3 = 111.5$

$$D_{T,A} = \frac{0.00143(312.6)^{1.75}}{(1)(44.1)^{1/2}[(19.7)^{1/3} + (111.5)^{1/3}]^2} = 0.0887 \text{ cm}^2/\text{s}$$

The predicted value is 4.3% less than the measured value. This is good agreement.

Exercise 3.7

Subject: Countercurrent molecular diffusion of hydrogen (H) and nitrogen (N) in a tube.

Given: Tube of 1 mm (0.1 cm) inside diameter and 6 inches (15.24 cm) long. At one end of the tube (1) is pure hydrogen (H) blowing past. At the other end of the tube (2) is pure nitrogen blowing past. The temperature is 75°C (348 K) and pressure is 1 atm.

Assumptions: Ideal gas law.

Find: (a) Estimate the diffusivity and the rate of diffusion of nitrogen in mol/s for equimolar, countercurrent diffusion.

(c) Plot of hydrogen mole fraction with distance.

Analysis: (a) Estimate diffusivity from (3-36), with T =348 K, P = 1 atm,

$$M_{\mathrm{H,N}} = \frac{2}{\frac{1}{2.02}+\frac{1}{28}} = 3.765$$

From Table 3.1, $\left(\sum v\right)_{\mathrm{H}} = 6.12, \quad \left(\sum v\right)_{\mathrm{N}} = 18.5$

$$D_{\mathrm{H,N}} = \frac{0.00143(348)^{1.75}}{(1)(3.765)^{1/2}[(6.12)^{1/3}+(18.5)^{1/3}]^2} = 1.033 \text{ cm}^2/\text{s}$$

From Eq. (3-18), Fick's law for equimolar, countercurrent diffusion, with,

$c = P/RT = 1/(82.06)(348) = 0.000035$ mol/cm^3

Δy_{N} = mole fraction driving force for nitrogen = 1 - 0 = 1

Δz = distance for diffusion = 15.24 cm

A = cross-sectional area for diffusion = $(3.14)(0.1)^2/4 = 0.00785$ cm^2

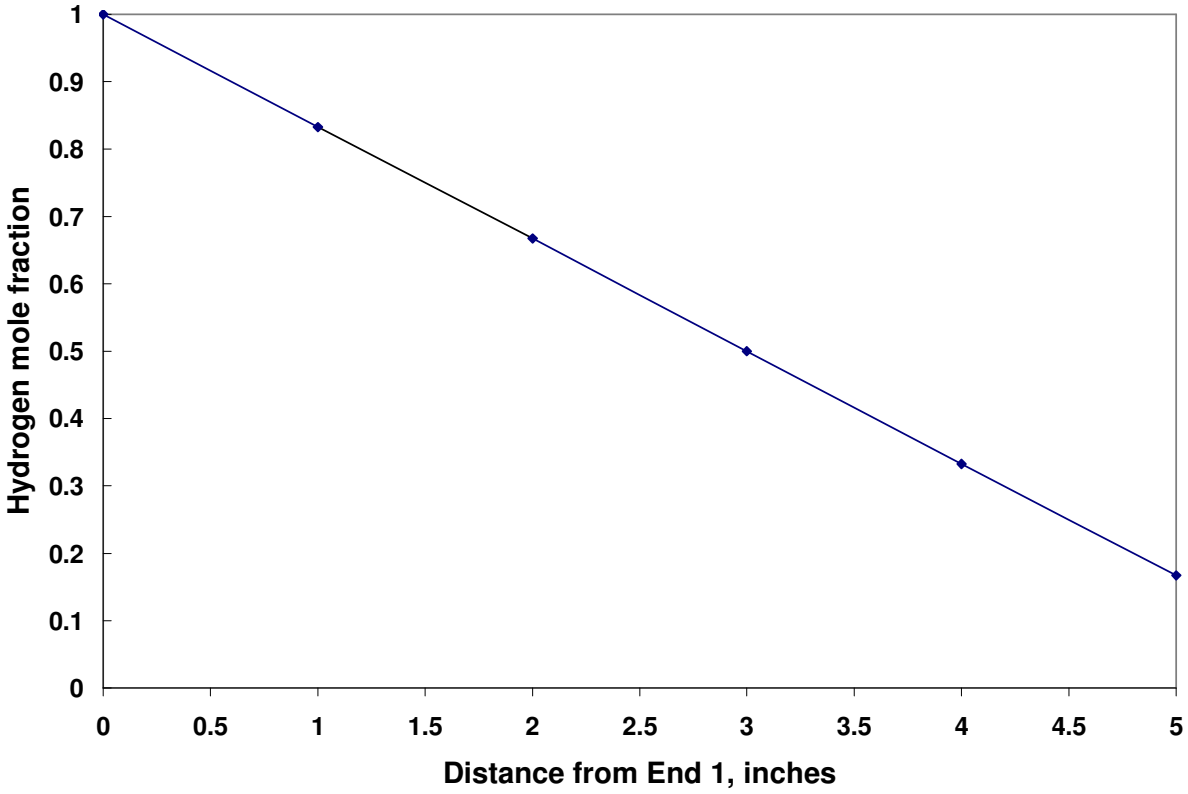
Nitrogen flow rate,

$$n_{\mathrm{N}} = J_{\mathrm{N}} A = \frac{cD_{\mathrm{H,N}}(\Delta y_{\mathrm{N}})}{\Delta z} A = \frac{(0.000035)(1.033)(1.0)}{15.24}(0.00785) = 1.86\times10^{-8} \text{ mol/s}$$

(c) The mole fraction of hydrogen varies linearly through the tube because of equimolar, countercurrent diffusion. Thus,

Exercise 3.7 (continued)

Distance from End 1, inches	Hydrogen mole fraction
0	1
1	0.833
2	0.667
3	0.500
4	0.333
5	0.167
6	0



Exercise 3.8

Subject: Molecular diffusion of HCl (H) across an air (A) film at 20°C.

Given: Air film of 0.1-inch (0.254 cm) thickness. HCl partial pressure of 0.08 atm on side 1 of the film and 0 on the other side 2. Diffusivity of HCl in air at 20°C (293 K) and 1 atm = 0.145 cm^2/s.

Assumptions: Ideal gas law. Unimolecular diffusion of HCl.

Find: Diffusion flux of HCl in mol/s-cm^2 for the following total pressures:
(a) 10 atm
(b) 1 atm
(c) 0.1 atm

Analysis: Fick's law applies. Use the form of Eq. (3-33).

Note that for an ideal gas, product $cD_{H,A}$ is independent of total pressure because c is directly proportional to P, while from Eq. (3-36), $cD_{H,A}$ is inversely proportional to P.

At P = 1 atm, $c = P/RT$ = 1/(82.06)(293) = 4.16 x 10^{-5} mol/cm^3.

Therefore, $cD_{H,A}$ = (4.16 x 10^{-5})(0.145) = 6.03 x 10^{-6}

(a) P = 10 atm. By Dalton's law, at $(y_H)_1$ = 0.08/10 = 0.008

From Eq. (3-33),

$$N_H = \frac{cD_{H,A}}{\Delta z}\ln\left(\frac{1-(y_H)_2}{1-(y_H)_1}\right) = \frac{(6.03\times10^{-6})}{(0.254)}\ln\left(\frac{1-0}{1-0.008}\right) = 1.91\times10^{-7} \text{ mol HCl/s-cm}^2$$

(b) For P = 1 atm, $(y_H)_1$ = 0.08/1 = 0.08, which gives, N_H = 1.98 x 10^{-6} mol/s-cm^2

(c) For P = 0.1 atm, $(y_H)_1$ = 0.08/0.1 = 0.8, which gives, N_H =3.82 x 10^{-5} mol/s-cm^2

Exercise 3.9

Subject: Estimation of the binary gas diffusivity for nitrogen (A) - toluene (B) at 25° C (298 K) and 3 atm

Assumptions: No need to correct diffusivity for high pressure with Takahashi method.

Find: Binary gas diffusivity using the method of Fuller, Shettler, and Giddings.

Analysis: Use Eq. (3-36), with,

$$M_{A,B} = \frac{2}{\frac{1}{28} + \frac{1}{92}} = 42.9$$

From Table 3.1,

$$\sum V_A = 18.5, \qquad \sum V_B = 7(15.9) + 8(2.31) - 18.3 = 111.5$$

$$D_{A,B} = \frac{0.00143(298)^{1.75}}{(3)(42.9)^{1/2}[18.5^{1/3} + 111.5^{1/3}]^2} = 0.028 \text{ cm}^2/\text{s}$$

Exercise 3.10

Subject: Correction of gas binary diffusivity for high pressure.

Given: Results of Example 3.3 for oxygen-benzene system at 38°C (311 K) and 2 atm, which give, $D_{AB} = 0.0494$ cm^2/s

Find: Diffusivity at 100 atm.

Analysis: If Eq. (3-36) is applied,

$D_{AB} = 0.0494\ (3/100) = 0.00148$ cm^2/s

Apply the Takahashi correlation of Fig. 3.3, based on reduced T and P.
For equimolar mixture, $T_r = T/T_c$ and $P_r = P/P_c$
where, $T_c = 0.5(154 + 563) = 359$ K and $P_c = 0.5(48.6+49.7) = 49.1$ atm
Therefore, $T_r = 311/359 = 0.866$, and $P_r = 100/49.1 = 2.04$

We are outside the range of the Takahashi correlation, but it appears that the correction would greatly decrease the diffusivity, by a factor of 10 or more.

Exercise 3.11

Subject: Estimation of infinite-dilution liquid diffusivity for carbon tetrachloride at 25°C (298 K) in four different solvents.

Given: Experimental values diffusivity for solvents of (a) methanol, (b) ethanol, (c) benzene, and (d) n-hexane.

Find: Diffusivities by the methods of Wilke and Chang (W-C), and of Hayduk and Minhas (H-M). Compare predicted values to given experimental values.

Analysis: Let:A = the solute, CCl_4; and B = solvent. The Wilke-Chang equation, Eq. (3-39), is

$$D_{A,B} = \frac{7.4\times10^{-8}\left(\phi_B M_B\right)^{1/2} T}{\mu_B v_A^{0.6}} \qquad (1)$$

From Table 3.3, v_A = 14.8 + 4(21.6) =101.2 cm^3/mol
Using Eq. (1) with the following parameters, values of diffusivity are computed.

Solvent, B	M_B	ϕ_B	μ_B , cP	$D_{A,B}$ (W-C)	$D_{A,B}$ (Expt.)
Methanol	32	1.9	0.57	1.89 x 10^{-5}	1.69 x 10^{-5}
Ethanol	46	1.5	1.17	0.98 x 10^{-5}	1.50 x 10^{-5}
Benzene	78	1.0	0.60	2.03 x 10^{-5}	1.92 x 10^{-5}
n-Hexane	86	1.0	0.32	4.00 x 10^{-5}	3.70 x 10^{-5}

Except for ethanol, the Wilke-Chang equation makes good predictions.

The applicable Hayduk-Minhas equation, Eq. (3-42), is,

$$D_{A,B} = 1.55\times10^{-8}\frac{T^{1.29}\left(P_B^{0.5}/P_A^{0.42}\right)}{\mu_B^{0.92} v_B^{0.23}} \qquad (2)$$

where, for the nonpolar solute, CCl_4 , with methanol and ethanol solvents, both P_B and v_B must be multipled by $8\mu_B$ in cP. Parachors for methanol and benzene are obtained from Table 3.5. Parachors for ethanol, n-Hexane, and carbon tetrachloride are obtained by structural contributions from Table 3.6. Using Eq. (2) with P_A= 229.8 and the following parameters, values of diffusivity are computed.

Solvent, B	P_B	v_B	μ_B , cP	$D_{A,B}$ (H-M)	$D_{A,B}$ (Expt.)
Methanol	88.8	37.0	0.57	2.55 x 10^{-5}	1.69 x 10^{-5}
Ethanol	125.3	59.2	1.17	1.70 x 10^{-5}	1.50 x 10^{-5}
Benzene	205.3	96.0	0.60	1.96 x 10^{-5}	1.92 x 10^{-5}
n-Hexane	271.0	140.6	0.32	3.05 x 10^{-5}	3.70 x 10^{-5}

Except for methanol and n-hexane, the predictions by the Hayduk-Minhas equation are good.

Exercise 3.12

Subject: Estimation of the diffusivity of benzene (A) at infinite dilution in formic acid (B) at 25°C and comparison to the experimental value for B at infinite dilution in A.

Given: Experimental value of 2.28 x 10^{-5} cm^2/s for the diffusivity of B at infinite dilution in A.

Find: Diffusivity by the Hayduk-Minhas equation, (3-42).

Analysis: The applicable H-M equation is,

$$D_{A,B} = 1.55\times10^{-8}\frac{T^{1.29}\left(P_B^{0.5}/P_A^{0.42}\right)}{\mu_B^{0.92}v_B^{0.23}} \qquad (1)$$

From Table 3.5, parachors for A and B are 205.3 and 93.7, respectively.
From Table 3.3, The molar volume of the solvent, B, is 2(3.7)+14.8+7.4+12.0 = 41.3 cm^3/mol.
From Perry's Handbook, the viscosity of B at 25°C is 1.7 cP.

Using Eq. (1),

$$D_{A,B} = 1.55\times10^{-8}\frac{298^{1.29}\left(93.7^{0.50}/205.3^{0.42}\right)}{(1.7)^{0.92}(41.3)^{0.23}} = 6.5\times10^{-6}\ cm^2/s$$

This is significantly less than the experimental value of 2.28 x 10^{-5} and the predicted value of 2.15 x 10^{-5} cm^2/s for the diffusivity of formic acid at infinite dilution in benzene.

Exercise 3.13

Subject: Estimation of the liquid diffusivity of acetic acid at 25°C (298 K) in dilute solutions of benzene, acetone, ethyl acetate, and water, and comparison with experimental values.

Given: Experimental values.

Find: Infinite dilution diffusivities for acetic acid (A) in the four solvents using the appropriate equation.

Analysis: For benzene, acetone, and ethyl acetate, Eq. (3-42) of Hayduk-Minhas applies:

$$D_{A,B} = 1.55\times10^{-8}\frac{T^{1.29}\left(P_B^{0.5}/P_A^{0.42}\right)}{\mu_B^{0.92}v_B^{0.23}} \qquad (1)$$

From Table 3.5, the parachor for acetic acid = P_A = 131.2. For all three solvents, this value is multiplied by 2 to give 262.4. Parachors for benzene and acetone are obtained from Table 3.5, and are listed below. The parachors for ethyl acetate, obtained by structural contributions from Table 3.6, is 2(55.5) + 40.0 + 63.8 = 214.8. Molecular volumes are obtained from Table 3.3, and are listed below. Solvent viscosities are obtained from Perry's Handbook. The results of applying Eq. (1) are as follows

Solvent, B	P_B	v_B	μ_B , cP	$D_{A,B}$ (H-M)	$D_{A,B}$ (Expt.)
Benzene	205.3	96	0.60	1.5×10^{-5}	2.09×10^{-5}
Acetone	161.5	74	0.32	2.5×10^{-5}	2.92×10^{-5}
Ethyl acetate	214.4	106.1	0.45	1.93×10^{-5}	2.18×10^{-5}

The predictions by the Hayduk-Minhas equation are low, but quite good for ethyl acetate.

For water, the Wilke-Chang equation, Eq. (3-39), is most applicable,

$$D_{A,B} = \frac{7.4\times10^{-8}\left(\phi_B M_B\right)^{1/2}T}{\mu_B v_A^{0.6}} \qquad (2)$$

From Table 3.3, v_A = (2)14.8 + 4(3.7) + 7.4 + 12 = 63.8 cm^3/mol.
Solvent viscosity = 0.95 cP, M_B = 18, and ϕ_B = 2.6. Substitution into Eq. (1) gives,

$$D_{A,B} = \frac{7.4\times10^{-8}\left(2.6\times18\right)^{1/2}298}{0.95(63.8)^{0.6}} = 1.3\times10^{-5}\ cm^2/s$$

This is close to the experimental value of 1.19×10^{-5} cm^2/s.

Exercise 3.14

Subject: Vapor diffusion through an effective film thickness.

Given: Water (A) at 11°C (284 K) evaporating into dry air (B) at 25°C (298 K) at the rate of 0.04 g/h-cm^2.

Assumptions: 1 atm pressure. Ideal gas law. Raoult's law for water vapor mole fraction.

Find: Effective stagnant air film thickness, assuming molecular diffusion of the water vapor through the air film.

Analysis: Apply Eq. (3-31) for Fick's law with the bulk flow effect. Solving for film thickness,

$$\Delta z = \frac{cD_{\mathrm{A,B}} \ln\left(\dfrac{1-y_{\mathrm{A}_b}}{1-y_{\mathrm{A}_I}}\right)}{N_{\mathrm{A}}} \qquad (1)$$

From the ideal gas law, using T = (284 + 298)/2 = 291 K, $c = P/RT$ = 1/(82.06)(284) = 4.29 x 10^{-5} mol/cm^3.

Molar flux of water vapor = $N_{\mathrm{A}} = 0.04/M_{\mathrm{A}} = 0.04/(18)(3600) = 6.17 \times 10^{-7}$ mol/s-cm^2.

Mole fraction of water vapor in the bulk dry air = $y_{\mathrm{A}_b} = 0$

Mole fraction of water vapor at the interface, $y_{\mathrm{A}_I} = P^s$ at 11°C/P = 0.191/14.7 = 0.013.

Estimate diffusivity of water vapor in air at 291 K and 1 atm from Eq. (3-36) of Fuller, Schettler, and Giddings, with,

$$M_{\mathrm{A,B}} = \frac{2}{\dfrac{1}{18}+\dfrac{1}{29}} = 22.2$$

From Table 3.1,

$$\sum V_{\mathrm{A}} = 13.1, \qquad \sum V_B = 19.7$$

$$D_{\mathrm{A,B}} = \frac{0.00143(291)^{1.75}}{(1)(22.2)^{1/2}[13.1^{1/3}+19.7^{1/3}]^2} = 0.24 \text{ cm}^2/\text{s}$$

Substitution into Eq. (1),

$$\Delta z = \frac{4.29\times10^{-5}\,(0.24)\ln\left(\dfrac{1-0}{1-0.013}\right)}{6.17\times10^{-7}} = 0.218 \text{ cm}$$

Note that the bulk flow has little effect here.

Exercise 3.15

Subject: Mass transfer of isopropyl alcohol (A) by molecular diffusion through liquid water and gaseous nitrogen at 35°C (308 K) and 2 atm

Given: Critical conditions for nitrogen and isopropyl alcohol and molar liquid volume of isopropyl alcohol.

Assumptions: Ideal gas law.

Find: (a) Diffusivity of A in liquid water by Wilke-Chang equation.
(b) Diffusivity of A in gaseous nitrogen by the Fuller, Schettler, Giddings equation.
(c) The product, $D_{AB}\rho_M = D_{AB}\,c$ for part (a).
(d) The product, $D_{AB}\rho_M = D_{AB}\,c$ for part (b).
(e) Comparison of diffusivities in parts (a) and (b).
(f) Comparison of results from parts (c) and (d).
(g) Conclusions about diffusion in the liquid versus the vapor phase.

Analysis: (a) For the Wilke-Chang equation (3-39), use $\phi_B = 2.6$ and $M_B = 18$.

From Perry's Handbook, $\mu_B = 0.78$ cP.

From Table 3.3, $v_A = 3(14.8) + 8(3.7) + 7.4 = 81.4$

From Eq. (3-39),

$$D_{A,B} = \frac{7.4\times10^{-8}\,(2.6\times18)^{1/2}\,308}{0.78(81.4)^{0.6}} = 1.43\times10^{-5}\ \text{cm}^2/\text{s}$$

(b) For the Fuller-Schettler-Giddings Eq. (3-36), use $T = 308$K and $P = 2$ atm, with,

$$M_{A,B} = \frac{2}{\frac{1}{60.4}+\frac{1}{28}} = 38.3$$

From Table 3.1,

$$\sum V_A = 3(15.9) + 8(2.31) + 6.11 = 72.3 \qquad \sum V_B = 18.5$$

$$D_{A,B} = \frac{0.00143(308)^{1.75}}{(2)(38.3)^{1/2}[72.3^{1/3} + 18.5^{1/3}]^2} = 0.056\ \text{cm}^2/\text{s}$$

Exercise 3.15 (continued)

Analysis: (continued)

(c) The molar density of liquid water = $\rho/M = 1/18 = 0.056$ mol/cm^3.
Therefore, $D_{AB}\rho_M = 1.43 \times 10^{-5}\ (0.056) = 8.01 \times 10^{-7}$ mol/s-cm

(d) From the ideal gas law, the molar density of gaseous nitrogen =
$P/RT = 2/(82.06)(308) = 7.91 \times 10^{-5}$ mol/cm^3.
Therefore, $D_{AB}\rho_M = 0.056\ (7.91 \times 10^{-5}) = 4.43 \times 10^{-6}$ mol/s-cm

(e) The diffusivity in the gas is about 3 orders of magnitude more than in the liquid.

(f) The product of diffusivity and molar density in the gas is less than one order of magnitude more than in the liquid.

(g) For equal mole fraction gradients, diffusion through the liquid phase is comparable to that in the gas phase.

Exercise 3.16

Subject: Liquid diffusivities for the ethanol (A) -benzene (B) system at 45°C (318 K) over the entire composition range.

Given: Experimental activity coefficients in Exercise 2.23.

Find: Effect of composition on diffusivities of both ethanol and benzene.

Analysis: Use Eq. (3-42) of Hayduk-Minhas to estimate the infinite-dilution liquid diffusivities, with liquid viscosities from Perry's Handbook. From Table 3.5, the parachor of benzene is given. The parachor for ethanol is estimated from Table 3.6. Table 3.3 is used to estimate molecular volumes. The resulting parameters are as follows:

Component	P	υ	μ , cP
Benzene	205.3	96	0.48
Ethanol	125.3	59.2	0.79

For benzene at infinite dilution in ethanol, values of molecular volume and the parachor for ethanol must be multiplied by 8 times the viscosity of ethanol. Thus, from Eq. (3-42), using $P = 8(0.79)(125.3) = 792$ and $\upsilon = 8(0.79)(59.2) = 374$ for ethanol, the solvent in this case,

$$\left(D_{\mathrm{B,A}}\right)_{\infty} = 1.55\times10^{-8}\,\frac{318^{1.29}\left(792^{0.5}/205.3^{0.42}\right)}{0.79^{0.92}\left(374\right)^{0.23}} = 2.51\times10^{-5}\,\mathrm{cm^2/s}$$

For ethanol at infinite dilution in benzene, Eq. (3-42) gives,

$$\left(D_{\mathrm{A,B}}\right)_{\infty} = 1.55\times10^{-8}\,\frac{318^{1.29}\left(205.3^{0.5}/125.3^{0.42}\right)}{0.48^{0.92}\left(96\right)^{0.23}} = 3.4\times10^{-5}\,\mathrm{cm^2/s}$$

Use Eqs. (3-45) and (3-46) of Vignes to compute $D_{\mathrm{A,B}}$ and $D_{\mathrm{B,A}}$ as a function of composition,

$$D_{\mathrm{A,B}} = \left(D_{\mathrm{A,B}}\right)_{\infty}^{x_{\mathrm{B}}}\left(D_{\mathrm{B,A}}\right)_{\infty}^{x_{\mathrm{A}}}\left(1+\frac{\partial\ln\gamma_{\mathrm{A}}}{\partial\ln x_{\mathrm{A}}}\right)_{T,P} \qquad (1)$$

$$D_{\mathrm{B,A}} = \left(D_{\mathrm{B,A}}\right)_{\infty}^{x_{\mathrm{A}}}\left(D_{\mathrm{A,B}}\right)_{\infty}^{x_{\mathrm{B}}}\left(1+\frac{\partial\ln\gamma_{\mathrm{B}}}{\partial\ln x_{\mathrm{B}}}\right)_{T,P} \qquad (2)$$

The partial derivatives are evaluated numerically with,

$$\frac{\partial\ln\gamma_{\mathrm{A}}}{\partial\ln x_{\mathrm{A}}} = \frac{\Delta\ln\gamma_{\mathrm{A}}}{\Delta\ln x_{\mathrm{A}}} \qquad \text{and} \qquad \frac{\partial\ln\gamma_{\mathrm{B}}}{\partial\ln x_{\mathrm{B}}} = \frac{\Delta\ln\gamma_{\mathrm{B}}}{\Delta\ln x_{\mathrm{B}}}$$

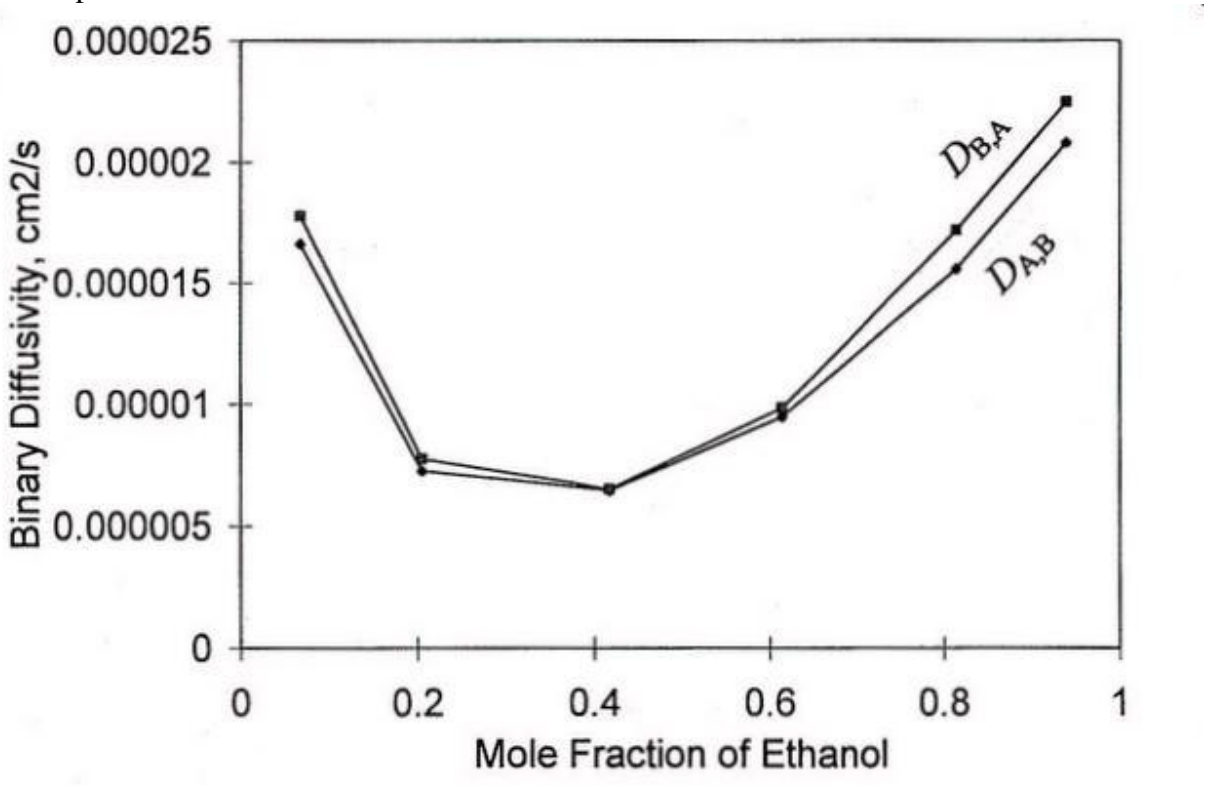
Exercise 3.16 (continued)

Analysis: (continued)

Using the data from Exercise 2.23,

x_A	$\ln \gamma_A$	$\ln \gamma_B$	$\frac{\Delta \ln \gamma_A}{\Delta \ln x_A}$	$\frac{\Delta \ln \gamma_B}{\Delta \ln x_B}$	$D_{A,B}$, cm^2/s	$D_{B,A}$, cm^2/s
0.0000					3.4×10^{-5}	
0.0374	2.0937	0.0220				
0.0673			-0.501	-0.466	1.66×10^{-5}	1.78×10^{-5}
0.0972	1.6153	0.0519				
0.2057			-0.773	-0.757	0.727×10^{-5}	0.777×10^{-5}
0.3141	0.7090	0.2599				
0.4170			-0.785	-0.783	0.645×10^{-5}	0.651×10^{-5}
0.5199	0.3136	0.5392				
0.6143			-0.664	-0.651	0.949×10^{-5}	0.985×10^{-5}
0.7087	0.1079	0.8645				
0.8140			-0.414	-0.353	1.56×10^{-5}	1.72×10^{-5}
0.9193	0.0002	1.3177				
0.9392			-0.186	-0.121	2.08×10^{-5}	2.25×10^{-5}
0.9591	-0.0077	1.3999				
1.0000						2.51×10^{-5}

These results give the following plot showing that the liquid diffusivities do not vary linearly with composition.



Exercise 3.17

Subject: Estimation of the diffusivity of an electrolyte.

Given: 1-M aqueous NaOH at 25°C (298 K).

Assumptions: Dilute solution.

Find: Diffusivity of the Na^+ (A) and OH^- (B) ions.

Analysis: Eq. (3-47) of Nernst and Haskell applies, with $n_+ = 1$ and $n_- = 1$.
From Table 3.7, $\lambda_+ = 50.1$ for Na^+, and $\lambda_- = 197.6$ for OH^-. From Eq. (3-47),

$$D_{A,B} = \frac{RT\left[\left(\frac{1}{n_+}\right)+\left(\frac{1}{n_-}\right)\right]}{F^2\left[\left(\frac{1}{\lambda_+}\right)+\left(\frac{1}{\lambda_-}\right)\right]} = \frac{8.314(298)\left[\left(\frac{1}{1}\right)+\left(\frac{1}{1}\right)\right]}{96{,}500^2\left[\left(\frac{1}{50.1}\right)+\left(\frac{1}{197.6}\right)\right]} = 2.1\times10^{-5}\,\text{cm}^2/\text{s}$$

Note that $D_{A,B}$ may be 10 to 20% higher for 1-M solution.

Exercise 3.18

Subject: Estimation of the diffusivity of an electrolyte and comparison with experiment.

Given: Experimental value of 1.28 x 10^{-5} cm^2/s for 2 M aqueous NaCl at 18°C (291 K).

Assumptions: Dilute solution

Find: Diffusivity of Na^+ (A) and Cl^- (B) ions.

Analysis: Eq. (3-47) of Nernst and Haskell applies, with $n_+ = 1$ and $n_- = 1$.
From Table 3.7, for 25°C, $\lambda_+ = 50.1$ for Na^+, and $\lambda_- = 76.3$ for Cl^-. Correction to ionic conductances for 18°C = $T/334$ $\mu_{water} = 291/(334)(1.05) = 0.83$

$$D_{A,B} = \frac{RT\left[\left(\frac{1}{n_+}\right)+\left(\frac{1}{n_-}\right)\right]}{F^2\left[\left(\frac{1}{\lambda_+}\right)+\left(\frac{1}{\lambda_-}\right)\right]} = \frac{8.314(291)\left[\left(\frac{1}{1}\right)+\left(\frac{1}{1}\right)\right]}{96{,}500^2\left[\left(\frac{1}{50.1(0.83)}\right)+\left(\frac{1}{76.3(0.83)}\right)\right]} = 1.3\times10^{-5}\,\text{cm}^2/\text{s}$$

This value compares very well with the experimental value.

Exercise 3.19

Subject: Estimation of diffusivity of N_2 (A) in H_2 (B) in pores of a solid catalyst.

Given: Catalyst at 300°C (573 K) and 20 atm, with porosity of 0.45 and tortuosity of 2.5.

Assumptions: Only mass transfer mechanism is ordinary molecular diffusion. Correction for high pressure is not necessary because of high temperature.

Find:. Diffusivity

Analysis: Use Eq. (3-49), with $\varepsilon = 0.45$ and $\tau = 2.5$. Estimate diffusivity of nitrogen in hydrogen at 573 K and 20 atm from Eq. (3-36) of Fuller, Schettler, and Giddings, with,

$$M_{A,B} = \frac{2}{\frac{1}{28} + \frac{1}{2.016}} = 3.76$$

From Table 3.1,

$$\sum V_A = 18.5, \qquad \sum V_B = 6.12$$

$$D_{A,B} = \frac{0.00143(573)^{1.75}}{(20)(3.76)^{1/2}[18.5^{1/3} + 6.12^{1/3}]^2} = 0.124 \text{ cm}^2/\text{s}$$

From Eq. (3-49),

$$D_{eff} = \frac{\varepsilon D_{A,B}}{\tau} = \frac{(0.45)(0.124)}{2.5} = 0.022 \text{ cm}^2/\text{s}$$

Exercise 3.20

Subject: Diffusion of hydrogen through the steel wall of a spherical pressure vessel.

Given: Gaseous hydrogen (A) stored at 150 psia and 80°F in a 4-inch inside diameter spherical pressure vessel of steel, with a 0.125-inch wall thickness. Solubility of hydrogen in steel at these conditions = 0.094 lbmol/ft^3. Diffusivity of hydrogen in steel at these conditions = 3.0 x 10^{-9} cm^2/s. Air outside the vessel with zero partial pressure of hydrogen.

Assumptions: Henry's law for solubility of hydrogen in steel. Ideal gas law.

Find:. (a) Initial rate of mass transfer of hydrogen.
(b) Initial rate of pressure decrease inside the vessel.
(c) Time in hours for the pressure inside the vessel to decrease to 50 psia at constant temperature of 80°F.

Analysis: As the hydrogen diffuses through the wall, the pressure in the vessel will decrease.
(a) Assume finite-difference form of Fick's law with no bulk flow effect.
For a spherical shell, Eq. (3-62) gives,

$$n_A = D_{A,B} A_{GM} \frac{\left(c_{A_1} - c_{A_2}\right)}{\left(r_2 - r_1\right)} \qquad (1)$$

$$D_{A,B} = 3\times10^{-9} \frac{(3600)}{(2.54\times12)^2} = 11.6\times10^{-9} \text{ ft}^2/\text{h}$$

$r_2 = (2 + 0.125)/12 = 0.1771$ ft, $r_1 = 2/12 = 0.1667$ ft
$A_{GM} = (A_2A_1)^{1/2}$, $A_2 = 4\pi(r_2)^2 = 4(3.14)(0.1771)^2 = 0.394$ ft^2 ,
$A_1 = 4\pi(r_1)^2 = 4(3.14)(0.1667)^2 = 0.349$ ft^2 , $A_{GM} = (0.394 \text{ x } 0.349)^{1/2} = 0.371$ ft^2
$c_{A_1} = 0.094$ lbmol / ft^3 , $c_{A_2} = 0$

Substituting into Eq. (1),

$$n_A = 11.6\times10^{-9}\,(0.371)\frac{(0.094-0)}{(0.1771-0.1667)} = 3.89\times10^{-8} \text{ lbmol/h}$$

(b) Let m = number of moles of hydrogen in the vessel at any time.

By the ideal gas law, $m = PV/RT$ (2)

$T = 540$°R , $V = \pi D^3/6 = 3.14(4/12)^3/6 = 0.233$ ft^3
Initially, $P = 150$ psia and $m = (150)(0.233)/(10.73)(540) = 0.00603$ mol

Exercise 3.20 (continued)

Analysis: (b) (continued)

Differentiating Eq. (2) with respect to time to determine the rate of change of pressure due to the decrease in the number of moles of hydrogen as it leaves the vessel by diffusion through the walls,

$$\frac{dm}{dt} = n = -\frac{V}{RT}\frac{dP}{dt} \qquad (3)$$

Solving Eq. (3) for the rate of change of pressure, the initial rate of change is,

$$\frac{dP}{dt} = -\frac{nRT}{V} = -\frac{(3.89\times10^{-8})(10.73)(540)}{0.233} = -0.00097 \text{ psia/h}$$

(c) As the pressure in the vessel decreases, the solubility of hydrogen in steel and, therefore, the rate of diffusion of hydrogen through the steel will decrease. Assume Henry's law for the solubility. Then,

$$c_{A_1} = 0.094\left(\frac{P}{150}\right) \qquad (4)$$

From Eqs. (1), (3), and (4), the rate of diffusion of hydrogen as a function of pressure is,

$$n = 3.89\times10^{-8}\left(\frac{P}{150}\right) = -\frac{V}{RT}\frac{dP}{dt} = -\frac{(0.233)}{(10.73)(540)}\frac{dP}{dt} = -0.000040\frac{dP}{dt} \qquad (5)$$

Integrating Eq. (5) from P = 150 psia to 50 psia,

$$\frac{3.89\times10^{-8}}{150(0.000040)}\int_0^t dt = -\int_{150}^{50}\frac{dP}{P} = \ln\left(\frac{150}{50}\right) = 1.0986$$

Therefore, t = 154,000 (1.0986) = 169,500 h , a very long time!

Exercise 3.21

Subject: Mass transfer of gases through a dense polymer membrane

Given: A 0.8-micron thick polyisoprene membrane. Partial pressures of methane and hydrogen on the two sides of the membrane. Membrane properties in Table 14.9.

Assumptions: Applicability of the solution-diffusion model.

Find:. Mass-transfer fluxes for methane and hydrogen

Analysis: The mass-transfer flux of a gas species is given by Eq. (3-52),

$$N_i = \frac{H_i D_i}{\Delta z}\left(\Delta p_i\right) \qquad (1)$$

Membrane thickness = 0.8 micron = 0.8 x 10^{-6} m

Values of D_i and $H_i = S_i$ are given in Table 14.9 and are used with the given partial pressures in Eq. (1) to give the following results:

Species	Δp, Pa	H, mol/m^3-Pa	D, m^2/s	Flux, N, mol/m^2-s
Methane	2.45 x 10^6	1.14 x 10^{-4}	8.0 x 10^{-11}	0.028
Hydrogen	1.80 x 10^6	0.17 x 10^{-4}	109 x 10^{-11}	0.042

Exercise 3.22

Subject: Diffusion of NaCl into stagnant water at 25°C (298 K).

Given: An initial 0.10-inch (0.254-cm) thickness of NaCl sitting below a 3-ft (91.44 cm) depth of water. Solubility of NaCl in water of 36 g NaCl/100 g water. Diffusivity of NaCl in water = 1.2 x 10^{-5} cm^2/s.

Assumptions: Water acts as a semi-infinite slab. Equilibrium at salt-water interface.

Find:. Time and concentration profile of salt in the water, when:
(a) 10% of the salt has dissolved.
(b) 50% of the salt has dissolved.
(c) 90% of the salt has dissolved.

Analysis: Basis: area for mass transfer = 1 $cm^2 = A$
Volume of salt = 1(0.254) = 0.254 cm^3
From Perry's Handbook, density of NaCl = 2.165 g/cm^3
Mass of salt = 2.165 (0.254) = 0.550 g
Molecular weight of NaCl = 58.44 g/mol
Moles of salt = 0.550/58.44 = 0.00941 mol/cm^3
At the solid-liquid interface, NaCl concentration = 36/(100 + 36) x 100% = 26.5 wt%
From Perry's Handbook, density of this solution at 25°C = 1.2 g/cm^3 or
c_s = 0.265 (1.2)/58.44 = 0.00544 mol NaCl/cm^3
Initial concentration of salt in the bulk of the water = $c_o = 0$
For diffusion into a semi-infinite slab, Eq. (3-79) applies, for the number of moles of NaCl, $\mathcal{N}$, transferred in time t. Solving that equation for time t gives,

$$t = \frac{\mathcal{N}^2 \pi}{4A^2 \left(c_s - c_o\right)^2 D_{\text{NaCl}}} = \frac{\mathcal{N}^2 (3.14)}{4(1)^2 \left(0.00544 - 0\right)^2 \left(1.2\times10^{-5}\right)} = 2.21\times10^{9}\ \mathcal{N}^2 \text{ s} \qquad (1)$$

Using Eq. (1), the following times are computed:

Part	Moles transferred	Time, s	Time, h
(a) 10% transferred	0.000941	1,960	0.544
(b) 50% transferred	0.004705	48,900	13.6
(c) 90% transferred	0.008469	159,000	44.0

Use Eq. (3-75) to compute concentration profiles, where $z = 0$ at the salt-water interface,

$$c = c_s \text{erfc}\left(\frac{z}{2\sqrt{D_{\text{NaCl}} t}}\right) = 0.00544\ \text{erfc}\left(\frac{z}{2\sqrt{\left(1.2\times10^{-5}\right)t}}\right) = 0.00544\ \text{erfc}(x) \qquad (2)$$

Exercise 3.22 (continued)

Analysis: (continued)

Solving Eq. (2) for values of x, which fixes the value of c, the following results are obtained:

			z, cm for value of c		
x	erfc (x)	c, mol/cm^3	10% transf.	50% transf.	90% transf.
0.5	0.4795	0.00261	0.157	0.782	1.408
1.0	0.1573	0.000856	0.313	1.565	2.816
1.5	0.0339	0.000184	0.470	1.173	4.224
2.0	0.0047	0.0000256	0.627	3.130	5.632

Since the water layer is 91.44 cm thick, we see that the penetration of the salt is far less than this, such that the assumption of a semi-infinite slab is valid.

Exercise 3.23

Subject: Diffusion of water into 4-inch (10.16-cm) thick wood, with sealed edges, from air of 40% relative humidity.

Given: Equilibrium moisture content for air conditions = 10 lb water/100 lb of dry wood. Diffusivity of water in wood = 8.3 x 10^{-6} cm^2/s. Initially, wood is dry.

Find:. Time for water to penetrate to the center of the wood

Analysis: To determine the time, apply the semi-infinite slab solution of Eq. (3-75). Consider center concentrations of moisture equal to 1%, 0.1%, and 0.01% of the equilibrium surface concentration.
From Eq. (3-75),

$$\theta = \frac{c_{\text{center}} - c_o}{c_s - c_o} = \frac{c_{\text{center}}}{c_s} = \text{erfc}\left(\frac{z}{2\sqrt{D_{\text{water}} t}}\right) = \text{erfc}\left(\frac{5.08}{2\sqrt{(8.3\times10^{-6})t}}\right) = \text{erfc}\,(x) \qquad (1)$$

Using Eq. (1), the following results are obtained,

θ	x	t, s	Time, h
0.01	1.82	234,000	65
0.001	2.33	144,000	40
0.0001	2.75	104,400	29

If the penetration depth is defined as x = 2, then time = 54 h. Regardless, it takes a long time

Exercise 3.24

Subject: Determination of moisture diffusivity in clay brick from measurements of drying rate.

Given: Brick dimensions of 2 in (5.08 cm) by 4 in (10.16 cm) by 6 in (15.24 cm). Uniform initial moisture content of 12 wt%. Equilibrium surface moisture content maintained at 2 wt%. After 5 h, average moisture content is 8 wt%.

Assumptions: Diffusivity is uniform in all directions.

Find: (a) Diffusivity of moisture in clay.
(b) Additional time for average moisture content to reach 4 wt%.

Analysis: (a) By definition in Eq. (3-80), the unaccomplished fractional moisture concentration change after 5 hours = $E_{avg} = (c_s - c_{avg})/(c_s - c_o) = (2\text{-}8)/(2\text{-}12) = 0.60$.

Apply Newman's method for a rectangular slab, given by Eq. (3-86). Thus,

$E_{avg} = E_x E_y E_z$ (1)

where the three E values are average values.

These values are plotted in Fig. 3.9 as a function of the Fourier number for mass transfer, using half dimensions, a, b, and c in the x, y, and z directions. Thus, using units of cm and seconds, the three Fourier numbers are:

$Dt/a^2 = D\ (5 \times 3600)/(2.54)^2 = 349\ D$ to get E_x
$Dt/b^2 = D\ (5 \times 3600)/(5.08)^2 = 698\ D$ to get E_y
$Dt/c^2 = D\ (5 \times 3600)/(7.62)^2 = 1047\ D$ to get E_z

An iterative procedure is used to determine the diffusivity, D.

1. Assume a value of D in cm^2/s.
2. Compute the three Fourier numbers.
3. From Fig. 3.9, read off values of E_x , E_y , and E_z for the corresponding Fourier numbers.
4. Calculate E_{avg} from Eq. (1). If it does not equal 0.60, repeat the four steps.

This procedure leads to the following results, where the first assumed value of D is obtained by reading the Fourier number for $E_{avg} = 0.6^{1/3} = 0.84$ for Fig. 3.9 and using it with the Fourier number for the y dimension to compute D.

Assumed D, cm^2/s	Dt/a^2	Dt/b^2	Dt/c^2	E_x	E_y	E_z	E_{avg}
3.2×10^{-5}	0.011	0.022	0.033	0.92	0.84	0.81	0.626
3.4×10^{-5}	0.012	0.024	0.036	0.91	0.83	0.80	0.604

Therefore, $D = 3.4 \times 10^{-5}\ cm^2/s$.

(b) At 4 wt% average moisture, $E_{avg} = (2\text{-}4)/(2\text{-}12) = 0.2$

The three Fourier numbers, with time in hours, are $2.37 \times 10^{-3}\ t$, $4.74 \times 10^{-3}\ t$, and $7.11 \times 10^{-3}\ t$. By iteration, to satisfy Eq. (1), using Fig. 3.9, time = 32 h or additional time = 27 h.

Exercise 3.25

Subject: Diffusion of moisture from a 2-inch (5.08 cm) diameter (a = 2.54 cm radius) spherical ball of clay into air.

Given: Initial moisture content of clay = 10 wt%. Equilibrium moisture content of clay-air interface = 3 wt%. Diffusivity of water in clay = $D = 5 \times 10^{-6}$ cm^2/s.

Assumptions: Diffusivity is uniform throughout clay.

Find: Time for average moisture content to drop to 5 wt%.

Analysis: By definition in Eq. (3-80), the unaccomplished fractional moisture concentration change after time, t is:

$$E_{avg} = (c_s - c_{avg})/(c_s - c_o) = (3\text{-}5)/(3\text{-}10) = 0.286$$

The lower curve in Fig. 3.9 relates that change to the Fourier number. From the figure,

$$N_{Fo_M} = 0.08 = \frac{Dt}{a^2} = \frac{\left(5\times10^{-6}\right)}{2.54^2}t = 7.75\times10^{-7}\,t$$

Solving Eq. (1), gives $t = 1.03 \times 10^5$ s = 28.7 h

Exercise 3.26

Subject: Absorption of pure oxygen into a downward flowing laminar water film

Given: Film, at 10 atm and 25°C, flows down a wall, with L = 1 m high and W = 6 cm (0.06 m) wide. Flow is laminar, without ripples, at a Reynolds number of 50.

Assumptions: Diffusivity of O_2 in water = 2.5 x 10^{-5} cm^2/s = 2.5 x 10^{-9} m^2/s. Solubility of O_2 in water = a mole fraction of 2.3 x 10^{-4} = x_{O_2}. Negligible vaporization of water.

Find: Rate of absorption

Analysis: The exercise is similar to Example 3.13. By material balance on the O_2 in the water film, Eq. (3-103) gives:

$$n_{O_2} = \bar{u}_y \delta W \left[\left(\bar{c}_{O_2} \right)_L - \left(\bar{c}_{O_2} \right)_o \right] \qquad (1)$$

where, W = 0.06 m and $\left(\bar{c}_{O_2} \right)_o$ = oxygen concentration in the water at the top of the film = 0.

From Eq. (3-92), the bulk average film velocity is,

$$\bar{u}_y = \frac{\rho g \delta^2}{3\mu} \qquad (2)$$

where from Eq. (3-92), film thickness = $\delta = \left(\frac{3\mu\Gamma}{\rho^2 g} \right)^{1/3}$ (3)

The Reynolds number for film flow is given by (3-93). For a water viscosity, μ_L= 0.89 cP = 0.00089 kg/m-s at 25°C, the film flow rate per unit width of film is,

$$\Gamma = N_{Re} \frac{\mu}{4} = 50 \frac{0.00089}{4} = 0.01112 \text{ kg/m-s}$$

From Eq. (3), the film thickness for ρ = 1,000 kg/m^3 and g = 9.807 m/s^2 is,

$$\delta = \left[\frac{3(0.00089)(0.01112)}{(1{,}000)^2 (9.807)} \right]^{1/3} = 1.45 \times 10^{-4} \text{ m}$$

$$\text{From Eq. (2), } \bar{u}_y = \frac{(1{,}000)(9.807)(1.45 \times 10^{-4})^2}{3(0.00089)} = 0.0772 \text{ m/s}$$

Combining Eqs. (3-103) and (3-113), we obtain an equation for the O_2 concentration in the water at the bottom of the film, noting that with pure oxygen gas, all of the mass-transfer resistance resides in the liquid water film:

$$\left(\bar{c}_{O_2} \right)_L = \left(c_{O_2} \right)_i - \left[\left(c_{O_2} \right)_i - \left(\bar{c}_{O_2} \right)_o \right] \exp \left[- \frac{k_{c_{avg}} \left(\frac{A}{W} \right)}{\bar{u}_y \delta} \right] \qquad (4)$$

Exercise 3.26 (continued)

Analysis: (continued)

The total concentration in the liquid is approximately that of water =

$$c = \rho/M_{\text{water}} = 1{,}000/18.02 = 55.5 \text{ kmol/m}^3.$$

The concentration of oxygen in the water at the interface =

$$\left(c_{O_2}\right)_i = x_{O_2}\, c = 2.3 \text{ x } 10^{-4}\ (55.5) = 0.0128 \text{ kmol/m}^3.$$

The average mass-transfer coefficient is given by (3-110), provided that the factor η, given by Eq. (3-100), is greater than 0.1. This equation requires the Schmidt number. From Eq. (3-101),

$$N_{Sc} = \frac{\mu}{\rho D_{O_2,H_2O}} = \frac{0.00089}{(1{,}000)(2.5\times10^{-9})} = 356$$

From Eq. (3-100),

$$\eta = \frac{8/3}{N_{Re}N_{Sc}(\delta/L)} = \frac{8/3}{(50)(356)\left(1.45\times10^{-4}/1\right)} = 1.033\ (>\ 0.1)$$

From Eq. (3-110),

$$k_{c_{avg}} = \frac{\overline{u}_y\delta}{L}\left(0.241+5.1213\eta\right) = \frac{0.0772(1.45\times10^{-4})}{1}\left[0.241+5.1213(1.033)\right] = 6.2\times10^{-5}\ \text{m/s}$$

Area for mass transfer = $A = LW = (1)(0.06) = 0.06$ m^2. From Eq. (4),

$$\left(\overline{c}_{O_2}\right)_L = 0.0128-(0.0128-0)\exp\left[-\frac{6.2\times10^{-5}\left(\frac{0.06}{0.06}\right)}{(0.0772)(1.45\times10^{-4})}\right] = 0.01275 \text{ kmol/m}^3$$

Thus, the water is better than 99% saturated with oxygen.

From Eq. (1),

$$n_{O_2} = (0.0772)\left(1.45\times10^{-4}\right)(0.06)(0.01275-0) = 8.6\times10^{-9} \text{ kmol/s}$$

Exercise 3.27

Subject: Absorption of pure carbon dioxide into a downward flowing laminar water film.

Given: Results in Example 3.13, including: D_{AB} = 1.96 x 10^{-5} cm^2/s, $\overline{u}_y$ = 0.0486 m/s, δ = 1.15 x 10^{-2} cm, and $\left(\overline{c}_{CO_2}\right)_o = 0$

Find: Height, y, from the top of the film where the water is 50% saturated with CO_2.

Analysis: At height, $y = L$, from the top of the film, $\left(\overline{c}_{CO_2}\right)_y / \left(c_{CO_2}\right)_i = 0.5$.

If we use Eqs. (3-99) and (3-100), we do not have to compute the average mass-transfer coefficient.

Compute the value of η from (3-99):

$$1-0.5 = 0.5 = 0.7857\exp\left(-5.1213\eta\right) + 0.09726\exp\left(-39.661\eta\right) + 0.036093\exp\left(-106.25\eta\right)$$

Solving this nonlinear equation for η with a spreadsheet, η = 0.0894

From a rearrangement of Eq. (3-100),

$$L = \frac{3\delta^2 \overline{u_y}\eta}{2D_{AB}} = \frac{3\left(1.15\times10^{-2}\right)^2 (4.86)(0.0894)}{2\left(1.96\times10^{-5}\right)} = 4.4 \text{ cm}$$

Exercise 3.28

Subject: Evaporation of water (A) from a film on a flat plate into air (B) at 1 atm (101.3 kPa) and 25°C (298 K) that is flowing past the plate.

Given: Free-stream air velocity = u_o = 2 m/s. Plate length = L = 2 inches = 0.0508 m. Diffusivity of water vapor in air = $D_{A,B}$ = 0.25 cm^2/s = 0.25 x 10^{-4} m^2/s

Assumptions: Ideal gas law. Laminar boundary-layer flow of the air. Negligible absorption of air by the water film. Equilibrium at the air-water interface.

Find: Evaporation flux at 50% of $L = x$ = 0.0254 m from the leading edge of the plate.

Analysis: First check to see if the boundary layer is laminar. From Perry's Handbook, for air at 25°C, μ = 0.018 cP = 1.8 x 10^{-5} kg/m-s. From the ideal gas law,

$\rho = PM/RT = (101.3)(29)/(8.314)(298) = 1.186$ kg/m^3

From Eq. (3-127), at x = 0.0254 m,

$$N_{\mathrm{Re}_x} = \frac{x u_o \rho}{\mu} = \frac{(0.0254)(2)(1.186)}{1.8\times10^{-5}} = 3{,}350$$

Therefore, the boundary layer is laminar, since the criterion is less than 5 x 10^5.

Since the liquid film is pure water, the only mass-transfer resistance for evaporation of water into air is in the air boundary layer. From Eq. (3-105), the molar mass-transfer flux of water is,

$$\frac{n_{\mathrm{H_2O}}}{A} = k_{c_x}\left[\left(c_{\mathrm{H_2O}}\right)_i - \left(c_{\mathrm{H_2O}}\right)_o\right] \qquad (1)$$

For a laminar boundary layer, the local mass-transfer coefficient can be obtained from Eq. (3-132), which can be rearranged to give:

$$k_{c_x} = 0.332\frac{D_{A,B}}{x}\left(N_{\mathrm{Re}_x}\right)^{1/2}\left(N_{\mathrm{Sc}}\right)^{1/3} \qquad (2)$$

From Eq. (3-101), $N_{\mathrm{Sc}} = \dfrac{\mu}{\rho D_{A,B}} = \dfrac{1.8\times10^{-5}}{(1.186)\left(0.25\times10^{-4}\right)} = 0.607$

From Eq. (2), $k_{c_x} = 0.332\dfrac{\left(0.25\times10^{-4}\right)}{(0.0254)}(3{,}350)^{1/2}(0.607)^{1/3} = 0.16$ m/s

At 25°C, vapor pressure of water = 0.46 psia, Therefore, mole fraction of water at the interface = $\left(y_{\mathrm{H_2O}}\right)_i$ = 0.46/14.7 = 0.0313. $\left(c_{\mathrm{H_2O}}\right)_i = \left(y_{\mathrm{H_2O}}\right)_i \rho/M_{\mathrm{air}}$ = 0.0313(1.186)/29 = 0.0128 kmol/m^3.From Eq. (1), $\dfrac{n_{\mathrm{H_2O}}}{A} = (0.016)[0.00128-0] = 2.05\times10^{-5}$ kmol/s-m^2

Exercise 3.29

Subject: Sublimation of a thin, flat plate of naphthalene (A) into air (B) at 100°C (373 K) and 1 atm (101.3 kPa) that is flowing past the plate.

Given: Length of plate, L, is 1m. Reynolds number at the trailing edge of the plate = $N_{\mathrm{Re}_L} = 5\times10^5$ = limit of laminar boundary-layer flow.

Find: (a) Average rate of sublimation.
(b) Local rate of sublimation at x = 0.5 m from leading edge of plate.

Analysis: This exercise is similar to Example 3.14, which also deals with the sublimation of naphthalene into air at the same temperature and pressure. Therefore, the physical properties used in Example 3.14 apply here. The only mass-transfer resistance is in the gas phase.
(a) From Eq. (3-105), the average rate of sublimation per unit area is,

$$n_{\mathrm{A,B}} / A = k_{c_{\mathrm{avg}}}\left[\left(c_{\mathrm{A}}\right)_i - \left(c_{\mathrm{A}}\right)_o\right] \qquad (1)$$

From Eqs. (3-137) and (3-138), the average mass-transfer coefficient is given by,

$$k_{c_{\mathrm{avg}}} = 0.664\frac{D_{\mathrm{A,B}}}{L}\left(N_{\mathrm{Re}_L}\right)^{1/2}\left(N_{\mathrm{Sc}}\right)^{1/3} = 0.664\frac{0.94\times10^{-5}}{1}\left(5\times10^5\right)^{1/2}\left(2.41\right)^{1/3} = 0.0059\ \mathrm{m/s}$$

From Example (3.14), $\left(c_{\mathrm{A}}\right)_i$ =4.3 x 10^{-2} kmkol/m^3 and $\left(c_{\mathrm{A}}\right)_o = 0$. From Eq. (1),

$$n_{\mathrm{A,B}} / A = 0.0059\left(4.3\times10^{-2} - 0\right) = 2.54\times10^{-4}\ \mathrm{kmol/s\text{-}m^2}$$

(b) From Eqs. (3-132) and (3-133), using physical properties in Example (3.14), with a Reynolds number of one-half of 5 x 10^5, since x = 0.5 m,

$$k_{c_x} = 0.332\frac{D_{\mathrm{A,B}}}{x}\left(N_{\mathrm{Re}_x}\right)^{1/2}\left(N_{\mathrm{Sc}}\right)^{1/3} = 0.332\frac{0.94\times10^{-5}}{0.5}\left(2.5\times10^5\right)^{1/2}\left(2.41\right)^{1/3} = 0.00417\ \mathrm{m/s}$$

From Eq. (3-105), the local rate of sublimation per unit area is,

$$n_{\mathrm{A,B}} / A = k_{c_x}\left[\left(c_{\mathrm{A}}\right)_i - \left(c_{\mathrm{A}}\right)_o\right] = 0.00417\left(4.3\times10^{-2} - 0\right) = 1.79\times10^{-4}\ \mathrm{kmol/s\text{-}m^2}$$

Exercise 3.30

Subject: Sublimation of a straight, circular tube of naphthalene (A) into air (B) at 100°C (373 K) and 1 atm that flows through it in laminar flow.

Given: Tube diameter, D, is 5 cm (0.05 m). Reynolds number = N_{Re} = 1,500. Physical properties in Example 3.14.

Assumptions: Fully established laminar-flow velocity profile for air entering the tube. Negligible pressure drop. Equilibrium at naphthalene-air interface.

Find: Tube length, x, for average naphthalene mole fraction in exiting air, $\bar{y}_{\mathrm{A}_L}$, to equal 0.005.

Analysis: From Example 3.14, $y_{\mathrm{A}_i} = P_{\mathrm{A}}^s / P = 10/760 = 0.0132$

By material balance for sublimation of naphthalene into air, the rate of mass transfer over the tube length must be:

$$n_{\mathrm{A}} = \bar{u}_x S\left[\left(c_{\mathrm{A}}\right)_x - \left(c_{\mathrm{A}}\right)_0\right] \qquad (1)$$

This rate of mass transfer is given by (3-105), which with a log-mean driving force is,

$$n_{\mathrm{A}} = k_{c_{\mathrm{avg}}} A \frac{\left\{\left[\left(c_{\mathrm{A}}\right)_i - \left(\bar{c}_{\mathrm{A}}\right)_0\right] - \left[\left(c_{\mathrm{A}}\right)_i - \left(\bar{c}_{\mathrm{A}}\right)_x\right]\right\}}{\ln \dfrac{\left[\left(c_{\mathrm{A}}\right)_i - \left(\bar{c}_{\mathrm{A}}\right)_0\right]}{\left[\left(c_{\mathrm{A}}\right)_i - \left(\bar{c}_{\mathrm{A}}\right)_x\right]}} \qquad (2)$$

For the entering air, $\left(\bar{c}_{\mathrm{A}}\right)_0 = 0$. Therefore, combining Eqs. (1) and (2), and solving for $k_{c_{\mathrm{avg}}}$,

$$k_{c_{\mathrm{avg}}} = \frac{\bar{u}_x S}{A} \ln \frac{\left[\left(c_{\mathrm{A}}\right)_i - \left(\bar{c}_{\mathrm{A}}\right)_0\right]}{\left[\left(c_{\mathrm{A}}\right)_i - \left(\bar{c}_{\mathrm{A}}\right)_x\right]} \qquad (3)$$

From the tube geometry, $S = \pi D^2/4 = (3.14)(0.05)^2/4 = 0.00196\ \mathrm{m}^2$

$A = \pi D x = (3.14)(0.05)x = 0.157\ x\ \mathrm{m}^2$

For laminar flow, Eq. (3-150) applies, which contains the Peclet number, Eq. (3-102):

$$N_{\mathrm{Pe}_M} = N_{\mathrm{Re}} N_{\mathrm{Sc}} = (1{,}500)(2.41) = 3{,}620$$

From Eq. (3-150), using the definition of the Sherwood number in Eq. (3-148), but for average conditions,

Exercise 3.30 (continued)

Analysis: (continued)

$$k_{c_{avg}} = \frac{D_{A,B}}{D} N_{Sh_{avg}} = \frac{D_{A,B}}{D}\left\{3.66 + \frac{0.0668\left[N_{Pe_M}/(x/D)\right]}{1+0.04\left[N_{Pe_M}/(x/D)\right]^{2/3}}\right\} = \frac{0.94\times10^{-5}}{0.05}\left\{3.66 + \frac{0.0668\left[3620/(x/0.05)\right]}{1+0.04\left[3620/(x/0.05)\right]^{2/3}}\right\} =$$

$$= 0.000688 + \frac{0.00227}{x\left[1+1.28/x^{2/3}\right]} \qquad (4)$$

$$N_{Re} = \frac{D\bar{u}_x\rho}{\mu}, \text{ therefore, } \bar{u}_x = \frac{N_{Re}\mu}{D\rho} = \frac{(1{,}500)(0.000215)}{(5)\left(\frac{0.0327(29)}{1{,}000}\right)} = 68 \text{ cm/s} = 0.68 \text{ m/s}$$

$$\ln\frac{\left[(c_A)_i - (\bar{c}_A)_0\right]}{\left[(c_A)_i - (\bar{c}_A)_x\right]} = \ln\frac{\left[(y_A)_i - (\bar{y}_A)_0\right]}{\left[(y_A)_i - (\bar{y}_A)_x\right]} = \ln\frac{[0.0132-0.0]}{[0.0132-0.005]} = 0.476$$

Combining Eqs. (3) and (4),

$$0.000688 + \frac{0.00227}{x\left[1+1.28/x^{2/3}\right]} = \frac{(0.68)(0.00196)}{0.157x}(0.476) = \frac{0.00404}{x} \qquad (5)$$

Rearranging Eq. (5),

$$f\{x\} = 0.000688 + \frac{0.00227}{x\left[1+1.28/x^{2/3}\right]} - \frac{0.00404}{x} = 0 \qquad (6)$$

Solving the nonlinear Eq. (6),

$x = 3.73$ m

Exercise 3.31

Subject: Evaporation of a spherical water (A) drop into still, dry air (B).

Given: Initial drop diameter = d_p = 1 mm = 0.1 cm. Air temperature = T = 38°C. Drop temperature = 14.4°C. Pressure = P = 1 atm.

Assumptions: Ideal gas law. Quasi-steady-state evaporation of water into air. That is, the rate of accumulation of water vapor in the air is negligible compared to the rate of diffusion of the water through the air.

Find: (a) A Sherwood number of 2 for mass transfer from the drop surface to the air.
(b) The initial mass of the drop.
(c) The initial rate of evaporation of the drop in g/s.
(d) The time in seconds for the drop diameter to be reduced to 0.2 mm = 0.02 cm.
(e) The initial rate of heat transfer to the drop. If insufficient to supply the necessary heat, what will happen?

Analysis: (a) With a pure water drop, the only resistance to mass transfer is in the air by ordinary molecular diffusion from the drop surface out to infinity. With the quasi-steady-state assumption, Eq. (3-74) for diffusion through a spherical region becomes,

$$\frac{\partial c_A}{\partial t} = \frac{D_{AB}}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial c_A}{\partial r}\right) = 0 \qquad (1)$$

Therefore,

$$\frac{d}{dr}\left(r^2 \frac{dc_A}{dr}\right) = 0 \qquad (2)$$

Integrating Eq. (2) twice,

$c_A = -\frac{C_1}{r} + C_2$ with boundary conditions of: $c_A = c_{A_s}$ at $r = r_s$ and $c_A = 0$ at $r = \infty$

With these boundary conditions, the two constants of integration are evaluated to give for the region outside the drop,

$$c_A = c_{A_s}\left(\frac{r_s}{r}\right) \qquad (3)$$

The rate of mass transfer from the drop surface to the bulk air in terms of a mass-transfer coefficient, Eq. (3-105), can be equated to the diffusion rate from the drop surface, as given by Fick's first law, as in Eq. (3-63), to give the following equation, which is similar to Eq. (3-106),

Exercise 3.31 (continued)

Analysis: (a) (continued)

$$n_A = k_c A\left(c_{A_s} - c_{A_\infty}\right) = -D_{AB} A \left.\frac{dc_A}{dr}\right|_{r=r_s} \qquad (4)$$

Differentiating Eq. (3), $$\left.\frac{dc_A}{dr}\right|_{r=r_s} = c_{A_s} r_s \left.\left(-\frac{1}{r^2}\right)\right|_{r=r_s} = -\frac{c_{A_s}}{r_s} \qquad (5)$$

Substituting Eq. (5) into Eq. (4),

$$k_c A\left(c_{A_s} - 0\right) = -D_{AB} A\left(-\frac{c_{A_s}}{r_s}\right) \qquad (6)$$

Simplifying and rearranging Eq. (6) into the form of a Sherwood number, like Eq. (3-112), with a characteristic length of the drop diameter,

$$N_{Sh} = \frac{k_c (2r_s)}{D_{AB}} = \frac{k_c d_p}{D_{AB}} = 2 \qquad (7)$$

(b) Initial mass of a spherical drop = $m = \rho V = \rho\left(\pi \frac{d_p^3}{6}\right) = (1.0)\left((3.14)\frac{(0.1)^3}{6}\right) = 5.23\times10^{-4}$ g

(c) Initial rate of evaporation can be obtained for Fick's law or from Eq. (3-105) with a mass-transfer coefficient. From Eq. (3-105),

$$n_A = k_c A\left(c_{A_s} - c_{A_\infty}\right) = k_c A c\left(y_{A_s} - 0\right) \quad (8)$$

The binary gas diffusivity is obtained from Eq. (3-36) using $T = 38^\circ$C = 311 K and P = 1 atm.

$$M_{A,B} = \frac{2}{\frac{1}{18} + \frac{1}{29}} = 22.2$$

From Table 3.1, $\left(\sum V\right)_A = 13.1$, $\left(\sum V\right)_B = 19.7$

$$D_{AB} = \frac{0.00143(311)^{1.75}}{(1)(22.2)^{1/2}\left[(13.1)^{1/3} + (19.7)^{1/3}\right]^2} = 0.273 \text{ cm}^2/\text{s}$$

Exercise 3.31 (continued)

Analysis: (c) (continued)

From Eq. (7),

$$k_c = \frac{2D_{AB}}{d_p} = \frac{(2)(0.273)}{0.1} = 5.46 \text{ cm/s}$$

Area for mass transfer = area of the drop = $A = \pi d_p^2 = (3.14)(0.1)^2 = 0.0314 \text{ cm}^2$

From the ideal gas law, the total gas concentration is,

$$c = \frac{P}{RT} = \frac{1}{(82.06)(311)} = 3.92 \times 10^{-5} \text{ mol/cm}^3$$

The mole fraction of water in the air at the surface of the drop is obtained from the vapor pressure of water at 14.4°C = 12.3 torr, with a total pressure of 1 atm = 760 torr,

$$y_{A_s} = \frac{P_A^s}{P} = \frac{12.3}{760} = 0.0162$$

Substituting into Eq. (8),

$$n_A = (5.46)(0.0314)(3.92 \times 10^{-5})(0.0162 - 0) = 1.09 \times 10^{-7} \text{ mol/s} = 1.96 \text{ x } 10^{-6} \text{ g/s}$$

(d) At any instant of time, the rate of evaporation by mass transfer = rate of loss of drop. Let $\mathcal{N}$ = moles of water drop at any time, t. Then,

$$k_c A c\left(y_{A_s} - 0\right) = -\frac{d\mathcal{N}}{dt} = -\frac{\rho_{water}}{M_{water}} \frac{dV_{drop}}{dt} \qquad (9)$$

$$V_{drop} = \frac{\pi d_p^3}{6}, \quad \text{Therefore,} \quad \frac{dV_{drop}}{dt} = \frac{3\pi d_p^2}{6} \frac{d\left(d_p\right)}{dt}$$

$$A = \pi d_p^2, \quad \text{From Eq. (7),} \quad k_c = \frac{2D_{AB}}{d_p}$$

Combining these equations and solving for dt,

$$dt = -\frac{\rho_{water} d_p}{4 M_{water} D_{AB} c y_{A_s}} d\left(d_p\right) \qquad (10)$$

Integrating Eq. (10) from the initial drop diameter, d_{p_1}, to the later drop diameter, d_{p_2},

Exercise 3.31 (continued)

Analysis: (continued)

$$t = \frac{\rho_{water}}{4M_{water}D_{AB}cy_{A_s}}\left(\frac{d_{p_1}^2 - d_{p_2}^2}{2}\right) = \frac{(1.0)}{4(18)(0.273)(3.92\times10^{-5})(0.0162)}\left[\frac{(0.1)^2-(0.02)^2}{2}\right] = 380 \text{ s}$$

(e) By analogy to mass transfer, the rate of heat transfer from the air to the drop is,

$$Q = hA(T_s - T_\infty), \quad \text{where } N_{Nu} = 2 = \frac{hd_p}{k} \text{ or } h = \frac{2k}{d_p}$$

From Perry's Handbook, thermal conductivity of air at 38°C = k = 58 x 10^{-6} cal/s-cm^2-(°C/cm)

h = 2(58 x 10^{-6})/0.1 = 0.00116 cal/s-cm^2-°C.

T_s - T_∞ = 38 - 14.4 = 23.6°C.

A = 0.0314 cm^2

Therefore, the initial rate of heat transfer = Q = 0.00116(0.0414)(23.6) = 0.00086 cal/s

The rate of heat transfer required to maintain the drop at 14.4°C, based on the initial drop diameter is,

$$Q_{needed} = (n_{evap}M_{water})\left[\Delta H_{vap} + (C_P)_{water\ vapor}(T_s - T_\infty)\right]$$
$$= (1.96\times10^{-6})\left[589 + 0.44(38-14.4)\right] = 0.001176 \text{ cal/s}$$

since, from Perry's Handbook, the heat of vaporization of water at 14.4°C is 589 cal/g and the specific heat of steam is 0.44 cal/g-°C.

Because the heat needed is greater than the rate of heat transfer, the temperature of the drop will decrease with time initially.

Exercise 3.32

Subject: Dissolution of benzoic acid when water flows in turbulent motion.through a straight, circular tube of it

Given: Tube has an initial inside diameter, D, of 2 inches (5.08 cm), with a length, L, of 10 ft (305 cm). Water at 25°C flows through the tube, with a velocity, $\overline{u}_x$, of 5 ft/s (152 cm/s). Physical properties in Example 3.15.

Assumptions: Fully developed turbulent flow.

Find: Average concentration of benzoic acid in the water exiting the tube.

Analysis: The rate of increase in benzoic acid (A) in the water (B), by the continuity equation, equals the rate of mass transfer. The only resistance to mass transfer is in the water. Using Eq. (3-105), with a log mean driving force,

$$n_{\mathrm{A}} = \overline{u}_x S\left(\overline{c}_{\mathrm{A_{out}}} - \overline{c}_{\mathrm{A_{in}}}\right) = k_c A\left(c_{\mathrm{A_{wall}}} - \overline{c}_{\mathrm{A}}\right)_{\mathrm{LM}} = k_c A \frac{\left[\left(c_{\mathrm{A_{wall}}} - \overline{c}_{\mathrm{A_{in}}}\right) - \left(c_{\mathrm{A_{wall}}} - \overline{c}_{\mathrm{A_{out}}}\right)\right]}{\ln \dfrac{\left(c_{\mathrm{A_{wall}}} - \overline{c}_{\mathrm{A_{in}}}\right)}{\left(c_{\mathrm{A_{wall}}} - \overline{c}_{\mathrm{A_{out}}}\right)}} \qquad (1)$$

Because $\overline{c}_{\mathrm{A_{in}}} = 0$, Eq. (1) simplifies to,

$$\frac{k_c A}{\overline{u}_x S} = \ln \frac{c_{\mathrm{A_{wall}}}}{c_{\mathrm{A_{wall}}} - \overline{c}_{\mathrm{A_{out}}}} \quad \text{or solving,}$$

$$\overline{c}_{\mathrm{A_{out}}} = c_{\mathrm{A_{wall}}}\left[1 - \exp\left(-\frac{k_c A}{\overline{u}_x S}\right)\right] \qquad (2)$$

Area for mass transfer = $A = \pi DL = 3.14(5.08)(305) = 4{,}870\ \mathrm{cm}^2$
Cross-sectional area for flow = $S = \pi D^2/4 = 3.14(5.08)^2/4 = 20.25\ \mathrm{cm}^2$
Use the Chilton-Colburn j-factor method to obtain k_c. Combining Eqs. (3-165) and (3-166),

$$k_c = \frac{0.023G}{\rho}\frac{\left(N_{\mathrm{Re}}\right)^{-0.2}}{\left(N_{\mathrm{Sc}}\right)^{2/3}} = \frac{0.023\overline{u}_x\rho}{\rho}\frac{\left(N_{\mathrm{Re}}\right)^{-0.2}}{\left(N_{\mathrm{Sc}}\right)^{2/3}} = 0.023\overline{u}_x\frac{\left(N_{\mathrm{Re}}\right)^{-0.2}}{\left(N_{\mathrm{Sc}}\right)^{2/3}} \qquad (3)$$

$$N_{\mathrm{Re}} = \frac{DG}{\mu} = \frac{D\overline{u}_x\rho}{\mu} = \frac{(5.08)(152)(1.0)}{0.0089} = 86{,}800 \text{ (confirms turbulent flow)} \qquad (4)$$

$$N_{\mathrm{Sc}} = \frac{\mu}{\rho D_{\mathrm{AB}}} = \frac{0.0089}{(1.0)(9.18\times10^{-6})} = 970 \qquad (5)$$

Exercise 3.32 (continued)

Analysis: (continued)

Substitution of the results of Eqs. (4) and (5) into (3) gives,

$$k_c = 0.023(152)\frac{(86{,}800)^{-0.2}}{(970)^{2/3}} = 0.00367 \text{ cm/s}$$

From Example 3.15, equilibrium exists at the inside wall of the tube such that the concentration of benzoic acid in the water is at its equilibrium value of $c_{A_{wall}} = 0.0034$ g/cm^3

From Eq. (2),

$$\overline{c}_{A_{out}} = 0.0034\left[1 - \exp\left(-\frac{(0.00367)(4{,}870)}{(152)(20.25)}\right)\right] = 0.000020 \text{ g/cm}^3$$

Therefore, the concentration of benzoic acid in the exiting water is way below the solubility value.

Exercise 3.33

Subject: Sublimation of a long, circular cylinder of naphthalene (A) to air (B) flowing normal to it.

Given: Long, circular cylinder of 1-inch (0.0254 m) diameter, D. Air at 100°C (373 K) and 1 atm flows at a Reynolds number, N_{Re} , of 50,000. Physical properties given in Example 3.14.

Assumptions: Negligible bulk flow effect.

Find: Average sublimation flux in kmol/s-m^2.

Analysis: Only mass-transfer resistance is in the air. From Eq. (3-105), the flux is,

$$n_A / A = N_A = k_c\left(c_{A_s} - c_{A_\infty}\right) \qquad (1)$$

Using the Chilton-Colburn analogy, Eq. (3-169) applies, which combined with Eq. (3-165) gives,

$$k_c = \frac{0.0266G}{\rho}\frac{\left(N_{Re}\right)^{-0.195}}{\left(N_{Sc}\right)^{2/3}} \qquad (2)$$

From the Reynolds number, mass velocity, G, is, using $\mu = 0.0215$ cP (2.15×10^{-5} kg/s-m^2),

$$G = \frac{N_{Re}\mu}{D} = \frac{(50{,}000)(2.15\times10^{-5})}{0.0254} = 42.3 \text{ kg/s-m}^2$$

From Example 3.14, gas density = 0.0327(29) = 0.948 kg/m^3 and $N_{Sc} = 2.41$.

From Eq. (2), $k_c = \dfrac{0.0266G}{\rho}\dfrac{\left(N_{Re}\right)^{-0.195}}{\left(N_{Sc}\right)^{2/3}} = \dfrac{0.0266(42.3)}{0.948}\dfrac{(50{,}000)^{-0.195}}{(2.41)^{2/3}} = 0.080$ m/s

Using properties in Example 3.14,

$$c_{A_s} = y_{A_s}c = \frac{P_A^s}{P}c = \frac{10}{760}(0.0327) = 4.3\times10^{-4} \text{ kmol/m}^3 \quad \text{and} \quad c_{A_\infty} = 0$$

From Eq. (1), $N_A = k_c\left(c_{A_s} - c_{A_\infty}\right) = (0.080)(4.3\times10^{-4} - 0) = 3.44\times10^{-5}$ kmol/s-m^2

Exercise 3.34

Subject: Sublimation of a sphere of naphthalene (A) into air (B) flowing past it.

Given: Sphere of 1-inch (0.0254 m) diameter, D. Air at 100°C (373 K) and 1 atm flows at a Reynolds number, N_{Re} , of 50,000. Physical properties given in Example 3.14.

Assumptions: Negligible bulk flow effect.

Find: Initial average sublimation flux in kmol/s-m^2 and comparison to that in a bed packed with the same spheres at a void fraction of 0.5.

Analysis: Only mass-transfer resistance is in the air. From Eq. (3-105), the flux is,

$$n_A / A = N_A = k_c\left(c_{A_s} - c_{A_\infty}\right) \qquad (1)$$

Using the Chilton-Colburn analogy, Eq. (3-170) applies, which combined with Eq. (3-165) gives,

$$k_c = \frac{0.37G}{\rho}\frac{\left(N_{Re}\right)^{-0.4}}{\left(N_{Sc}\right)^{2/3}} \qquad (2)$$

From the Reynolds number, mass velocity, G, is, using $\mu = 0.0215$ cP (2.15 x 10^{-5} kg/s-m^2),

$$G = \frac{N_{Re}\mu}{D} = \frac{(50{,}000)(2.15\times10^{-5})}{0.0254} = 42.3 \text{ kg/s-m}^2$$

From Example 3.14, gas density = 0.0327(29) = 0.948 kg/m^3 and $N_{Sc} = 2.41$.

From Eq. (2), $k_c = \dfrac{0.37(42.3)}{0.948}\dfrac{(50{,}000)^{-0.4}}{(2.41)^{2/3}} = 0.121$ m/s

Using properties in Example 3.14,

$$c_{A_s} = y_{A_s}c = \frac{P_A^s}{P}c = \frac{10}{760}(0.0327) = 4.3\times10^{-4} \text{ kmol/m}^3 \quad \text{and} \quad c_{A_\infty} = 0$$

From Eq. (1), $N_A = k_c\left(c_{A_s} - c_{A_\infty}\right) = (0.121)(4.3\times10^{-4} - 0) = 5.20\times10^{-5}$ kmol/s-m^2

From Eq. (3-171), packed bed correlation can't used with N_{Re} = 50,000.

Exercise 3.35

Subject: Experimental data for stripping of CO_2 (A) from water by air (B) in a wetted-wall tube.

Given: Location in the tube where P = 10 atm, T =25°C (298 K), CO_2 flux from water into air = N_A = 1.62 lbmol/h-ft^2, partial pressure of CO_2 at gas-liquid interface = p_{A_i} = 8.2 atm, and partial pressure of CO_2 in bulk air = p_{A_b} = 0.1 atm. Diffusivity of CO_2 in air = D_{AB} = 1.6 x 10^{-2} cm^2/s.

Assumptions: Neglect stripping of water, but account for the bulk flow effect. Mass-transfer resistance of the water film does not need to be considered. Ideal gas law.

Find: Using the film theory, find the mass-transfer coefficient, k_c , for the gas phase and the film thickness, δ.

Analysis: Solve the problem in cgs units. From Eq. (3-105) and a rearrangement of Eq. (3-189),

$$k_c = \frac{N_A (1-y_A)_{LM}}{c\left(y_{A_i} - y_{A_b}\right)} = \frac{D_{AB}}{\delta} \qquad (1)$$

N_A = 1.62 lbmol/h-ft^2 = 0.00022 mol/s-cm^2

From the ideal gas law, $c = P/RT$ = (10)/(82.06)(298) = 0.000409 mol/cm^3

$$y_{A_i} = \frac{p_{A_i}}{P} = \frac{8.2}{10} = 0.82 \qquad y_{A_b} = \frac{p_{A_b}}{P} = \frac{0.1}{10} = 0.01$$

$$(1-y_A)_{LM} = \frac{(1-y_{A_b}) - (1-y_{A_i})}{\ln \dfrac{(1-y_{A_b})}{(1-y_{A_i})}} = \frac{(1-0.01) - (1-0.82)}{\ln \dfrac{(1-0.01)}{(1-0.82)}} = 0.475$$

From Eq. (1), $k_c = \dfrac{(0.00022)(0.475)}{(0.000409)(0.82-0.01)} = 0.315$ cm/s

From Eq. (1), δ = D_{AB} / k_c = 1.6 x 10^{-2}/0.315 = 0.051 cm

Exercise 3.36

Subject: Experimental data for absorption of CO_2 (A) from air into water (B) using a packed column of Pall rings.

Given: Location in a packed column where $p_{A_i} = 150$ psia, $c_{A_b} = 0$, and $N_A = 0.017$ lbmol/h-ft^2 (2.31 x 10^{-6} mol/s-cm^2). Diffusivity of CO_2 in water = D_{AB} = 2.0 x 10^{-5} cm^2/s. Henry's law for CO_2 between air and water is p, psia = 9,000 x.

Assumptions: Negligible bulk flow effect. Only the mass-transfer resistance in the water need be considered. Neglect stripping of water.

Find: (a) Liquid-phase mass-transfer coefficient, k_c, and film thickness, δ, for the film theory.
(b) Contact time for penetration theory.
(c) Average eddy residence time and probability distribution for surface renewal theory.

Analysis: Solve the problem in cgs units.

(a) From Eq. (3-105) and a rearrangement of Eq. (3-189),

$$k_c = \frac{N_A}{c\left(x_{A_i} - x_{A_b}\right)} = \frac{D_{AB}}{\delta} \qquad (1)$$

Total liquid-phase concentration, since almost pure water, = $c = \rho/M_B = 1.0/18 = 0.0556$ mol/cm^3
From given Henry's law, $x_{A_i} = p_{A_i}/9{,}000 = 150/9{,}000 = 0.0167$ and $x_{A_b} = 0.0$.

From Eq. (1), $$k_c = \frac{2.31\times10^{-6}}{(0.0556)\left(0.0167-0\right)} = 0.0025 \text{ cm/s}$$

From Eq. (1), $\delta = D_{AB}/k_c = 2 \text{ x } 10^{-5}/0.0025 = 0.0080$ cm

(b) From a rearrangement of Eq. (3-194),

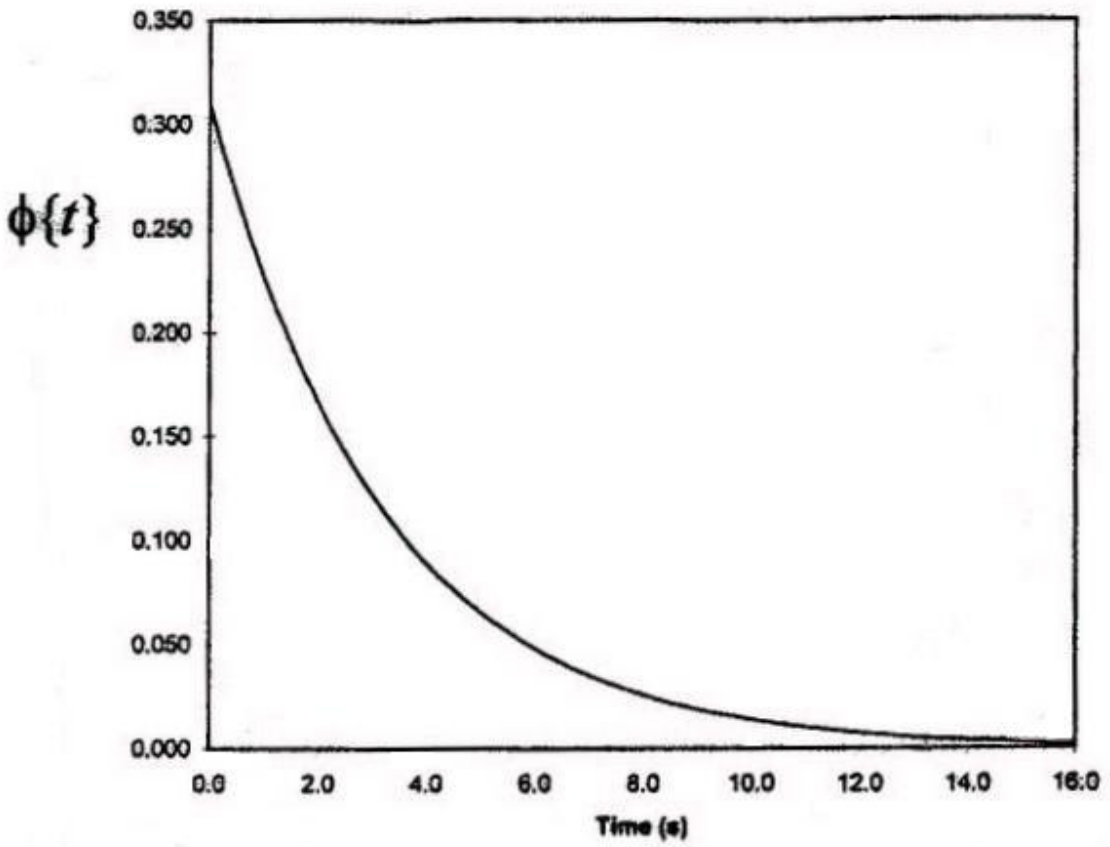
$$t_c = \frac{4D_{AB}}{\pi k_c^2} = \frac{4(2\times10^{-5})}{(3.14)(0.0025)^2} = 4.08 \text{ s}$$

(c) From Eq. (3-201), $$\bar{t} = \frac{1}{s} = \frac{D_{AB}}{k_c^2} = \frac{2\times10^{-5}}{(0.0025)^2} = 3.2 \text{ s}$$

From Eq. (3-196), the probability distribution is:

$$\phi\{t\} = s\exp(-st) = 0.313\exp(-0.313t)$$

Exercise 3.36 (continued)



Exercise 3.37

Subject: Determination of diffusivity of H_2S (A) in water (B) from experimental data for absorption into a laminar jet, using the penetration theory.

Given: Laminar jet of D = 1 cm and L = 7 cm. Temperature, T = 20°C (293 K). Solubility of H_2S in water = c_{A_i} = 100 mol/m^3 (100 x 10^{-6} mol/cm^3). Absorption rates, n_A, as a function of jet volumetric flow rate, Q.

Assumptions: Jet is contacted by pure H_2S. Therefore, all mass-transfer resistance is in the liquid. Negligible bulk flow effect. Concentration of H_2S in bulk water $c_{A_b} = 0$.

Find: Diffusivity by penetration theory.

Analysis: Use cgs units. From a rearrangement of Eq. (3-192),

$$D_{AB} = \left[\frac{n_A}{2A\left(c_{A_i} - c_{A_i}\right)}\right]^2 \pi\, t_c \qquad (1)$$

Surface area of jet = $A = \pi DL = (3.14)(1)(7) = 22.0$ cm^2

Assume the contact time is the time of exposure of the jet = jet volume/jet flow rate = V/Q

Jet volume = $V = \pi D^2 L/4 = (3.14)(1)^2(7)/4 = 5.5$ cm^3. Therefore, $t_c = 5.5/Q$.

Therefore, Eq. (1) becomes, $D_{AB} = \left[\dfrac{n_A}{2(22)\left(100\times10^{-6} - 0\right)}\right]^2 \dfrac{(3.14)(5.5)}{Q} = 89.2\times10^4\, \dfrac{n_A^2}{Q}$

Jet rate, cm^3/s	Absorption rate, mol/s x 10^6	Diffusivity, D_{AB}, cm^2/s
0.143	1.5	1.40 x 10^{-5}
0.568	3.0	1.41 x 10^{-5}
1.278	4.25	1.26 x 10^{-5}
2.372	6.15	1.42 x 10^{-5}
3.571	7.20	1.29 x 10^{-5}
5.142	8.75	1.33 x 10^{-5}

Average D_{AB} = 1.35 x 10^{-5} cm^2/s. Experimental value at 25°C is 1.61 x 10^{-5} cm^2/s.

Note that a material balance shows that the bulk concentration of H_2S in the water only reaches a high of 10.5 x 10^{-6} mol/cm^3. Thus, the diffusivities would only be slightly higher than above.

Exercise 3.38

Subject: Vaporization of water (A) into air (B) in a wetted-wall column.

Given: Column inside diameter = D = 1.46 cm and length = L = 82.7 cm. Air volumetric flow rate = Q = 720 cm^3/s at 24°C and 1 atm (760 torr). Water enters at 25.15°C and exits at 25.35°C. Partial pressures of water vapor in the air are 6.27 torr entering and 20.1 torr leaving. Diffusivity of water vapor in air = D_{AB} = 0.22 cm^2/s at 0°C and 1 atm.

Assumptions: Negligible bulk flow effect. Ideal gas law. Negligible pressure drop in column.

Find: (a) Rate of mass transfer of water into air.
(b) Overall mass transfer coefficient, K_G.

Analysis: Use cgs units. No mass transfer resistance in the liquid phase because pure water.

(a) The rate of mass transfer can be obtained from a material balance on the water content of the air using the entering and exiting partial pressures of the water vapor.

For the entering air:

Mole fraction of water vapor = $y_A = p_A / P = 6.27/760 = 0.00825$

Molecular weight = M = 0.00825(18) + (1-0.825)(29) = 28.9

Density = $\rho = PM/RT$ = (1)(28.9)/(82.06)(298) = 0.00118 g/cm^3

Mole flow rate of gas = $n = Q\rho/M$ =(720)(0.00118)/28.9 = 0.02941 mol/s

Mole flow rate of water in entering air = $n\, y_A$ = 0.02941(0.00825) = 2.426 x 10^{-4} mol/s

For the exiting air:

Mole fraction of water vapor = $y_A = p_A / P$ =20.1/760 = 0.02645

By ratio with entering gas, mole flow rate of gas = $m = 0.02941\dfrac{(1-0.00825)}{(1-0.02645)} = 0.02996$ mol/s

Mole flow rate of water in exiting air = $m\, y_A$ = 0.02996(0.02645) = 7.924 x 10^{-4} mol/s

Increase in water content of the gas = rate of mass transfer of water =
n_A = 7.924 x 10^{-4} - 2.426 x 10^{-4} = 5.5 x 10^{-4} mol/s

(b) From Eqs. (3-211) and (3-218), noting that there is no resistance in the liquid phase,

$$K_G = k_p = \frac{N_A}{\left(p_{A_i} - p_{A_b}\right)_{LM}} = \frac{n_A}{AP\left(y_{A_i} - y_{A_b}\right)_{LM}} \qquad (1)$$

Exercise 3.38 (continued)

Analysis: (b) (continued)

$$A = \pi DL = 3.14(1.46)(82.7) = 379 \text{ cm}^2$$

At 25°C, the interface mole fraction of water vapor $= y_{A_i} = \dfrac{P_A^s}{P} = \dfrac{0.46 \text{ psi}}{14.7 \text{ psi}} = 0.0313$

$$\left(y_{A_i} - y_{A_b}\right)_{LM} = \frac{\left[\left(y_{A_i} - y_{A_{in}}\right) - \left(y_{A_i} - y_{A_{out}}\right)\right]}{\ln \dfrac{\left(y_{A_i} - y_{A_{in}}\right)}{\left(y_{A_i} - y_{A_{out}}\right)}} = \frac{\left[(0.0313 - 0.00825) - (0.0313 - 0.02645)\right]}{\ln \dfrac{(0.0313 - 0.00825)}{(0.0313 - 0.02645)}} = 0.0117$$

From Eq. (1),

$$K_G = \frac{5.5 \times 10^{-4}}{(379)(1)(0.0117)} = 1.24 \times 10^{-4} \text{ mol/s-cm}^2\text{-atm}$$

Note that the correction for bulk flow amounts to only about 2.5% because the average mole fraction of air between the interface and the bulk is 0.975.

Exercise 3.39

Subject: Absorption of ammonia (A) from air (B) into 2 N H_2SO_4 in a wetted-wall column, with countercurrent flow.

Given: Column inside diameter = D = 0.575 inch (0.0479 ft) and length = L = 32.5 in. (2.71 ft) Air flow rate = n = 0.260 lbmol/h at 1 atm. Partial pressures of ammonia in the air are 0.0807 atm entering and 0.0205 leaving. Air enters at 77°F and exits at 84°F. Aqueous acid enters at 76°F and exits at 81°F. Change in acid strength is negligible.

Assumptions: Reaction of the basic ammonia with the sulfuric acid is instantaneous such that the partial pressure, p_{A_i}, of ammonia at the gas-liquid interface is zero. Therefore, the only mass transfer resistance is in the gas phase. Air flow rate refers to the total entering gas.

Find: Mass-transfer coefficient, k_p, for the gas phase. Negligible bulk flow effect.

Analysis: From a rearrangement of Eq. (3-207),

$$k_p = \frac{n_A}{A\left(p_{A_b} - p_{A_i}\right)_{LM}} = \frac{n_A}{A\left(p_{A_b} - 0\right)_{LM}} = \frac{n_A}{A\left(p_{A_b}\right)_{LM}} \qquad (1)$$

The rate of mass transfer is obtained by material balance for the decrease in partial pressure of the ammonia in the air. First compute the flow rate of just the air in the gas.

$$n_B = n\frac{\left(P - p_{A_{in}}\right)}{P} = 0.260\frac{\left(1.0 - 0.0807\right)}{1.0} = 0.239 \text{ lbmol/h}$$

$$\text{Ammonia in entering gas} = \frac{p_{A_{in}}}{p_{B_{in}}} n_B = \frac{0.0807}{\left(1.0 - 0.0807\right)} 0.239 = 0.021 \text{ lbmol/h}$$

$$\text{Ammonia in exiting gas} = \frac{p_{A_{out}}}{p_{B_{out}}} n_B = \frac{0.0205}{\left(1.0 - 0.0205\right)} 0.239 = 0.005 \text{ lbmol/h}$$

Rate of mass transfer of ammonia = n_A = 0.021 - 0.005 = 0.016 lbmol/h
Area for mass transfer = $A = \pi DL$ = 3.14(0.0479)(2.71) = 0.408 ft^2

$$\left(p_{A_b}\right)_{LM} = \frac{p_{A_{in}} - p_{A_{out}}}{\ln\dfrac{p_{A_{in}}}{p_{A_{out}}}} = \frac{0.0807 - 0.0205}{\ln\dfrac{0.0807}{0.0205}} = 0.0439 \text{ atm}$$

From Eq. (1), $k_p = n_A / A\left(p_{A_b}\right)_{LM} = 0.016/(0.408)(0.0439) = 0.893$ lbmol/h-ft^2-atm

The bulk flow effect amounts to a correction of about 5%.

Exercise 3.40

Subject: Overall mass-transfer coefficient for a packed cooling tower, where water (A) is evaporated into air (B).

Given: Cross-sectional area for air flow = $S = 0.5$ ft^2. Height over which data were taken = $H =$ 7 ft. Air rate = $n = 0.401$ lbmol/h. Water rate = 20 lbmol/h. At the bottom, $P = 14.1$ psia, $T =$ 120°F, $P_A^s = 1.69$ psia, and $y_{A_b} = 0.001609$. At the top, $P_A^s = 1.995$ psia, $y_{A_b} = 0.0882$, $T = 126$°F, and $P = 14.3$ psia.

Assumptions: All mass-transfer resistance resides in the gas phase because pure water is used. Assume air rate pertains to moisture-free air. Bulk-flow effect may be appreciable.

Find: Overall mass-transfer coefficient, K_y

Analysis: From a rearrangement of Eq. (3-234) and including the bulk-flow effect,

$$K_y = \frac{n_A (1.0 - y_A)_{LM}}{A\left(y_{A_i} - y_{A_b}\right)_{LM}} \qquad (1)$$

However, no data are given on the packing to enable the determination of the area, A. Therefore, let a = area, A, for mass transfer per unit volume, V, of tower. Then Eq. (1) becomes,

$$K_y a = \frac{n_A (1.0 - y_A)_{LM}}{V\left(y_{A_i} - y_{A_b}\right)_{LM}} \qquad (2)$$

Therefore, $K_y a$ will be determined instead of K_y .

The rate of mass transfer of water into the air is obtained by material balance, with the water mole fraction data and the air flow rate (water-free basis), where,

$$n_A = n\left[\frac{y_{A_{top}}}{1.0 - y_{A_{top}}} - \frac{y_{A_{bottom}}}{1.0 - y_{A_{bottom}}}\right] = 0.401\left[\frac{0.0882}{1.0 - 0.0882} - \frac{0.001609}{1.0 - 0.001609}\right] = 0.0381 \text{ lbmol/h}$$

The volume over which the data were taken = $V = SH = 0.5(0.7) = 0.35$ ft^2

Interface mole fractions of water vapor are,

$$y_{A_{i_{top}}} = P_{A_{top}}^s / P_{top} = 1.995/14.3 = 0.1395 \qquad y_{A_{i_{bottom}}} = P_{A_{bottom}}^s / P_{bottom} = 1.69/14.1 = 0.1199$$

Exercise 3.40 (continued)

Analysis: (continued)

$$\left(y_{A_i} - y_{A_b}\right)_{LM} = \frac{\left[\left(y_{A_{i_{top}}} - y_{A_{b_{top}}}\right) - \left(y_{A_{i_{bottom}}} - y_{A_{b_{bottom}}}\right)\right]}{\ln \dfrac{\left(y_{A_{i_{top}}} - y_{A_{b_{top}}}\right)}{\left(y_{A_{i_{bottom}}} - y_{A_{b_{bottom}}}\right)}} = \frac{\left[(0.1395 - 0.0882) - (0.1199 - 0.001609)\right]}{\ln \dfrac{(0.1395 - 0.0882)}{(0.1199 - 0.001609)}} = 0.0802$$

For the bulk-flow effect,

$$(1.0 - y_A)_{LM} \text{ at the top} = \frac{\left[\left(1 - y_{A_{i_{top}}}\right) - \left(1 - y_{A_{b_{top}}}\right)\right]}{\ln \dfrac{\left(1 - y_{A_{i_{top}}}\right)}{\left(1 - y_{A_{b_{top}}}\right)}} = \frac{\left[(1 - 0.1395) - (1 - 0.0882)\right]}{\ln \dfrac{(1 - 0.1395)}{(1 - 0.0882)}} = 0.886$$

$$(1.0 - y_A)_{LM} \text{ at the bottom} = \frac{\left[\left(1 - y_{A_{i_{bottom}}}\right) - \left(1 - y_{A_{b_{bottom}}}\right)\right]}{\ln \dfrac{\left(1 - y_{A_{i_{bottom}}}\right)}{\left(1 - y_{A_{b_{bottom}}}\right)}} = \frac{\left[(1 - 0.1199) - (1 - 0.001609)\right]}{\ln \dfrac{(1 - 0.1199)}{(1 - 0.001609)}} = 0.938$$

The average value of $(1.0 - y_A)_{LM}$ is 0.912.

From Eq. (2),

$$K_y a = \frac{0.0381(0.912)}{(0.35)(0.0802)} = 1.24 \text{ lbmol/h-ft}^3\text{-unit mole fraction}$$

For the same packing and gas and liquid velocities, this value can be used to design a large unit.

Exercise 4.1

Subject: Degrees of freedom analysis for a three-phase equilibrium stage.

Given: Equilibrium stage of Figure 4.35, with two feeds (one vapor, one liquid), vapor entering from stage below, liquid entering from stage above, three exiting streams (one vapor, two liquid), and heat transfer.

Assumptions: Equilibrium stage

Find: (a) List and count of variables.
(b) List and count of equations.
(c) Number of degrees of freedom.
(d) List of reasonable set of design variables.

Analysis: (a) With 4 streams in and 3 streams out, and heat transfer,

Number of variables = $N_V = 7(C+3) + 1 = 7C + 22$

The variables are 7 total flow rates, 7 temperatures, 7 pressures, 1 heat transfer rate and C mole fractions for each of the 7 streams.

(b) The equations are:

C	Component material balances
1	Energy balance
2	Pressure identity equations for the 3 exiting streams
2	Temperature identity equations for the 3 exiting streams
7	Mole fraction sums (one for each stream)
$2C$	Phase equilibrium equations: $K_i^{\mathrm{I}} = \frac{y_i}{x_i^{\mathrm{I}}}$ and $K_i^{\mathrm{II}} = \frac{y_i}{x_i^{\mathrm{II}}}$

Total number of equations = $N_E = 3C + 12$

(c) Degrees of freedom = $N_D = N_V - N_E = (7C + 22) - (3C + 12) = 4C + 10$

(d) A possible set of specifications is:
For each entering stream: Total flow rate, temperature, pressure, and C-1 mole fractions, which totals $4(C + 2) = 4C + 8$
For the remaining 2 variables, choose any combination of Q, temperature of one of the three exiting streams, and/or pressure of one of the three exiting streams.

Exercise 4.2

Subject: Determination of uniqueness of three different operations.

Given: (a) An adiabatic equilibrium stage with known vapor and liquid feed streams, and known stage temperature and pressure.

(b) Same as (a), except that stage is not adiabatic.

(c) Partial condenser using cooling water, with known vapor feed (except for flow rate), outlet pressure, and inlet cooling water flow rate.

Assumptions: Exiting streams in equilibrium.

Find: (a) Whether composition and amounts of exiting vapor and liquid can be computed.

(b) Same as part (a).

(c) Whether cooling water rate can be computed.

Analysis: (a) With two steams in and two out, number of variables = $N_V = 4(C + 3) = 4C + 12$

Equations are:

C	Component material balances
1	Energy balance
1	Pressure identity for 2 exiting streams
1	Temperature identity for 2 exiting streams
4	Mole fraction sums for 4 streams
C	Phase equilibrium equations

Therefore, number of equations = $N_E = 2C + 7$

Degrees of freedom = $N_D = N_V - N_E = (4C + 12) - (2C + 7) = 2C + 5$

Given specifications are: $2C + 4$ variables for the two feed streams. Only one specification left. Therefore can not specify both T and P for exiting streams.

(b) If stage in part (a) is not adiabatic, add Q as a variable to give $N_V = 4C + 13$.

The number of equations stays the same, i. e. $N_E = 2C + 7$.

Thus, have one additional degree of freedom, giving, $N_D = N_V - N_E = 2C + 6$.

Can now specify both T and P for exiting streams.

(c) First, consider just the partial condensation of the vapor into two exiting streams by heat transfer, Q, without considering the cooling water.

For three streams, $N_V = 3(C + 3) + 1$ (for Q) $= 3C + 10$.

Equations are:

C	Component material balances
1	Energy balance
1	Pressure identity for 2 exiting streams
1	Temperature identity for 2 exiting streams
3	Mole fraction sums for 3 streams
C	Phase equilibrium equations

Therefore, $N_E = 2C + 6$ and $N_D = N_V - N_E = C + 4$

Exercise 4.2 (continued)

Analysis: (c) (continued)

Specified for the feed vapor are only $C + 1$ variables, because the feed rate is not specified. Also the outlet pressure of the condenser is specified. This give $C + 2$. We are short two variables from being able to compute Q.

An energy balance on the cooling water gives:

$$Q = mC_P\left(T_{\text{out}} - T_{\text{in}}\right)$$

But only T_{in} is given. Thus, with Q unknown and T_{out} not given, we are three variable short of being able to compute the water rate, m. Thus, the problem can not be solved uniquely. We could solve it if the vapor feed rate, the outlet temperature of the partial condensate, and the cooling water outlet temperature were specified.

Exercise 4.3

Subject: Degrees of freedom analysis for an adiabatic, two-phase flash.

Given: Continuous, adiabatic flash of one feed into vapor and liquid products

Assumptions: Exiting streams are in equilibrium

Find: (a) Number of variables.
(b) All equations relating variables.
(c) Number of equations.
(d) Number of degrees of freedom
(e) Preferred specifications

Analysis: (a) Variables are those appearing in Figure 4.36

$N_V = 3C + 9$

(b) C Component material balances
1 Energy balance
1 Pressure identity for two exiting streams
1 Temperature identity for two exiting streams
3 Mole fraction sums for three streams
C Vapor-liquid equilibrium equations

(c) $N_E = 2C + 6$

(d) $N_D = N_V - N_E = (3C + 9) - (2C + 6) = C + 3$

(e) Specify the feed completely (feed rate, temperature, pressure and C - 1 mole fractions) plus exiting pressure.

Exercise 4.4

Subject: Degrees of freedom analysis for a non-adiabatic three-phase flash.

Given: Continuous, non-adiabatic flash of a liquid feed to produce a vapor and two liquid phases as shown in Figure 4.33.

Assumptions: The three exiting phases are in equilibrium.

Find: Number of degrees of freedom.

Analysis: The variables are the heat transfer rate and four each of stream flow rates, temperatures, pressures, and C mole fractions. Thus, $N_V = 4C + 13$.

The equations are:

C	Component material balances
1	Energy balance
2	Pressure identities for three exiting streams
2	Temperature identities for three exiting streams
4	Mole fraction sums for four streams
$2C$	Phase equilibrium relations: $K_i^{\mathrm{I}} = y_i / x_i^{\mathrm{I}}$ and $K_i^{\mathrm{II}} = y_i / x_i^{\mathrm{II}}$

Therefore, $N_E = 3C + 9$

Number of degrees of freedom $= N_D = N_V - N_D = (4C + 13) - (3C + 9) = C + 4$

Exercise 4.5

Subject: Application of Gibbs phase rule to seven-phase system of Figure 4.31.

Given: One gas and six liquid phases in equilibrium.

Assumptions: Gas phase includes N_2 , O_2 , and argon.

Find: Number of degrees of freedom by Gibbs phase rule.
Possible set of specifications to fix system.

Analysis: From Eq. (4-1), Number of degrees of freedom = *C* - number phases + 2
Number of components = 9 (N_2 , O_2 , argon, n-hexane, aniline, water, phosphorus, gallium, and mercury.
Number of phases = 7
Number of degrees of freedom = 9 - 7 + 2 = 4
Specify *T*, *P*, and mole fractions of argon and oxygen in the air.

Exercise 4.6

Subject: Partial vaporization of a mixture of benzene and ethyl alcohol.

Given: Vapor-liquid equilibrium data (*T*-*x*-*y*) for benzene-ethyl alcohol at 1 atm and vapor pressure data for benzene and ethyl alcohol. Initial mixture contains 25 mol% benzene.

Assumptions: Phase equilibrium

Find: (a) Bubble point.
(b) Composition of vapor at bubble point.
(c) Composition of liquid at 25 mol% vaporization.
(d) Composition of liquid at 90 mol% vaporization.
(e) Same as part (c), except vapor is removed and then additional 35 mol% is vaporized.
(f) Plot of temperature vs. mol% vaporized for parts (c) and (e).
(g) Repeat of parts (a) to (f) assuming ideal solutions

Analysis: See plot of *T*-*x*-*y* data on next page, as drawn with a spreadsheet. Curved (instead of straight) lines connecting the points would be a good improvement.

(a) For a benzene mole fraction of 0.25, a vertical line from M intersects the liquid line at N at 69.4°C, which is the bubble point.

(b) The benzene mole fraction in the vapor at 69.4°C, obtained from the left-most vapor line at P, is 0.56.

(c) To find the benzene mole fraction in the liquid at 25 mol% vaporization, extend a dashed, vertical line upward from the bubble point at N, as shown in the figure on the next page, until point B is reached. At this point, using the inverse lever-arm rule, the ratio of the AB line length to the BC line length is 25/75. The benzene mole fraction in the equilibrium liquid at point A is 0.175 at a temperature of 71.2°C.

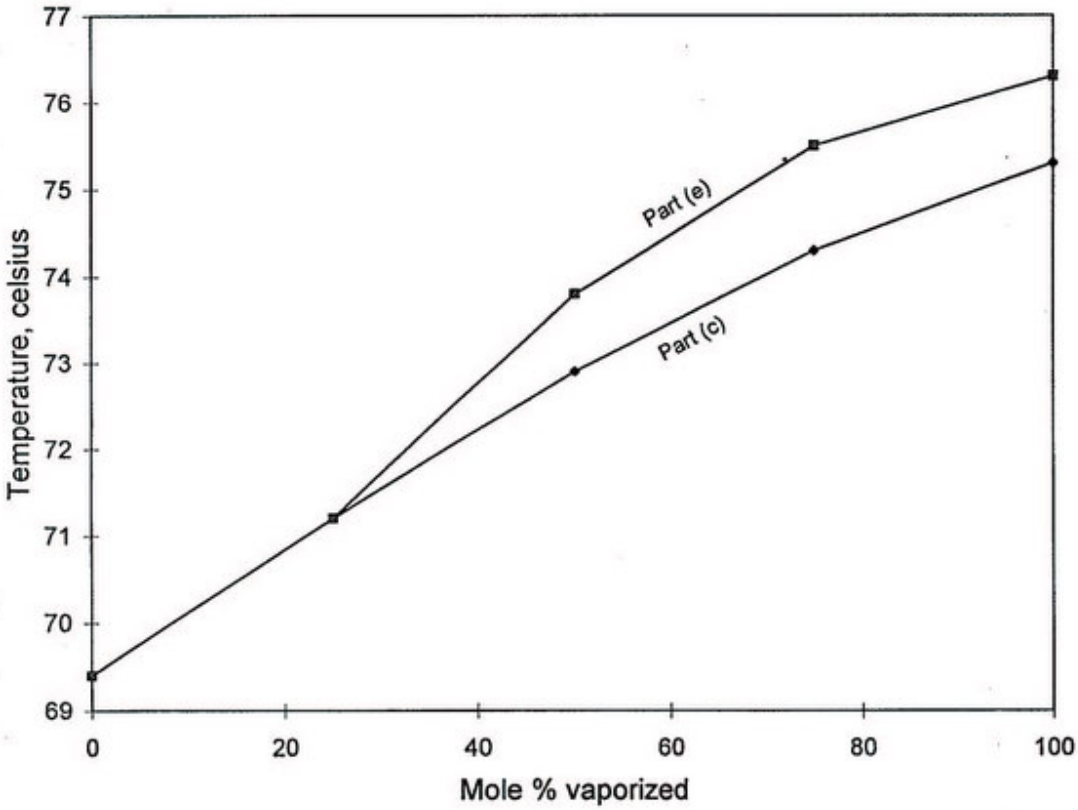
(d) To find the benzene mole fraction in the liquid at 90 mol% vaporization, extend a dashed, vertical line upward from the bubble point, as shown in the figure on the next page, until point Eis reached. At this point, using the inverse lever-arm rule, the ratio of the DE line length to the EF line length is 90/10. The benzene mole fraction in the equilibrium liquid at point D is 0.045 at a temperature of 75.1°C.

(e) To find the benzene mole fraction in the liquid when the liquid from part (c) is removed from the vapor and further vaporized, proceed as follows. If we start with 100 moles, then the liquid at 25 mol% vaporized is 75 moles with a benzene mole fraction of 0.17. If an additional 35 mol% is vaporized, we will have 35 moles of vapor in equilibrium with 40 moles of liquid. Therefore, extend a dashed, vertical line upward from point A, as shown in the figure on the next page, until point H is reached. At this point, using the inverse lever-arm rule, the ratio of the GH line length to the HI line length is 35/40. The benzene mole fraction in the liquid at G is 0.05 at a temperature of 74.9°C.

Exercise 4.6 (continued)

Analysis: (f) Extending parts (c) and (e) to other percent vaporizations, the following data are obtained, where for the extension of part (e), the first 25 mol% of vapor is removed in each case.

Mol% vaporization	Part (c) temperature, ^{o}C	Part (e) temperature, ^{o}C
0	69.4	69.4
25	71.2	71.2
50	72.9	73.8
75	74.3	75.5
100	75.3	76.3



(g) To calculate *T-x-y* curves from vapor pressure data, using Raoult's and Dalton's laws, Eq. (2-44) applies, as well as the sum of the mole fractions in the phases in equilibrium.

Thus,

letting A = benzene and B = ethyl alcohol,

$$K_A = \frac{y_A}{x_A} = \frac{P_A^s\{T\}}{P} \quad , \quad K_B = \frac{y_B}{x_B} = \frac{P_B^s\{T\}}{P} \qquad (1,\ 2)$$

$$y_A + y_B = 1 \quad , \quad x_A + x_B = 1 \qquad (3,\ 4)$$

Exercise 4.6 (continued)

Analysis: (g) (continued)

Equations (1) to (4) can be reduced to the following equations for the mole fractions of benzene in terms of the *K*-values:

$$x_A = \frac{1 - K_B}{K_A - K_B} \quad , \quad y_A = K_A x_A \qquad (5, 6)$$

If the given vapor pressure data are fitted to Antoine equations, we obtain:

$$P_A^s = \exp\left(15.5645 - \frac{2602.34}{T + 211.271}\right) \qquad (7)$$

$$P_B^s = \exp\left(21.0192 - \frac{5051.06}{T + 272.702}\right) \qquad (8)$$

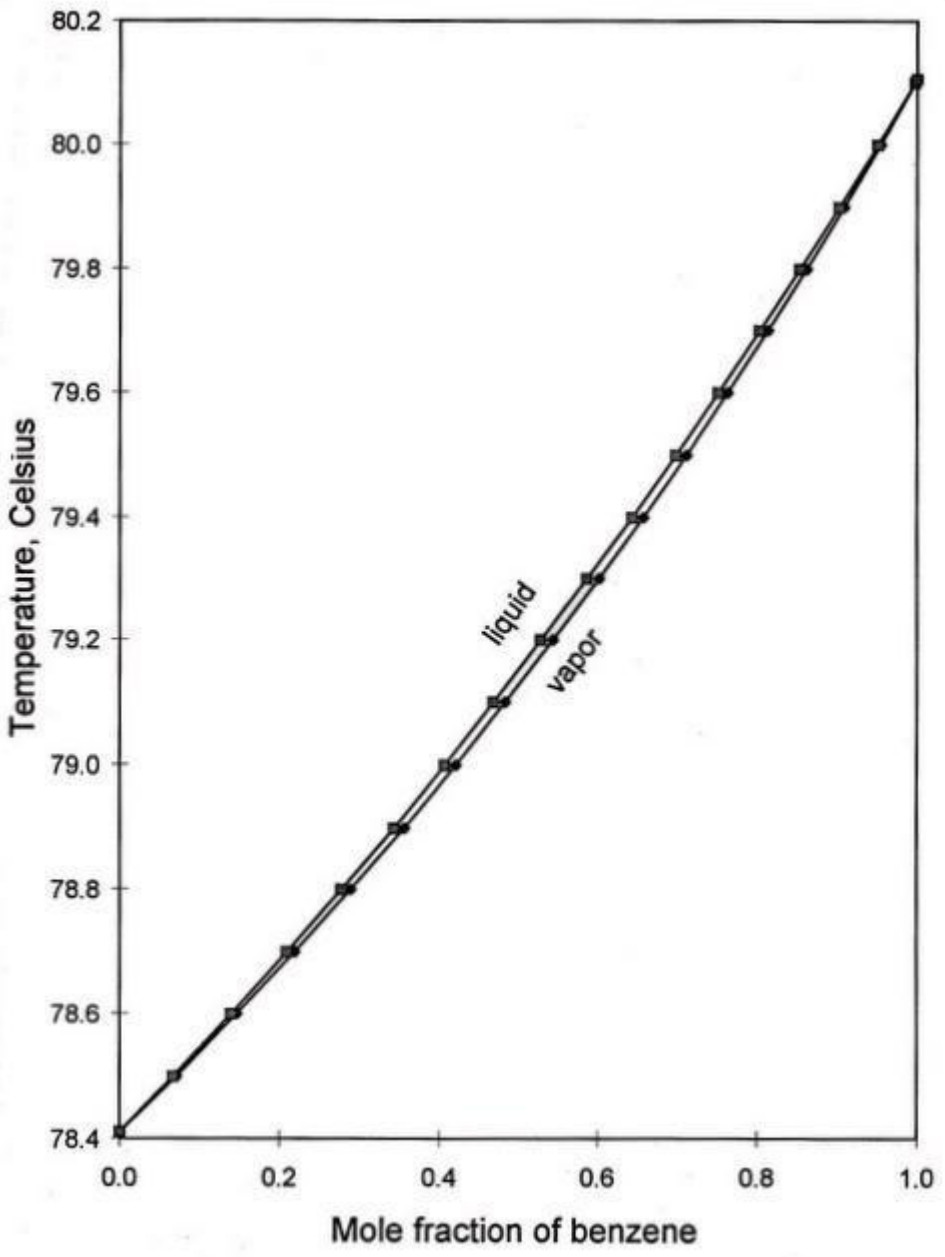
Where vapor pressure is in torr and temperature is in ^oC. Solving, Eqs. (1) to (8),

T, ^oC	P^s of A, torr	P^s of B, torr	K_A	K_B	x_A	y_A
78.41	721.3	760.0	0.9491	1.0000	0.000	0.000
78.50	723.3	762.8	0.9517	1.0037	0.071	0.067
78.60	725.5	765.9	0.9547	1.0078	0.147	0.140
78.70	727.8	769.1	0.9576	1.0119	0.220	0.210
78.80	730.0	772.2	0.9606	1.0161	0.290	0.278
78.90	732.3	775.4	0.9636	1.0202	0.357	0.344
79.00	734.6	778.6	0.9665	1.0244	0.422	0.408
79.10	736.8	781.7	0.9695	1.0286	0.484	0.469
79.20	739.1	784.9	0.9725	1.0328	0.544	0.529
79.30	741.4	788.1	0.9755	1.0370	0.602	0.587
79.40	743.7	791.4	0.9785	1.0413	0.658	0.644
79.50	746.0	794.6	0.9816	1.0455	0.712	0.699
79.60	748.3	797.8	0.9846	1.0498	0.764	0.752
79.70	750.6	801.1	0.9876	1.0541	0.814	0.804
79.80	752.9	804.3	0.9907	1.0584	0.862	0.854
79.90	755.2	807.6	0.9937	1.0627	0.909	0.903
80.00	757.5	810.9	0.9968	1.0670	0.954	0.951
80.10	759.9	814.2	0.9998	1.0713	0.997	0.997
80.11	760.0	814.4	1.0000	1.0716	1.000	1.000

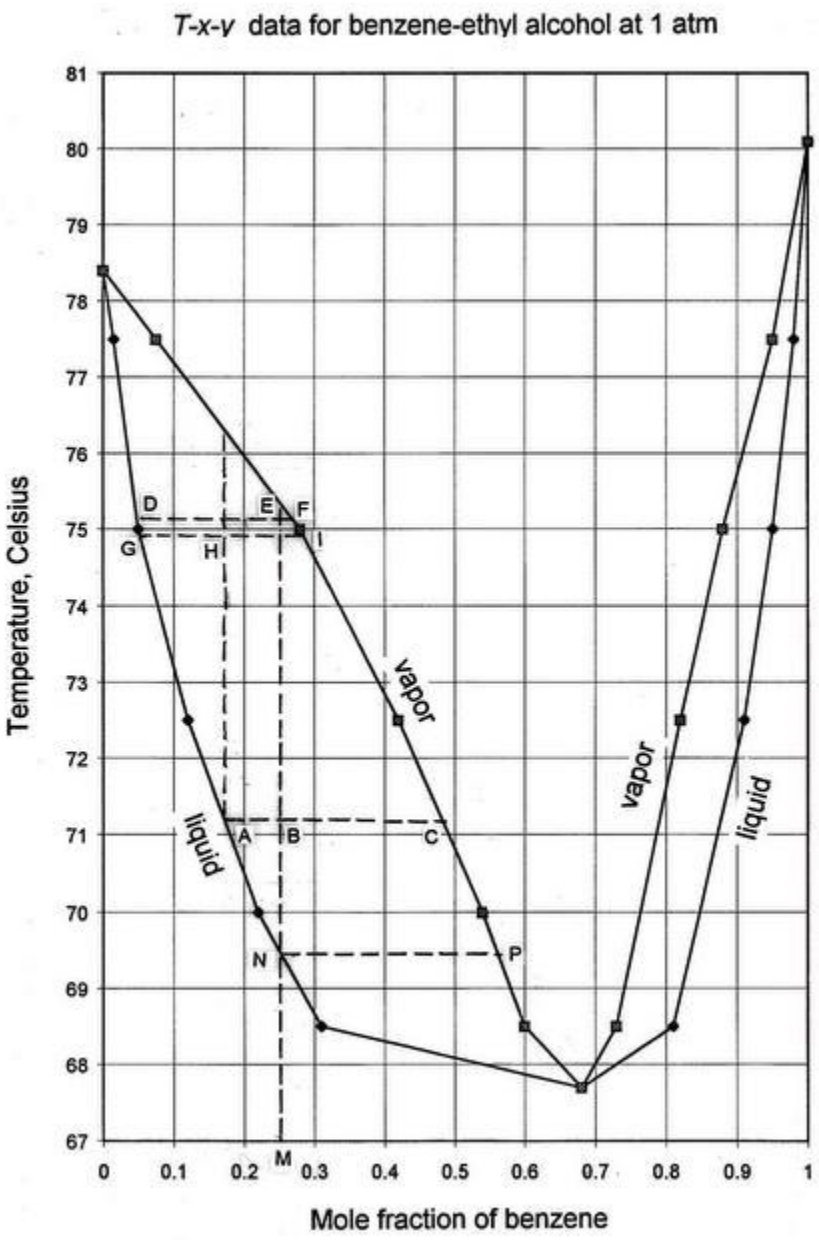
The *T*-*x*-*y* plot is shown on the next page. It is drastically different from the one based on experimental data. Thus, Raoult's law *K*-values for the benzene-ethyl benzene system are greatly in error. Consequently, no calculations are made for parts (a) to (f). They would predict only very small differences between y_A and x_A over a very small temperature range.

Exercise 4.6 (continued)

Raoult's law prediction of *T-x-y* curves for Benzene-Ethyl alcohol at 1 atm



Exercise 4.6 (continued)



Exercise 4.7

Subject: Steam (B) distillation of stearic acid (A).

Given: $T = 200^{\circ}C$. Vapor pressure of pure stearic acid at $200^{\circ}C = 0.40$ kPa.

Assumptions: Partial pressure of stearic acid in vapor = 70% of the pure vapor pressure.

Find: Kilograms of acid distilled per kilogram of steam added as a function of total pressure from 3.3 kPa to 101.3 kPa.

Analysis: $p_A = 0.7(0.4) = 0.28$ kPa

$$p_B = P - p_A = P - 0.28 \qquad (1)$$

$$y_i = p_i / P \qquad (2)$$

$$M_A = 284.5 \quad , \quad M_B = 18.02$$

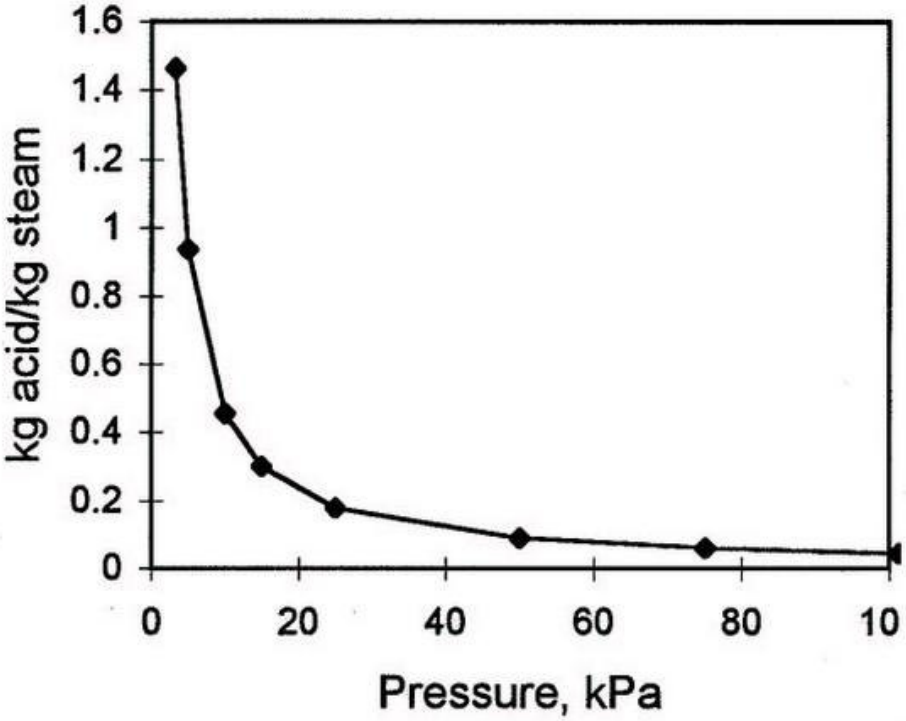
Using Eqs. (1) and (2),

$$\frac{\text{kg A}}{\text{kg B}} = \frac{y_A M_A}{y_B M_B} = \frac{p_A M_A}{p_B M_B} = \frac{0.28(284.5)}{(P\text{-}0.28)(18.02)} = \frac{4.42}{P - 0.28} \qquad (3)$$

Solving Eq. (3) for values of P from 3.3 to 101.3 kPa gives the following results:

***P*, kPa**	**kg A/kg B**
101.3	0.0438
75	0.0592
50	0.0890
25	0.1790
15	0.3006
10	0.4553
5	0.9376
3.3	1.4650

Exercise 4.7 (continued)



Exercise 4.8

Subject: Vapor-liquid equilibrium for benzene (A) - toluene (B) system at 1 atm

Given: Average relative volatility = 2.5. Vapor pressure data.

Assumptions: Raoult's and Dalton's laws.

Find: *x-y* diagram for $\alpha_{A,B} = 2.5$.

x-y diagram for Raoult's law using vapor pressure data.

(a) Temperature for 25 mol% vaporization of a 70 mol% A/30 mol% B mixture. Composition of condensed vapor and liquid residue.

(b) Plot of Raoult's law *K*-values as a function of temperature.

Analysis: For a constant relative volatility, Eq. (4-8) applies. For $\alpha_{A,B} = 2.5$,

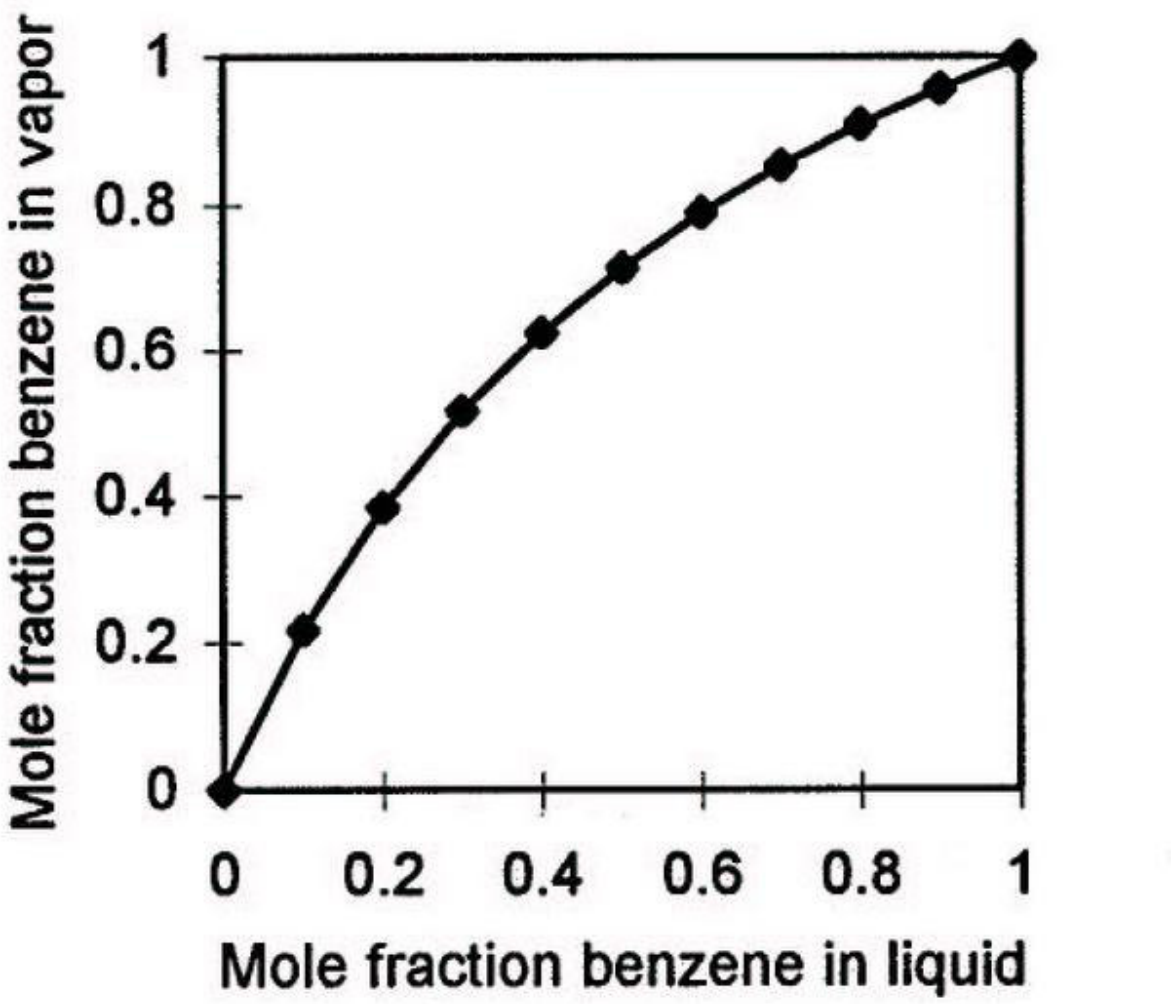
$$y_A = \frac{\alpha_{A,B} x_A}{1 + x_A(\alpha_{A,B} - 1)} = \frac{2.5 x_A}{1 + 1.5 x_A}$$

Solving this equation for values of $x_A = 0$ to 1.0 gives the following:

x_A	y_A
0.0	0.0000
0.1	0.2174
0.2	0.3846
0.3	0.5172
0.4	0.6250
0.5	0.7143
0.6	0.7895
0.7	0.8536
0.8	0.9091
0.9	0.9574
1.0	1.0000

Exercise 4.8 (continued)

Analysis: (continued)



To calculate *y-x* and *T-x-y* curves from vapor pressure data, using Raoult's and Dalton's laws, Eq. (2-44) applies, as well as the sum of the mole fractions in the phases in equilibrium. Thus,

$$K_A = \frac{y_A}{x_A} = \frac{P_A^s\{T\}}{P} \quad , \quad K_B = \frac{y_B}{x_B} = \frac{P_B^s\{T\}}{P} \qquad (1,\ 2)$$

$$y_A + y_B = 1 \quad , \quad x_A + x_B = 1 \qquad (3,\ 4)$$

Exercise 4.8 (continued)

Analysis: (continued)

Equations (1) to (4) can be reduced to the following equations for the mole fractions of benzene (A) in terms of the *K*-values:

$$x_A = \frac{1 - K_B}{K_A - K_B} \quad , \quad y_A = K_A x_A \qquad (5, 6)$$

If the given vapor pressure data in Exercise 4.6 for benzene, and this exercise for toluene are fitted to Antoine equations, we obtain:

$$P_A^s = \exp\left(15.5645 - \frac{2602.34}{T + 211.271}\right) \qquad (7)$$

$$P_B^s = \exp\left(17.2741 - \frac{3896.3}{T + 255.67}\right) \qquad (8)$$

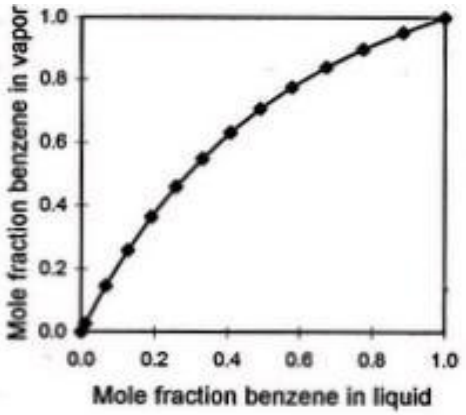
Where vapor pressure is in torr and temperature is in ^oC. Solving, Eqs. (1) to (8),

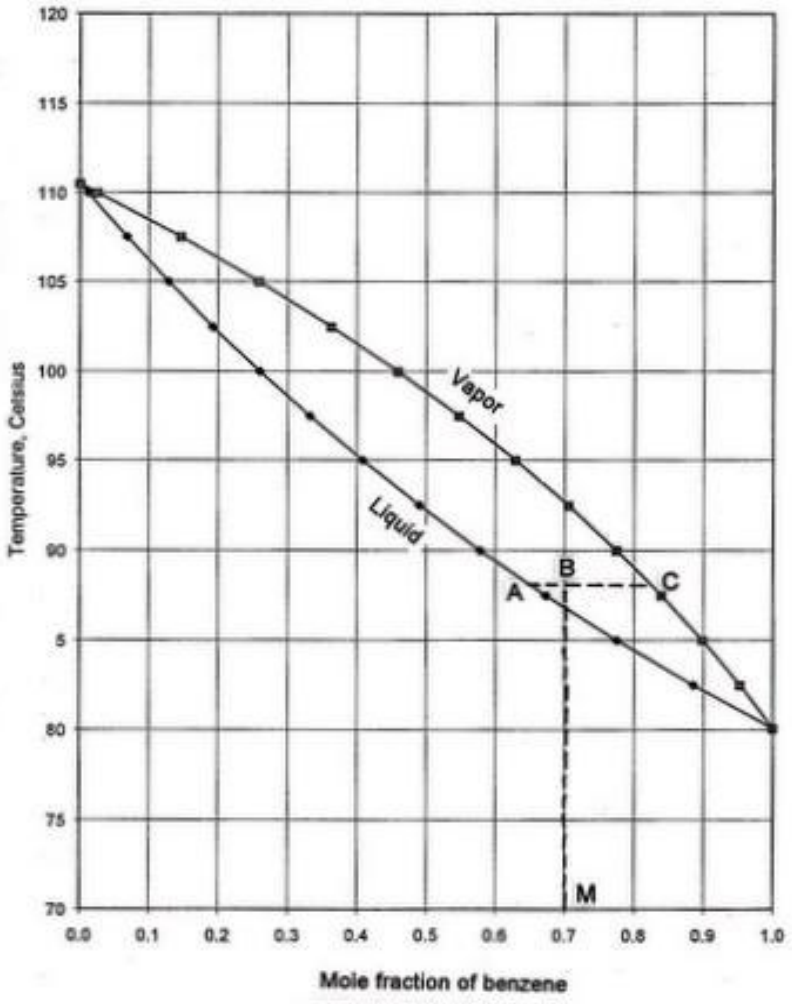
T, ^oC	P^s of A, torr	P^s of B, torr	K_A	K_B	x_A	y_A
80.1	759.9	290.0	0.9998	0.3816	1.000	1.000
82.5	817.4	314.9	1.0755	0.4144	0.886	0.953
85.0	880.8	342.7	1.1590	0.4510	0.775	0.899
87.5	948.0	372.5	1.2474	0.4901	0.673	0.840
90.0	1019.1	404.4	1.3409	0.5321	0.579	0.776
92.5	1094.1	438.5	1.4396	0.5769	0.490	0.706
95.0	1173.4	474.9	1.5439	0.6249	0.408	0.630
97.5	1256.9	513.7	1.6539	0.6760	0.331	0.548
100.0	1345.0	555.2	1.7697	0.7305	0.259	0.459
102.5	1437.6	599.3	1.8916	0.7885	0.192	0.363
105.0	1535.0	646.2	2.0198	0.8503	0.128	0.259
107.5	1637.3	696.1	2.1544	0.9159	0.068	0.146
110.0	1744.7	749.1	2.2957	0.9856	0.011	0.025
110.5	1766.8	760.1	2.3248	1.0001	0.000	0.000

Plots of *y*-*x* and *T*-*x*-*y* based on the above table from Raoult's law calculations are shown on the next page. When the *y*-*x* plot is compared to the previous *y*-*x* plot based on a constant relative volatility, it is seen that, for a given value of *x* for benzene, the values of *y* for benzene are in fairly close agreement. From the above table, the Raoult's law $\alpha_{A,B} = P_A^s / P_B^s$ ranges from 2.62 at 80.1^{o}C to 2.32 at 110.5^{o}C.

Exercise 4.8 (continued)

Analysis: (continued)



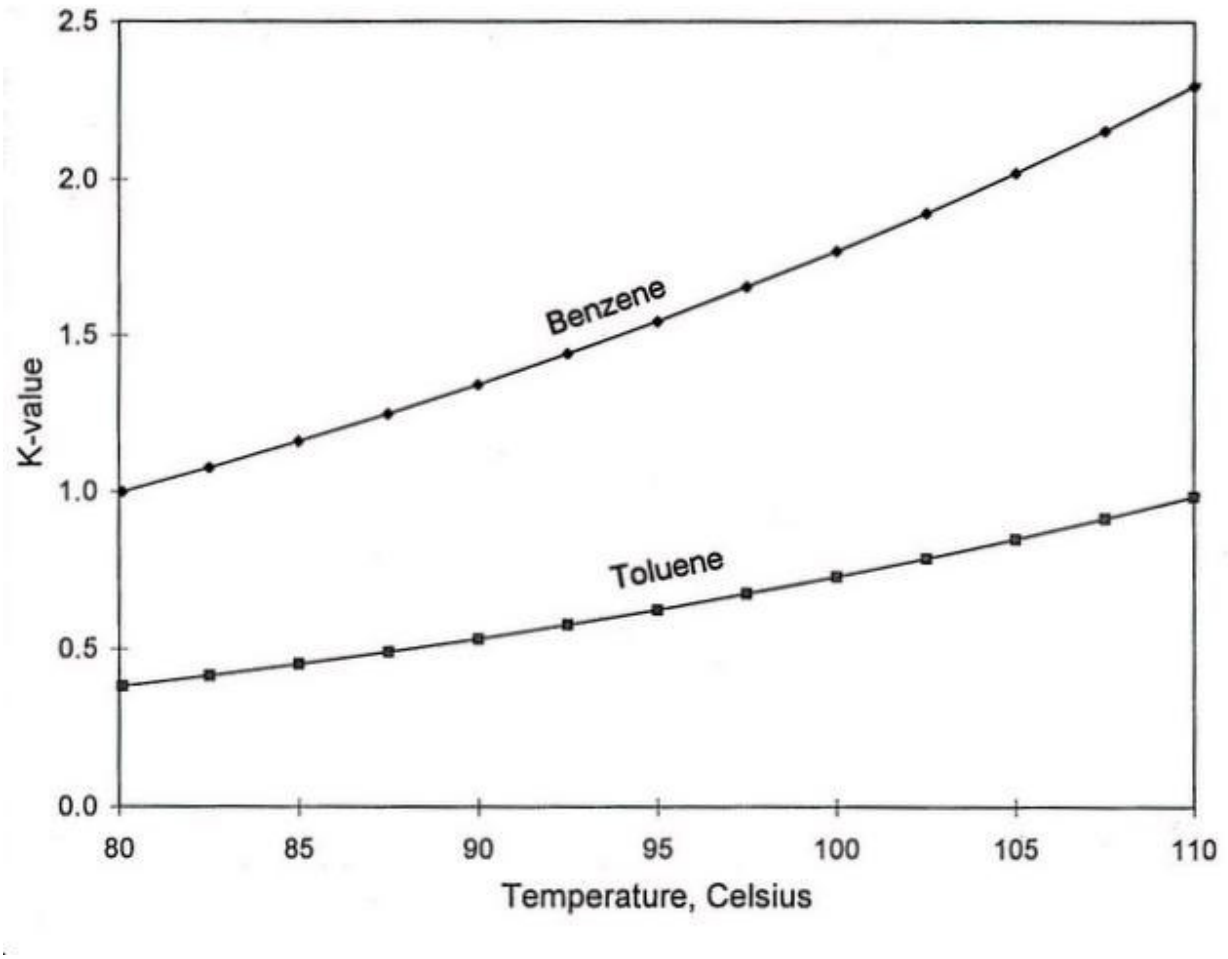


Exercise 4.8 (continued)

Analysis: (continued)

(a) To find the temperature at 25 mol% vaporization, starting with a liquid mixture of 70 mol% benzene and 30 mol% toluene, extend a dashed, vertical line upward from point M on the *T*-*y*-*x* diagram on the previous page until point B is reached. At this point, using the inverse lever-arm rule, the ratio of the AB line length to the BC line length is 25/75. The temperature is 88°C. The benzene mole fraction of the equilibrium vapor when condensed is the same as the equilibrium vapor at point C or 0.88. The benzene mole fraction in the residue liquid is the same as the equilibrium liquid at point A or 0.65.

(b) The Raoult's law *K*-values are included in the above table, and are plotted below.



Exercise 4.9

Subject: Vapor-liquid equilibrium for n-heptane (A) - toluene (B) system at 1 atm

Given: Vapor pressure data for n-heptane and toluene, and experimental *T*-*y*-*x* data.

Assumptions: Raoult's and Dalton's laws

Find: (a) *x*-*y* plot based on n-heptane, the most volatile component.
(b) *T*-*x* bubble-point plot.
(c) $\alpha_{A,B}$ and *K*-values plotted against temperature.
(d) *x*-*y* plot based on the average $\alpha_{A,B}$.
(e) Comparison of *x*-*y* and *T*-*x*-*y* plots with experimental data.

Analysis: (a) To calculate *y*-*x* and *T*-*x*-*y* curves from vapor pressure data, using Raoult's and Dalton's laws. Eq. (2-44) applies, as well as the sum of the mole fractions in the phases in equilibrium. Thus,

$$K_A = \frac{y_A}{x_A} = \frac{P_A^s\{T\}}{P} \quad , \quad K_B = \frac{y_B}{x_B} = \frac{P_B^s\{T\}}{P} \qquad (1,\ 2)$$

$$y_A + y_B = 1 \quad , \quad x_A + x_B = 1 \qquad (3,\ 4)$$

Equations (1) to (4) can be reduced to the following equations for the mole fractions of n-heptane (A) in terms of the *K*-values:

$$x_A = \frac{1 - K_B}{K_A - K_B} \quad , \quad y_A = K_A x_A \qquad (5,\ 6)$$

If the given vapor pressure data in Exercise 4.8 for toluene, and this exercise for n-heptane are fitted to Antoine equations, we obtain:

$$P_A^s = \exp\left(15.7831 - \frac{2855.27}{T + 213.64}\right) \qquad (7)$$

$$P_B^s = \exp\left(17.2741 - \frac{3896.3}{T + 255.67}\right) \qquad (8)$$

Where vapor pressure is in torr and temperature is in ^{o}C. Solving, Eqs. (1) to (8),

Exercise 4.9 (continued)

Analysis: (a) (continued)

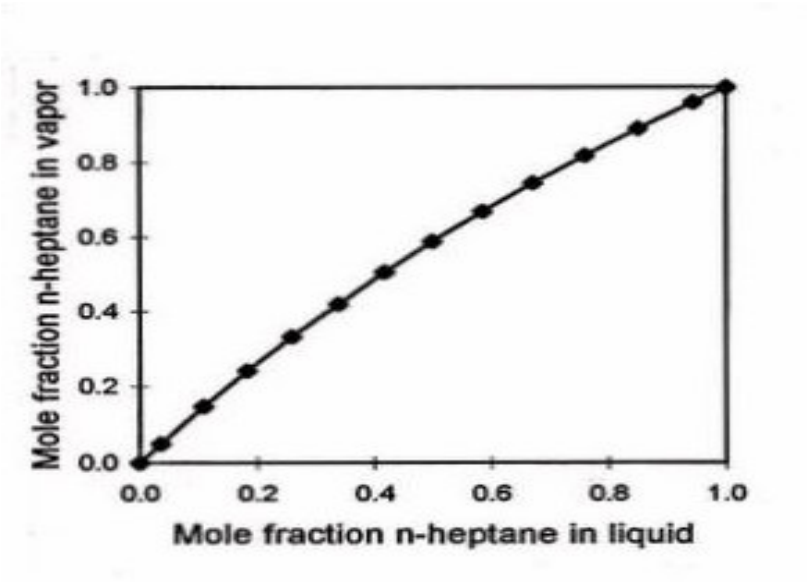
T, °C	P^s of A, torr	P^s of B, torr	K_A	K_B	x_A	y_A	$\alpha_{A,B}$
98.4	760.0	528.7	1.0000	0.6956	1.000	1.000	1.438
99.0	773.0	538.3	1.0172	0.7083	0.944	0.961	1.436
100.0	795.9	555.2	1.0472	0.7305	0.851	0.891	1.434
101.0	819.2	572.5	1.0780	0.7533	0.760	0.819	1.431
102.0	843.1	590.2	1.1094	0.7766	0.671	0.745	1.428
103.0	867.6	608.4	1.1415	0.8006	0.585	0.668	1.426
104.0	892.6	627.1	1.1744	0.8251	0.501	0.588	1.423
105.0	918.1	646.2	1.2080	0.8503	0.418	0.506	1.421
106.0	944.2	665.8	1.2424	0.8761	0.338	0.420	1.418
107.0	970.9	685.9	1.2775	0.9025	0.260	0.332	1.415
108.0	998.1	706.5	1.3133	0.9296	0.184	0.241	1.413
109.0	1026.0	727.5	1.3500	0.9573	0.109	0.147	1.410
110.0	1054.4	749.1	1.3874	0.9856	0.036	0.050	1.408
110.5	1068.9	760.1	1.4064	1.0001	0.000	0.000	1.406

From this table, an *x*-*y* plot is given below.

(b) From the above table, a *T*-*x*-*y* plot is given below. The *x*-curve is the bubble-point curve, while the *y*-curve is the dew-point curve.

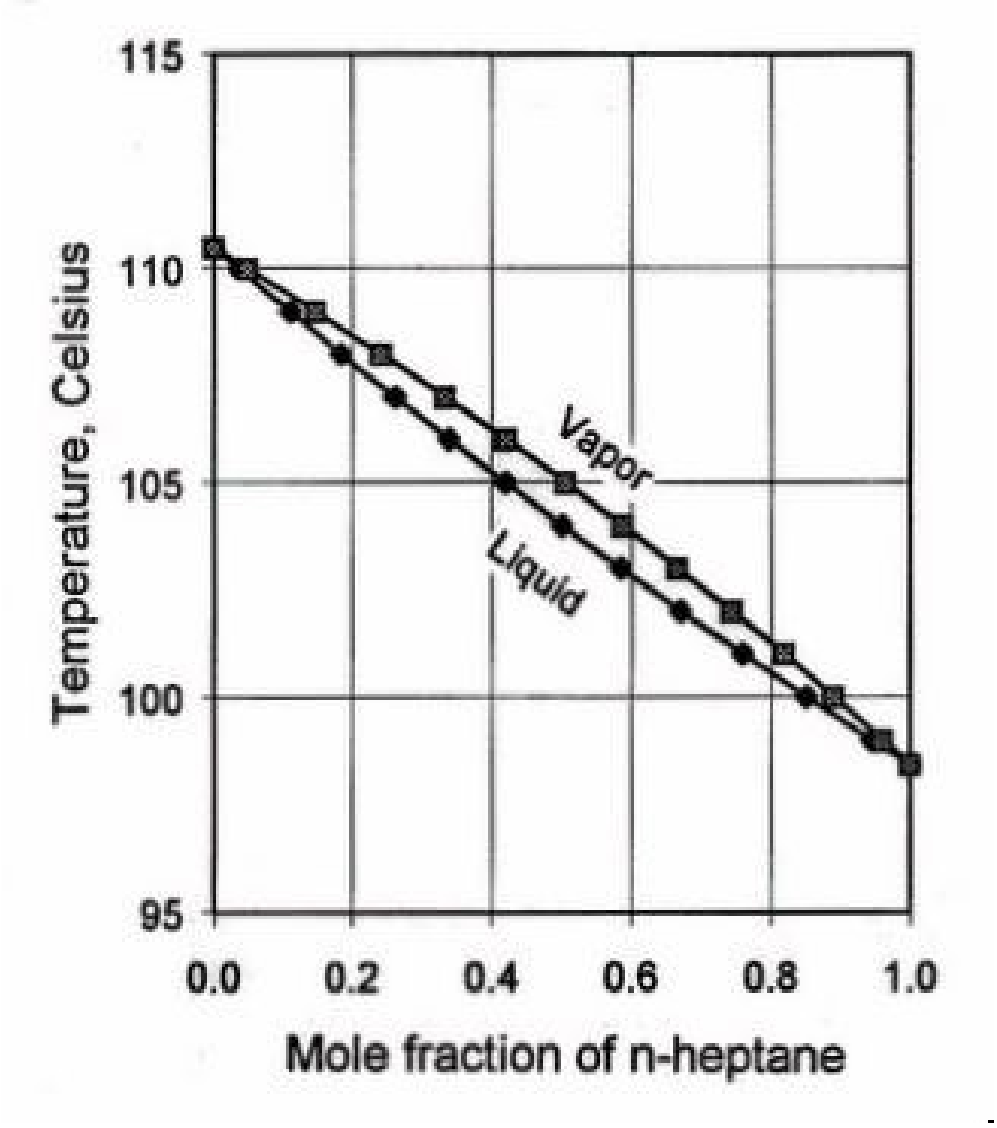
(c) A graph of relative volatility and *K*-values as a function of temperature is given on the next page.

(d) From the above table, the arithmetic average relative volatility, using the extreme values is: $(\alpha_{A,B})_{avg} = (1.438 + 1.406)/2 = 1.422$



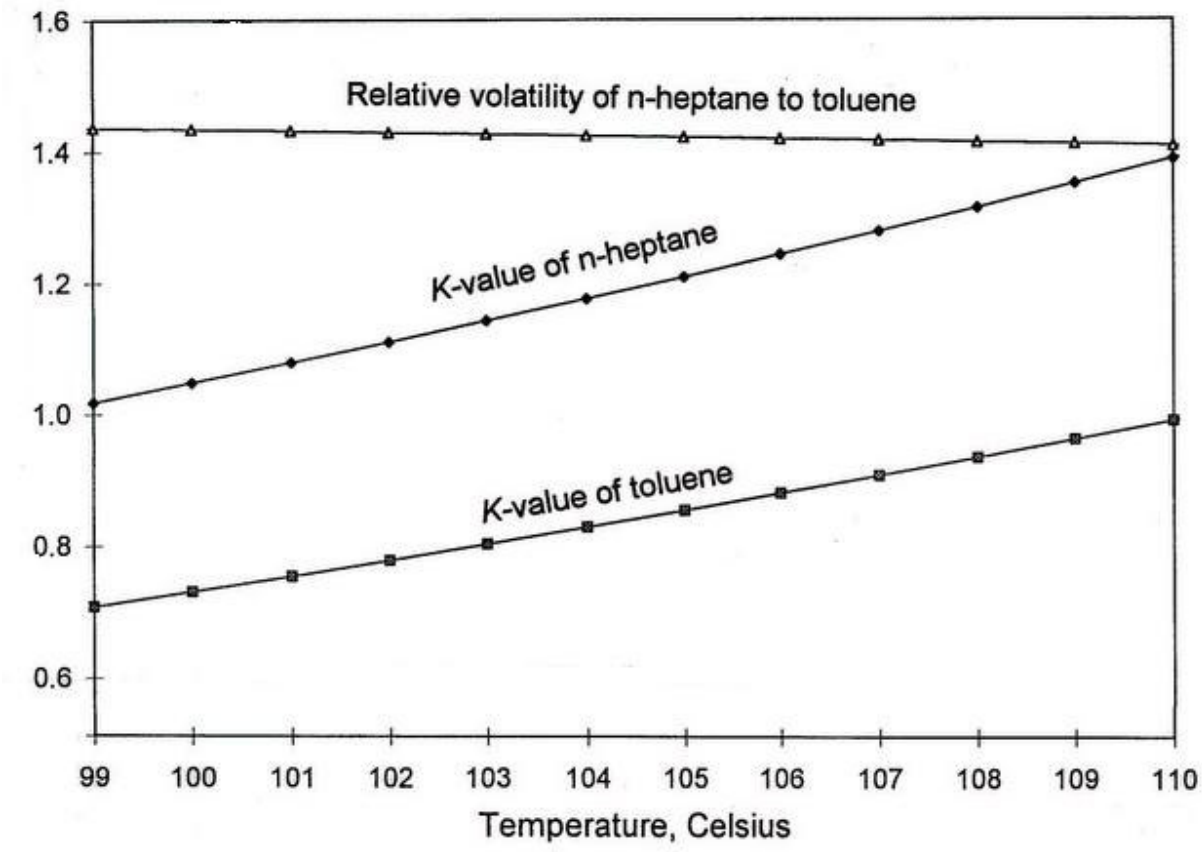
Exercise 4.9 (continued)

Analysis: (a) (continued)



Exercise 4.9 (continued)

Analysis: (c) and (d) (continued) **Relative Volatility and *K*-Values**



For a constant relative volatility, Eq. (4-8) applies. For $\alpha_{A,B} = 1.422$,

$$y_A = \frac{\alpha_{A,B} x_A}{1 + x_A(\alpha_{A,B} - 1)} = \frac{1.422 x_A}{1 + 0.422 x_A}$$

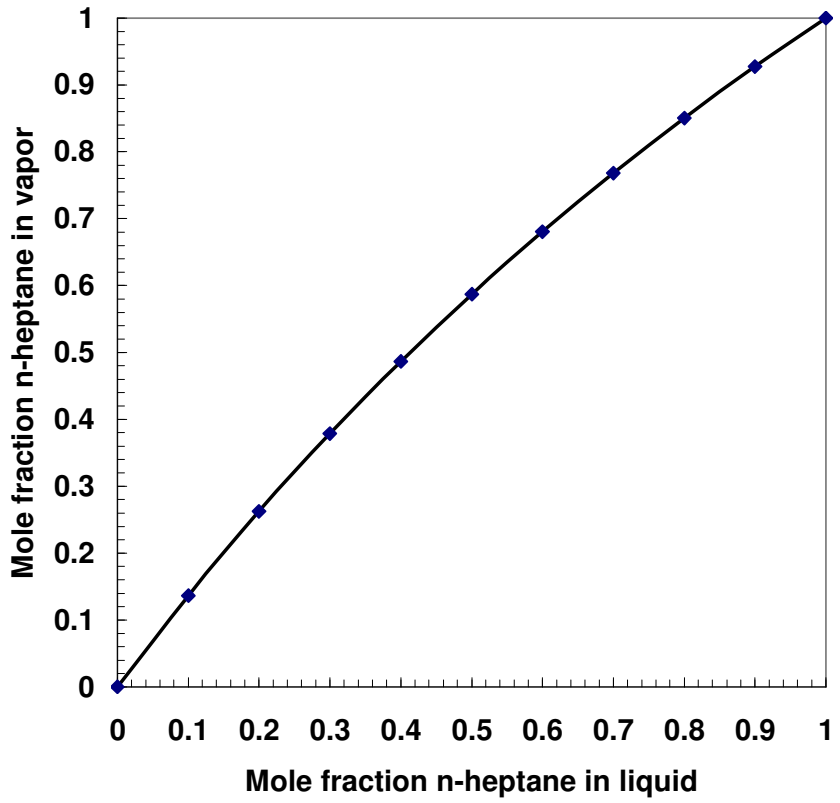
Solving this equation for values of x_A = 0 to 1.0 gives the following:

x_A	y_A
0	0.0000
0.1	0.1364
0.2	0.2623
0.3	0.3787
0.4	0.4867
0.5	0.5871
0.6	0.6808
0.7	0.7684
0.8	0.8505
0.9	0.9275
1	1.0000

Exercise 4.9 (continued)

Analysis: (c) and (d) (continued)

***y*-*x* Plot for an average relative volatility**



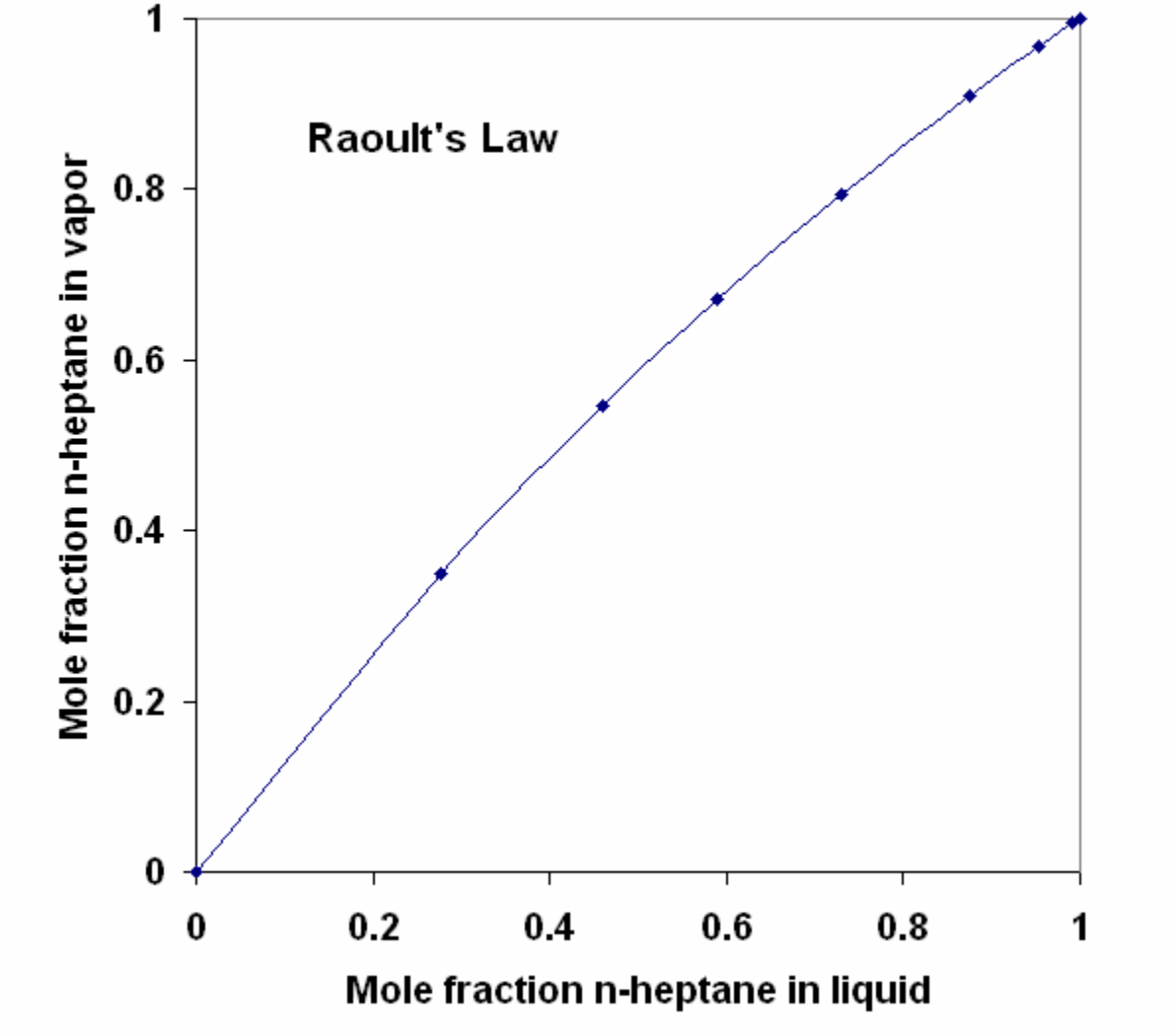
(e) Raoult's law calculations compared to experimental are as follows:

	Raoult's law		Experimental	
T, °C	x_A	y_A	x_A	y_A
110.75	-0.018	-0.026	0.025	0.048
106.80	0.276	0.350	0.129	0.205
104.50	0.459	0.547	0.250	0.349
102.95	0.589	0.672	0.354	0.454
101.35	0.729	0.793	0.497	0.577
99.73	0.876	0.910	0.692	0.742
98.90	0.954	0.967	0.843	0.864
98.50	0.992	0.995	0.940	0.948
98.35	1.007	1.005	0.994	0.993

The Raoult's law values are in very poor agreement with the experimental values.

Exercise 4.9 (continued)

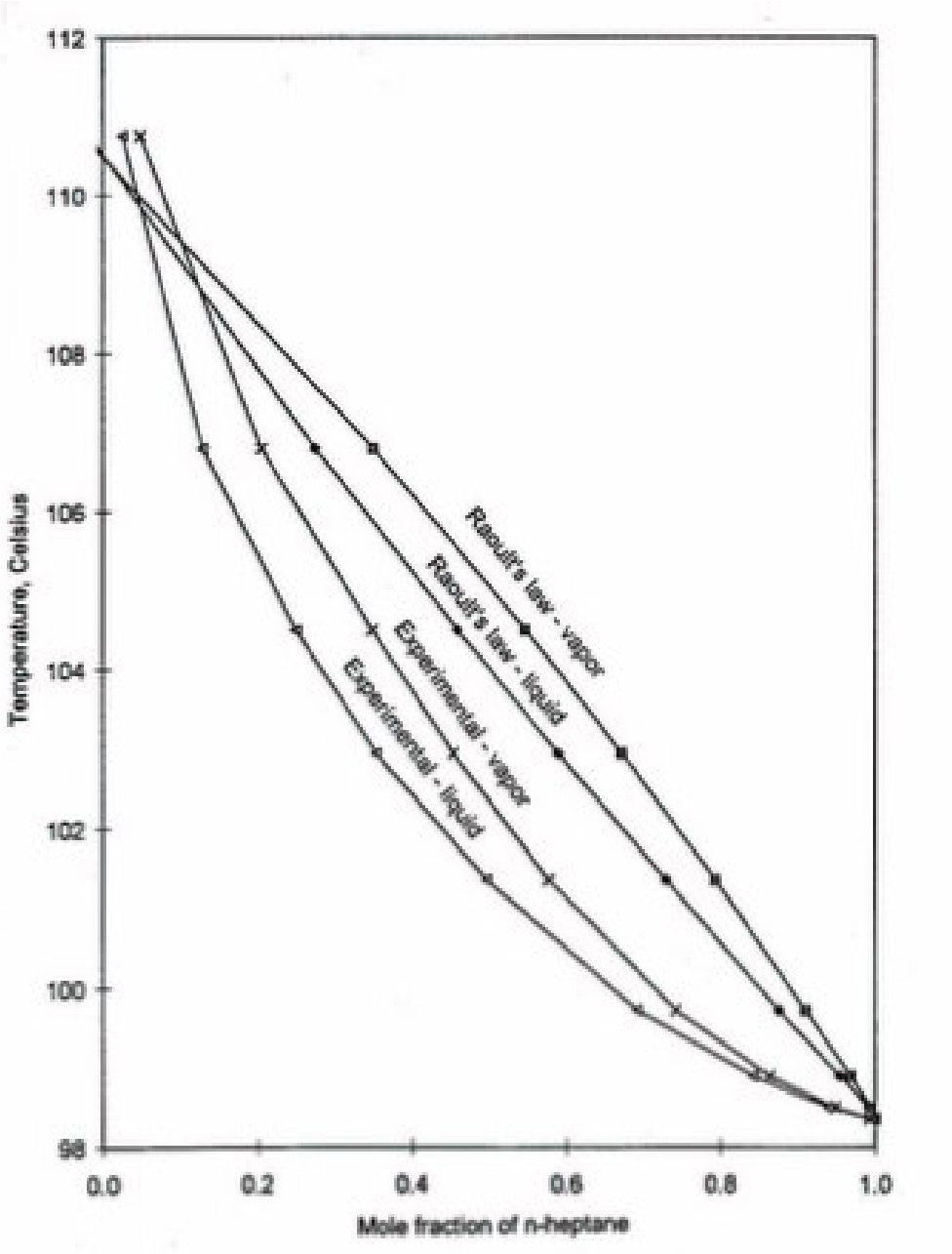
Analysis: (e) (continued)



Exercise 4.9 (continued)

Analysis: (e) (continued)

Comparison with Experimental Data



Exercise 4.10

Subject: Continuous, single stage distillation of A and B to produce a distillate and bottoms.

Given: Saturated liquid feed of 50 mol% A and 50 mol% B fed to a still at 40 mol/h.
Relative volatility = $\alpha_{A,B} = 2$. Bottoms rate = 30 mol/h
(a) Total condenser with a reflux ratio = 1.
(b) No reflux.

Assumptions: Still is an equilibrium stage.

Find: (a) Composition of the two products.
(b) Composition of the two products.

Analysis: From the definition of the relative volatility,

$$\alpha_{A,B} = \frac{y_A x_B}{x_A y_B} = \frac{y_A(1-x_A)}{x_A(1-y_A)} = 2 \qquad (1)$$

(a) Distillate = $D = F - W = 40 - 30 = 10$ mol/h
Material balance for A: $0.5(40) = 20 = y_A(10) + x_A(30)$ (2)
Solving Eqs. (1) and (2) simultaneously by eliminating y_A, we obtain:

$$3x_A^2 + 3x_A - 2 = 0 \qquad (3)$$

Solving Eq. (3), a quadratic equation, get only one postive root:

$x_A = 0.4575$, $x_B = 0.5425$ for the bottoms

Substitution into Eq. (2), gives,

$y_A = 0.6275$, $y_B = 0.3725$ for the distillate

(b) Note that the solution to Part (a) was independent of the reflux ratio. Accordingly, the solution to Part (b) is the as for Part (a)

Exercise 4.11

Subject: Distillation of an acetone (A) - water (B) mixture that is partially vaporized.

Given: Feed is 57 mol% A and 43 mol% B as a liquid at 125°C and 687 kPa. It is flashed across a valve to the column pressure of 101.3 kPa, with a resulting temperature of 60°C. Vapor-liquid equilibrium data at column pressure. Enthalpy data at column conditions. Compositions of the distillate and bottoms.

Assumptions: Feed is at equilibrium downstream of the feed valve. Will have to check if feed valve operates adiabatically. Given heat capacities are for the liquid and are constant. Heats of vaporization are constant. No effect of pressure on enthalpy.

Find: Mole ratio of liquid to vapor in the feed downstream of the valve. Construct an *H-x-y* diagram.

Analysis: From the equilibrium data, at 60°C, $x_A = 0.50$ and $y_A = 0.85$.

Take a basis of F = feed rate = 1 kmol/s.

Total material balance around feed valve: $F = 1 = V + L$ (1)

Acetone material balance around feed valve: $0.57(1) = 0.85V + 0.50L$ (2)

Solving Eqs. (1) and (2) simultaneously,

$V = 0.2$ kmol/s and $L = 0.8$ kmol/s

Therefore, after the valve, moles L/moles $V = 0.8/0.2 = 4$

Now check whether valve is operating adiabatically.

Enthalpy of liquid entering valve = 0 (as given)

Enthalpy of feed after the valve, using given enthalpies =

27,200(0.2) + (-5,270)(0.8) = 1224 kJ/s

Therefore, the enthalpy increases across the valve by 1224 kJ/s

To construct an enthalpy diagram for 1 atm pressure, take as an enthalpy datum, A and B as liquids at 25°C. This is a different datum than that used to get the given enthalpy of the hot feed.

Pure A: boils at 56.7°C.

Since C_P of liquid =134 kJ/kmol-K, h_L at 56.7°C = 134(56.7-25)=4248 kJ/kmol-K

h_V at 56.7°C =4248 + latent heat = 4248 + 29750 = 33998 kJ/kmol-K

Pure B: boils at 100°C.

Since C_P of liquid =75.3 kJ/kmol-K, h_L at 100°C = 75.3(100-25)=5648 kJ/kmol-K

h_V at 100°C =5648 + latent heat = 5648 + 42430 = 48078 kJ/kmol-K

Equilibrium liquid mixture of 50 mol% A and 50 mol% B has a bubble point at 60°C. Therefore,

$h_L = 0.5(134)(60-25) + 0.5(75.3)(60-25) = 3663$ kJ/kmol-K

Equilibrium vapor mixture of 85 mol% A and 15 mol% B has dew point of 60°C. Therefore,

$h_V = 0.85[(134)(60-25) + 29750] + 0.15[(75.3)(60-25) + 42430] = 36034$ kJ/kmol-K

Calculations for other equilibrium mixtures are done in a similar manner and are summarized in the following table:

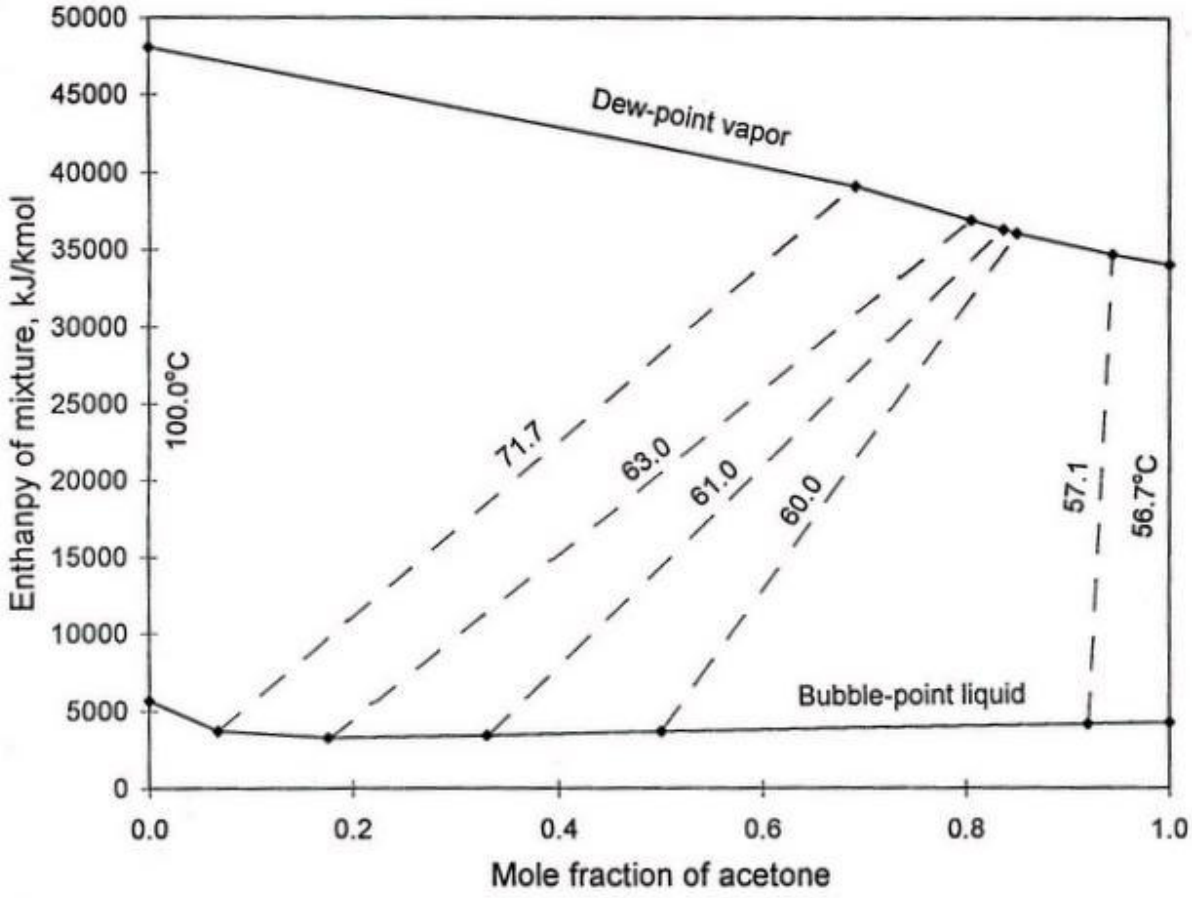
Exercise 4.11 (continued)

Analysis: (continued)

T, °C	x_A	x_B	h_L, kJ/kmol	y_A	y_B	h_V, kJ/kmol
56.7	1.000	0.000	4248	1.000	0.000	33998
57.1	0.920	0.080	4151	0.944	0.056	34656
60.0	0.500	0.500	3663	0.850	0.150	36034
61.0	0.330	0.670	3408	0.837	0.163	36296
63.0	0.176	0.824	3254	0.805	0.195	36880
71.7	0.068	0.932	3703	0.692	0.308	39069
100.0	0.000	1.000	5648	0.000	1.000	48078

From this table, the *h-x-y* plot follows, with tie lines to connect the vapor-liquid equilibrium along the dew-point and bubble-point lines.

Enthalpy-Composition Plot



Exercise 4.12

Subject: Vaporizer and condenser heat duties for benzene (A) -toluene (B) mixtures, using an enthalpy-concentration diagram.

Given: P = 1 atm. Vapor pressure data. Saturated liquid and vapor enthalpy data.

Assumptions: Raoult's law.

Find: (a) Construct an *h*-*x*-*y* plot.
(b) Heat duty for 50 mol% vaporization of a 30 mol% A mixture, starting from liquid saturation temperature. Heat duty to condense the vapor and subcool it 10°C.

Analysis: (a) First, compute the vapor and liquid equilibrium compositions at 1 atm and temperatures from 60 to 100°C using Raoult's law with the vapor pressure data. Eq. (2-44) applies, as well as the sum of the mole fractions in the phases in equilibrium. Thus,

$$K_A = \frac{y_A}{x_A} = \frac{P_A^s\{T\}}{P} \quad , \quad K_B = \frac{y_B}{x_B} = \frac{P_B^s\{T\}}{P} \qquad (1,\ 2)$$

$$y_A + y_B = 1 \quad , \quad x_A + x_B = 1 \qquad (3,\ 4)$$

Equations (1) to (4) can be reduced to the following equations,

$$x_A = \frac{1 - K_B}{K_A - K_B} \quad , \quad y_A = K_A x_A \qquad (5,\ 6)$$

Vapor pressure data in Exercises 4.6 for benzene, and 4.8 for toluene give Antoine equations,

$$P_A^s = \exp\left(15.5645 - \frac{2602.34}{T + 211.271}\right), \quad P_B^s = \exp\left(17.2741 - \frac{3896.3}{T + 255.67}\right) \qquad (7,\ 8)$$

Where vapor pressure is in torr and temperature is in °C. Solving, Eqs. (1) to (8),

T, °C	P^s of A, torr	P^s of B, torr	K_A	K_B	x_A	y_A
80.1	759.9	290.0	0.9998	0.3816	1.000	1.000
85.0	880.8	342.7	1.1590	0.4510	0.775	0.899
90.0	1019.1	404.4	1.3409	0.5321	0.579	0.776
95.0	1173.4	474.9	1.5439	0.6249	0.408	0.630
100.0	1345.0	555.2	1.7697	0.7305	0.259	0.459
105.0	1535.0	646.2	2.0198	0.8503	0.128	0.259
110.5	1766.8	760.1	2.3248	1.0001	0.000	0.000

This covers the temperature range of co-existence of vapor and liquid.

Exercise 4.12 (continued)

Analysis: (a) (continued)

Molecular weights are $M_A = 78$ and $M_B = 92$

For a given temperature, compute saturated liquid-phase mixture enthalpies in kJ/kg of mixture from,

$$h_L = \frac{x_A M_A h_{L_A} + (1 - x_A) M_B h_{L_B}}{x_A M_A + (1 - x_A) M_B} \qquad (9)$$

Similarly for the vapor, $$h_V = \frac{y_A M_A h_{V_A} + (1 - y_A) M_B h_{V_B}}{y_A M_A + (1 - y_A) M_B} \qquad (10)$$

Will have to interpolate and extrapolate given saturated enthalpy data. Liquid enthalpy data are linear with temperature, therefore, it is found that:

$$h_{L_A} = 1.85T - 32 \quad , \qquad h_{L_B} = 1.85T - 34 \qquad (11, 12)$$

Vapor enthalpy data are not quite linear, but fit the following quadratic equations:

$$h_{V_A} = 427 + 0.85T + 0.0025T^2 \quad , \quad h_{V_B} = 411 + 0.85T + 0.0025T^2 \qquad (13, 14)$$

T, °C	x_A	y_A	$(h_L)_A$, kJ/kg	$(h_L)_B$, kJ/kg	$(h_V)_A$, kJ/kg	$(h_V)_B$, kJ/kg	h_L, kJ/kg	h_V, kJ/kg
80.1	1.000	1.000	116.2	114.2	511.1	495.1	116.2	511.1
85.0	0.775	0.899	125.3	123.3	517.3	501.3	124.7	515.4
90.0	0.579	0.776	134.5	132.5	523.8	507.8	133.6	519.7
95.0	0.408	0.630	143.8	141.8	530.3	514.3	142.5	523.8
100.0	0.259	0.459	153.0	151.0	537.0	521.0	151.5	527.7
105.0	0.128	0.259	162.3	160.3	543.8	527.8	160.5	531.5
110.5	0.000	0.000	172.4	170.4	551.5	535.5	170.4	535.5

Plots of h in kJ/kg mixture as a function of saturated vapor and liquid mole fractions, and y-x are given on the next page.

(b) Take a basis of 1 kmol of 30 mol% A - 70 mol% B feed mixture. Then, kg A = (0.30)(78) = 23.4 kg and kg B = (0.70)(92) = 64.4 kg or 87.8 kg total feed.

Use y-x diagram to obtain compositions of vapor and liquid for 50 mol% vaporized. From the equation above Eq. (4-6), the slope of the q-line is $[(V/F)-1]/(V/F) = (0.5-1.0)/0.5 = -1$. The construction is shown on the y-x diagram, where the intersection with the equilibrium curve gives $x_A = 0.22$ and $y_A = 0.38$. The mass of liquid = (0.22)(0.5)(78) + (0.78)(0.5)(92) = 44.5 kg. The mass of vapor = 87.8 - 44.5 = 43.3 kg. On the h-x-y diagram, Point A is the saturated liquid feed with h_L = 150 kJ/kg of feed. Point C is the liquid remaining after 50 mol% vaporization, withh_L, = 158 kJ/kg. Since 44.5/87.8 or 0.507 of the feed is left as liquid, this is equivalent to (0.507)(158) = 80 kJ/kg feed. Point D is the vapor, with h_V = 540 kJ/kg vaporized. Since 0.493

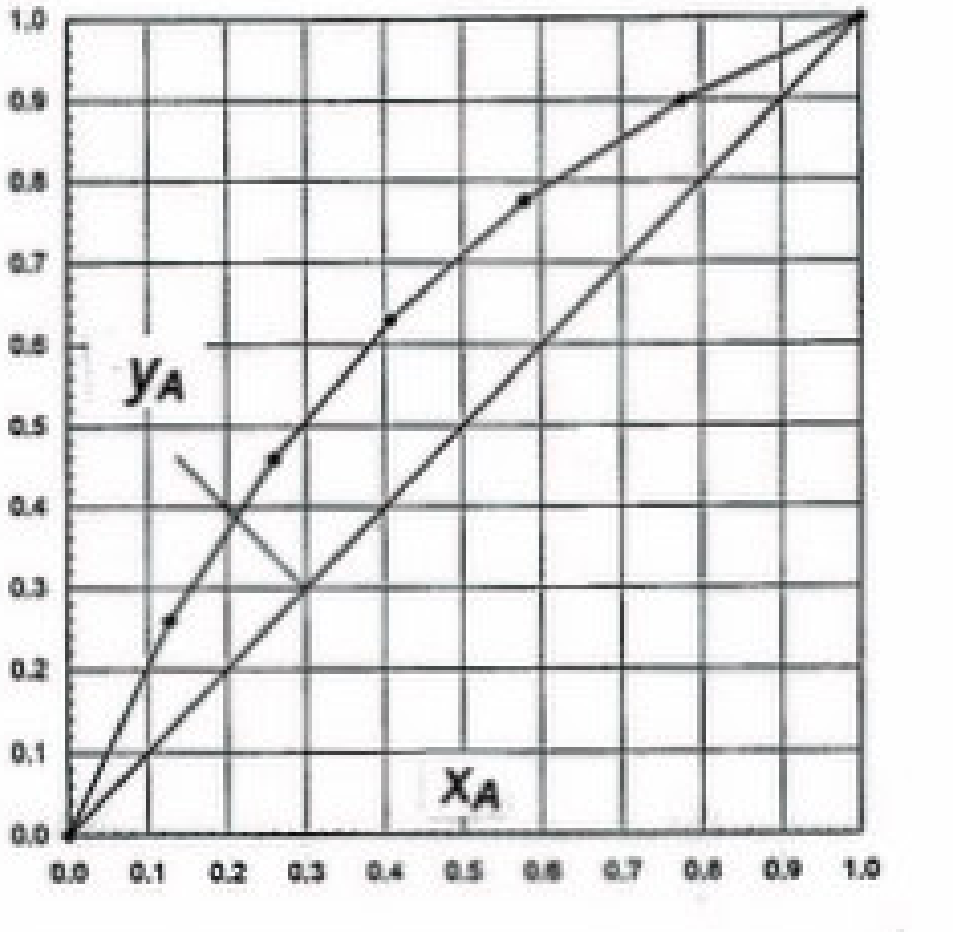
Exercise 4.12 (continued)

Analysis: (b) (continued)

of the feed is vaporized, this is equivalent to (0.493)(540) = 266 kJ/kg feed. Therefore, the energy required for partial vaporization = 266 + 80 - 150 = 196 kJ/kg of feed.

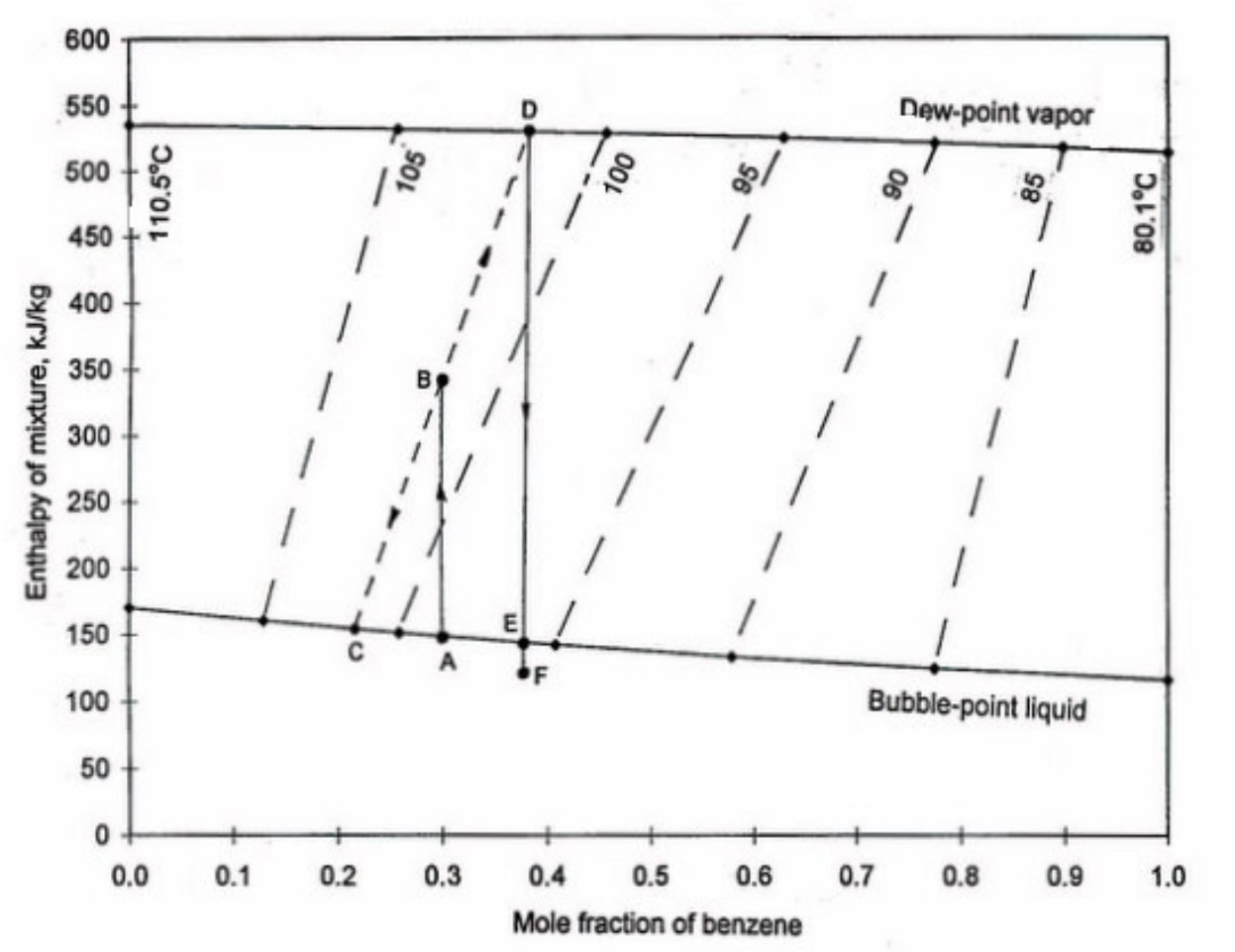
Point B is the combined vapor and liquid phases after partial vaporization. Point E is condensed vapor as saturated liquid, with an enthalpy of 145 kJ/kg. This is equivalent to (0.493)(145) = 71 kJ/kg of feed. Therefore, the condenser duty = 266 - 71 = 195 kJ/kg feed.

Point F is 10°C subcooled condensate, where the enthalpy change from saturation, based on a liquid specific heat of 1.85 kJ/kg-°C, is 1.85(10)(0.493) = 9 kJ/kg feed. Therefore, the condenser duty is now 195 + 9 = 204 kJ/kg feed.



Exercise 4.12 (continued)

Analysis: (a) Enthalpy – Composition Diagram



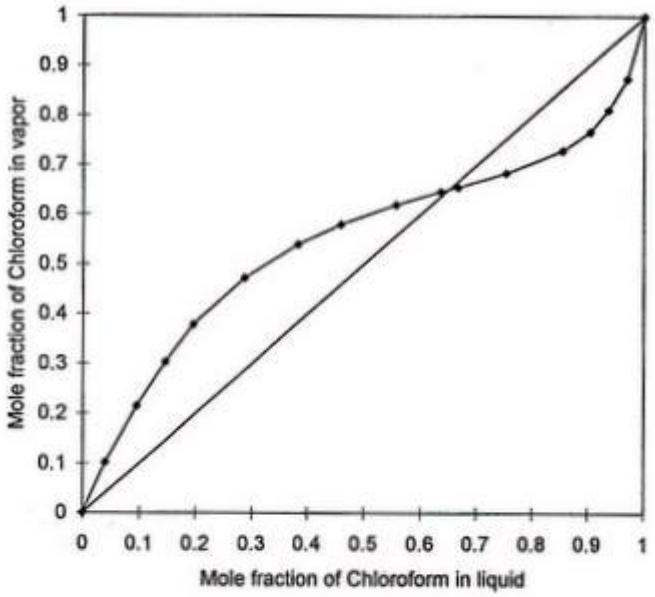
Exercise 4.13

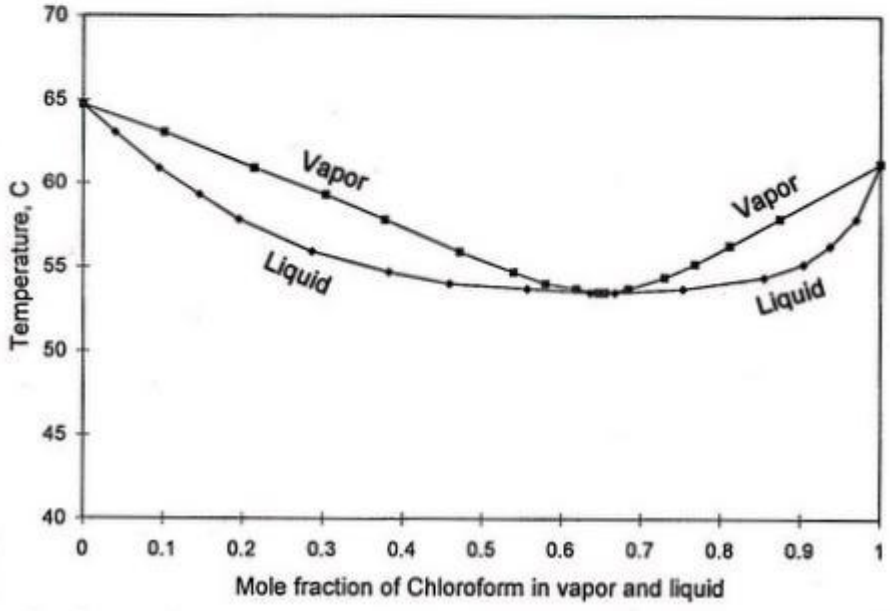
Subject: Azeotrope for the chloroform-methanol system at 101.3 kPa.

Given: Vapor-liquid equilibrium data from Section 13, p. 11 of Perry's Handbook, 6th edition.

Find: From data, construct *y-x* and *T-x-y* plots. Azeotrope conditions

Analysis: See plots below. From these plots, a minimum-boiling azeotrope occurs at 53.5°C with a composition of 65 mol% chloroform and 35 mol% methanol.





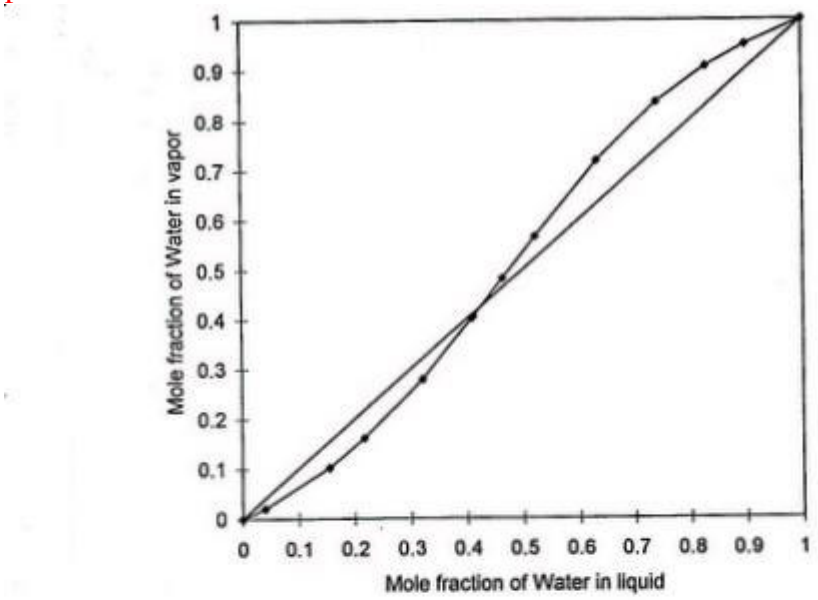
Exercise 4.14

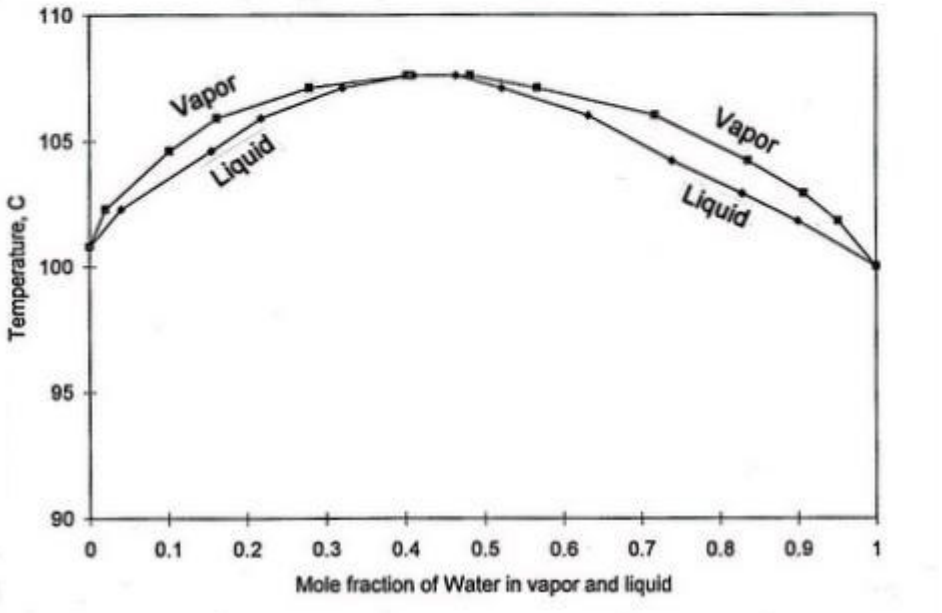
Subject: Azeotrope for the water-formic acid system at 101.3 kPa.

Given: Vapor-liquid equilibrium data from Section 13, p. 14 of Perry's Handbook, 6th edition.

Find: From data, construct *y-x* and *T-x-y* plots. Azeotrope conditions

Analysis: See plots below. From these plots, a maximum-boiling azeotrope occurs at 107.6°C with a composition of 42 mol% water and 58 mol% formic acid.





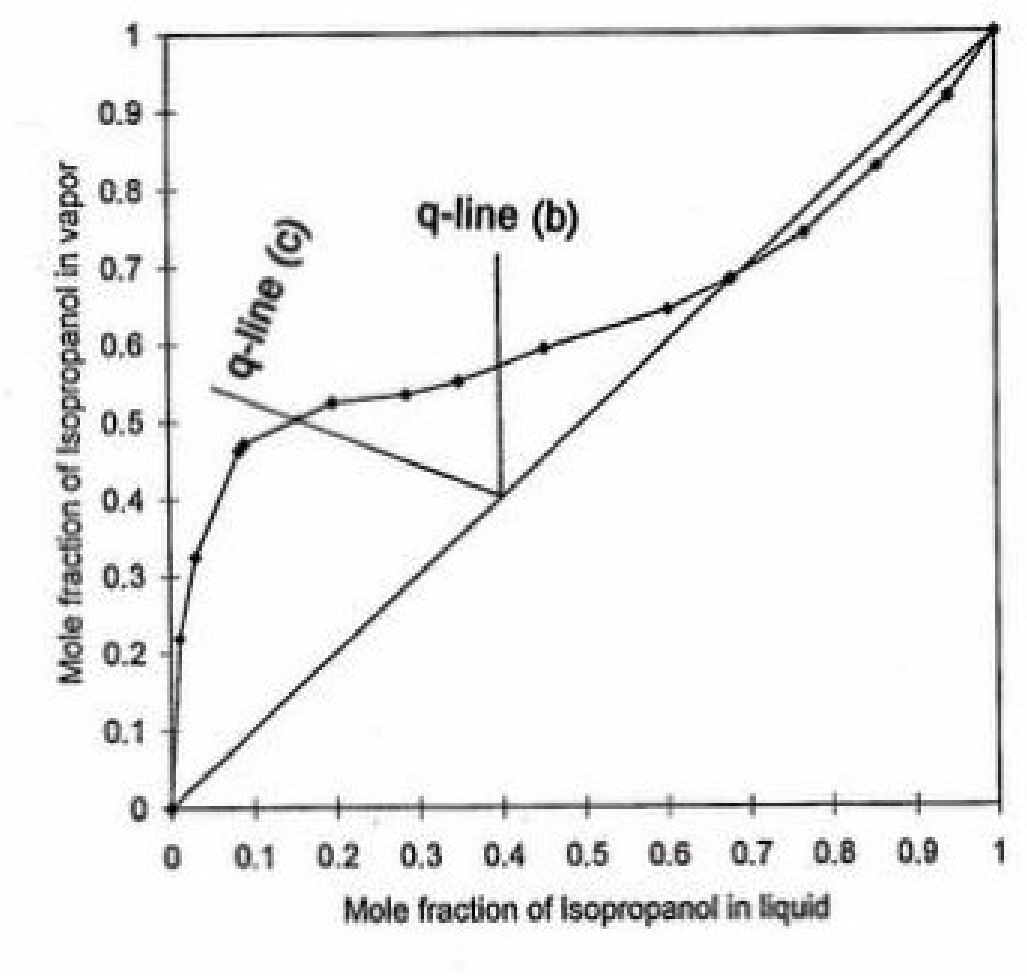
Exercise 4.15

Subject: Partial vaporization of a water (A) -isopropanol (B) mixture at 1 atm.

Given: Vapor-liquid equilibrium data at 1 atm and vapor-pressure data.

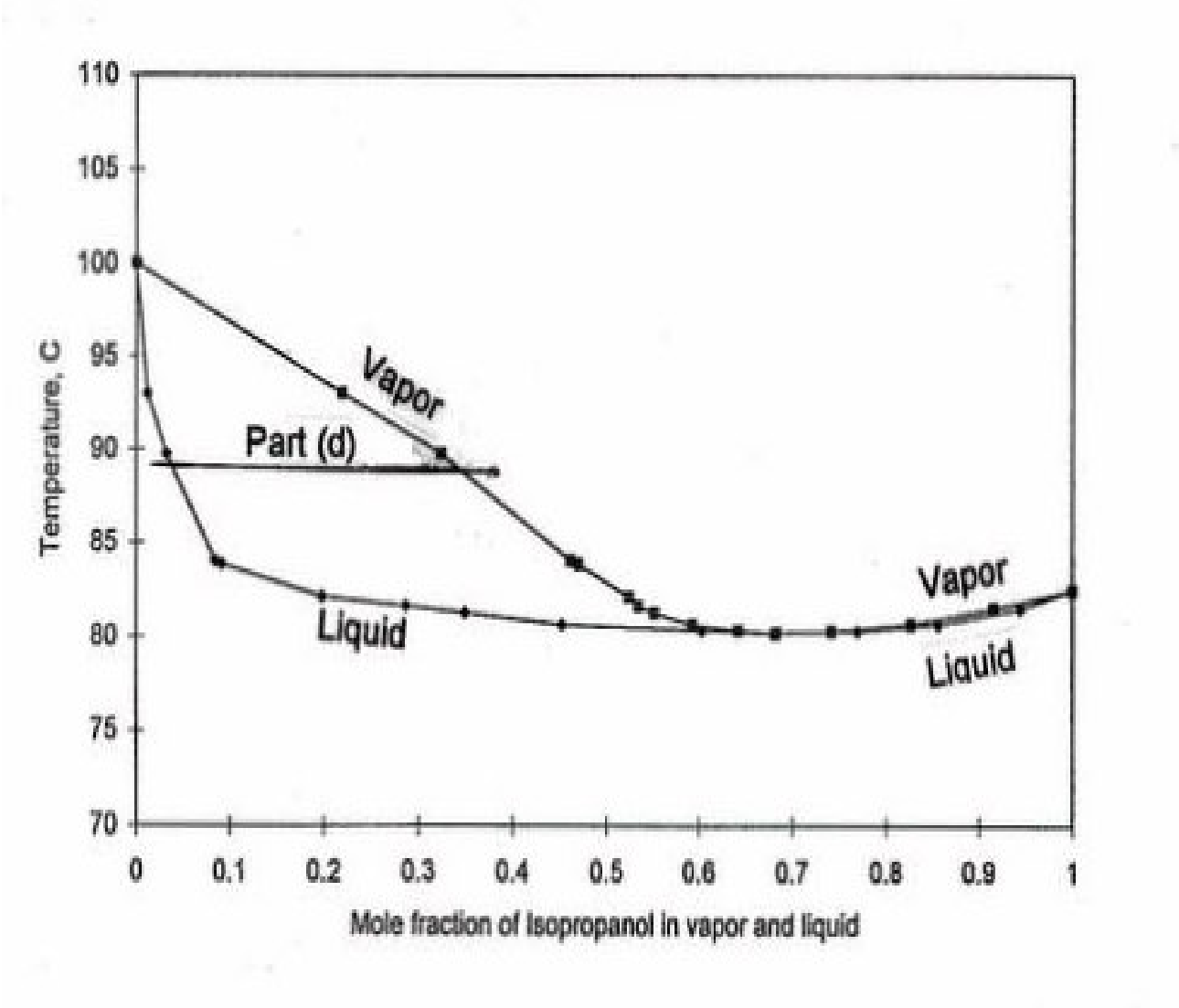
Find: (a) Construct *T-x-y* and *y-x* diagrams.
(b) Composition of vapor when a 60 mol% A - 40 mol% B mixture is at its bubble point.
(c) Composition of vapor and liquid for 75 mol% vaporization of mixture in Part (a).
(d) *K*-values and α-values at 80 and 89°C.
(e) Comparison of parts (a), (b), and (c) to results from using Raoult's and Dalton's laws.

Analysis: (a) The following are plots of the given equilibrium data, including the pure-component normal boiling points.



Exercise 4.15 (continued)

Analysis: (a) continued



Exercise 4.15 (continued)

Analysis: (b) From the *y-x* plot on the previous page, the composition of the first bubble of vapor is 57 mol% isopropanol and 43 mol% water. See the q-line on the diagram.

(c) For 75 mol% vaporization, use the inverse lever-arm rule on the *T-x-y* diagram or plot a q-line on the *y-x* diagram. For the latter, from the equation above Eq. (4-6), the slope of the q-line is $[(V/F)-1]/(V/F) = (0.75-1.0)/0.75 = -0.333$. The construction is shown on the *y-x* diagram, where the intersection with the equilibrium curve gives $x_A = 0.14$ and $y_A = 0.50$.

(d) Can not compute the *K*-values or α at 80°C, because this temperature is below the lowest boiling mixture, which is the azeotrope.

At 89°C, the *T-x-y* diagram gives the following compositions from the line shown on the above diagram:

$$y_B = 0.35,\ y_A = 0.65 \qquad x_B = 0.035,\ x_A = 0.965$$

From Eq. (2-19) for the definition of the *K*- value,

$$K_B = \frac{y_B}{x_B} = \frac{0.35}{0.035} = 10 \qquad K_A = \frac{y_A}{x_A} = \frac{0.65}{0.965} = 0.67$$

From Eq. (2-21) for the definition of the relative volatility, α, noting that at 89°C and 1 atm, isopropanol is more volatile,

$$\alpha_{B,A} = \frac{K_B}{K_A} = \frac{10}{0.67} = 15$$

(e) To calculate *T-x-y* curves from vapor pressure data, using Raoult's and Dalton's laws, Eq. (2-44) applies, as well as the sum of the mole fractions in the phases in equilibrium. Thus,

$$K_A = \frac{y_A}{x_A} = \frac{P_A^s\{T\}}{P} \quad , \quad K_B = \frac{y_B}{x_B} = \frac{P_B^s\{T\}}{P} \qquad (1,\ 2)$$

$$y_A + y_B = 1 \quad , \quad x_A + x_B = 1 \qquad (3,\ 4)$$

Equations (1) to (4) can be reduced to the following equations for the mole fractions of benzene in terms of the *K*-values:

$$x_A = \frac{1 - K_B}{K_A - K_B} \quad , \quad y_A = K_A x_A \qquad (5,\ 6)$$

If the given vapor pressure data are fitted to Antoine equations, we obtain:

Exercise 4.15 (continued)

Analysis: (e) continued

$$P_A^s = \exp\left(18.4854 - \frac{3921.96}{T + 230.91}\right) \quad (7)$$

$$P_B^s = \exp\left(25.0173 - \frac{8010.6}{T + 353.238}\right) \quad (8)$$

Where vapor pressure is in torr and temperature is in °C. Solving, Eqs. (1) to (8),

T, °C	P^s of B	P^s of A	K_B	K_A	x_B	y_B	$\alpha_{B\text{-}A}$
82.5	760.0	392.1	1.0000	0.5159	1.000	1.000	1.938
84.0	809.5	416.2	1.0651	0.5476	0.874	0.931	1.945
86.0	879.9	450.2	1.1578	0.5924	0.721	0.835	1.954
88.0	955.7	486.6	1.2575	0.6402	0.583	0.733	1.964
90.0	1037.3	525.3	1.3649	0.6912	0.458	0.626	1.975
92.0	1125.0	566.6	1.4803	0.7456	0.346	0.513	1.985
94.0	1219.3	610.6	1.6043	0.8035	0.245	0.394	1.997
96.0	1320.5	657.4	1.7375	0.8650	0.155	0.269	2.009
98.0	1429.1	707.2	1.8804	0.9305	0.073	0.138	2.021
100.0	1545.6	760.0	2.0336	1.0000	0.000	0.000	2.034

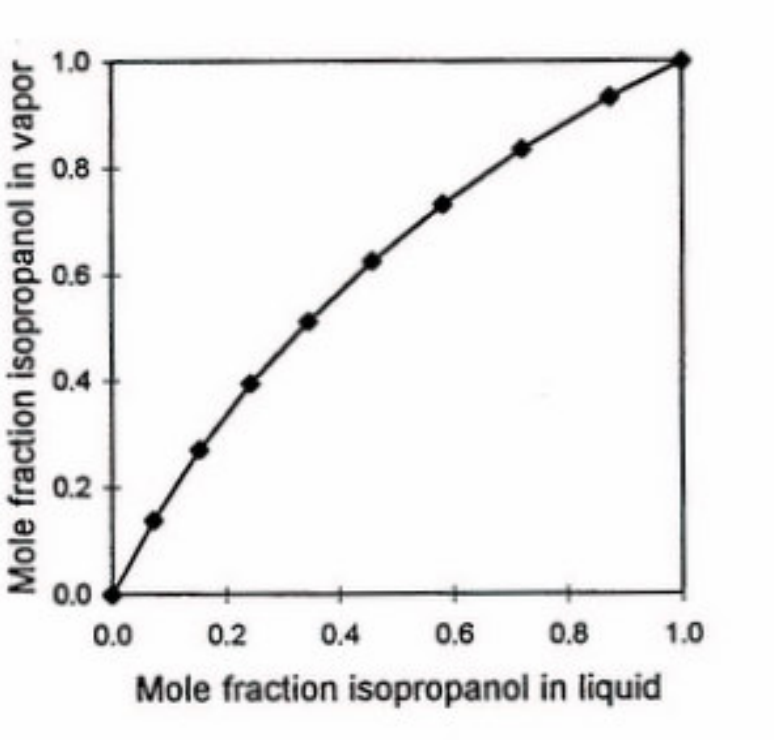
These results are plotted below. Raoult's law is badly in error when compared to the experimental data.

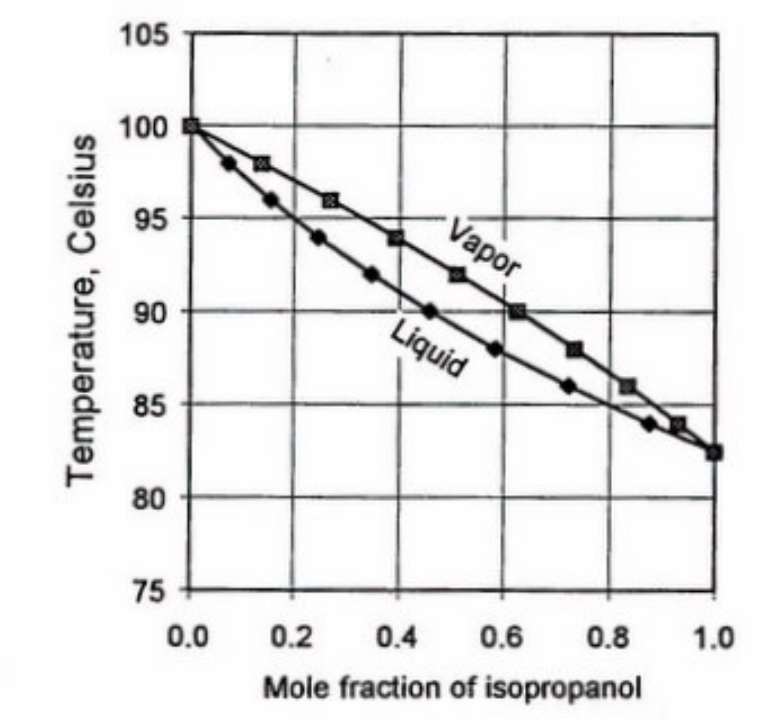
For part (b), Raoult's law predicts a bubble-point vapor with an isopropanol mole fraction of 0.56.

By coincidence, this compares well with the result determined with the experimental data.
For part (c), however, Raoult's law predicts isopropanol mole fractions of 0.28 for the liquid and 0.43 for the vapor. These are drastically different from the values of 0.14 and 0.50, respectively from the experimental data. Raoult's law can not be used for the isopropanol-water system, for which it also fails to predict an azeotrope.

Exercise 4.15 (continued)

Analysis: (e) continued





Exercise 4.16

Subject: Vaporization of mixtures of n-hexane (H) and n-octane (C) at 1 atm

Given: *T*-*x*-*y* diagram in Fig. 4.3, and *y*-*x* diagram in Fig. 4.4. 100 kmol mixture.

Find: Temperature, kmol of vapor, mole fractions of H in liquid and vapor at equilibrium for various flash conditions.

Analysis: Let z_H = mole fraction of n-hexane in the feed and $\Psi = V/F$.
Use inverse lever-arm rule as displayed by Line DEF in Fig. 4.3.
The results for parts (a) through (f) are as follows:

Given	T, °F	V, kmol	y_H	x_H
(a) $z_H = 0.5$, $\Psi = 0.2$	196	20	0.80	0.43
(b) $z_H = 0.4$, $y_H = 0.6$	220	48.6	0.60	0.21
(c) $z_H = 0.6$, $x_C = 0.7$	210	73.7	0.70	0.30
(d) $z_H = 0.5$, $\Psi = 0.0$	188	0.0	0.84	0.50
(e) $z_H = 0.5$, $\Psi = 1.0$	230	100	0.50	0.14
(f) $z_H = 0.5$, $T = 200$°F	200	31	0.77	0.38

Exercise 4.17

Subject: Derivation of equilibrium flash equations for a binary mixture (1, 2).

Given: Eqs. (5), (6), and (3) of Table 4.4.

Find: Derive given equations for x_1, x_2, y_1, y_2, and $\Psi = V/F$.

Analysis: First derive the equation for $\Psi = V/F$. From Eq. (3), Table 4.4,

$$\frac{z_1(1-K_1)}{1+\Psi(K_1-1)}+\frac{(1-z_1)(1-K_2)}{1+\Psi(K_2-1)}=0 \qquad (1)$$

Solving Eq. (1) for Ψ, and simplifying,

$$\Psi=\frac{-z_1(1-K_1)-(1-z_1)(1-K_2)}{z_1(1-K_1)(K_2-1)+(1-z_1)(1-K_2)(K_1-1)}=\frac{z_1\left[(K_1-K_2)/(1-K_2)\right]-1}{K_1-1} \qquad (3)$$

Substituting Eq. (3) into Eq. (5) of Table 4.4 and simplifying gives the required equation for x_1.
Then use $y_1 = K_1x_1$ and simplify, followed by $x_2 = 1 - x_1$ and $y_2 = 1- y_1$.

Exercise 4.18

Subject: Conditions for Rachford-Rice equation to be satisfied.

Given: Eq. (3), Table 4.4, which is the Rachford-Rice equation.

Find: Conditions under which the equation can be satisfied for $0 \le \frac{V}{F} \le 1$.

Analysis: A necessary, but not sufficient, condition is that at least one K-value is < 1 and at least one K-value is > 1. If all K-values are > 1, the sum:

$$\sum_{i=1}^{C} \frac{z_i(1-K_i)}{1+\Psi(K_i-1)}$$ will be negative and can not be zero.

If all K-values are < 1, the numerator in the sum will be positive for each term. With Ψ between 0 and 1, the term $\Psi(K_i - 1)$ will always be < 1. Therefore, the denominator will be positive also and the sum will be positive and can not be zero.

Exercise 4.19

Subject: Flash vaporization of a benzene (A) - toluene (B) mixture for $\alpha_{A\text{-}B} = 2.3$.

Given: Feed is 40 mol% A and 60 mol% B.

Find: Percent of A in the equilibrium vapor if 90% of the toluene leaves in the liquid by graphical means.

Analysis: For constant relative volatility, Eq. (4-8) applies, $$y_A = \frac{\alpha_{A,B} x_A}{1 + x_A(\alpha_{A,B} - 1)}$$

Solving this equation for y_A as a function of x_A ,

x_A	y_A
0.1	0.2035
0.2	0.3651
0.3	0.4964
0.4	0.6053
0.5	0.6970
0.6	0.7753
0.7	0.8429
0.8	0.9020
0.9	0.9539

A plot of the calculated equilibrium curve is given below. To use this plot for a graphical solution of the equilibrium, draw a q-line, using the following equation above Eq. (4-6), for an assumed value of $\Psi = V/F$ and check the resulting % recovery of toluene in the liquid. Vary Ψ until the % recovery = 90%. Then compute, for the corresponding Ψ , the % recovery of benzene in the vapor.

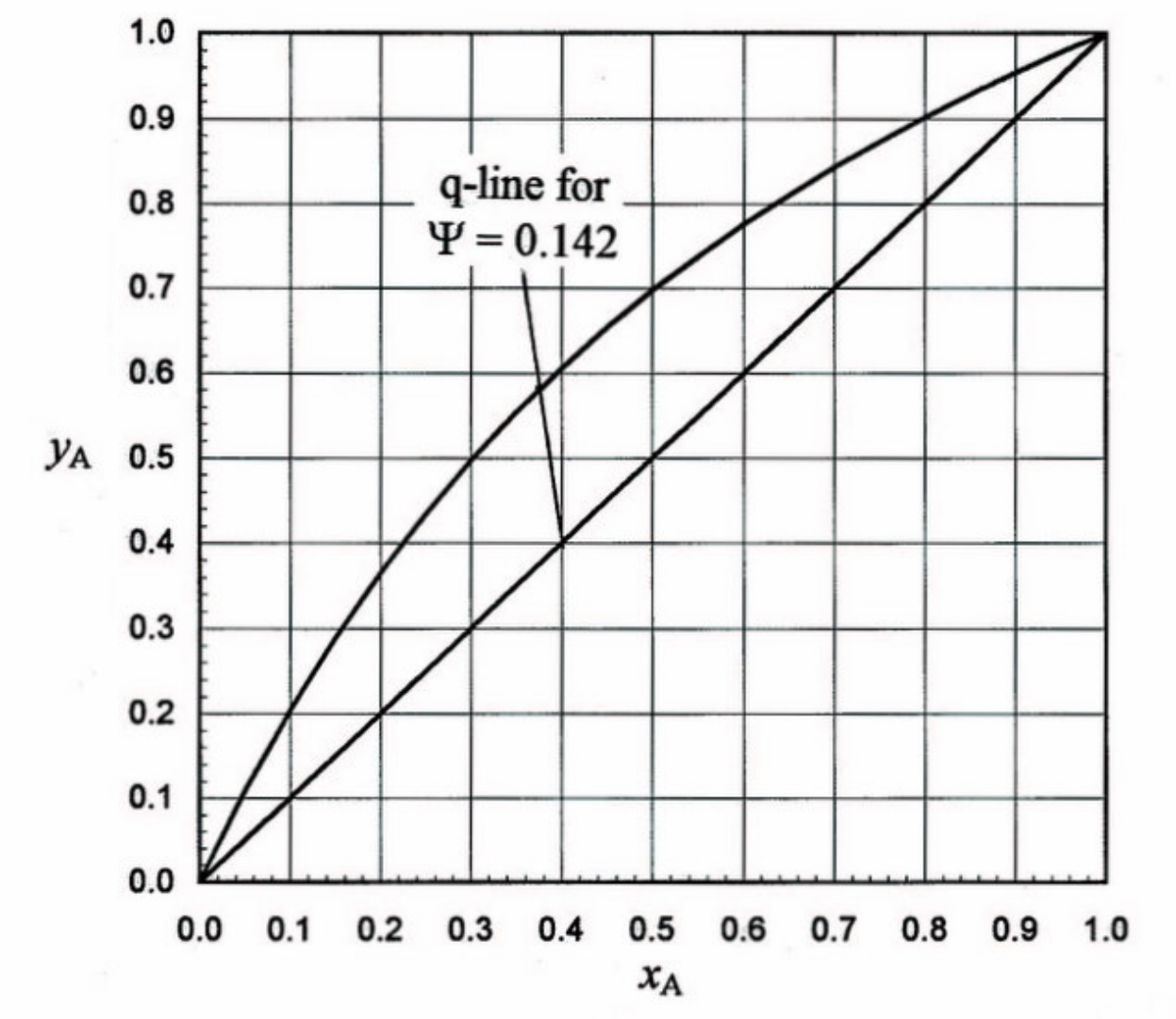
$$y_A = \left(\frac{\Psi - 1}{\Psi}\right) x_A + \left(\frac{1}{\Psi}\right) z_A = \left(\frac{\Psi - 1}{\Psi}\right) x_A + \left(\frac{1}{\Psi}\right) 0.40 \qquad (1)$$

Exercise 4.19 (continued)

Analysis: (continued)

Basis: F = 100 moles, 60 moles toluene (B). Want 0.9(60) = 54 moles B in liquid. Therefore, 60 - 54 = 6 moles B in vapor. Therefore, want $(n_B)_V = y_B V = (1 - y_A)100\Psi = 6$. Then compute % recovery of benzene in vapor = $(n_A)_V/40$ x 100% = $y_A V/40$ x 100% = 2.5 $y_A\Psi$ x 100%. The following are typical values for the trial and error procedure, with the final result at the bottom.

Assumed Ψ	y_A	x_A	$(n_B)_V$, moles	% recovery of A in vapor
0.3	0.54	0.35	13.8	40.5
0.2	0.56	0.36	8.8	28.0
0.15	0.575	0.37	6.4	21.6
0.142	0.58	0.375	6.0	20.6



Exercise 4.20

Subject: Flash vaporization of a benzene (A) - toluene (B) mixture.

Given: Feed is 40 mol% A and 60 mol% B. Vapor pressure data.

Assumptions: Raoult's law (ideal solutions). Pressure = 1 atm.

Find: Percent of A in the equilibrium vapor if 90% of the toluene leaves in the liquid.

Analysis: Basis: F = 100 mole with 60 moles B and 40 moles A. Want 0.9(60) = 54 moles B in liquid. Therefore, 60 - 54 = 6 moles B in vapor. Therefore, want $(n_B)_V = y_B V = (1 - y_A)100\Psi = 6$. Then compute % recovery of benzene in vapor = $(n_A)_V/40$ x 100% = $y_A V/40$ x 100% = 2.5 $y_A\Psi$ x 100%. The following trial and error procedure can be used, based on material balance and equilibrium equations:
(1) Guess a temperature. (2) Read vapor pressures from Fig. 2.4 and compute K-values from Raoult's law (Eq. (3), Table 2.3), $K_i = P_i^s / P$. (3) Solve for $\Psi = V/F$ using the fifth equation in Exercise 4.17,

$$\Psi = \frac{z_A\left[\left(K_A - K_B\right)/\left(1-K_B\right)\right]-1}{K_A - 1} = \frac{0.40\left[\left(K_A - K_B\right)/\left(1-K_B\right)\right]-1}{K_A - 1}$$

(4) Solve for y_A from the third equation in Exercise 4.17,

$$y_A = \left(K_A K_B - K_A\right)/\left(K_B - K_A\right)$$

(5) Compute $(n_B)_V = (1 - y_A)100\Psi$. If the value is 6, then temperature guess is correct. Otherwise, guess another T, and repeat steps (1) to (5). If 6, compute % recovery of benzene in the vapor from 2.5 $y_A\Psi$ x 100%.

Guess T, °F	P^s of A, psia	P^s of B, psia	K_A	K_B	Ψ	y_A	Moles B in vapor
195	20.0	8.0	1.36	0.544	-0.79		
205	23.4	9.5	1.59	0.646	0.113	0.596	4.6
205.5	23.6	9.6	1.605	0.653	0.161	0.585	6.7

By interpolation, T = 205.3°F to obtain 6 moles of B in the vapor. This corresponds to Ψ = 0.145 and y_A = 0.588. From above,

% recovery of benzene in the vapor = 2.5(0.588)(0.145)100% = 21.3%

Exercise 4.21

Subject: Equilibrium flash of a seven-component mixture.

Given: Feed mole fractions and *K*-values.

Find: $\Psi = V/F$ by:

(a) Rachford- Rice equation, $f_1\{\Psi\} = \sum_{i=1}^{C} \frac{z_i(1-K_i)}{1+\Psi(K_i-1)} = \sum_{i=1}^{C} g_1\{i,\Psi\}$

(b) Alternative flash equation, $f_2\{\Psi\} = \sum_{i=1}^{C} \frac{z_i K_i}{1+\Psi(K_i-1)} = \sum_{i=1}^{C} g_2\{i,\Psi\}$

Make plots of $f\{\Psi\}$ vs. Ψ for each method and compare.

Analysis: Calculations with a spreadsheet, for values of Ψ from 0 to 1.0 in intervals of 0.1:

(a)

I	z_F	*K*	$\Psi = 0$	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1
			g{i,Ψ}:										
1	0.0079	16.2	-0.120	-0.048	-0.030	-0.022	-0.017	-0.014	-0.012	-0.010	-0.009	-0.008	-0.007
2	0.1321	5.2	-0.555	-0.391	-0.302	-0.245	-0.207	-0.179	-0.158	-0.141	-0.127	-0.116	-0.107
3	0.0849	2.6	-0.136	-0.117	-0.103	-0.092	-0.083	-0.075	-0.069	-0.064	-0.060	-0.056	-0.052
4	0.2690	1.98	-0.264	-0.240	-0.220	-0.204	-0.189	-0.177	-0.166	-0.156	-0.148	-0.140	-0.133
5	0.0589	0.91	0.005	0.005	0.005	0.005	0.005	0.006	0.006	0.006	0.006	0.006	0.006
6	0.1321	0.72	0.037	0.038	0.039	0.040	0.042	0.043	0.044	0.046	0.048	0.049	0.051
7	0.3151	0.28	0.227	0.244	0.265	0.289	0.319	0.354	0.399	0.457	0.535	0.645	0.810
		f{Ψ}:	-0.805	-0.508	-0.345	-0.227	-0.130	-0.042	0.045	0.137	0.245	0.380	0.568

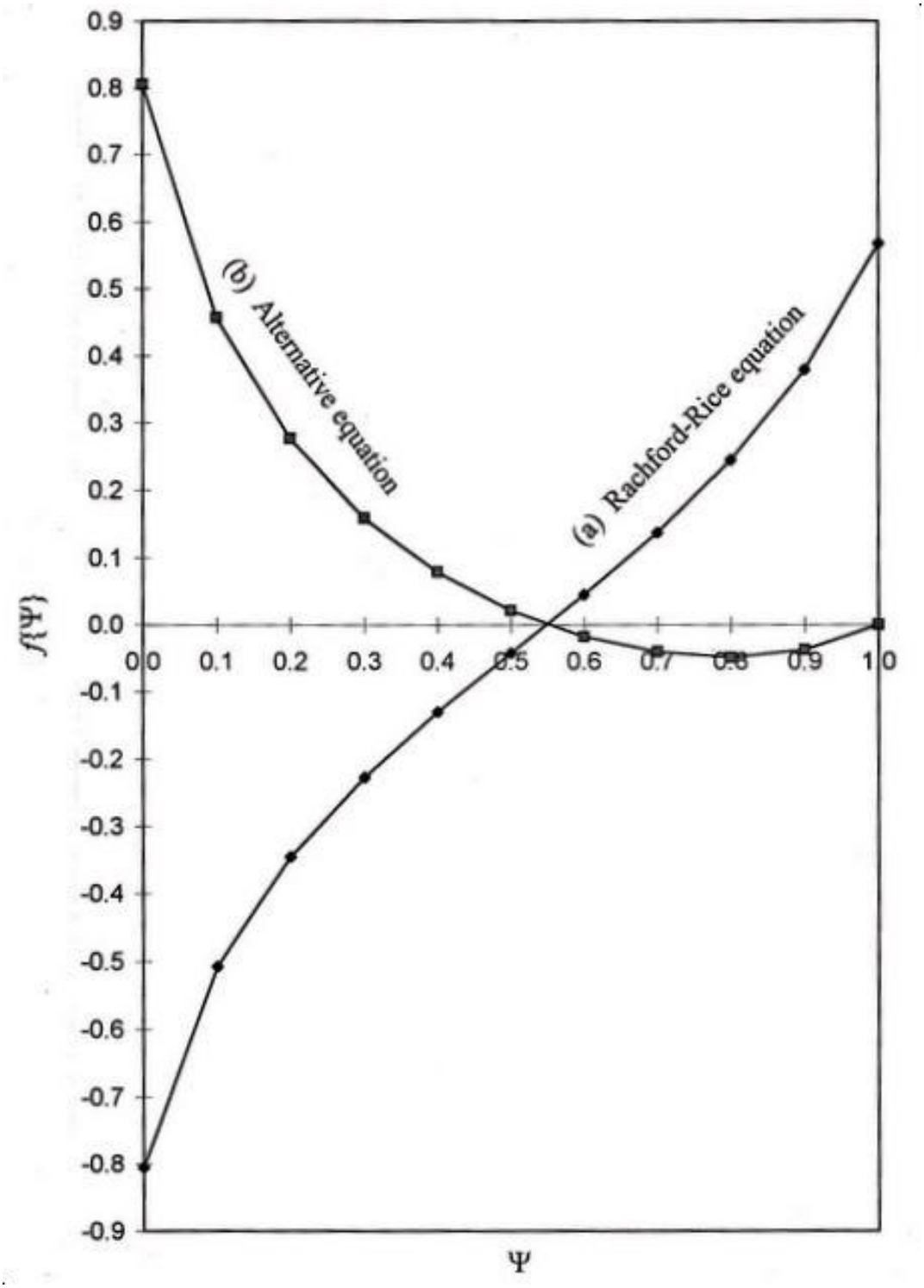
(b)

I	z_F	*K*	$\Psi = 0$	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1
			g{i,Ψ}:										
1	0.0079	16.2	0.128	0.051	0.032	0.023	0.018	0.015	0.013	0.011	0.010	0.009	0.008
2	0.1321	5.2	0.687	0.484	0.373	0.304	0.256	0.222	0.195	0.174	0.158	0.144	0.132
3	0.0849	2.6	0.221	0.190	0.167	0.149	0.135	0.123	0.113	0.104	0.097	0.090	0.085
4	0.2690	1.98	0.533	0.485	0.445	0.412	0.383	0.357	0.335	0.316	0.299	0.283	0.269
5	0.0589	0.91	0.054	0.054	0.055	0.055	0.056	0.056	0.057	0.057	0.058	0.058	0.059
6	0.1321	0.72	0.095	0.098	0.101	0.104	0.107	0.111	0.114	0.118	0.123	0.127	0.132
7	0.3151	0.28	0.088	0.095	0.103	0.113	0.124	0.138	0.155	0.178	0.208	0.251	0.315
		f{Ψ}:	0.805	0.457	0.276	0.159	0.078	0.021	-0.018	-0.041	-0.049	-0.038	0.000

The values of $f\{\Psi\}$ are plotted on the next page, where it is observed that the Rachford-Rice and Alternative equations give the same result of $\Psi = 0.55$. However, the alternative equation also has a trivial root at $\Psi = 1.0$. With a Newton procedure, the alternative equation may converge to the trivial root. Therefore, the Rachford-Rice equation is preferred because of its uniqueness.

Exercise 4.21 (continuous)

Analysis: (continued)



Exercise 4.22

Subject: Equilibrium flash of a hydrocarbon mixture.

Given: 100 kmoles of 25 mo1% nC_4, 40 mol% nC_5, and 35 mol% nC_6. *K*-values in Fig. 2.8

Assumptions: Amounts are per hour.

Find: Pressure and liquid and vapor compositions for equilibrium at 240°F to recover, in the liquid phase, 80% of the nC_6 in the feed.

Analysis: For 80% recovery of nC_6, the liquid product must contain (0.35)(0.80)(100) = 28 kmole/h of nC_6. Must solve by trial and error by assuming values of pressure to obtain the *K*-values from Fig. 2.8. Then solve the Rachford-Rice equation (Eq. (3), Table 4.4),

$$f\{\Psi\} = \sum_{i=1}^{C} \frac{z_i(1-K_i)}{1+\Psi(K_i-1)} = 0$$

for $\Psi = V/F$ by a nonlinear solver, such as Newton's method. Compute *V* from Eq. (4), Table 4.4. Then solve Eqs. (5) and (6), Table 4.4 for the equililbrium vapor and liquid compositions. Solve for the liquid, *L,* from Eq. (7). Repeat this procedure until 28 kmol/h of nC_6 are found in the equilibrium liquid as computed from $(n_{nC_6})_L = x_{nC_6} L$, noting that each assumed pressure requires an iterative procedure to solve for Ψ from the Rachford-Rice equation. The calculations are summarized in the following table:

Assumed *P*, psia		100	110	117
K-values:	nC_4	2.40	2.30	2.25
	nC_5	1.20	1.08	1.00
	nC_6	0.53	0.50	0.48
V/F		0.706	0.482	0.335
L, kmol/h		29.4	51.8	66.5
x of nC_4		0.524	0.461	0.424
n_L of nC_4, kmol/h		15	24	28

Therefore, the converged pressure is 117 psia. The equilibrium vapor and liquid compositions in terms of amounts are:

Component	Vapor flows, kmol/h	Liquid flows, kmol/h
nC_4	13	12
nC_5	13	27
nC_6	7	28

.

Exercise 4.23

Subject: Equilibrium flash vaporization of a hydrocarbon mixture.

Given: Equimolar mixture of C_2, C_3, nC_4, and nC_5. *K*-values from Fig. 2.8 and 2.9

Find: Amounts and compositions of equilibrium liquid and vapor at 150°F and 205 psia. Conditions of *T* and *P* where 70% of C_2 and no more than 5% of nC_4 is in the vapor.

Analysis: Take as a basis, a feed of 100 lbmol/h. From Fig. 2.8, at 150°F and 205 psia, the *K*-values are as given in the table below. Then solve the Rachford-Rice equation (Eq. (3), Table 4.4),

$$f\{\Psi\} = \sum_{i=1}^{C} \frac{z_i(1-K_i)}{1+\Psi(K_i-1)} = 0$$

for $\Psi = V/F$ by a nonlinear solver, such as Newton's method. Compute *V* from Eq. (4), Table 4.4. Then solve Eqs. (5) and (6), Table 4.4 for the equililbrium vapor and liquid compositions. The calculations are summarized in table below, which also includes other conditions of *T* and *P* to obtain 70% of C_2 and no more than 5% of nC_4 in the vapor. Thus, we desire (0.7)(25) = 17.5 lbmol/h of C_2 in the vapor and 25 - 17.5 = 7.5 lbmol/hr of C_2 in the liquid. At the same time we desire no more than (0.05)(25) = 1.25 lbmol/h of nC_4 in the vapor, corresponding to 25 - 1.25 = 23.75 lbmol/h of nC_4 in the liquid. In searching for these other conditions, we note that at the base conditions, 75.8% of the C_2 goes to the vapor, which is very close to the desired 70%. But 30% of the nC_4 also goes to the vapor, which is much higher than the desired 5%. The relative volatility of C_2 to nC_4 at the base conditions is:

$$\alpha_{C_2,nC_4} = \frac{K_{C_2}}{K_{nC_4}} = \frac{y_{C_2}/x_{C_2}}{y_{nC_4}/x_{nC_4}} = \frac{(n_{C_2})_V/(n_{C_2})_L}{(n_{nC_4})_V/(n_{nC_4})_L} = \frac{(19.0/6.0)}{(7.5/17.5)} = 7.39$$

But we need a relative volatility of:

$$\alpha_{C_2,nC_4} = \frac{(n_{C_2})_V/(n_{C_2})_L}{(n_{nC_4})_V/(n_{nC_4})_L} = \frac{(17.5/7.5)}{(1.25/23.75)} = 44.3$$

For ideal solutions, where the Raoult's law *K*-value applies, Eq. (2-21) combined with Eq. (3 in Table 2.3, gives relative volatility as independent of pressure and equal to the ratio of vapor pressures, which depend only on temperature. In general, as the temperature is reduced, the relative volatility increases. Assume that the hydrocarbon mixture, although not an ideal solution,

Exercise 4.23 (continued)

Analysis: (continued)

follows these same trends. Thus, to increase the relative volatility, the pressure has little effect. We must decrease the temperature to obtain the desired relative volatility, and then adjust the pressure to obtain the required compositions. The base case and calculations leading to the desired separation are summarized in the following table:

	Base Case			Desired Case
T, °F	150	-70	-40	-40
P, psia	205	14.7	14.7	16.4
K-values: C_2	4.1	4.0	7.5	6.7
C_3	1.5	0.46	1.11	1.00
nC_4	0.56	0.055	0.165	0.148
nC_5	0.215	0.077	0.028	0.025
α of C_2 to nC_4	7.3	73	45	45
% C_2 to vapor	75.8			70
% nC_4 to vapor	30			4.9

Thus, at -40°F and 16.4 psia, the desired 70% of the ethane is found in the vapor product, with only 5% of the n-butane.

The compositions of the vapor and liquid products for the base case and the desired case are as follows:

	Base Case:				Desired Case:			
Component	v, lbmol/h	y	l, lbmol/h	x	v, lbmol/h	y	l, lbmol/h	x
C_2	19.0	0.44	6.0	0.11	17.5	0.69	7.5	0.10
C_3	13.4	0.31	11.6	0.20	6.4	0.25	18.6	0.25
nC_4	7.5	0.17	17.5	0.31	1.22	0.05	23.78	0.32
nC_5	3.5	0.08	21.5	0.38	0.22	0.01	24.78	0.33
Total:	43.4	1.00	56.6	1.00	25.34	1.00	74.66	1.00

Exercise 4.24

Subject: Cooling of a reactor effluent with recycle liquid from a partial condensation.

Given: Reactor effluent temperature of 1000°F and composition in lbmol/h of 2000 H_2, 2000 CH_4, 500 benzene, and 100 toluene. Partial condensation conditions or 100°F and 500 psia, and component *K*-values at these conditions. Two heat exchangers in a recycle loop.

Find: (a) Composition and flow rate of vapor leaving flash drum in Fig. 4.38.
(b) Proof that vapor flow rate is independent of quench rate.

Analysis: (a) Assume that vapor rate is independent of quench rate. Therefore, conduct the flash calculation on just the reactor effluent at the flash drum conditions of temperature and pressure. Use the Rachford-Rice equations (Eqs. (3) and (6), Table 4.4):

$$f\{\Psi\} = \sum_{i=1}^{C} \frac{z_i(1-K_i)}{1+\Psi(K_i-1)} = 0 \qquad (1)$$

$$y_i = \frac{z_i K_i}{1+\Psi(K_i-1)} \qquad (2)$$

Nonlinear Eq. (1) is solved for $\Psi = V/F$, followed by calculation of $V = \Psi F$, and then calculations of vapor mole fractions from Eq. (2). The given input for Eq. (1) is:

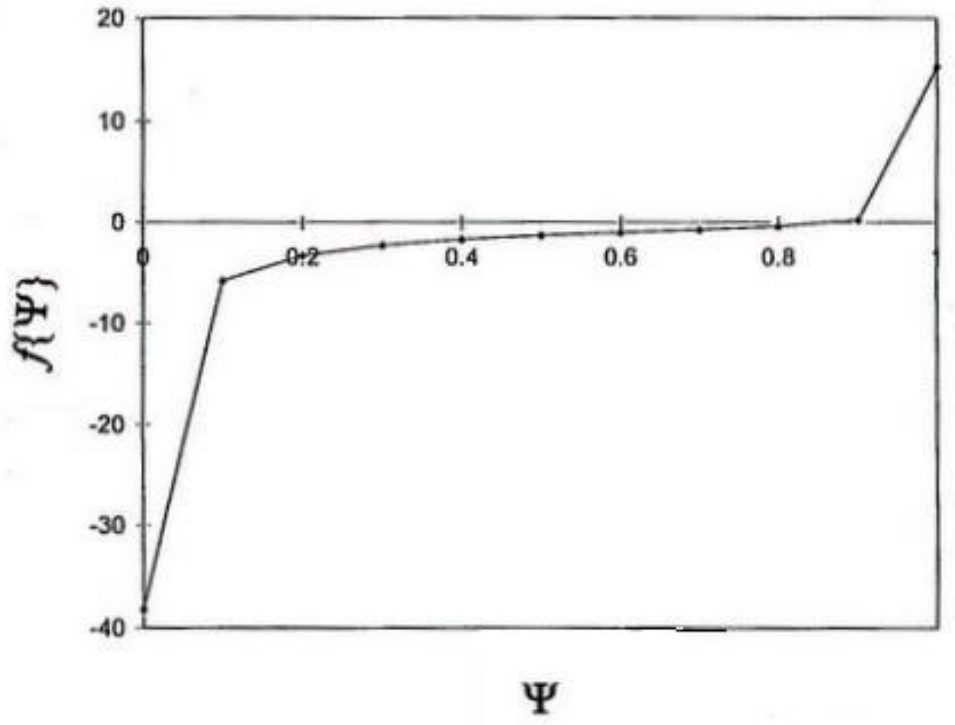
Component	f, lbmol/h	z_i	K_i
Hydrogen	2,000	0.4348	80
Methane	2,000	0.4348	10
Benzene	500	0.1087	0.010
Toluene	100	0.0217	0.004

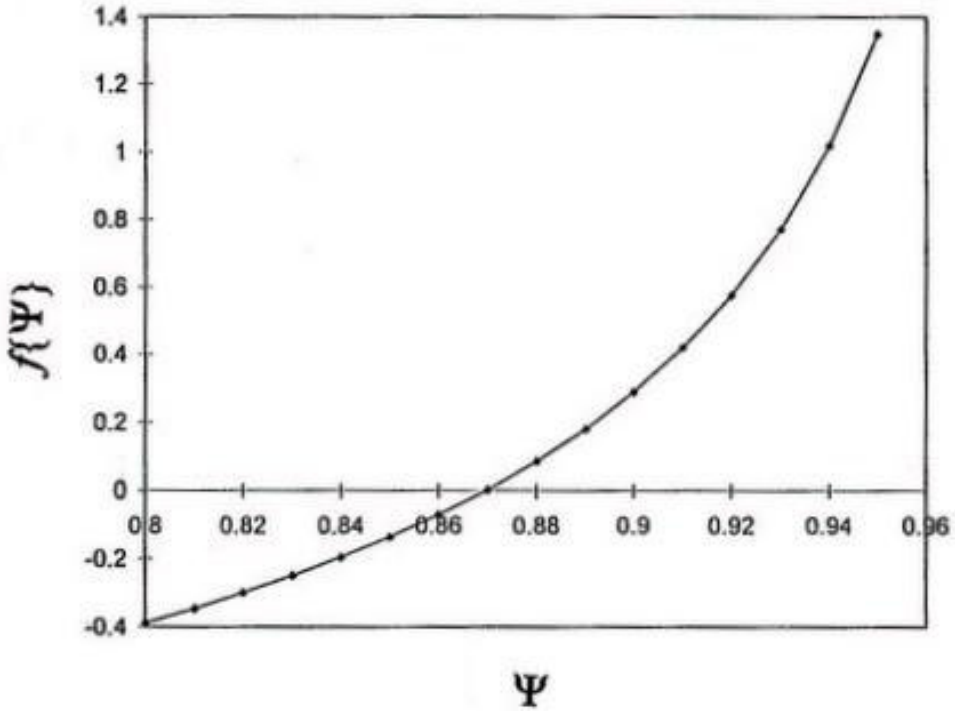
One method for solving Eq. (1) is to use a spreadsheet to make a plot of $f\{\Psi\}$ vs. Ψ in increments of 0.1 from 0.0 to 1.0. Then, use smaller increments in Ψ in the vicinity of $f\{\Psi\} = 0$ to obtain the solution. The results are shown in the two figures on the next page. The converged solution is
$\Psi = 0.8697$. Therefore, $V = 0.8697(4{,}600) = 4{,}000.6$ lbmol/h. The composition of the equilibrium vapor from Eq. (2) is as follows:

Component	z_i	y_i	x_i
Hydrogen	0.4348	0.4990	0.0062
Methane	0.4348	0.4925	0.0493
Benzene	0.1087	0.0078	0.7820
Toluene	0.0217	0.0007	0.1625

Exercise 4.24 (continued)

Analysis: (a) (continued)

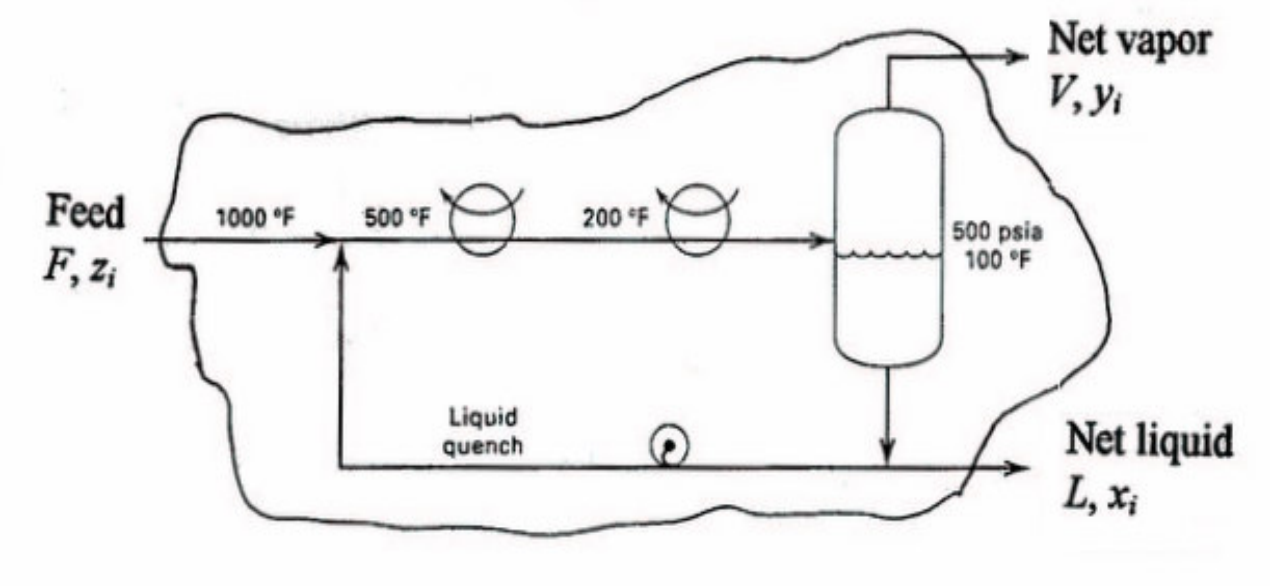




Exercise 4.24 (continued)

Analysis:

(b) When the flash conditions of temperature and pressure are fixed, the compositions of the equilibrium vapor and liquid are independent of any recycle of equilibrium liquid or vapor. To prove this, draw a material balance envelope around the system in Fig. 4.38 as shown below. Now, the flash equations are the same as in Table 4.3, except for the energy balance, Eq. (6). But, that equation is only solved after all of the other equations are solved. Thus, the results for the compositions of the net vapor and liquid products are the same as when there is no recycle.



Exercise 4.25

Subject: Partial condensation of a gas mixture at 120°F and 300 psia.

Given: Gas at 392°F and 315 psia, with a composition in kmol/h of 72.53 N_2, 7.98 H_2, 0.13 benzene, and 150 cyclohexane. The gas is cooled and partial condensed to 120°F and 300 psia, followed by phase separation.

Find: Equilibrium vapor and liquid flow rates and compositions.

Analysis: The flash calculations are made conveniently with a process simulator, using an appropriate *K*-value correlation. The following results were obtained with CHEMCAD, using the Chao-Seader, Grayson-Streed (CSGS) method for *K*-values.

Component	CSGS K_i	f_i, kmol/h	v_i, kmol/h	l_i, kmol/h
Hydrogen	79.7	72.53	70.82	1.71
Nitrogen	7.54	7.98	6.36	1.62
Benzene	0.024	0.13	0.0016	0.1284
Cyclohexane	0.022	150.00	1.67	148.33

Exercise 4.26

Subject: Rapid determination of phase condition without making a flash calculation.

Given: A hydrocarbon mixture at 200°F and 200 psia, with a composition in lbmol/h of 125 C_3, 200 nC_4, and 175 nC_5, and *K*-values at these conditions.

Find: Phase(s) present without making a flash condition.

Analysis: From Eq. (4-12), have a subcooled liquid if $\sum_{i=1}^{C} z_i K_i < 1$.

From Eq. (4-13), have a superheated vapor if $\sum_{i=1}^{C} \frac{z_i}{K_i} < 1$.

Component	f_i	z_i	K_i	z_iK_i	z_i/K_i
C_3	125	0.25	2.056	0.514	0.122
nC_4	200	0.40	0.925	0.370	0.432
nC_5	175	0.35	0.520	0.182	0.673
Total:	500	1.00		1.066 > 1	1.227 > 1

Therefore stream is partially vaporized. Both vapor and liquid phases present.

Exercise 4.27

Subject: Determination of reflux-drum pressure for a specified temperature and total distillate (vapor and liquid phases) composition

Given: Overhead partial condensing system of a distillation column that produces vapor distillate, liquid distillate, and liquid reflux. Of the total distillate, 10 mol% is vapor. Reflux drum temperature is 100°F, and composition of total distillate in mole fractions is 0.10 C_2, 0.20 C_3, and 0.70 nC_4. Reflux pressure is not given, but *K*-values at 100°F and 200 psia are given.

Assumptions: ***K***-values are inversely proportional to pressure.

Find: Pressure in the reflux drum.

Analysis: As shown in Exercise 4.24, the compositions of net equilibrium vapor and liquid are independent of recycle or, in this case, reflux. Therefore, the flash equations can be applied using the total distillate composition as the feed composition. Therefore, $\Psi = V/F = 0.10$. The *K*-values

are given by: $$K_{C_2} = 2.7\left(\frac{200}{P}\right), \quad K_{C_3} = 0.95\left(\frac{200}{P}\right), \quad K_{nC_4} = 0.34\left(\frac{200}{P}\right)$$

Substituting these equations into Eq. (3), Table 4.4,

$$f\{P\} = \frac{0.1\left[1-2.7\left(\frac{200}{P}\right)\right]}{1+0.1\left[2.7\left(\frac{200}{P}\right)-1\right]} + \frac{0.1\left[1-0.95\left(\frac{200}{P}\right)\right]}{1+0.1\left[0.95\left(\frac{200}{P}\right)-1\right]} + \frac{0.1\left[1-0.34\left(\frac{200}{P}\right)\right]}{1+0.1\left[0.34\left(\frac{200}{P}\right)-1\right]} = 0 \qquad (1)$$

Eq. (1) is a nonlinear equation that can be solved by various means. Using a spreadsheet, in a manner similar to that used to solve Exercise 4.24, we obtain $P = 126$ psia.

Exercise 4.28

Subject: Comparison of flash calculations using three different *K*-value correlations.

Given: A stream at 7.2°C and 2,620 kPa with the overall composition given below.

Find: Phase conditions

Analysis: Using the CHEMCAD process simulator, the following results are obtained using the Soave-Redlich-Kwong (SRK), Peng-Robinson (PR), and Benedict-Webb-Rubin-Starling (BWRS) correlations:

K-values:

Component	SRK	PR	BWRS
N_2	17.5	17.6	16.3
C_1	5.73	5.71	6.00
C_2	1.07	1.12	0.99
C_3	0.327	0.337	0.292
nC_4	0.098	0.102	0.087
nC_5	0.036	0.032	0.029
nC_6	0.0096	0.0110	0.0071

The *K*-values for the SRK and PR correlations are in reasonably good agreement, deviating from each other by less than 15 %. Except for C_1, the BWRS correlation predicts lower values, with the biggest deviation for nC_6.

Product compositions:

		SRK:		**PR:**		**BWR:**	
Component	***f*, kmol/h**	***v*, kmol/h**	***l*, kmol/h**	***v*, kmol/h**	***l*, kmol/h**	***v*, kmol/h**	***l*, kmol/h**
N_2	1.0	0.70	0.30	0.69	0.31	0.67	0.33
C_1	124.0	52.92	71.08	52.06	71.94	53.04	70.96
C_2	87.6	11.13	76.46	10.45	77.15	9.63	77.97
C_3	161.6	6.81	154.79	6.42	155.18	5.67	155.93
nC_4	176.2	2.31	173.89	2.16	174.04	1.88	174.32
nC_5	58.5	0.25	58.25	0.26	58.24	0.21	58.29
nC_6	33.7	0.05	33.65	0.04	33.66	0.03	33.67
Total:	642.60	74.17	568.43	72.08	570.52	71.13	571.47

All three correlations predict about the same *V/F* ratio, which ranges from 0.1107 to 0.1154.

Exercise 4.29

Subject: Equilibrium flash calculations at different temperatures and pressures

Given: Mixture of 100 kmol of 60 mol% benzene (A), 25 mol% toluene (B), and 15 mol% o-xylene (C). Sources of vapor pressure data.

Assumptions: Ideal solutions using vapor pressure with Raoult's law.

Find: Amounts and compositions of vapor and liquid products at:
(a) 100°C and 1 atm.
(b) 100°C and 2 atm.
(c) 105°C and 0.1 atm.
(d) 150°C and 1 atm.

Analysis: Instead of Figure 2.4 for the vapor pressures of benzene and toluene and three vapor-pressure data points for o-xylene, use the built-in vapor pressure data in the CHEMCAD process simulator with ideal *K*-values. The results are as follows:

Case	**(a) 100°C, 1 atm**	**(b) 100°C, 2 atm.**	**(c)105°C, 0.1 atm.**	**(d) 150°C, 1 atm**
Vapor, kmol	67.64	0	100	100
Liquid, kmol	32.36	100	0	0
Vapor mol frac:				
Benzene	0.698		0.60	0.60
Toluene	0.224		0.25	0.25
o-Xylene	0.078		0.15	0.15
Liquid mol frac:				
Benzene	0.395	0.60		
Toluene	0.305	0.25		
o-Xylene	0.300	0.15		

Only in the Case (a), are two phases formed. At 1 atm, the bubble point is 91.3°C and the dew point is 107.5°C.

Exercise 4.30

Subject: Prove that, at equilibrium, vapor is at its dew point and liquid is at its bubble point.

Analysis: After equilibrium is achieved, separate the vapor from the liquid and analyze the separate phases.

For the liquid: Apply Eq. (5), Table 4.4, $$x_i = \frac{z_i}{1+\Psi(K_i-1)} \qquad (1)$$

At the bubble point, $\Psi = V/F = 0$ and, therefore, from Eq. (1), $x_i = z_i$. Also, then, $K_i x_i = K_i z_i = y_i$ and, therefore, $\sum_{i=1}^{C} K_i x_i = \sum_{i=1}^{C} K_i z_i = \sum_{i=1}^{C} y_i = 1$, which is the bubble-point equation, Eq. (4-12).

For the vapor: Apply Eq. (6), Table 4.4, $$y_i = \frac{K_i z_i}{1+\Psi(K_i-1)} \qquad (2)$$

At the dew point, $\Psi = V/F = 1$ and, therefore, from Eq. (2), $y_i = z_i$. Also, then, $x_i = y_i/K_i = z_i/K_i$ and, therefore, $\sum_{i=1}^{C} \frac{y_i}{K_i} = \sum_{i=1}^{C} \frac{z_i}{K_i} = \sum_{i=1}^{C} x_i = 1$, which is the bubble-point equation, Eq. (4-12).

Exercise 4.31

Subject: Bubble-point temperature of feed to a distillation column.

Given: Feed at 1.72 MPa (250 psia) with a composition in kmol/h below. *K*-values in Fig. 2.8.

Find: Bubble-point temperature.

Analysis: Iterate on temperature until the bubble-point equation, Eq. (4-12), is satisfied,

$$\sum_{i=1}^{C} K_i z_i = 1 \qquad (1)$$

For the first guess, take the temperature that gives the *K*-value for $nC_4 = 1.0$, that is 225°F. This result and one for 200°F is as follows:

			T = 225°F		T = 200°F	
Component	f_i, kmol/h	z_i	K_i	$K_i z_i$	K_i	$K_i z_i$
C_2	1.5	0.03	4.8	0.144	4.3	0.129
C_3	10.0	0.20	2.1	0.420	1.9	0.380
nC_4	18.5	0.36	1.0	0.360	0.81	0.292
nC_5	17.5	0.34	0.44	0.150	0.34	0.116
nC_6	3.5	0.07	0.21	0.015	0.15	0.011
Sum:	51.0	1.00		1.089		0.928

By linear interpolation, $T = 211$°F for Eq. (1) to be satisfied.

Exercise 4.32

Subject: Bubble and dew point pressures of binary mixture at constant temperature.

Given: Mixture of 50 mol% benzene (A) and 50 mol% toluene (B) at 90°C (194°F). Vapor pressures from Fig. 2.4 (19.5 psia for A and 7.9 psia for B).

Assumptions: Raoult's law for *K*-values.

Find: Bubble and dew point pressures.

Analysis: Substitution of Raoult's law, Eq. (3) in Table 2.3, into Eqs. (4-12) and (4-13) for the bubble and dew points, respectively, gives,

Bubble point: $$\sum_{i=1}^{C} K_i z_i = \sum_{i=1}^{C} \frac{P_i^s z_i}{P} = 1.0 \quad \text{or} \quad \sum_{i=1}^{C} P_i^s z_i = P \qquad (1)$$

Dew point: $$\sum_{i=1}^{C} \frac{z_i}{K_i} = \sum_{i=1}^{C} \frac{z_i P}{P_i^s} = 1.0 \quad \text{or} \quad \sum_{i=1}^{C} \frac{z_i}{P_i^s} = \frac{1}{P} \qquad (2)$$

Eq. (1) gives 13.70 psia for the bubble point. Eq. (2) gives 15.8 psia for the dew point.

Exercise 4.33

Subject: Bubble point, dew point, and flash of a water (W) - acetic acid (A) mixture.

Given: Equimolar mixture of W and A at 1 atm. Correlations of liquid-phase activity coefficients for W and A as a function of liquid-phase mole fractions and temperature:

Assumptions: Modified Raoult's law, Eq. (4), Table 2.3 applies.

Find: Dew point, bubble point, and equilibrium vapor and liquid at a temperature halfway between the bubble and dew points.

Analysis: The Rachford-Rice flash equations can be used from Table 4.4:

$$f\{\Psi\} = \sum_{i=1}^{C} \frac{z_i(1-K_i)}{1+\Psi(K_i-1)} = 0 \qquad (1)$$

$$y_i = \frac{z_i K_i}{1+\Psi(K_i-1)} \qquad (2)$$

$$x_i = \frac{z_i}{1+\Psi(K_i-1)} \qquad (3)$$

where, $z_W = 0.5$ and $z_A = 0.5$ and the modified Raoult's law is:

$$K_i = \frac{\gamma_{iL} P_i^s}{P} \qquad (4)$$

Antoine vapor pressure equations are given in Perry's Handbook for water and acetic acid:

$$\log P_W^s = 8.07131 - \frac{1730.63}{T(^oC) + 233.426} \qquad (5)$$

$$\log P_A^s = 8.02100 - \frac{1936.01}{T(^oC) + 258.451} \qquad (6)$$

The equations for the liquid-phase activity coefficients, given in the Chemical Engineering Science article of 1967 by Sebastiani and Lacquaniti, are incorrect. They are of the Redlich-Kister form (see Walas, S. M., "Phase Equilibria in Chemical Engineering", Butterworth, 1985, page 184) and should be:

$$\log \gamma_W = x_A^2\left[B + C(4x_W - 1) + C(x_W - x_A)(6x_W - 1)\right] \qquad (7)$$

$$\log \gamma_A = x_W^2\left[B + C(4x_W - 3) + C(x_W - x_A)(6x_W - 5)\right] \qquad (8)$$

Exercise 4.33 (continued)

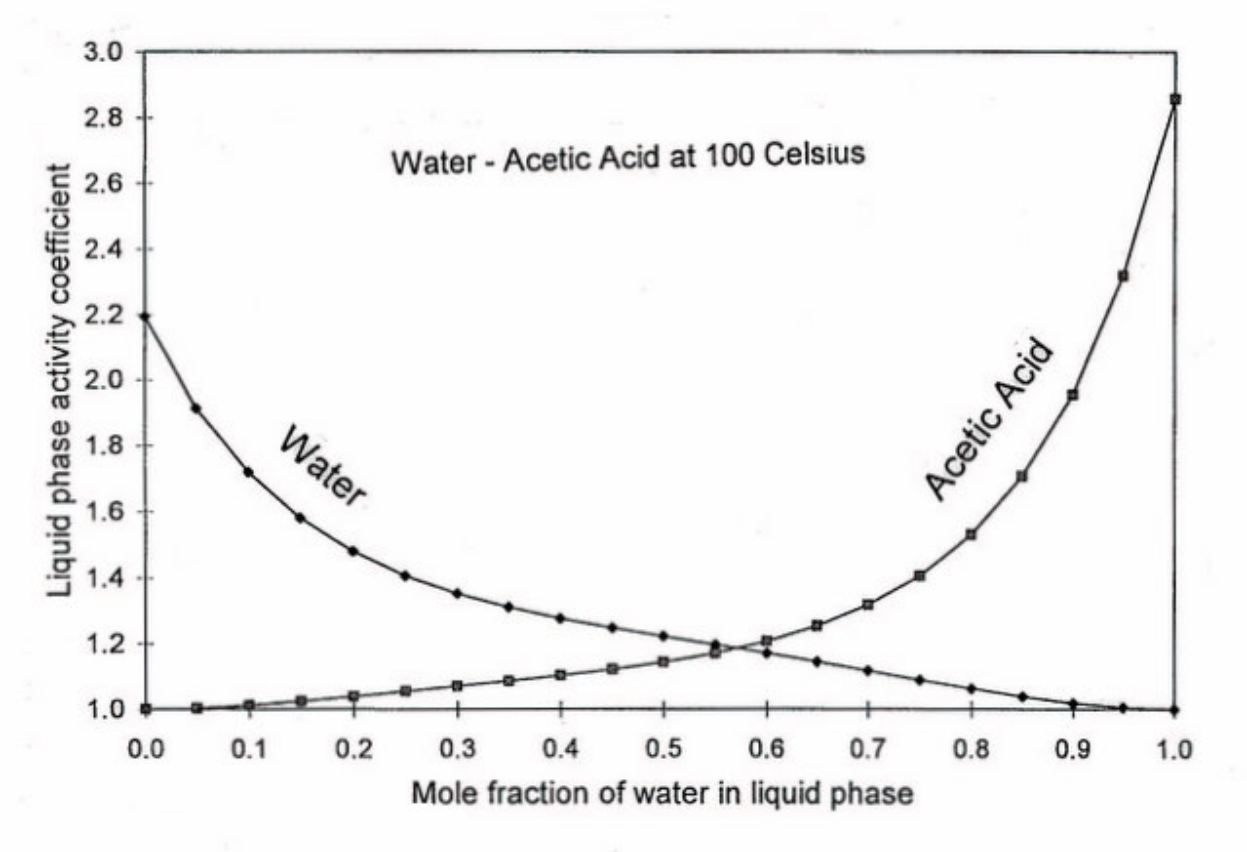
Analysis: (continued)

$$\text{where,} \quad A = 0.1182 + \frac{64.24}{T(\text{K})} \tag{9}$$

$$B = 0.1735 - \frac{43.27}{T(\text{K})} \tag{10}$$

$$C = 0.1081 \tag{11}$$

Since P = 1 atm and the normal boiling points of water and acetic acid are 100°C and 118.1°C, respectively, it might be expected that the dew and bubble point of the mixture would be in the vicinity of 100°C, unless the liquid-phase activity coefficients are much different from 1. To check this, activity coefficients are computed from Eqs. (7) and (8) with a spread sheet at 100°C, with the following result as a plot. It is seen that in the vicinity of mole fractions equal to 0.5, the coefficients are not large, but are about 1.2.



Exercise 4.33 (continued)

Analysis: (continued)

At the bubble point, $\Psi = V/F = 0$, and Eq. (1), combined with (4), becomes:

$$f\{T\} = z_W\left(1 - \frac{\gamma_W P_W^s\{T\}}{P}\right) + z_A\left(1 - \frac{\gamma_A P_A^s\{T\}}{P}\right) = 0 \qquad (12)$$

Also, at the bubble point, $x_i = z_i = 0.5$. Then, the only unknown in Eq. (12) is T. Solving nonlinear Eq. (12), with Eqs. (5) to (11), by trial and error with a spreadsheet, starting from a guess of $T = 100^oC$, quickly leads to a bubble-point temperature of 101.6^oC. The composition of the vapor bubble is obtained from Eq. (2), which at the bubble point reduces to $y_i = x_iK_i = z_iK_i$.. The K-values at the bubble point are computed to be $K_W = 1.364$ and $K_A = 0.636$, giving $y_W = 0.682$ and $y_A = 0.318$.

At the dew point, $\Psi = V/F = 1$, and Eq. (1), combined with (4), becomes:

$$f\{x_W, x_W, T\} = z_W\left(\frac{P}{\gamma_W\{x_W, x_A, T\}P_W^s\{T\}} - 1\right) + z_A\left(\frac{P}{\gamma_A\{x_W, x_A, T\}P_A^s\{T\}} - 1\right) = 0$$

where because $y_i = z_i = 0.5$, T , x_W , and $x_A = (1 - x_W)$ are left as unknowns. The liquid phase mole fractions are from Eq. (3), $x_i = z_i/K_i$. Solving these equations by trial and error with a spread sheet, starting from $T = 105^oC$, $x_W = 0.4$ and $x_A = 0.6$, quickly leads to a dew-point temperature of 105.8^oC. The K-values at the dew point are computed to be $K_W = 1.578$ and $K_A = 0.732$, with $x_W = 0.3169$ and $x_A = 0.6832$.

The equilibrium flash calculation is carried out at $T = (101.6 + 105.8)/2 = 103.7^oC$. In this case, the values of Ψ, x_W, and x_A are computed from Eqs. (1) and (3), where the vapor pressures are computed from Eqs. (5) and (6) to be 867 torr for W and 473 for A. Values of y_W and y_A are obtained from Eq. (2). Using, again, a spreadsheet with a trial and error procedure, the following result is quickly obtained:

$V/F = 0.49$ $x_W = 0.4100$ $x_A = 0.5900$ $y_W = 0.5937$ $y_A = 0.4063$

Exercise 4.34

Subject: Bubble point, dew point, and flash of a toluene (1) - n-butanol (2) mixture.

Given: Feed of z_1 =0.4 and z_2 =0.6 at 1 atm. Liquid-phase activity coefficients for 1 and 2 as a function of liquid-phase mole fractions from the van Laar equations.

Assumptions: Modified Raoult's law, Eq. (2-72) applies.

Find: Dew point, bubble point, and equilibrium vapor and liquid at a temperature halfway between the bubble and dew points.

Analysis: The Rachford-Rice flash equations can be used from Table 4.4:

$$f\{\Psi\} = \sum_{i=1}^{C} \frac{z_i(1-K_i)}{1+\Psi(K_i-1)} = 0 \qquad (1)$$

$$y_i = \frac{z_i K_i}{1+\Psi(K_i-1)} \qquad (2)$$

$$x_i = \frac{z_i}{1+\Psi(K_i-1)} \qquad (3)$$

The modified Raoult's law is:

$$K_i = \frac{\gamma_{iL} P_i^s}{P} \qquad (4)$$

Antoine vapor pressure (in torr) equations are obtained by fitting the vapor pressure data for toluene that are given in Exercise 4.8 and from Perry's Handbook for n-butanol:

$$P_1^s = \exp\left[17.2741 - \frac{3896.3}{T(^oC)+255.67}\right] \qquad (5)$$

$$\log P_2^s = 7.36366 - \frac{1305.198}{T(^oC)+173.427} \qquad (6)$$

The van Laar equations, Table 2.9, with the given constants are:

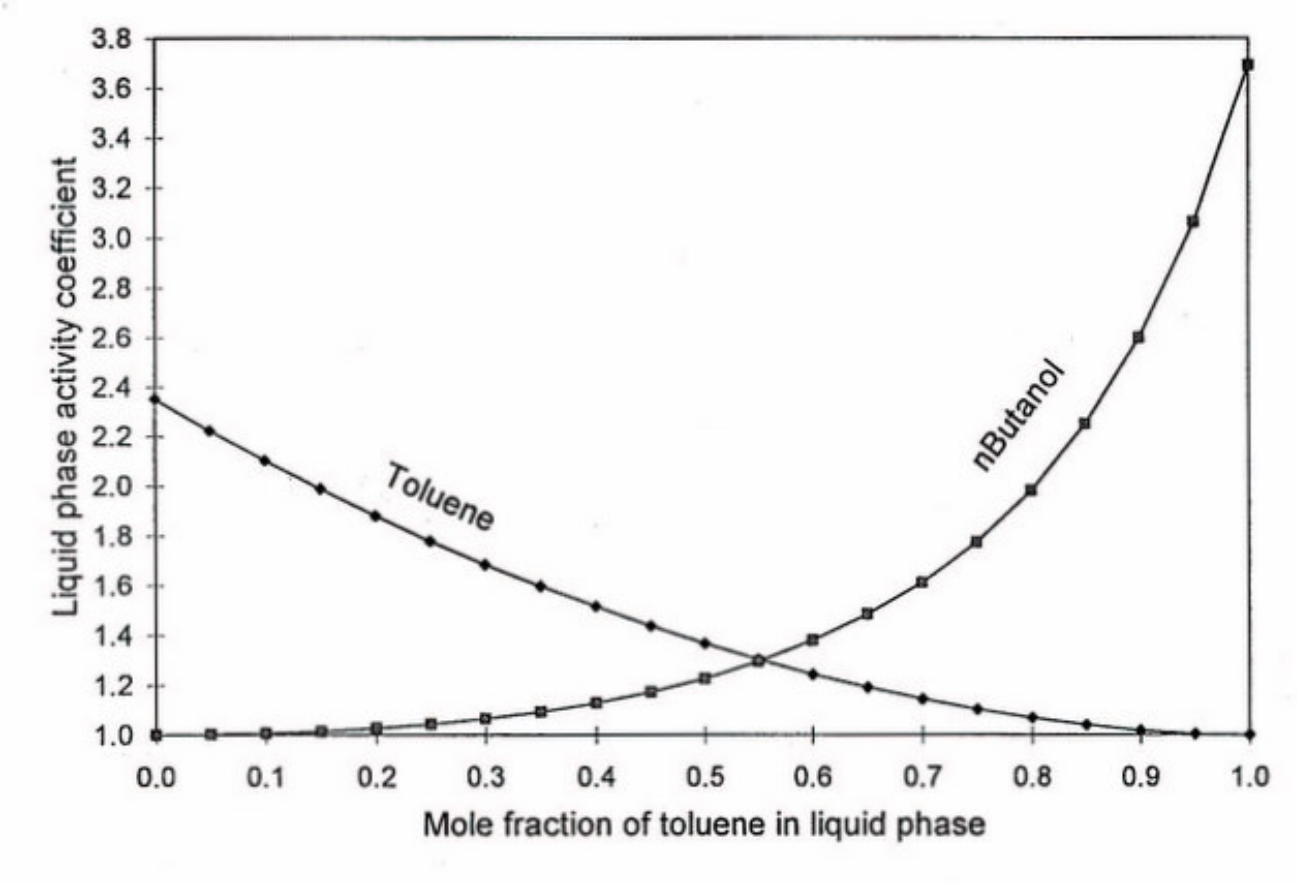
$$\ln\gamma_1 = \frac{0.855}{\left[1+\frac{0.855x_1}{1.306x_2}\right]} \qquad (7)$$

$$\ln\gamma_2 = \frac{1.306}{\left[1+\frac{1.306x_2}{0.855x_1}\right]} \qquad (8)$$

Exercise 4.34 (continued)

Analysis: (continued)

Since P = 1 atm and the normal boiling points of toluene and n-butanol are 110.8°C and 117°C, respectively, it might be expected that the dew and bubble point of the mixture would be in the vicinity of 110°C, unless the liquid-phase activity coefficients are much different from 1. To check this, activity coefficients are computed from Eqs. (7) and (8), with a spread sheet, with the following result as a plot. It is seen that in the vicinity of mole fractions equal to 0.5, the coefficients are not large, but are about 1.3.



At the bubble point, $\Psi = V/F = 0$, and Eq. (1), combined with (4), becomes:

$$f\{T\} = z_1\left(1 - \frac{\gamma_1 P_1^s\{T\}}{P}\right) + z_2\left(1 - \frac{\gamma_2 P_2^s\{T\}}{P}\right) = 0 \qquad (9)$$

Exercise 4.34 (continued)

Analysis: (continued)

Also, at the bubble point, $x_1 = z_1 = 0.4$ and $x_2 = z_2 = 0.6$. Then, the only unknown in Eq. (9) is T. Solving nonlinear Eq. (9), by trial and error with a spreadsheet, starting from a guess of $T = 100^{\circ}$C, quickly leads to a bubble-point temperature of 106.9°C. The composition of the vapor bubble is obtained from Eq. (2), which at the bubble point reduces to $y_i = x_i K_i = z_i K_i$.. The K-values at the bubble point are computed to be $K_1 = 1.363$ and $K_2 = 0.758$, giving $y_1 = 0.545$ and $y_2 = 0.455$.

At the dew point, $\Psi = V/F = 1$, and Eq. (1), combined with (4), becomes:

$$f\{x_1, x_2, T\} = z_1\left(\frac{P}{\gamma_1\{x_1, x_2\}P_1^s\{T\}} - 1\right) + z_2\left(\frac{P}{\gamma_2\{x_1, x_2\}P_2^s\{T\}} - 1\right) = 0$$

where because $y_1 = z_1 = 0.4$ and $y_2 = z_2 = 0.6$, x_1 , and $x_2 = (1 - x_1)$ are left as unknowns. The liquid phase mole fractions are from Eq. (3), $x_i = z_i / K_i$. Solving these equations by trial and error with a spread sheet, starting from $T = 105^{\circ}$C, $x_1 = 0.2$ and $x_2 = 0.8$, quickly leads to a dew-point temperature of 109.7°C. The K-values at the dew point are computed to be $K_1 = 1.793$ and $K_2 = 0.772$, with $x_1 = 0.2231$ and $x_2 = 0.7769$.

The equilibrium flash calculation is carried out at $T = (109.7 + 106.9)/2 = 108.3^{\circ}$C. In this case, the values of Ψ, x_1, and x_2 are computed from Eqs. (1) and (3), where the vapor pressures are computed from Eqs. (5) and (6) to be 714 torr for 1 and 539 torr for 2. Values of y_1 and y_2 are obtained from Eq. (2). Using, again, a spreadsheet with a trial and error procedure, the following result is quickly obtained:

$V/F = 0.604$ $x_1 = 0.2949$ $x_2 = 0.7051$ $y_1 = 0.4689$ $y_2 = 0.5311$

Exercise 4.35

Subject: Bubble point, dew point, and azeotrope of an ethyl acetate (A) - ethyl alcohol (E) mixture.

Given: Liquid mixture of 80 mol% A - 20 mol% E at 101.3 kPa (1 atm). Liquid-phase activity coefficients for A and E as a function of liquid-phase mole fractions from the van Laar equations.

Assumptions: Modified Raoult's law, Eq. (2-72) applies.

Find: (a) Bubble-point temperature and vapor composition. (b) Dew point. (c) Temperature and composition of possible azeotrope.

Analysis: The Rachford-Rice flash equations can be used from Table 4.4:

$$f\{\Psi\} = \sum_{i=1}^{C} \frac{z_i(1-K_i)}{1+\Psi(K_i-1)} = 0 \qquad (1)$$

$$y_i = \frac{z_i K_i}{1+\Psi(K_i-1)} \qquad (2)$$

$$x_i = \frac{z_i}{1+\Psi(K_i-1)} \qquad (3)$$

The modified Raoult's law from Eq. (2-72) is:

$$K_i = \frac{\gamma_{iL} P_i^s}{P} \qquad (4)$$

Antoine vapor pressure (in torr) equations are obtained from Section 13 of Perry's Handbook:

$$\log P_{\mathrm{A}}^s = 7.10179 - \frac{1244.951}{T(^oC)+217.881} \qquad (5)$$

$$\log P_{\mathrm{E}}^s = 7.58670 - \frac{1281.590}{T(^oC)+193.768} \qquad (6)$$

The van Laar equations, Table 2.9, with the given constants are:

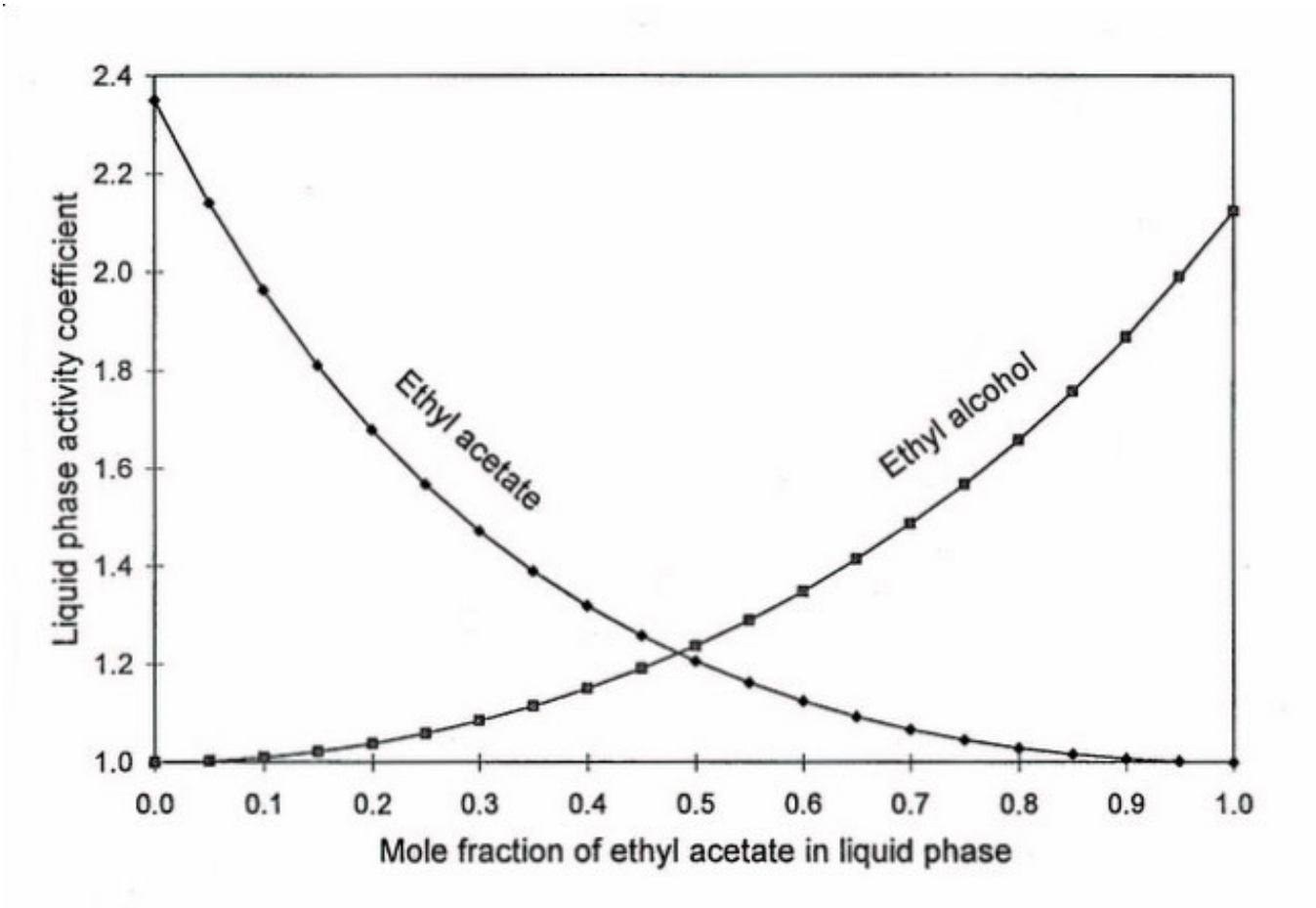
$$\ln \gamma_{\mathrm{A}} = \frac{0.855}{\left[1+\frac{0.855x_{\mathrm{A}}}{0.753x_{\mathrm{E}}}\right]} \qquad (7)$$

$$\ln \gamma_{\mathrm{E}} = \frac{0.753}{\left[1+\frac{0.753x_{\mathrm{E}}}{0.855x_{\mathrm{A}}}\right]} \qquad (8)$$

Exercise 4.35 (continued)

Analysis: (continued)

(a) Since P = 1 atm and the normal boiling points of ethyl acetate and ethyl alcohol are 77.1°C and 78.4°C, respectively, it might be expected that the bubble and dew points of the mixture would be in the vicinity of 70°C, unless the liquid-phase activity coefficients are much different from 1. To check this, activity coefficients are computed from Eqs. (7) and (8), with a spread sheet, with the following result as a plot. It is seen that the coefficients are not large, but are as high as 2.35.



At the bubble point, $\Psi = V/F = 0$, and Eq. (1), combined with (4), becomes:

$$f\{T\} = z_A\left(1 - \frac{\gamma_A P_A^s\{T\}}{P}\right) + z_E\left(1 - \frac{\gamma_E P_E^s\{T\}}{P}\right) = 0 \qquad (9)$$

Exercise 4.35 (continued)

Analysis: (continued)

Also, at the bubble point, $x_A = z_A = 0.8$ and $x_E = z_E = 0.2$. Then, the only unknown in Eq. (9) is T. Solving nonlinear Eq. (9), by trial and error with a spreadsheet, starting from a guess of $T = 70^oC$, quickly leads to a bubble-point temperature of 73.5^oC. The composition of the vapor bubble is obtained from Eq. (2), which at the bubble point reduces to $y_i = x_i K_i = z_i K_i$.. The K-values at the bubble point are computed to be $K_A = 0.913$ and $K_E = 1.350$, giving $y_A = 0.730$ and $y_E = 0.270$.

(b) At the dew point, $\Psi = V/F = 1$, and Eq. (1), combined with (4), becomes:

$$f\{x_A, x_E, T\} = z_A\left(\frac{P}{\gamma_A\{x_A, x_E\}P_A^s\{T\}} - 1\right) + z_E\left(\frac{P}{\gamma_E\{x_A, x_E\}P_E^s\{T\}} - 1\right) = 0$$

where because $y_A = z_A = 0.8$ and $y_E = z_E = 0.2$, x_A , and $x_E = (1 - x_A)$ are left as unknowns. The liquid phase mole fractions are from Eq. (3), $x_i = z_i / K_i$. Solving these equations by trial and error with a spread sheet, starting from $T = 70^oC$, $x_A = 0.8$ and $x_E = 0.2$, quickly leads to a dew-point temperature of 74.3^oC. The K-values at the dew point are computed to be $K_A = 0.922$ and $K_E = 1.508$, with $x_A = 0.8674$ and $x_E = 0.1326$.

(c) To determine the existence of an azeotrope, where $y_i = x_i$, a series of bubble-point calculations can be made, using the procedure in part (a), starting from say, $x_A = 0.05$ in increments of 0.05. If, in the range of x_A from 0.05 to 0.95, the K-value of A switches from more than 1 to less than 1, then an azeotrope exists in this range. The calculations can then be refined. The result from a spreadsheet is a minimum-boiling azeotrope at 72.46^oC with a composition of 54.4 mol% A and 45.6 mol% B. This compares to experimental values from Perry's Handbooof 71.8^oC at a composition of 54 mol% A.

Exercise 4.36

Subject: Bubble point, dew point, and azeotrope of a water (W) - formic acid (F) mixture.

Given: Liquid mixture of 50 mol% W - 50 mol% F at 107°C. Liquid-phase activity coefficients for W and F as a function of liquid-phase mole fractions from the van Laar equations.

Assumptions: Modified Raoult's law, Eq. (2-72) applies.

Find: (a) Bubble-point pressure. (b) Dew point pressure. (c) Azeotropic pressure and composition at 107°C.

Analysis: The Rachford-Rice flash equations can be used from Table 4.4:

$$f\{\Psi\} = \sum_{i=1}^{C} \frac{z_i(1-K_i)}{1+\Psi(K_i-1)} = 0 \qquad (1)$$

$$y_i = \frac{z_i K_i}{1+\Psi(K_i-1)} \qquad (2)$$

$$x_i = \frac{z_i}{1+\Psi(K_i-1)} \qquad (3)$$

The modified Raoult's law from Eq. (2-72) is:

$$K_i = \frac{\gamma_{iL} P_i^s}{P} \qquad (4)$$

Antoine vapor pressure (in torr) equations are obtained from Section 13 of Perry's Handbook:

$$\log P_{\mathrm{W}}^s = 8.07131 - \frac{1730.630}{T(^oC) + 233.426} \qquad (5)$$

$$\log P_{\mathrm{F}}^s = 6.94459 - \frac{1295.260}{T(^oC) + 218.00} \qquad (6)$$

The van Laar equations, Table 2.9, with the given constants are:

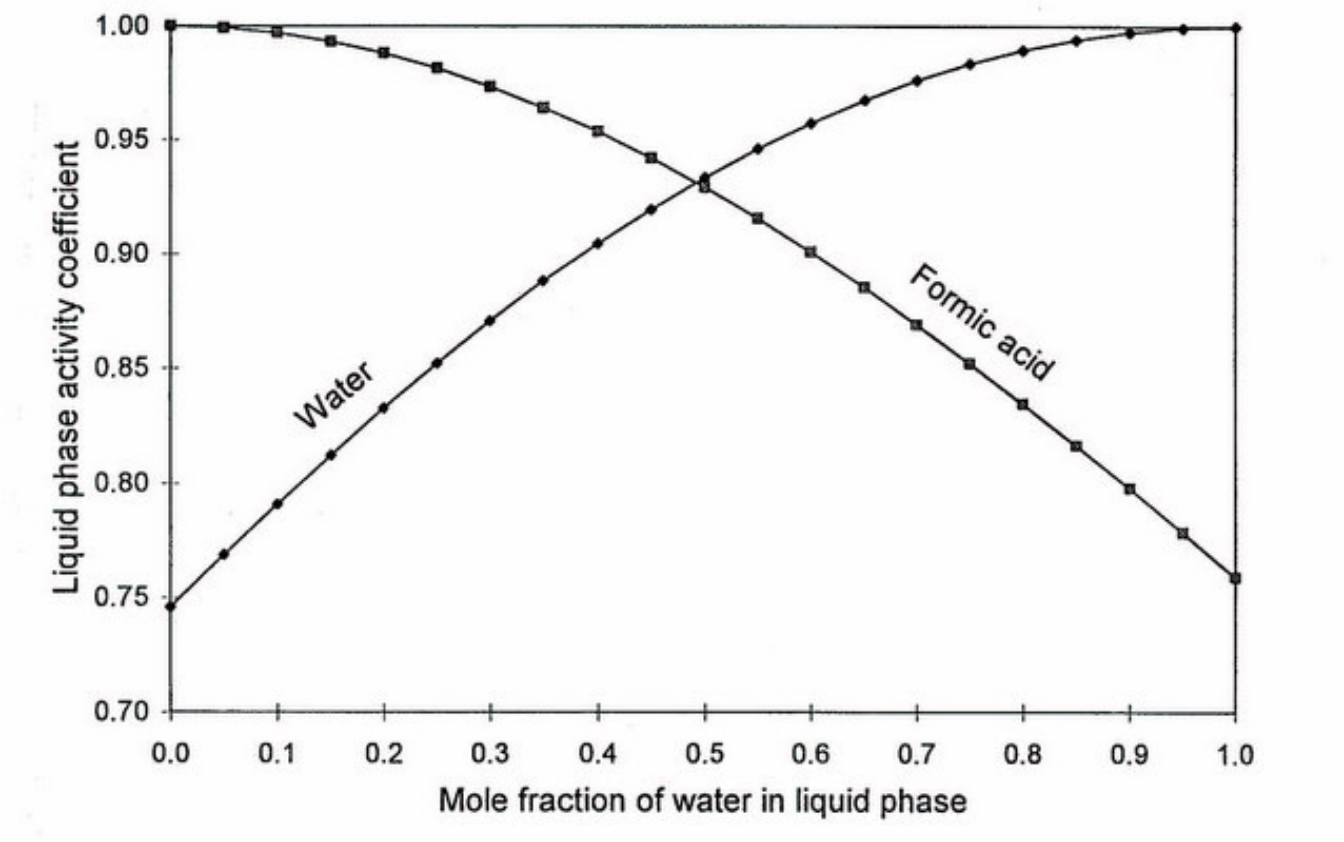
$$\ln \gamma_{\mathrm{W}} = \frac{-0.2935}{\left[1 + \frac{(-0.2935)x_{\mathrm{A}}}{(-0.2757)x_{\mathrm{E}}}\right]} \qquad (7)$$

$$\ln \gamma_{\mathrm{F}} = \frac{-0.2757}{\left[1 + \frac{(-0.2757)x_{\mathrm{E}}}{(-0.2935)x_{\mathrm{A}}}\right]} \qquad (8)$$

Exercise 4.36 (continued)

Analysis: (continued)

(a) Since $T = 107^{o}C$ and the normal boiling points of water and formic acid are $100^{o}C$ and $100.8^{o}C$, respectively, it might be expected that the bubble and dew point pressures of the mixture would be in the vicinity of 1 atm, unless the liquid-phase activity coefficients are much different from 1. To check this, activity coefficients are computed from Eqs. (7) and (8), with a spread sheet, with the following result as a plot. It is seen that the coefficients lie between 0.7 and 1.0



At the bubble point, $\Psi = V/F = 0$, and Eq. (1), combined with (4), becomes:

$$f\{P\} = z_{W}\left(1 - \frac{\gamma_{W} P_{W}^{s}\{107^{O}C\}}{P}\right) + z_{F}\left(1 - \frac{\gamma_{F} P_{F}^{s}\{107^{O}C\}}{P}\right) = 0 \qquad (9)$$

Exercise 4.36 (continued)

Analysis: (continued)

Also, at the bubble point, $x_W = z_W = 0.5$ and $x_F = z_F = 0.5$. Then, the only unknown in Eq. (9) is P. Equation (9) is linear in P and, thus, can be solved directly to give a bubble-point pressure of 719 torr. The K-values at the bubble point are 1.015 for W and 0.984. The composition of the vapor bubble is obtained from Eq. (2), which at the bubble point reduces to $y_i = x_i K_i = z_i K_i$. This gives $y_W = 0.508$ and $y_F = 0.492$.

(b) At the dew point, $\Psi = V/F = 1$, and Eq. (1), combined with (4), becomes:

$$f\{x_W, x_F, P\} = z_W\left(\frac{P}{\gamma_W\{x_W, x_F\}P_W^s\{107^\circ C\}} - 1\right) + z_F\left(\frac{P}{\gamma_F\{x_W, x_F\}P_F^s\{107^\circ C\}} - 1\right) = 0$$

where because $y_W = z_W = 0.5$ and $y_F = z_F = 0.5$, x_W, and $x_F = (1 - x_W)$ are left as unknowns. The liquid phase mole fractions are from Eq. (3), $x_i = z_i / K_i$. Solving these equations by trial and error with a spread sheet, starting from $P = 760$ torr, $x_W = 0.5$ and $x_F = 0.5$, quickly leads to a dew-point pressure of 725.2 torr. The K-values at the dew point are computed to be $K_W = 1.006$ and $K_F = 0.977$, with $x_W = 0.497$ and $x_F = 0.512$.

(c) To determine the existence of an azeotrope, where $y_i = x_i$, a series of bubble-point calculations can be made, using the procedure in part (a), starting from say, $x_W = 0.05$ in increments of 0.05. If, in the range of x_W from 0.05 to 0.95, the K-value of W switches from more than 1 to less than 1, then an azeotrope exists in this range. The calculations can then be refined. The result from a spreadsheet is a maximum-boiling azeotrope at 718.2 torr with a composition of 44.5 mol% W and 55.5 mol% F.

Exercise 4.37

Subject: Bubble point, dew point, and equilibrium flash of a ternary mixture.

Given: Mixture of 45 mol% n-hexane (1), 25 mol% n-heptane, and 30 mol% n-octane.

Assumptions: Applicability of S-R-K method for estimating *K*-values.

Find: (a) Bubble-point temperature at pressures of 5, 1, and 0.5 atm.
Dew-point temperature at pressures of 5, 1, and 0.5 atm.
(b) Temperature and phase compositions for flash of *V/F* = 0.5 at 5, 1, and 0.5 atm.
(c) n-octane in the vapor if 90% of the n-hexane is vaporized at 1 atm.

Analysis: The following results are obtained with the CHEMCAD simulator.

(a) Bubble-point and dew-point temperatures:

Pressure, atm	0.5	1	5
Bubble-point *T*, °F	147	187	307
Dew-point *T*, °F	178	216	330

(b) 50 mol% vaporization of feed:

Pressure, atm	0.5	1	5
Temperature, °F	162	201	318
Vapor mole fractions:			
n-Hexane	0.615	0.599	0.554
n-Heptane	0.231	0.233	0.239
n-Octane	0.154	0.168	0.207
Liquid mole fractions:			
n-Hexane	0.285	0.301	0.346
n-Heptane	0.269	0.267	0.261
n-Octane	0.446	0.432	0.393
Moles V/mole F	0.5	0.5	0.5
Moles L/mole F	0.5	0.5	0.5

(c) By iteration on the isothermal flash calculation, for 90 mol% of n-hexane to vapor, need a temperature of 210.2°F at 1atm. This gives 80.1 mol% vaporization with 65% vaporization of n-octane.

Exercise 4.38

Subject: Vaporization of column bottoms in a partial reboiler.

Given: 150 kmol/h of bubble-point liquid, L_1, at 758 kPa, with a molar composition of 10% propane, 40% n-butane, and 50% n-pentane leaving bottom stage of a distillation column and passing to a reboiler where all by 50 kmol/h is vaporized to V_B.

Assumptions: Pressure in reboiler = 758 kPa. S-R-K method for *K*-values and enthalpies.

Find: Compositions and amounts of boilup and bottoms, B, and reboiler duty, Q_R, from a simulation program

Analysis: Use flash module of the CHEMCAD simulator. Feed (L_1) temperature is computed from a bubble-point calculation at 758 kPa to be 74.9°C. Flash conditions are P = 758 kPa and V/F = (150 - 50)/150 = 0.6667. The result is a temperature of 87.5°C with a reboiler duty of 2.22 x 10^6 kJ/h, and compositions as follows in terms of component flow rates:

Component:	Bottoms, kmol/h	Boilup, kmol/h
Propane	1.94	13.06
n-Butane	15.39	44.61
n-Pentane	32.67	42.33
Total	50.00	100.00

Exercise 4.39

Subject: Bubble-point and equilibrium flash temperatures for a ternary mixture.

Given: Mixture at 50 psia with a composition in mole fractions of 0.005 methane, 0.595 ethane, and 0.400 n-butane.

Find: (a) Bubble-point temperature.
(b) Temperature and phase compositions for 25 mol% vaporization.

Analysis: Instead of using Figs. 2.8 and 2.9 for *K*-values, use S-R-K method with the CHEMCAD simulator, with the following results:

(a) Bubble-point temperature = -61°F. Use of Figs. 2.8 and 2.9 gives -60°F.
(b) Flash temperature for 25 mol% vaporization = -43.6°F, with compositions:

Component	Vapor mole fraction	Liquid mole fraction
Methane	0.0179	0.0007
Ethane	0.9559	0.4747
n-Butane	0.0262	0.5246

Exercise 4.40

Subject: Heating and expansion of a hydrocarbon mixture.

Given: 100 lbmol/h of a mixture at 150°F and 260 psia, with a mole fraction composition of 0.03 ethane, 0.20 propane, 0.37 n-butane, 0.35 n-pentane, and 0.05 n-hexane. Mixture is heated to 260°F at 250 psia, followed by expansion to 100 psia.

Assumptions: Expansion is adiabatic. S-R-K method for *K*-values and enthalpies

Find: Using a simulation program, find for each stream in the process, the mol% vapor, and vapor and liquid phase mole fractions.

Analysis: Using the CHEMCAD process simulator, the following results are obtained.
The feed is all liquid. The streams leaving the heater and the valve are all vapor.
The final temperature is 235°F.

Exercise 4.41

Subject: Equilibrium vapor and liquid streams leaving the feed stage of a distillation column

Given: Feed stream, F, and streams V_{F+1} and L_{F-1} as summarized below. Pressure = 785 kPa.

Assumptions: V_{F+1} is at its dew point and L_{F-1} is at its bubble point. Adiabatic conditions.

Find: Composition and amounts of streams V_F and L_F.

Analysis: Using the S-R-K method for *K*-values, with the CHEMCAD process simulator, the following results are obtained:

Stream	F	V_{F+1}	L_{F-1}	V_F	L_F
Temperature, °C	64.3	73.1	68.5	70.0	70.0
Phase condition	Liquid	Vapor	Liquid	Vapor	Liquid
Flow rate, kmol/h:					
Propane	32.0	58.8	15.0	69.6	36.2
n-Butane	64.0	98.0	45.0	89.9	117.1
n-Pentane	64.0	39.2	40.0	34.5	108.7
Total	160.0	196.0	100.0	194.0	262.0

Exercise 4.42

Subject: Adiabatic flash across a valve of a hydrocarbon mixture.

Given: Feed mixture, of composition below, at 250°F and 500 psia. Pressure exiting valve = 300 psia.

Find: (a) Phase condition of feed.
(b) Temperature downstream of valve.
(c) Mole fraction vaporized across valve.
(d) Mole fraction compositions of vapor and liquid phases downstream of valve.

Analysis: Use CHEMCAD process simulator with S-R-K method for *K*-values and enthalpies. Results are as follows:

Stream	Feed	Vapor from valve	Liquid from valve
Temperature, °F	250	207.6	207.6
Pressure, psia	500	300	300
Phase condition	Liquid	Vapor	Liquid
Mole fraction of feed	1.00	0.4043	0.5957
Mole fractions:			
Ethylene	0.02	0.0348	0.0099
Ethane	0.03	0.0491	0.0171
Propylene	0.05	0.0658	0.0393
Propane	0.10	0.1260	0.0823
Isobutane	0.20	0.1953	0.2032
n-Butane	0.60	0.5290	0.6482

Exercise 4.43

Subject and to Find: Algorithm for flash calculation when $\Psi = V/F$ and P are specified.

Given: Isothermal flash algorithm of Fig. 4-19a, and equations of Table 4.4.

Analysis: Specify feed rate and composition, and values of $\Psi = V/F$ and P. Use the isothermal flash algorithm of Fig. 4-19a as an inner loop. Guess the flash temperature and enter the inner loop. If the calculated $\Psi = V/F$ is not the specified value, guess a new value of T = say 1.05 times the initial guess of T, and repeat the inner loop. For the next and subsequent iterations, k, apply the false position method to provide a new guess of T:

$$T^{k+2} = T^{k+1} + \left(\Psi_{\text{spec}} - \Psi^{k+1}\right)\left(T^{k+1} - T^{k}\right) / \left(\Psi^{k+1} - \Psi^{k}\right)$$

This assumes that T is a linear function of $\Psi = V/F$. Iterate until the computed $\Psi = V/F$ is within say 0.1% of the specified value.

Exercise 4.44

Subject and to Find: Algorithms for flash calculations with 6 different sets of specified variables given in the table below.

Given: Isothermal flash algorithm of Fig. 4-19a, and equations of Table 4.4.

Assumption: All flashes are adiabatic.

Analysis: The equations to be solved for each algorithm are those for the standard adiabatic flash procedure, where the specifications are outlet P and $Q = 0$.

Rachford-Rice Eq. (3), Table 4.4:
$$f_1 = \sum_{i=1}^{C} \frac{z_i(1-K_i)}{1+\Psi(K_i-1)} = 0 \qquad (1)$$

Adiabatic energy balance, Eq. (4-19):
$$f_2 = \frac{\Psi h_V + (1-\Psi)h_L - h_F}{1{,}000} \qquad (2)$$

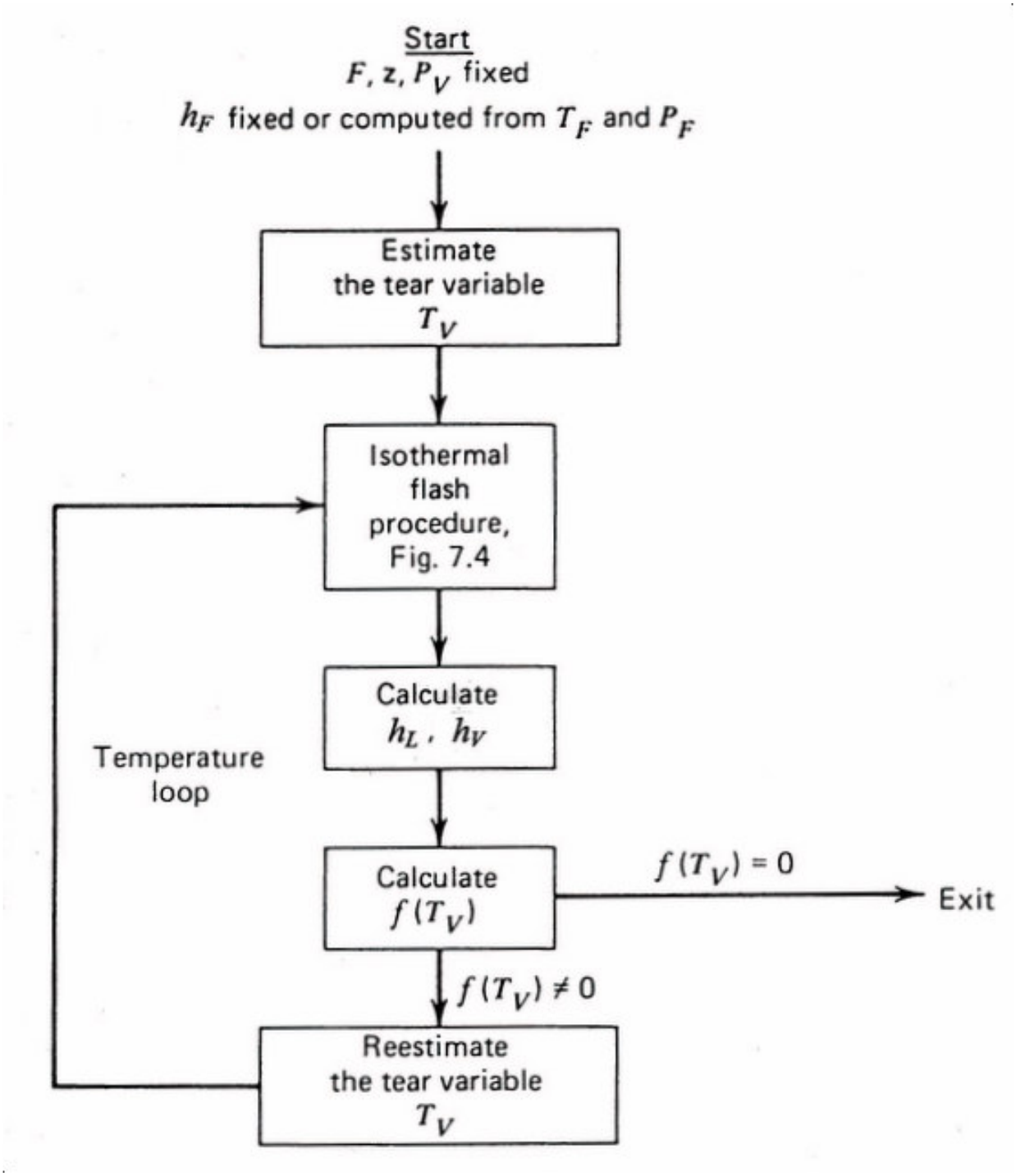
For each of the 6 algorithms, we must choose a tear variable, the output variable for f_1, and the output variable for f_2. If K-values are composition-dependent, then outer loop iterations with f_1 are necessary as in Fig. 4.19. Note that the specification of h_F is equivalent to specifying T_F or $Q = 0$. In some cases, it may be necessary to solve f_1 and f_2 simultaneously.

Case	Specifications	Find	Tear Variable	Output Variable in f_1	Output Variable in f_2
1	h_F, P	Ψ, T	T_V	Ψ	T_V
2	h_F, T	Ψ, P	Ψ	P_V	Ψ
3	h_F, Ψ	T, P	T_V	P_V	T_V
4	Ψ, T	h_F, P	$h_F\{T_F\}$	P_V	h_F
5	Ψ, P	h_F, T	$h_F\{T_F\}$	T_V	h_F
6	T, P	h_F, Ψ	$h_F\{T_F\}$	Ψ	h_F

As an example of one of the algorithms, consider Case 1, which is equivalent to the standard adiabatic flash specification. The algorithm is shown in diagram form on the following page.

Exercise 4.44 (continued)

Analysis: (continued)



Exercise 4.45

Subject: Comparison of solvents for single-equilibrium-stage liquid-liquid extraction.

Given: Feed, F = 13,500 kg/h of 8 wt% acetic acid (B) in water (A) at 25°C. Four solvents (C), each with a different distribution coefficient, K_C, in mass fractions, x_B, for acetic acid, as given in the table below, according to Eq. (2-20), where (1) is the extract of flow rate E and (2) is the raffinate of flow rate R, where for a single equilibrium stage, the raffinate is to contain only 1 wt% B

$$K_{D_B} = x_B^{(E)} / x_B^{(R)} \qquad (1)$$

Assumptions: Water is insoluble in the solvent and the solvent is insoluble in water.

Find: The kg/h, S, of each solvent required.

Analysis: In Eq. (1), $x_B^{(R)} = 0.01$. Therefore, $x_B^{(E)} = 0.01\ K_{D_B}$ (2)

A total material balance gives: $F = 13{,}500 = E + R - S$ (3)

An acetic acid material balance gives:

$$x_B^{(F)} F = (0.08)(13{,}500) = 1{,}080 = x_B^{(E)} E + x_B^{(R)} R = x_B^{(E)} E + 0.01R \qquad (4)$$

92 wt% of the feed is water, or (0.92)(13,500) = 12,420 kg/h. Since all of the water appears in the raffinate, which is 99 wt% water, R = 12,420/0.99 = 12,546 kg/h. Eq. (3) becomes:

$$S = E - 954 \qquad (5)$$

and Eq. (4) becomes: $$x_B^{(E)} E = 954.5 \qquad (6)$$

Eqs. (2), (5), (6) are three equations in three unknowns: S, E, and $x_B^{(E)}$. For each solvent, solve Eq. (2) for $x_B^{(E)}$. Solve (6) for E. Solve (5) for S. The results are:

Solvent	K_D	$x_B^{(E)}$	**E, kg/h**	**S, kg/h**
Methyl acetate	1.273	0.01273	74.984	74,030
Isopropyl ether	0.429	0.00429	222,500	221,500
Heptadecanol	0.312	0.00312	305,940	305,000
Chloroform	0.178	0.00178	536,260	535,300

Although methyl acetate is the best solvent, the solvent rates required are very large. To reduce the solvent rate, use a countercurrent, multiple-stage system.

Exercise 4.46

Subject: Liquid-liquid extraction of ethylene glycol from water by furfural with one stage.

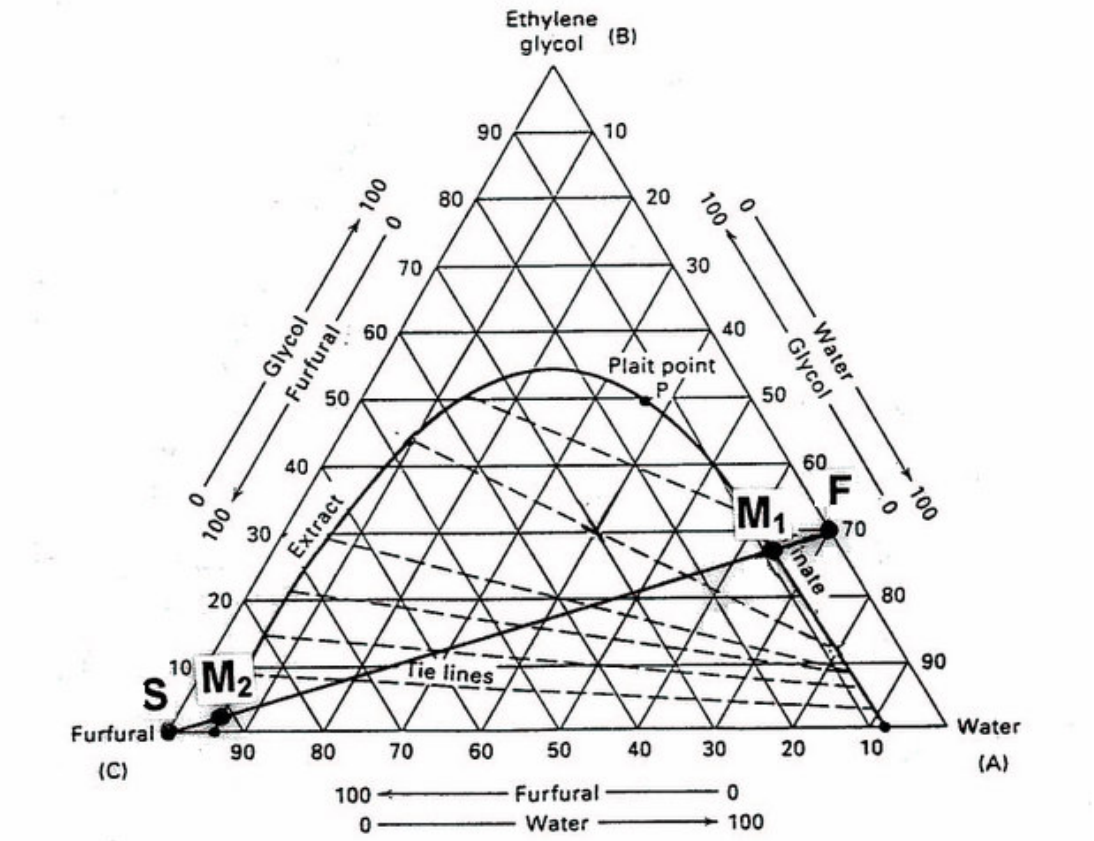
Given: Feed, F = 45 kg, of 30 wt% ethylene glycol (B) and 70 wt% water (A). Phase equilibrium diagrams of Fig. 4.14a and 4.14e for 25°C.

Find: (a) Minimum amount of solvent.
(b) Maximum amount of solvent.
(c) % glycol extraction and amounts of solvent-free extract and raffinate for 45 kg solvent.
(d) Maximum possible glycol purity in extract. Maximum purity of water in raffinate.

Analysis: For a single stage, all mixtures of feed, F, and solvent, S, lie on a straight line between these two points as shown in the following ternary diagram of Fig. 4.14a.

(a) The minimum amount of solvent corresponds to the maximum solubility of the solvent in the feed. This is point M_1 in the diagram below. By the inverse lever arm rule, S/F = 0.097. Therefore, S_{min} = 0.0972(45) = 4.4 kg. In this case, no extract is obtained.

(b) The maximum amount of solvent corresponds to maximum solubility of the feed in the solvent. This is point M_2 in the diagram below. By the inverse lever arm rule, S/F = 11.15. Thus, S_{max} = 11.2(45) = 504 kg. In this case, no raffinate is obtained.



Exercise 4.46 (continued)

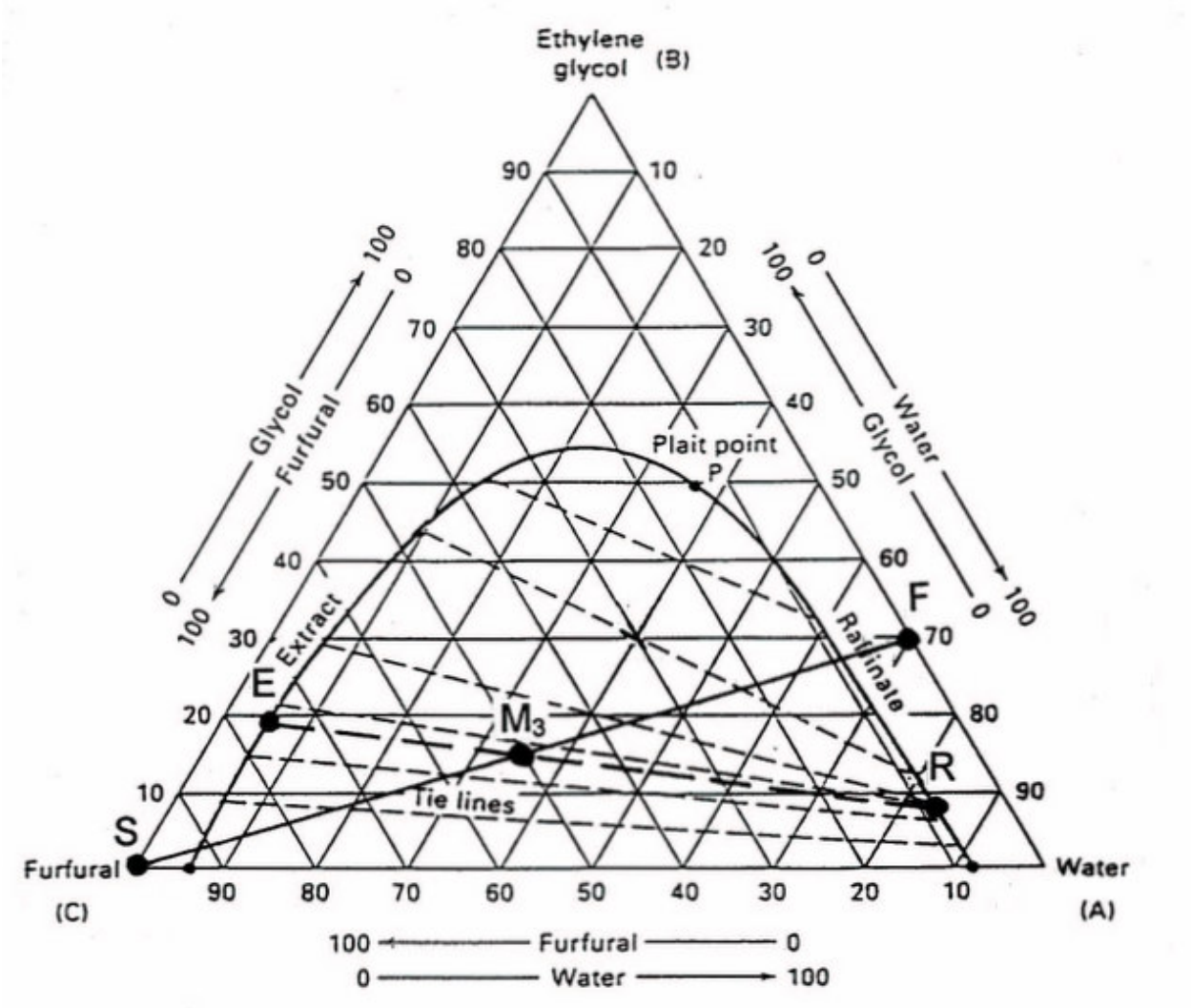
Analysis: (continued)

(c) With 45 kg of solvent, $S/F = 1$. Therefore, the mixing point, M_3 is at the mid point between F and S in the diagram below. A tie line drawn through point M_3 determines the raffinate, R, and the extract, E. By total material balance, $R + E = F + S = 45 + 45 = 90$. By the inverse lever arm rule, R/E = 0.61. Combining these equations gives: $E = 55.9$ kg, $R = 34.1$ kg. From the diagram, the composition of the extract is: 19 wt% B, 76 wt % C, and 5 wt% A. Therefore, the extract contains (0.19)(55.9) = 10.62 kg B. The composition of the raffinate is 8 wt% B, 84 wt% A, and 8 wt% C.

The % extraction of glycol (B) = 10.62/[(0.30)(45)] x 100% = 78.7%.

The amount of solvent-free extract = (55.9)(1 - 0.76) = 13.4 kg.

The amount of solvent-free raffinate = (34.1)(1 - 0.08) = 31.4 kg.

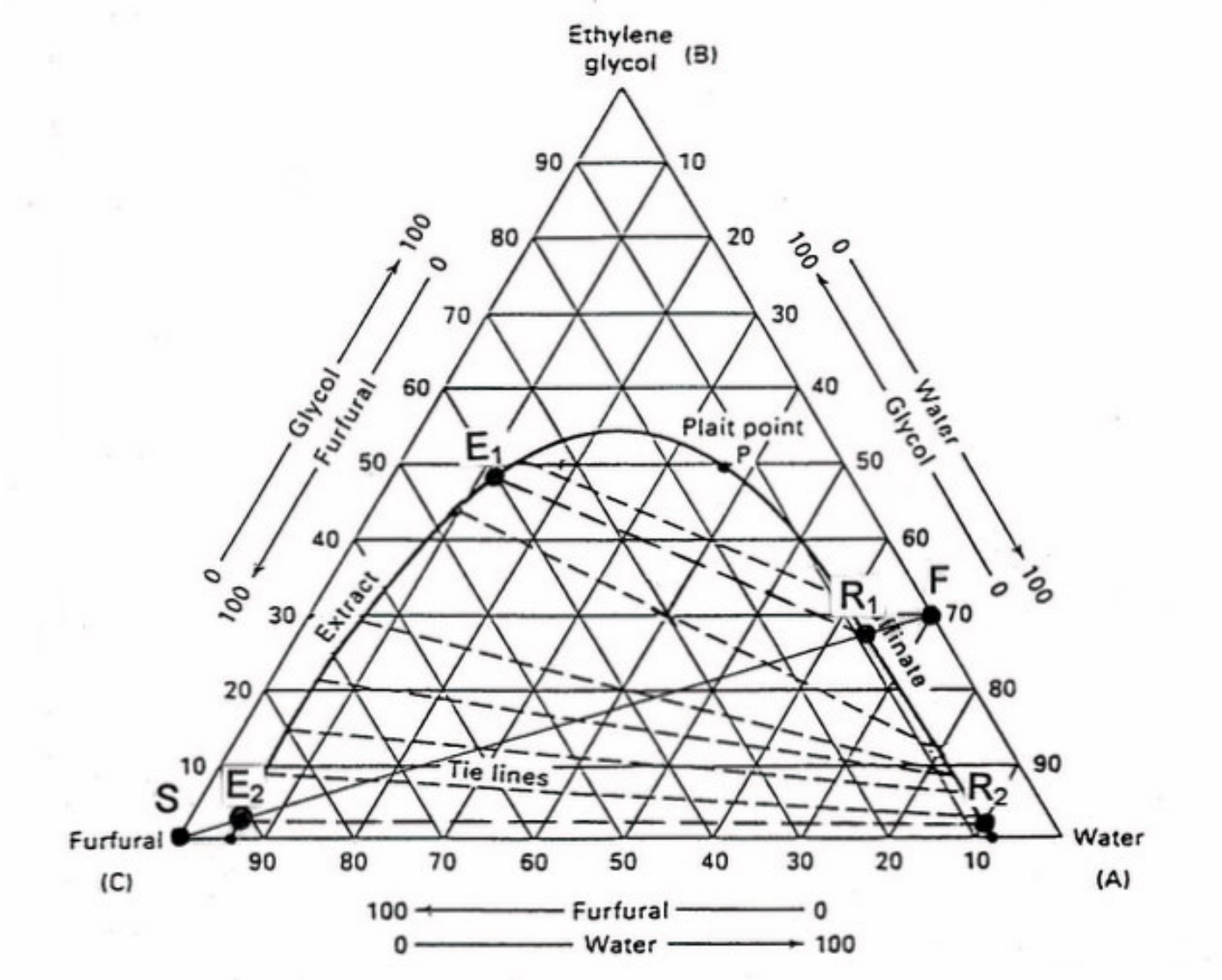


Exercise 4.46 (continued)

Analysis: (continued)

(d) The maximum possible glycol purity in the extract occurs when the minimum amount of solvent is used, as discussed in part (a), giving raffinate R_1. In this case, have say just one drop of extract, corresponding to point E_1, which connects to R_1 by a tie line in the diagram below. At point E_1, have 48 wt% glycol.

The maximum purity of water in the raffinate occurs when the maximum amount of solvent is used, as discussed in part (b), giving extract E_2. In this case, have say just one drop of raffinate, corresponding to point R_2, which connects to E_2 by a tie line in the diagram below. At point R_2, have 90 wt% water.



Exercise 4.47

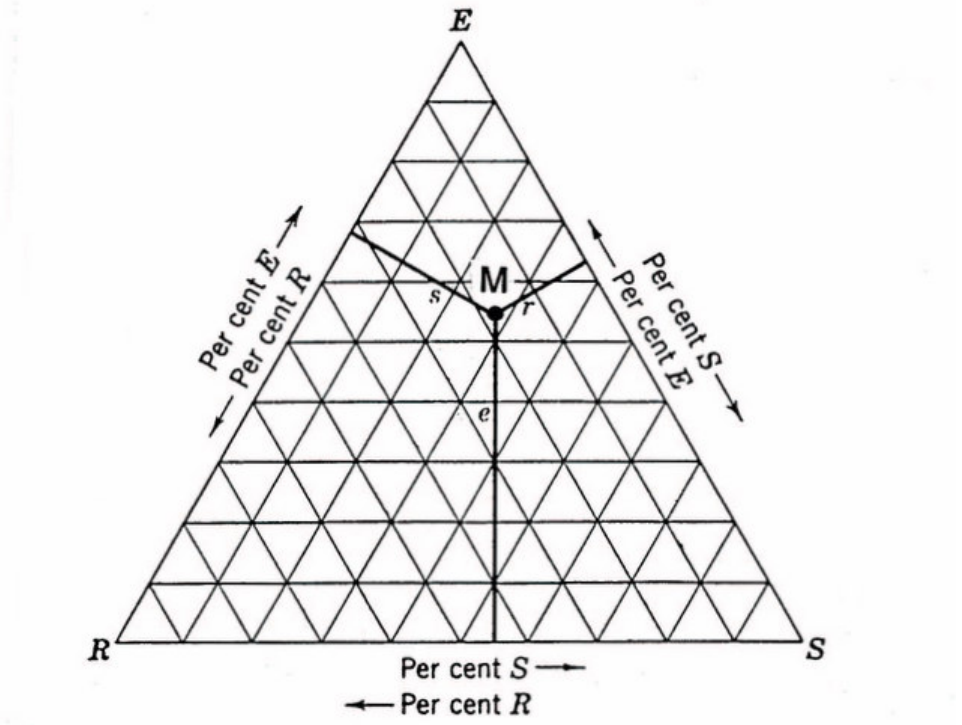
Subject: Representation of the composition of a ternary mixture on a triangular diagram.

Given: A triangular diagram where each vertex represents a pure component.

Assumptions: Consider the case of an equilateral triangular diagram.

Prove: The composition of any point inside the triangle is proportional to the length of the respective perpendicular drawn from the point to the side of the triangle opposite the vertex in question.

Analysis: In the triangular diagram below, the pure components are E, R, and S. A mixture of these components is represented by the point M. For the equilateral triangle shown, the sum of the lengths of the three perpendiculars drawn from an interior point, such as M, to the three sides equals the altitude, is the same length from each side. Therefore, divide each altitude into 100 divisions and number these divisions starting with 0 at the base to 100 at the apex. Thus, if the divisions represent wt% (or mol%), the sum of the perpendiculars equals 100%. In the diagram below, each division is 10%. The perpendicular s measures 28% and is the composition of S. The perpendicular r measures 18% and is the composition of R. The perpendicular e measures 54% and is the composition of E. This proof is extended to a triangle of any shape on pages 11 to 18 of "Chemical Process Principles, Part I" by Hougen, Watson, and Ragatz.



Exercise 4.48

Subject: Liquid-liquid extraction of acetic acid from chloroform by water at 18°C and 1 atm.

Given: Equilibrium data for the ternary mixture

Assumptions: Equilibrium stages.

Find: (a) Compositions and weights of raffinate and extract when 45 kg of a 35 wt% chloroform (C) and 65 wt% acetic acid (A) feed mixture (F) is extracted with 22.75 kg of water (S) in a single-stage extraction.

(b) Compositions and weights of raffinate and extract if the raffinate from part (a) is extracted again with half its weight of water.

(c) Composition of the raffinate from part (b) if all the water is removed from it.

Analysis: Use a right-triangle diagram of the equilibrium data, which is easily produced with a spreadsheet.

(a) In the diagram on the next page, the feed and solvent are represented by points F and S, respectively. The mixing point is M_1, which is the sum of the feed and solvent (67.75 kg) with an overall composition of 33.58 wt% S, 23.25 wt% C, and 43.17 wt% A. A tie line passing through point M_1 locates, on the equilibrium curve, the extract E_1 and the raffinate R_1. If the inverse lever arm rule is used to obtain E_1 and R_1, and their compositions are read from the diagram, the following results are obtained:

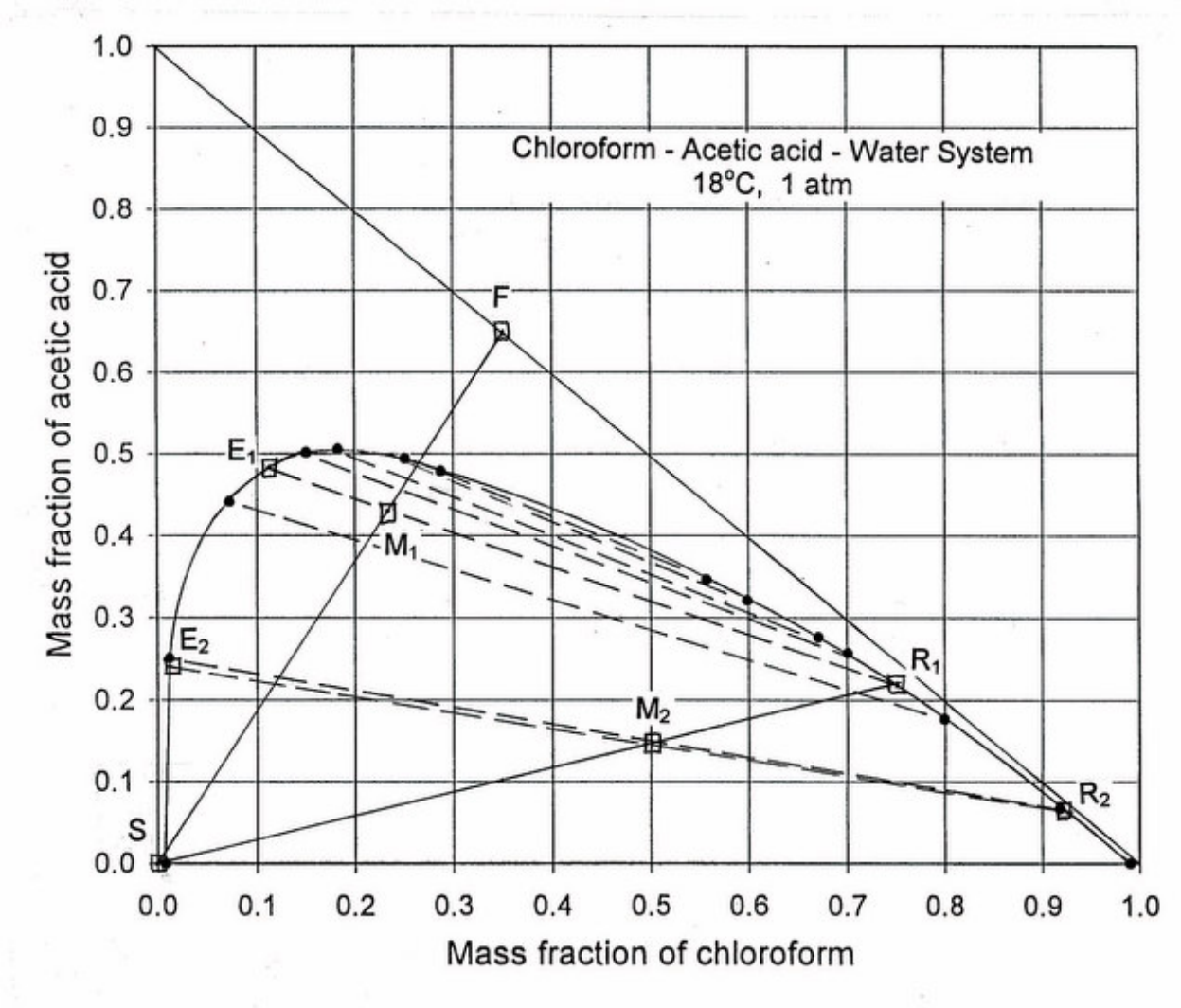
	Feed F	Solvent S	Extract E_1	Raffinate R_1
Amount, kg	45	22.75	55	12.75
Composition, wt%:				
Chloroform	35	0	11.5	74.5
Acetic acid	65	0	48.0	22.0
Water	0	100	40.5	3.5

(b) If R_1 is mixed with half its weight of solvent (6.375 kg), the mixing point is M_2, shown in the diagram on the next page, with an overall composition of 14.6 wt% A, 49.7 wt% C, and 35.7 wt% S. . A tie line passing through point M_2 locates, on the equilibrium curve, the extract E_2 and the raffinate R_2. If the inverse lever arm rule is used to obtain E_2 and R_2, and their compositions are read from the diagram, the following results are obtained:

	Feed (R_1)	Solvent S	Extract E_2	Raffinate R_2	Water-free Raffinate
Amount, kg	12.75	6.375	8.895	10.23	10.10
Composition, wt%:					
Chloroform	74.5	0	1.0	91.0	93.2
Acetic acid	22.0	0	24.0	6.7	6.8
Water	3.5	100	74.9	1.3	0.0

(c) The water-free raffinate is included in the above table.

Exercise 4.48 (continued)



Exercise 4.49

Subject: L-L extraction of acetic acid from water by isopropyl ether at 25°C and 1 atm.

Given: Equilibrium data for the ternary mixture

Assumptions: Equilibrium stages.

Find: (a) Compositions and weights of raffinate and extract when 100 kg of a 30 wt% acetic acid (A) and 70 wt% water (W) feed mixture (F) is extracted with 120 kg of isopropyl ether (E) in a single-stage extraction. Weight % of A in the extract if E is removed.

(b) Compositions and weights of raffinate and extract if 52 kg of A and 48 kg of W are contacted with 40 kg of E

Analysis: Use a right-triangle diagram of the equilibrium data, which is easily produced with a spreadsheet.

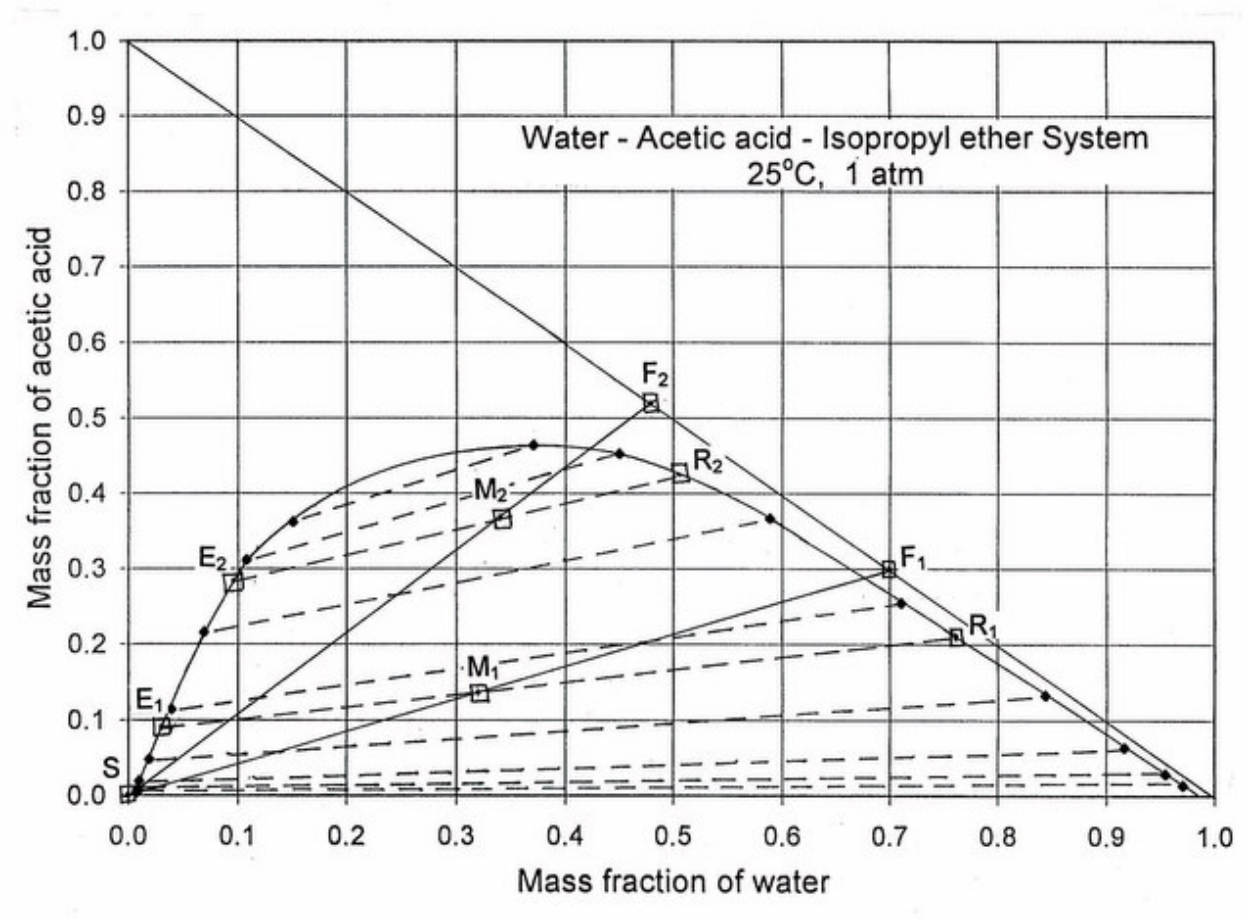
(a) In the diagram on the next page, the feed and solvent are represented by points F_1 and S, respectively. The mixing point is M_1, which is the sum of the feed and solvent (220 kg) with an overall composition of 13.6 wt% A, 31.8 wt% W, and 54.6 wt% E. A tie line passing through point M_1 locates, on the equilibrium curve, the extract E_1 and the raffinate R_1. If the inverse lever arm rule is used to obtain E_1 and R_1, and their compositions are read from the diagram, the following results are obtained, including the amount and composition of the ether-free extract.

	Feed F_1	Solvent S	Extract E_1	Raffinate R_1	Ether-free Extract
Amount, kg	100	120	133.4	86.6	16.1
Composition, wt%:					
Water	70	0	2.9	76.3	24.2
Acetic acid	30	0	9.1	20.6	75.8
Isopropyl ether	0	100	88.0	3.1	0.0

(b) In the diagram on the next page, the feed and solvent are represented by points F_2 and S, respectively. The mixing point is M_2, which is the sum of the feed and solvent (140 kg) with an overall composition of 37.1 wt% A, 34.3 wt% W, and 28.6 wt% E. A tie line passing through point M_2 locates, on the equilibrium curve, the extract E_2 and the raffinate R_2. If the inverse lever arm rule is used to obtain E_2 and R, and their compositions are read from the diagram, the following results are obtained:

	Feed F_2	Solvent S	Extract E_2	Raffinate R_2
Amount, kg	100	40	55.0	85.0
Composition, wt%:				
Water	48	0	9.3	50.5
Acetic acid	52	0	28.9	42.5
Isopropyl ether	0	100	61.8	7.0

Exercise 4.49 (continued)



Exercise 4.50

Subject: Separation of paraffins from aromatics by liquid-liquid extraction with 90 mol% diethylene glycol (DEG) and 10 mol% water at 325°F and 300 psia.

Given: 280 lbmol/h of 42.86 mol% nC_6, 28.57 mol% nC_7, 17.86 mol% benzene, and 10.71 mol% toluene. 500 lbmol/h of solvent solution.

Assumptions: One equilibrium stage. UNIFAC L/L method for activity coefficients.

Find: Flow rates and compositions of extract and raffinate phases. Selectivity of DEG.

Analysis: Using the LLVF (three-phase flash) model of CHEMCAD, the result is:

Flow rate, lbmol/h:	Feed	Solvent	Extract	Raffinate
Diethylene glycol	0	450	447.5	2.5
Water	0	50	49.8	0.2
nC_6	120	0	18.7	101.3
nC_7	80	0	8.8	71.2
Benzene	50	0	31.6	18.4
Toluene	30	0	16.5	13.5
Total	280	500	572.9	207.1

DEG is more selective for aromatics.

Exercise 4.51

Subject: Liquid-liquid extraction of organic acids from water with ethyl acetate (EA).

Given: 110 lbmol/h of feed containing 5, 3, and 2 lbmol/h, respectively, of formic, acetic, and propionic acids in water. 100 lbmol/h of ethyl acetate solvent. One equilibrium stage.

Assumptions: UNIFAC method for liquid-phase activity coefficients. $T = 25°C$.

Find: Flow rates and compositions of extract and raffinate. Order of selectivity of EA.

Analysis: Using the LLVF (three-phase flash) model of the CHEMCAD simulation program:

Flow rate, lbmol/h:	Feed	Solvent	Extract	Raffinate
Ethyl acetate	0	100	99.6	0.4
Water	100	0	14.7	85.3
Formic acid	5	0	2.1	2.9
Acetic acid	3	0	2.6	0.4
n-Propionic acid	2	0	1.9	0.1
Total	110	100	120.9	89.1

The order of selectivity is n-propionic acid highest, then acetic acid, and then formic acid.

Exercise 4.52

Subject: Leaching of oil from soybean flakes by a hexane solvent

Given: 100,000 kg/h of soybean flakes, containing 19% by weight oil.
200,000 kg/h of a hexane solvent.
Oil content of the flakes to be reduced to 0.5 wt% in a single stage.
Expected contents of the variable underflow in Example 4.9.

Assumptions: Ideal leaching stage so that compositions of overflow and underflow liquids are equal.

Find: Using an algebraic method, the compositions and flow rates, of overflow and underflow, and the percentage of oil in the feed that is recovered in the overflow.

Analysis:

The flakes contain (0.19)(100,000) = 19,000 kg/h of oil and (100,000 – 19,000) = 81,000 kg/h of oil-free solids. However, all of the oil is not leached. For convenience in the calculations, lump the unleached oil with the oil-free solids to give an effective solids.

The flow rate of unleached oil = (81,000)(0.5/99.5) = 407 kg/h.

Therefore, take the solids flow rate as (81,000 + 407) = 81,407 kg/h.

Take the oil in the feed as just the amount that is leached or (19,000 – 407) = 18,593 kg/h.

Therefore, in the feed, F,

$$Y_A = (81{,}407/18{,}593) = 4.38$$

$$X_B = 1.0$$

The sum of the liquid solutions in the underflow and overflow include 200,000 kg/h of hexane and 18,593 kg/h of leached oil. Therefore, for the underflow and overflow,

$$X_B = Y_B = [18{,}593/(200{,}000 + 18{,}593)] = 0.0851$$

This is a case of variable solution underflow. Using data in the table that accompanies Example 4.9, and the conversion shown there of that table to X_A as a function of X_B, we obtain $X_A = 2.09$.

Using the algebraic method, since the flow rate of solids in the underflow = 81,407 kg/h, the flow rate of liquid in the underflow = 81,407/2.09 = 38,950 kg/h. The total flow rate of underflow is U = 81,407 + 38,950 = 120,357 kg/h. By mass balance, the flow rate of overflow = 300,000 – 120357 = 179,643 kg/h.

Exercise 4.52 (continued)

Now compute the compositions of the underflow and overflow. In the overflow, with $X_B = 0.0851$, the mass fractions of solute B and solvent C are, respectively, 0.0851 and $(1 - 0.0851) = 0.9149$. In the underflow, using $X_A = 2.09$ and $X_B = 0.0851$, the mass fractions of solids, B, and C, are, respectively, $[2.09/(1 + 2.09)] = 0.676$, $0.0851(1 - 0.676) = 0.0276$, and $(1 - 0.676 - 0.0276) = 0.2964$.

From above, the oil flow rate in the feed is 19,000 kg/h. The oil flow rate in the overflow $= Y_B V = 0.0851(179{,}643) = 15{,}288$ kg/h. Thus, the percentage of the oil in the feed that is recovered in the overflow = 15,288/19,000 = 0.805 or 80.5%.

Exercise 4.53

Subject: Leaching of Na_2CO_3 from a solid by water.

Given: L_o = 3,750 kg/h of a solid containing 1,350 kg/h Na_2CO_3, contacted with S_o = 4,000 kg/h of water.

Assumptions: Ideal leaching stage so that compositions of overflow and underflow liquid are equal. Underflow contains 40 wt% water on a solute-free basis.

Find: Compositions and flow rates, L_1 and S_1, respectively, of overflow and underflow.

Analysis: Let x = mass fraction of Na_2CO_3 (solute).

(a) Total balance: $L_o + S_o = 3{,}750 + 4{,}000 = 7{,}750 = L_1 + S_1$ (1)

Na_2CO_3 balance: $x_{L_o} L_o = 1{,}350 = x_{L_1} L_1 + x_{S_1} S_1$ (2)

Insoluble solids balance:

$$(3{,}750 - 1{,}350) = 2{,}400 = (1 - 0.40)\left(1 - x_{S_1}\right)S_1 = 0.60\left(1 - x_{S_1}\right)S_1 \quad (3)$$

Equilibrium: $$x_{L_1} = \frac{x_{S_1} S_1}{S_1 - (0.60)\left(1 - x_{S_1}\right)S_1} = \frac{x_{S_1}}{0.4 + 0.6x_{S_1}} \quad (4)$$

Eqs. (1) to (4) can be reduced to one quadratic equation in x_{S_1}. Solving,

$x_{S_1} = 0.1189$; $x_{L_1} = 0.2523$; $S_1 = 4{,}540$ kg / h ; and $L_1 = 3{,}210$ kg / h

The material balance may be summarized as follows:

Component	L_o , Solids, kg/h	S_o , Solvent, kg/h	L_1 , Overflow, kg/h	S_1 , Underflow, kg/h
Insoluble oxide	2.400	0	0	2,400
Na_2CO_3	1,350	0	810	540
Water	0	4,000	2,400	1,600
Total	3,750	4,000	3,210	4,540

The % extraction of Na_2CO_3 = 810/1,350 x 100% = 60%

Exercise 4.54

Subject: Leaching of Na_2CO_3 from a solid by water.

Given: L_o = 3,750 kg/h of a solid containing 1,350 kg/h Na_2CO_3, contacted with S_o = 4,000 kg/h of water.

Assumptions: Ideal leaching stage so that compositions of overflow and underflow liquid are equal. Underflow contains 40 wt% water on a solute-free (dissolved Na_2CO_3-free) basis. Only 80% of the Na_2CO_3 is dissolved.

Find: Compositions and flow rates, L_1 and S_1, respectively, of overflow and underflow.

Analysis: Because only 80% of the Na_2CO_3 is dissolved, the underflow will contain (3,750 - 1,350) = 2,400 kg/h of insoluble oxide plus (0.20)(1,350) = 270 kg/h of solid Na_2CO_3 or a total of 2,670 kg/h of total solids. Let:

V = kg/h of overflow

L = kg/h of liquid in the underflow. Total underflow = L + 2,670 kg/h

y = mass fraction of dissolved Na_2CO_3 in overflow or underflow liquid (equilibrium)

Total mass balance: $L_o + S_o = 4{,}000 + 3{,}750 = 7{,}750 = V + L + 2{,}670$ (1)

Na_2CO_3 mass balance: $1{,}350 = 270 + y(V + L)$ (2)

Solving Eqs. (1) and (2), $V + L$ = 5,080 kg/h and y = 0.2126

Flow rate of underflow on a solute-free basis = $(1 - y)L + 2{,}670 = 0.7874\,L + 2{,}670$ kg/h

Therefore the flow rate of water in the underflow = $0.40(0.7874\,L + 2{,}670)$

Water mass balance: $4{,}000 = (1 - 0.2126)V + 0.40(0.7874\,L + 2{,}670)$ (3)

Solving linear Eqs. (1) and (3), L = 2,260 kg/h and V = 2,820 kg/h

The material balance may be summarized as follows:

Component	L_o, Solids, kg/h	S_o, Solvent, kg/h	Overflow, kg/h	Underflow, kg/h
Insoluble oxide	2.400	0	0	2,400
Insoluble Na_2CO_3	1,350	0	0	270
Soluble Na_2CO_3	-	0	600	480
Water	0	4,000	2,220	1,780
Total	3,750	4,000	2,820	4,930

The % extraction of Na_2CO_3 = 600/1,350 x 100% = 44.4%

Exercise 4.55

Subject: Crystallization from a mixture of benzene and naphthalene.

Given: 6,000 lb/h of 40 wt% benzene and 60 wt% naphthalene in liquid state at 50°C, which is cooled to 15°C.

Assumptions: Equilibrium at 15°C. Equilibrium phase diagram of Fig. 4.23.

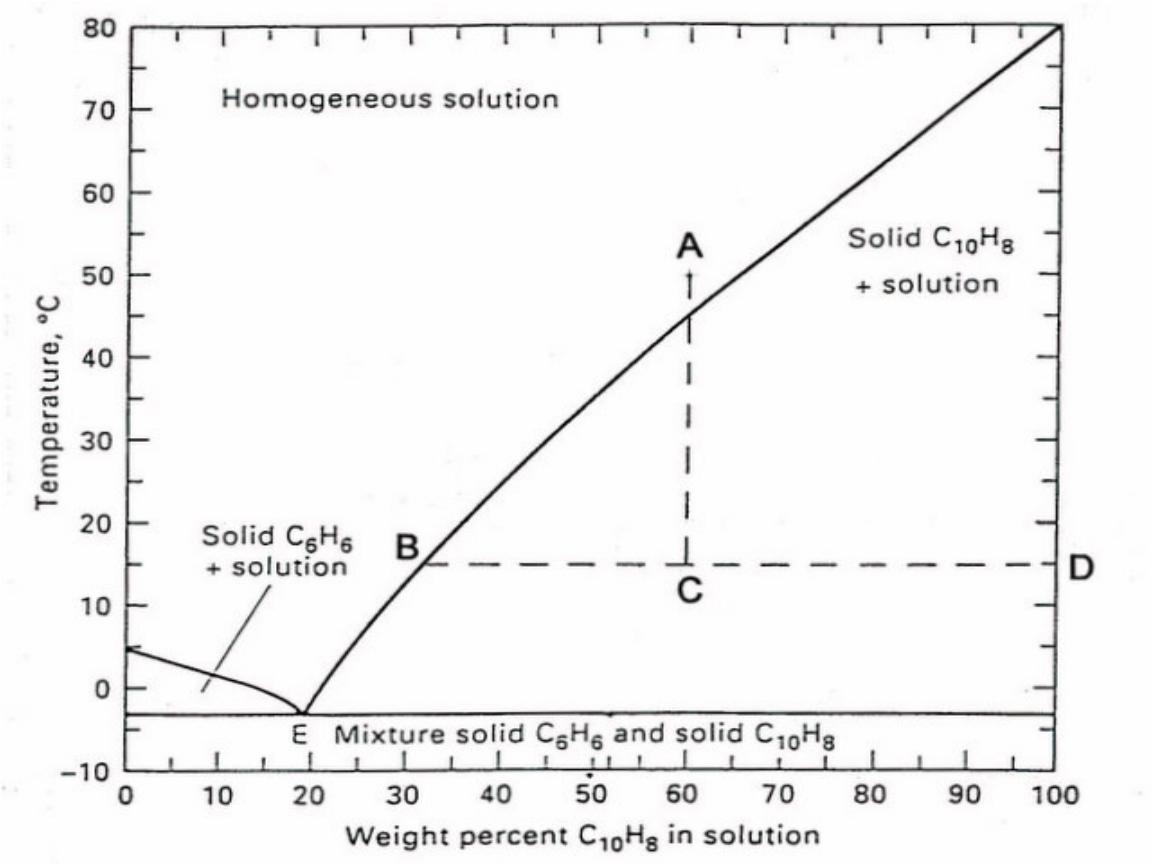
Find: Flow rates and compositions of crystals and mother liquor.

Analysis: The feed is (0.60)(6,000) = 3,600 lb/h of naphthalene and 2,400 lb/h of benzene. In the figure below:

A is the feed solution at 50°C. It lies in the homogeneous solution region.

C is the feed solution at 15°C. It now lies in the two-phase region and separates into naphthalene crystals at D and mother liquor at B.

From the diagram, the mother liquor at 15°C contains 31.5wt% naphthalene and, therefore, 68.5 wt% benzene. Because all of the benzene is in the mother liquor, the mother liquor flow rate is 2,400/(0.685) = 3,500 lb/h. Therefore, the naphthalene crystals flow rate is 6,000 - 3,500 = 2,500 lb/h. The % crystallization of naphthalene is 2,500/3,600 x 100% = 69.4%.



Exercise 4.56

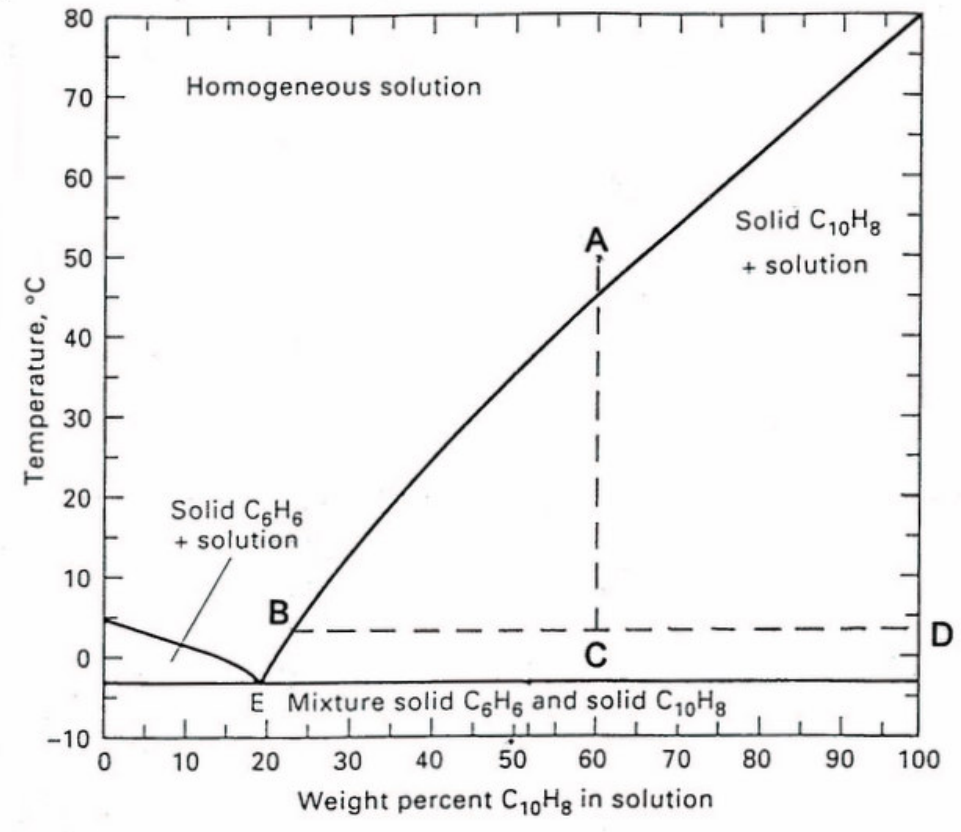
Subject: Crystallization from a mixture of benzene and naphthalene.

Given: 6,000 lb/h of 40 wt% benzene and 60 wt% naphthalene in liquid state at 50°C to be cooled to obtain crystals of naphthalene.

Assumptions: Equilibrium upon cooling, using phase diagram of Fig. 4.23.

Find: Temperature necessary to crystallize 80% of the naphthalene. Flow rates and compositions of crystals and mother liquor.

Analyze: The feed is (0.60)(6,000) = 3,600 lb/h of naphthalene and 2,400 lb/h of benzene. If 80% of the naphthalene is crystallized, the crystals flow rate will be (0.8)(3,600) = 2,880 lb/h. This leaves (3,600 - 2,880) = 720 lb/h of naphthalene in the mother liquor, with 2,400 lb/h of benzene. The total flow rate of mother liquor is 720 + 2,400 = 3,120 lb/h. Therefore, the naphthalene concentration in the mother liquor is 720/3,120 x 100% = 23 wt%. In the figure below, A is the feed solution at 50°C. It lies in the homogeneous solution region
C is the feed solution in the two-phase region, which separates into naphthalene crystals at D and mother liquor at B, with the 23 wt% solubility.
It is seen that a temperature of 3°C is needed to achieve a naphthalene solubility of 23 wt%.



Exercise 4.57

Subject: Crystallization from a mixture of benzene and naphthalene.

Given: 10,000 kg/h of 90 wt% benzene and 10 wt% naphthalene in liquid state at 30°C to be cooled to 0°C to obtain crystals.

Assumptions: Equilibrium upon cooling to 0°C, using phase diagram of Fig. 4.23.

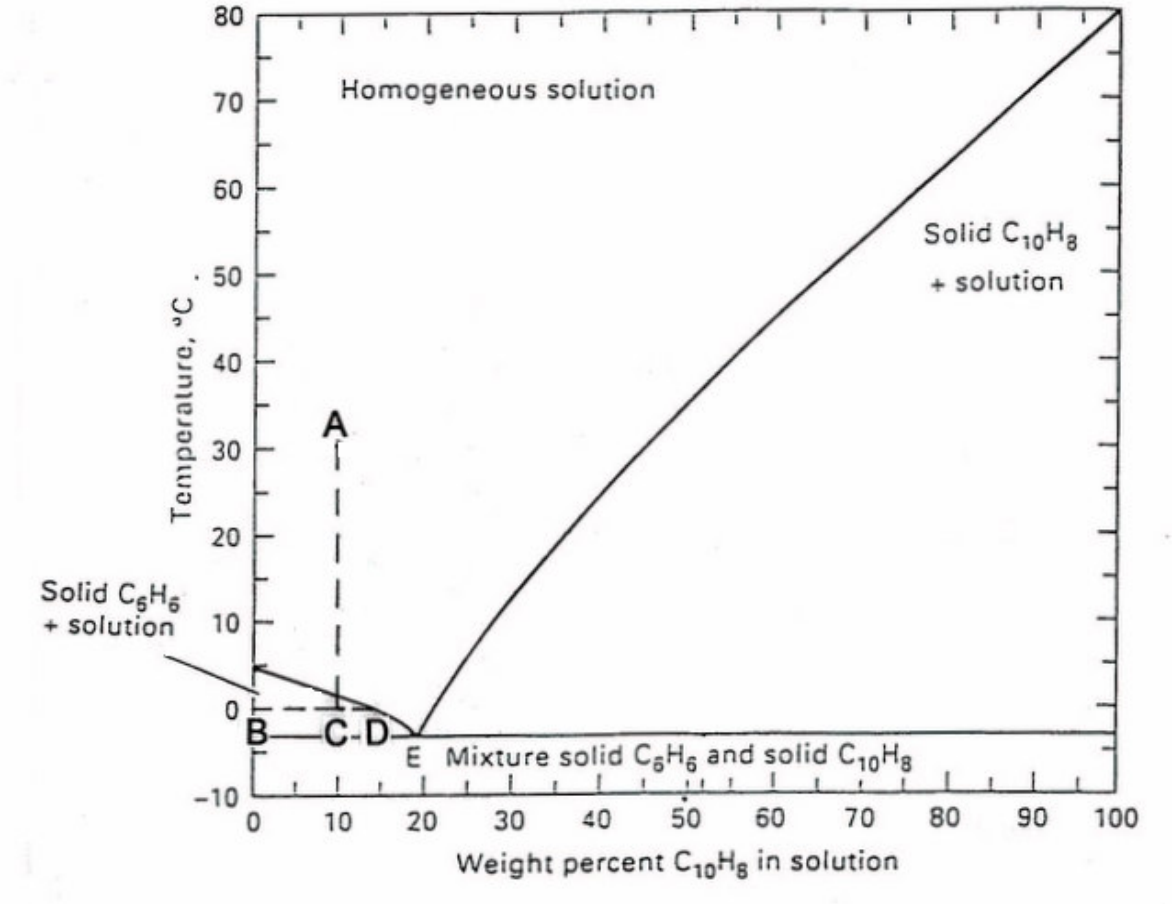
Find: Flow rates and compositions of crystals and mother liquor.

Analyze: The feed is (0.10)(10,000) = 1,000 kg/h of naphthalene and 9,000 kg/h of benzene. In the figure below:

A is the feed solution at 30°C. It lies in the homogeneous solution region.

C is the feed solution at 0°C. It now lies in the two-phase region and separates into benzene crystals at B and mother liquor at D.

From the diagram, the mother liquor at 0°C contains 15 wt% naphthalene and, therefore, 85 wt% benzene. Because all of the naphthalene is in the mother liquor, the mother liquor flow rate is 1,000/(0.15) = 6,667 kg/h. Therefore, the benzene crystals flow rate is 10,000 - 6,667 = 3,333 kg/h. The % crystallization of benzene is 3,333/9,000 x 100% = 37.0%.



Exercise 4.58

Subject: Crystallization of Na_2SO_4 from an aqueous solution by cooling.

Given: 1,000 lb/h of Na_2SO_4 dissolved in 4,000 lb/h of H_2O at 50°C.

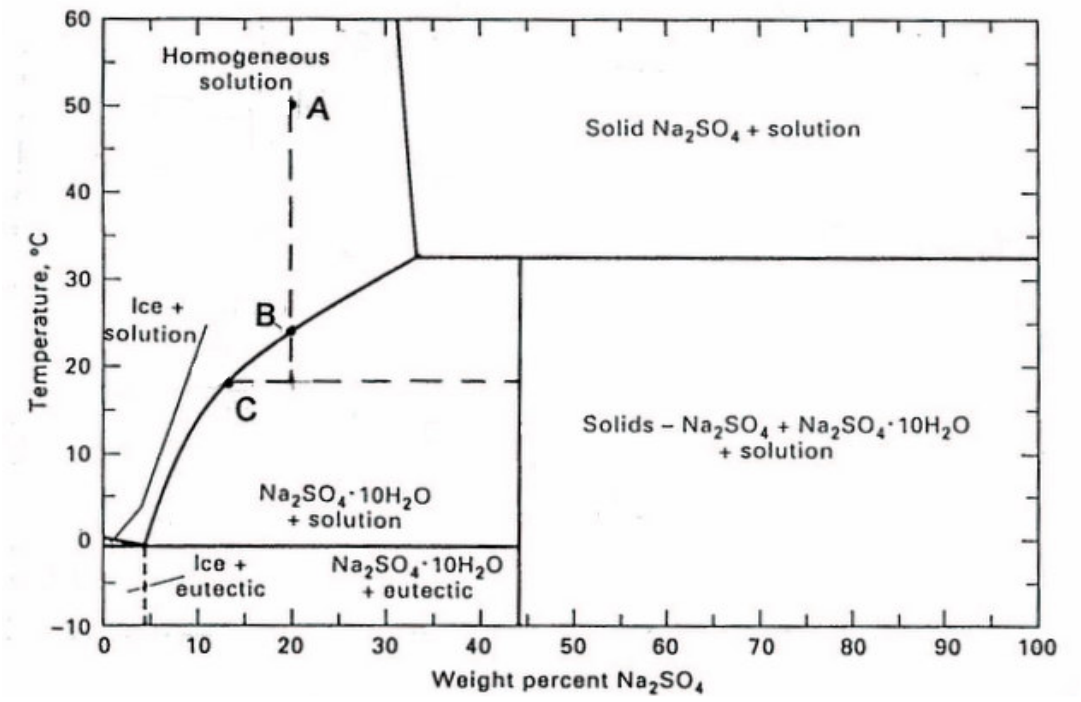
Assumptions: Equilibrium according to phase diagram of Fig. 4.24.

Find: Temperature at which crystallization begins. Temperature to obtain 50% crystallization of the sulfate. Hydrate form of the crystals.

Analysis: In the diagram below, the feed of 20 wt% sulfate, at point A, is in the homogeneous solution region at 50°C. Crystallization begins at point B, corresponding to a temperature of 24°C. As the temperature is lowered further, crystals of the decahydrate, $Na_2SO_4 \cdot 10H_2O$ form. For 50% crystallization of Na_2SO_4 , must crystallize 0.5(1,000) = 500 lb/h. For the decahydrate, with molecular weights of 18 for water and 142 for the sulfate, the crystals contain:

$$500\frac{(10)(18)}{142} = 634 \text{ lb/h or water of crystallization}$$

Therefore, the total flow rate of crystals = 500 + 634 = 1,134 lb/h.
This leaves 4,000 - 634 = 3,366 lb/h of water and 1,000 - 500 = 500 lb/h of sulfate in the mother liquor. The total flow rate of mother liquor is 3,366 + 500 = 3,866 lb/h. Thus, the concentration of sulfate in the mother liquor = 500/3,866 x 100% = 12.9 wt% Na_2SO_4. From the diagram below, the required temperature for this concentration at C in the mother liquor is 18°C.



Exercise 4.59

Subject: Dissolving crystals of Na_2SO_4 with water.

Given: 500 kg of $Na_2SO_4 \cdot 10H_2O$ crystals and 500 kg of Na_2SO_4 crystals at 20°C.

Assumptions: Equilibrium according to phase diagram of Fig. 4.24.

Find: Amount of water to dissolve the crystals at 20°C.

Analysis: From Fig. 4.24, the solubility of Na_2SO_4 in water at 20°C is 15 wt% Na_2SO_4.
Molecular weight of Na_2SO_4 = 142. Molecular weight of $Na_2SO_4 \cdot 10H_2O$ = 322.
Therefore, the kg of Na_2SO_4 in $Na_2SO_4 \cdot 10H_2O$ = 500(142/322) = 220 kg.
The water in $Na_2SO_4 \cdot 10H_2O$ = 500 - 220 = 280 kg.
Total Na_2SO_4 in the crystals = 500 + 220 = 720 kg.
Therefore, need a total of 720(85/15) = 4,080 kg water.
Additional water needed = 4,080 - 280 = 3,800 kg.

Exercise 4.60

Subject: Adsorption of phenol (B) from an aqueous solution at 20°C with activated carbon.

Given: One liter of aqueous solution containing 0.01 mol phenol. Freundlich isotherm equation for adsorption of phenol from aqueous solution by activated carbon at 20°C.

Assumptions: Attainment of equilibrium.

Find: Grams of activated carbon for (a) 75%, (b) 90%, and (c) 98% adsorption of phenol

Analysis: At equilibrium, Eq. (1) in Example 4.12 is: $q_B^* = 2.16 c_B^{0.233}$ (1)
where, q_B^* = mmol phenol adsorbed/g carbon
c_B = mmol phenol in solution/liter solution
For each case, c_B = 0.01(1,000 mmol/mol)(1-fraction adsorbed)
mmol adsorbed = 0.01(1,000 mmol/mol)(1 liter)(fraction adsorbed)
g activated carbon needed = mmol adsorbed/ q_B^*
Using these equations, the results are as follows:

Case	c_B at equilib, mmol/L	mmol phenol adsorbed	q_B^*, mmol/g	g activated carbon
(a) 75% adsorbed	2.5	7.5	2.67	2.81
(b) 90% adsorbed	1.0	9.0	2.16	4.17
(c) 98% adsorbed	0.2	9.8	1.48	6.62

Exercise 4.61

Subject: Adsorption of a colored substance (B) from an oil by clay particles at 25°C.

Given: Oil with a color index of 200 units/100 kg oil. Adsorption equilibrium data

Assumptions: One adsorption equilibrium contact.

Find: (a) Freundlich equation for the adsorption equilibrium data.
(b) kg clay to reduce color index to 20 units/100 kg oil for 500 kg of oil

Analysis: (a) From Eq. (4-30), the Freundlich equation is $q_B^* = Ac_B^{1/n}$, where here,

q_B^* = color units/100 kg clay and c_B = color units/100 kg oil

By nonlinear regression of the data, $A = 0.6733$ and $(1/n) = 0.5090$

The linearized form of the Freundlich equation is $\log q_B^* = \log A + (1/n)\log c_B$

By linear regression of the data with the linearized form, $A = 0.6853$, $(1/n) = 0.5050$

The two results are close and both fit the data quite well. Use the nonlinear regression result:

$$q_B^* = 0.6733 c_B^{0.509} \qquad (1)$$

(b) $Q = 500$ kg oil S = kg clay $c_B^{(F)} = 200$ units/kg oil

Need, at equilibrium, $c_B = 20$ units/kg oil

From Eq. (1), $q_B^* = 0.6733(20)^{0.509} = 3.09$ units/kg clay

Apply Eq. (4-29 for a material balance on the color units:

$$q_B^* = 3.09 = -\frac{Q}{S}c_B + c_B^{(F)}\frac{Q}{S} = -\frac{500}{S}(20) + (200)\frac{500}{S} \qquad (2)$$

Solving Eq. (2), $S = 29{,}100$ kg of clay

Exercise 4.62

Subject: Absorption of acetone (A) from air by water at 1 atm.

Given: *y-x* data for the distribution of acetone between air and water.

Assumptions: Only acetone undergoes mass transfer so that there is no water in the gas phase and no air in the liquid phase.

Find: (a) Plots of the equilibrium data as (1) *Y-X* , (2) *p-X'* (in mass units) , and (3) *y-x*.
(b) Compositions of the exiting streams when 20 moles of gas containing 0.015 mole fraction of acetone is brought to equilibrium with 15 moles of water.

Analysis: (a) Equilibrium data are given in acetone mole fractions (*y* and *x*). To convert to acetone mole ratios (*Y* and *X*), acetone partial pressure (*p*), and acetone mass ratio in the liquid (*X'*), the following equations are used, with molecular weight of acetone = 58:

$$Y_A = \frac{y_A}{1-y_A}\ , \qquad X_A = \frac{x_A}{1-x_A}\ , \qquad p_A = y_A P\ , \qquad X'_A = \frac{58}{18} X_A$$

Using these four equations, the following values are obtained from the given data:

y_A	x_A	Y_A, mol A/mol air	X_A, mol A/mol water	p_A, atm	X'_A, g A/g water
0.004	0.002	0.00402	0.002004	0.004	0.00645
0.008	0.004	0.00807	0.00402	0.008	0.01294
0.014	0.006	0.0142	0.00604	0.014	0.01945
0.017	0.008	0.0173	0.00807	0.017	0.02599
0.019	0.010	0.0194	0.0101	0.019	0.0325
0.020	0.012	0.0204	0.01215	0.020	0.0391

Plots are given on the next page.

(b) Solve by the intersection of the acetone material balance line with the equilibrium curve on the *Y-X* plot. Feed gas contains (0.015)(20) = 0.30 moles acetone and 20 - 0.3 = 19.7 moles air. The acetone material balance is:

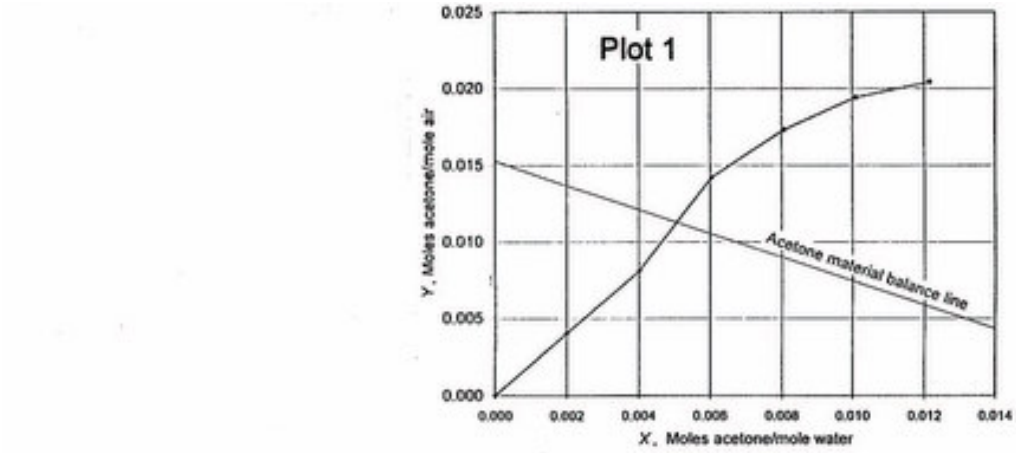
$$0.30 = 19.7Y_A + 15X_A \quad \text{or by rearrangement ,} \quad Y_A = -0.761X_A + 0.01523 \qquad (1)$$

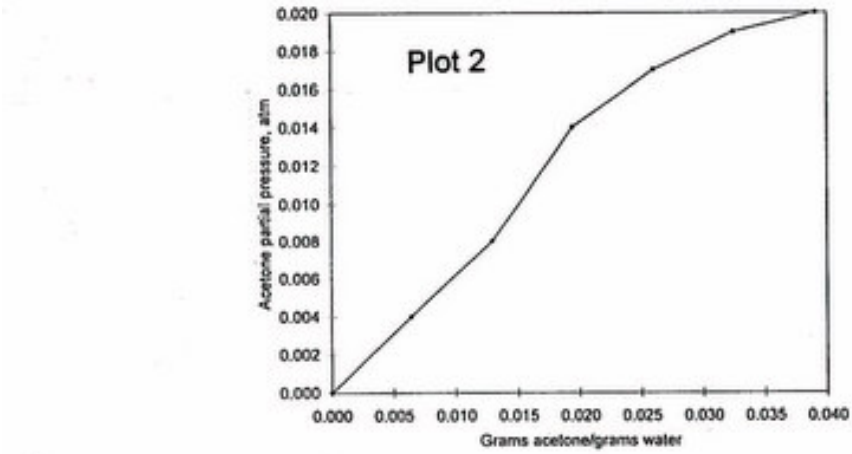
This equation is plotted on the *Y-X* plot on the next page and gives an intersection at $Y_A = 0.0114$ moles acetone/mole air and $X_A = 0.0051$ moles acetone/mole water. The material balance is:

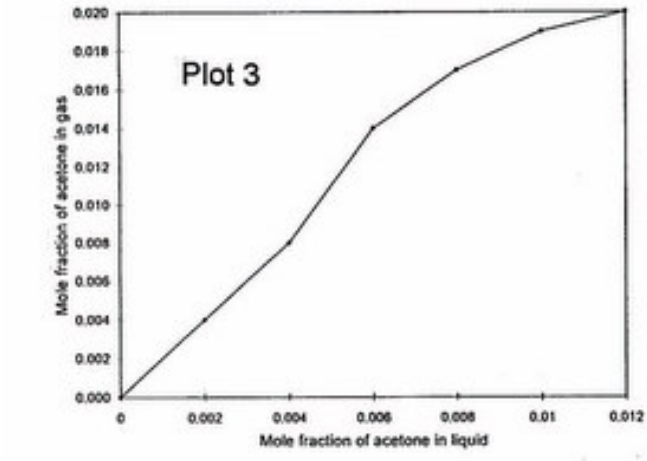
Component:	Gas in, moles	Liquid in, moles	Gas out, moles	Liquid out, moles
Air	19.7	0.0	19.7	0.0
Water	0.0	15.0	0.0	15.0
Acetone	0.3	0.0	0.224	0.076

Exercise 4.62 (continued)

Analysis: (a) (continued)







Exercise 4.63

Subject: Separation of air into O_2 and N_2 by absorption into water followed by desorption.

Given: Air containing 79 mol% N_2 and 21 mol O_2. Pressures ranging from 101.3 kPa (1 atm) to 10,130 kPa (100 atm), and temperatures ranging from 0 to 100°C.

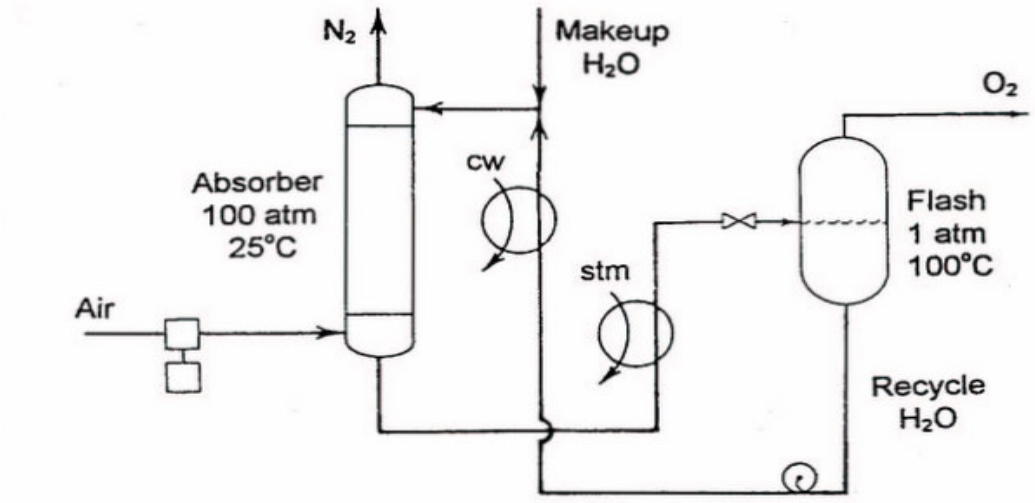
Assumptions: Applicability of Henry's law for solubility of H_2 and O_2 in water.

Find: (a) A workable process.
(b) Number of batch absorption steps to make 90 mol% pure O_2 and the corresponding yield of O_2.

Analysis: Henry's law constants are given in Fig. 4.27 as $(1/H)$ as function of temperature, where from Eq. (4-32), $x_i = (1/H_i)y_iP$ with pressure in atm. Absorption is most efficient at high pressures, while desorption is best at low pressures. From Henry's law in this form, $K_i = y_i/x_i = 1/[(1/H_i)P]$. Using Fig. 4.27, the following are calculated:

	P = 100 atm, 25°C:			P = 1 atm, 100°C:		
Component	$1/H_i$, atm^{-1}	K_i	$\alpha_{N2\text{-}O2}$	$1/H_i$, atm^{-1}	K_i	$\alpha_{N2\text{-}O2}$
Nitrogen	1.1×10^{-5}	910	2.02	7.5×10^{-6}	133,000	1.60
Oxygen	2.2×10^{-5}	450		1.2×10^{-5}	83,000	

(a) A possible continuous scheme is the following, where air is compressed to 100 atm, followed by absorption with water at 25°C. Because the K-value for O_2 is lower than that of N_2, the O_2 is more easily absorbed. The bottoms liquid is heated to 100°C and flashed at 1 atm to release the dissolved O_2. However, because of the large K-value for oxygen in the absorber, the process may require huge amounts of water to obtain a high yield of oxygen. Furthermore, the much higher concentration of nitrogen in the entering air and the fact that the relative volatility of nitrogen with respect to oxygen is not very high will make it very difficult to obtain a sharp split with absorption, as compared to distillation. Thus, the process may not be capable of either high yield or high purity of oxygen. The flash is capable of releasing any dissolved organic.



Exercise 4.63 (continued)

Analysis: (continued)

(b) For batch absorption, the yield and purity of the oxygen, after it flashed off from the water, depends upon the amount of water used. Let the amount of air be 100 kmol (79 kmol N_2 and 21 kmol O_2). Consider amounts of water equal to 100, 1000, 10000, 50000, and 100000 kmol/h. Add this to the air and flash it at 100 atm and 25°C. Using the isothermal flash equations of Table 4.4 (with the exception of the energy balance, which is not needed) with the *K*-values of 910 for nitrogen and 450 for oxygen from the table above, the following results are obtained for a single equilibrium absorption, neglecting the mass transfer of water (stripping into the gas phase), i.e. assigning a *K*-value of 0 to water:

Equilibrium conditions:

Water, kmol	kmol N_2 in V	kmol O_2 in V	kmol N_2 in L	kmol O_2 in L	Mol fraction O_2 in flashed vapor
100	78.92	20.95	0.08	0.05	0.349
1,000	78.15	20.55	0.85	0.45	0.347
10,000	70.33	16.81	8.67	4.19	0.326
50,000	32.95	5.49	46.05	15.51	0.252
100,000	0.00	0.00	79.00	21.00	0.210

These results show that for small amounts of water very little absorption occurs, but the greatest increase in O_2 purity occurs. If additional stages were used with small amounts of water to absorb the flashed vapor so as to reach 90 mol% purity of O_2 ,the yield would be extremely small. At the highest liquid rate in the table above, all of the air is absorbed and, therefore, no separation between nitrogen and oxygen occurs. If 50,000 kmol of water is used, about 75% of the O_2 is absorbed along with about 60% of the N_2, with a resulting O_2 mole fraction of 0.252 in the flashed vapor. If we start with 30,000 kmol of water and continue at this level using 300 kmol of water per kmol of flashed vapor for each batch absorption stage, the following results are obtained, using the isothermal flash equations for absorption at 100 atm and 25°C, followed by complete release of N_2 and O_2 at 1 atm and 100°C, but neglecting the vaporization of water:

Equilibrium conditions:

Stg.	Water, kmol	kmol N_2 in V	kmol O_2 in V	kmol N_2 in L	kmol O_2 in L	y of O_2 in flashed vapor
1	30,000	52.07	10.27	26.93	10.73	0.285
2	11,300	17.54	5.16	9.38	5.58	0.373
3	4,490	6.02	2.62	3.36	2.96	0.468
4	1,895	2.12	1.35	1.24	1.60	0.563
6	411	0.287	0.383	0.189	0.510	0.729
8	113	0.045	0.120	0.033	0.179	0.844
10	37	0.008	0.042	0.006	0.068	0.913

For these conditions, it takes 10 batch stages of absorption and flashing to obtain a vapor of at least 90 mol% O_2. However, the yield of O_2 is very low, 0.068/21 x 100% = 0.32%. It is doubtful that any processing conditions exist that can deliver 90 mol% O_2 with a high yield by absorption with water, followed by flash desorption.

Exercise 4.64

Subject: Absorption of ammonia from nitrogen into water at 20^0C and 1 atm (760 torr).

Given: 14 m^3 of gas containing equimolar NH_3 (A) and N_2 (N)to be contacted in one equilibrium stage with 10 m^3 of water (W). Equilibrium data for partial pressure of NH_3 over water at 20^oC.

Assumptions: No mass transfer of water and nitrogen.

Find: % absorption of NH_3.

Analysis: First compute the kmol of water. Density = 1000 kg/m^3. *M* of water = 18.02. Therefore, we have (10)(1000)/18.02 = 555 kmol = *L*. Next, compute the kmol of gas. *M* of ammonia = 17.03. Assume the 14 m^3 are at 1 atm and 20^oC. At 1 atm and 0^oC, have 22.4 m^3/kmol. At 20^oC and 1 atm, have 22.4(293/273) = 24.04 m^3/kmol or 14/24.04 = 0.582 kmol.

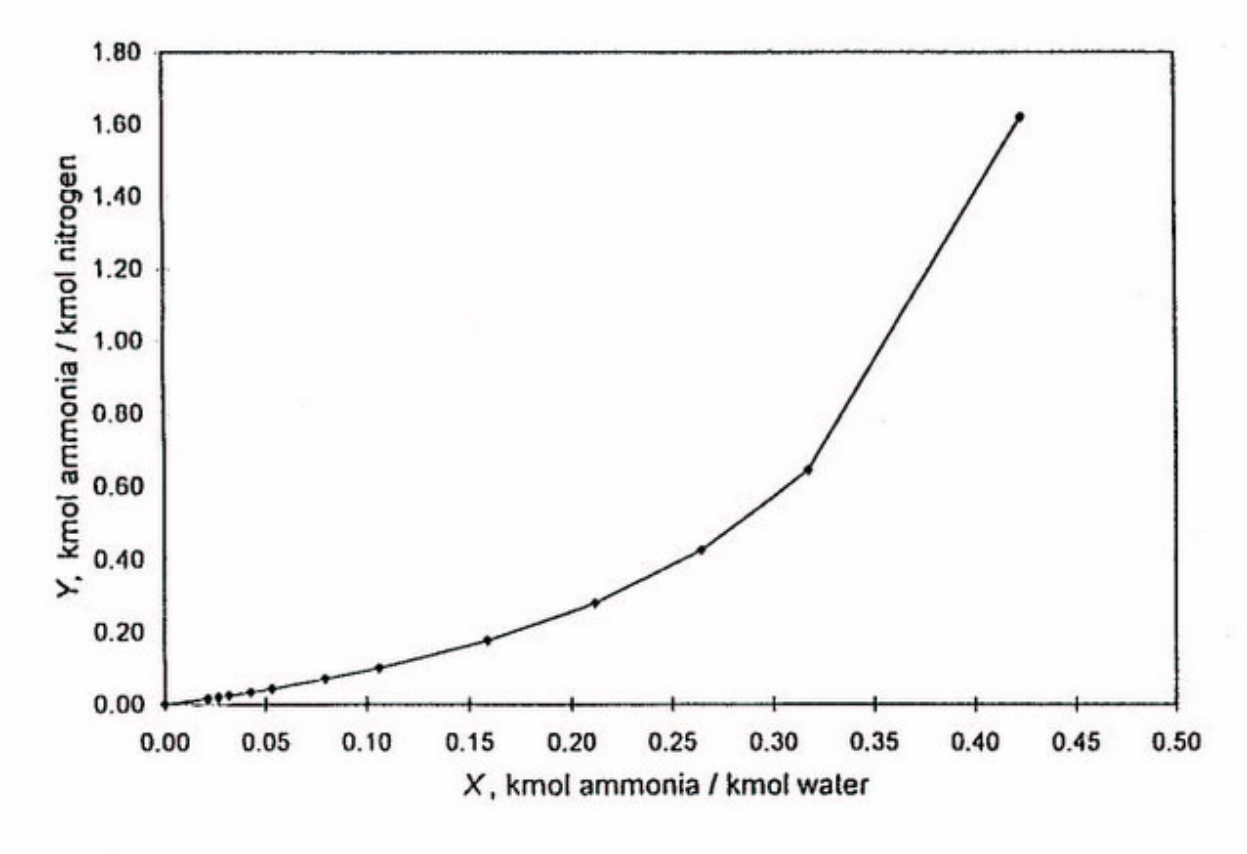
Because NH_3 is the only component being transferred use mole ratios, with: X = moles NH_3 / mole H_2O and Y = moles NH_3 / mole N_2. Convert equilibrium data to these variables, using: $Y = p_A/(760 \text{ torr} - p_A)$, where p_A is in torr.

$$X = \left(\frac{\text{grams } NH_3}{100 \text{ grams } H_2O}\right)\left(\frac{18.02}{17.03}\right)\frac{1}{100} = 0.0106\left(\frac{\text{grams } NH_3}{100 \text{ grams } H_2O}\right)$$

p of NH_3 ,torr	g NH_3 / 100 g H_2O	*Y*	*X*
470	40	1.6207	0.4240
298	30	0.6450	0.3180
227	25	0.4259	0.2650
166	20	0.2795	0.2120
114	15	0.1765	0.1590
69.6	10	0.1008	0.1060
50.0	7.5	0.0704	0.0795
31.7	5	0.0435	0.0530
24.9	4	0.0339	0.0424
18.2	3	0.0245	0.0318
15	2.5	0.0201	0.0265
12	2	0.0160	0.0212
0	0	0.0000	0.0000

Exercise 4.64 (continued)

Analysis: (continued)



The kmol of N_2 = 0.5(0.582) = 0.291 kmol = G.
Material balance for NH_3 , where 0 = inlet and 1 = outlet, with $Y_0 = 1.0$, and $X_0 = 0.0$:

$$LX_0 + GY_0 = G = 0.291 = LX_1 + GY_1 = 555X_1 + 0.291Y_1 \qquad (1)$$

Rearranging Eq. (1), $Y_1 = 1 - 1907X_1$ (2)

Because Y_1 at the outlet must be less than the inlet value of 1, X_1 must be a very small number.

Assume that at small values of X, the equilibrium curve is linear. Using the lowest point at Y = 0.0160 and X = 0.0212, then:

$$Y_1 = (0.0160/0.0212)X_1 = 0.755X_1 \qquad (3)$$

Solving Eqs. (2) and (3) simultaneously, $Y_1 = 3.96 \times 10^{-4}$ mol NH_3/mol N_2

$X_1 = 5.25 \times 10^{-4}$ mol NH_3/mol H_2O

Therefore, in the final gas, have $Y_1G = (3.96 \times 10^{-4})(0.291) = 0.000115$ kmol NH_3
Therefore, NH_3 not absorbed = 0.000115/0.291 x 100% = 0.04%.

Therefore, % NH_3 absorbed = 100 - 0.04 = 99.96.

Exercise 4.65

Subject: Desublimation of phthalic anhydride (PA) from a gas by cooling.

Given: 8,000 lbmol/h of a gas containing 67 lbmol/h of PA cooled at 770 torr.

Assumptions: Only PA desublimes. Dalton's law. At equilibrium, $p_{PA} = P^s_{PA}$.

Find: % recovery of PA for temperatures where the vapor pressure of PA, are (a) 0.7 torr, (b) 0.4 torr, and (c) 0.1 torr.

Analysis: Let n_{PA} = lbmol/h of PA still in the gas at equilibrium. Then by Dalton's law,

$$n_{PA} = \frac{P^s_{PA}}{P}[(8{,}000 - 67) + n_{PA}] \qquad (1)$$

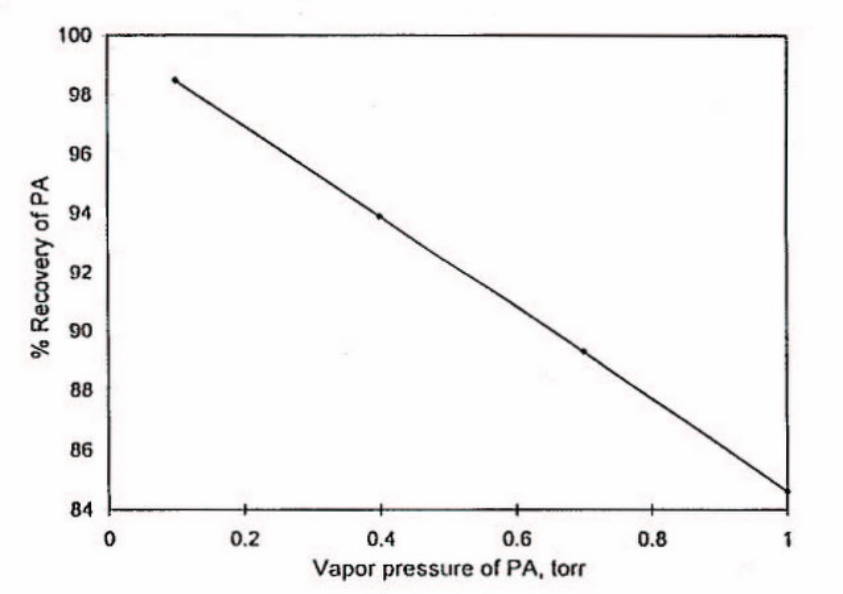
Solving for n_{PA}, with P = 770 torr,

$$n_{PA} = \frac{\frac{P^s_{PA}}{770}(7{,}933)}{1 - \frac{P^s_{PA}}{770}} \qquad (2)$$

and the percent recovery = (97 - n_{PA})/97 x 100% (3)

Solving Eqs. (2) and (3),

P^s, torr	n_{PA}, lbmol/h in gas	% Recovery of PA
0.7	7.2	89.3
0.4	4.1	93.9
0.1	1.03	98.5



Exercise 4.66

Subject: Desublimation of anthraquinone (A) from nitrogen (N).

Given: Gas containing 10 mol% A and 90 mol% N at 760 torr and 300°C is cooled to 200°C.

Assumptions: Given vapor pressure data for solid A can be fitted to Antoine equation

Find: % desublimation of A assuming no change in total pressure.

Analysis: Using Polymath, the given vapor pressure data are fitted to the following Antoine eq.:

$$P_A^s = 10^{\left(32.8653 - \frac{49{,}762.2}{1327.24+T}\right)} \qquad (1)$$

where P_A^s is in torr and T is in °C. From Eq. (1), $P_A^s = 1.915$ torr at 200°C. Assume 100 moles of initial gas, containing 90 moles N and 10 moles A. Let n_A = moles of A still in the gas at equilibrium at 200°C. Then by Dalton's law, where $p_A = P_A^s$,

$$n_A = \frac{p_A}{P} n_{total} = \frac{P_A^s}{P}(90 + n_A) = \frac{1.915}{760}(90 + n_A) \qquad (2)$$

Solving for n_A,

$$n_A = \frac{\frac{1.915}{760}(90)}{1 - \frac{1.915}{770}} = 0.227 \text{ mole} \qquad (3)$$

and the percent recovery = (10 - 0.227)/10 x 100% = 97.73%

Exercise 4.67

Subject: Separation of a gas mixture of propylene (A) and propane (P) by adsorption.

Given: $T = 25^{o}$C, P = 101 kPa, gas containing 0.7 mole A and 1.3 mole P, and S = 0.1 kg silica gel. Equilibrium adsorption data in Fig. 4.30.

Find: Equilibrium compositions and amounts of adsorbate and final gas.

Analysis: Let y and x be the mole fractions of P in the vapor and adsorbate, respectively. Let G and W be the moles of equilibrium vapor and adsorbate, respectively. Then a propane material balance is: $1.3 = Wx + Gy$. A total material balance is: $2.0 = W + G$. Combining balances,

$$y = \frac{1.3 - Wx}{2 - W} \qquad (1)$$

To solve, assume W, plot the equation on Fig. 4.30a and find intersection with the equilibrium curve to find y and x. Read the mmole adsorbate/g adsorbent = moles adsorbate/kg adsorbent from Fig. 4.30b. Calculate kg adsorbent. If it is not 0.1 kg, repeat with a new guess of W.

For W = 0.195 moles, G = 1.805 moles, y = 0.72 - 0.108x, y = 0.67, x = 0.41, S = 0.10 kg.

Exercise 4.68

Subject: Separation of a gas mixture of propylene (A) and propane (P) by adsorption.

Given: Gas containing 50 mol% A and 50 mol% P, and S = 1,000 lb of less of silica gel/lbmol of feed gas. Equilibrium adsorption data in Fig. 4.30 apply.

Find: If one equilibrium stage can produce a vapor with 90 mol% P and an adsorbate of 75 mol% A. If not, what separation can be achieved.

Analysis: With a basis of 1 lbmole of feed gas, let y and x be the mole fractions of P in the equilibrium vapor and adsorbate, respectively. Then we desire, $y = 0.9$ and $x = 0.25$. Let G and W be the lbmol of equilibrium vapor and adsorbate, respectively. Then a propane material balance is: $0.5 = Wx + Gy$. A total material balance is: $1.0 = W + G$. Combining balances,

$$y = \frac{0.5 - Wx}{1 - W} \qquad (1)$$

From the equilibrium curve in Fig. 4.30a, it is seen that when $x = 0.25$, $y = 0.47$, which is far from the desired value of 0.90. Therefore, cannot achieve the desired separation. So, calculate what can be achieved. To solve, assume W, plot the equation on Fig. 4.30a and find intersection with the equilibrium curve to find y and x. Read the mmole adsorbate/g adsorbent = lbmoles adsorbate/1000 lb adsorbent from Fig. 4.30b. However, we see in Fig. 4.30b that the smallest adsorbate amount is 1.57 lbmol adsorbate/1000 lb adsorbent. But we only have a total of 1.0 lbmol of feed gas. Therefore, we can use a lot less adsorbent. Assume a value of $W = 0.5$ lbmole (50% of the feed gas and equal to the amount of A in the feed gas). Then Eq. (1) becomes:

$$y = 1 - x.$$

From Fig. 4.30a, the intersection with the equilibrium curve is $y = 0.635$ and $x = 0.365$. From Fig. 4.30b, for $x = 0.365$, we have 2.0 lbmoles adsorbate/1000 lb of silica gel. Since we only have 0.5 lbmol of adsorbate, we only need 250 lb of silica gel. The separation achieved is far less than desired. Multiple stages might achieve the desired separation. Other values of W will give other separations.

Exercise 4.69

Subject: Crystallization of $MgSO_4$ from an aqueous by evaporation.

Given: 1,000 lb of $MgSO_4$ dissolved in 4,000 lb of water at 160°F. 90% of the water is evaporated at 160°F, causing the monohydrate to crystallize. At 160°F, $MgSO_4$ has a solubililty of 36 wt%.

Assumptions: Equilibrium.

Find: (a) Pounds of water evaporated.
(b) Pounds of monohydrate, $MgSO_4 \cdot H_2O$, crystals produced.
(c) Crystallizer pressure.

Analysis: (a) Evaporate 0.9(4,000) = 3,600 lb of water
Therefore, water left = 4,000 - 3,600 = 400 lb

(b) MW of water = 18 and MW of $MgSO_4$ = 120.4
Let W = lb of $MgSO_4$ remaining in solution.
Then $MgSO_4$ in the crystals = 1,000 - W.
From crystal stoichiometry, water of hydration in the crystals =

$$(1{,}000 - W)\left(\frac{18}{120.4}\right) = 0.15(1{,}000 - W) \qquad (1)$$

Therefore, the water in solution = 400 - 0.15(1,000 - W) = 250 + 0.15W
The total solution (water + dissolved sulfate) = 250 + 0.15W + W = 250 + 1.15W
From solubility of the sulfate,

$$0.36 = \frac{W}{250 + 1.15W} \qquad (2)$$

Solving Eq. (2), W = 153.6 lb $MgSO_4$ dissolved.
$MgSO_4$ in the crystals = 1,000 - 153.6 = 846.4 lb

$$\text{Water of crystallization} = \frac{18}{120.4}(846.4) = 126.5 \text{ lb}$$

Total crystals = 846.4 + 126.5 = 972.9 lb of $MgSO_4 \cdot H_2O$

(c) Since the crystallizer pressure depends only on temperature and the composition of the mother liquor in the crystallizer, it is the same as in Example 4.17 or 4.38 psia.

Exercise 4.70

Subject: Crystallization of Na_2SO_4 from an aqueous solution by evaporation.

Given: 1,000 kg/h of Na_2SO_4 dissolved in 4,000 kg/h of water. Water is evaporated at 60°C to crystallization 80% of the Na_2SO_4. Solubility data in Fig. 4.24.

Assumptions: Equilibrium. Raoult's law for the mother liquor.

Find: (a) The kg/h of water that must be evaporated.
(b) The crystallizer pressure in torr.

Analysis: (a) From Fig. 4.24, at 60°C, the stable crystals are Na_2SO_4 with no water of crystallization. The solubility of Na_2SO_4 at 60°C is 0.315 wt. Fraction.

C = rate of crystal formation = 0.8(1,000) = 800 kg/h

Therefore, sulfate dissolved in the mother liquor = 1,000 - 800 = 200 kg/h.

From the solubility of the sulfate, water in the mother liquor = $\frac{(1-0.315)}{0.315}(200) = 435$ kg/h

Therefore, we must evaporate, 4,000 - 435 = 3,565 kg/h

(b) MW of Na_2SO_4 = 142.05

Therefore, have 200/142.05 = 1.41 kmol/h of Na_2SO_4 in the mother liquor.

Also, we have 435/18.02 = 24.14 kmol/h of water in the mother liquor.

The mole fraction of water in the mother liquor = $\frac{24.14}{24.14+1.41} = 0.945$

At 60°C, the vapor pressure of water = 2.89 paia.

From Raoult's law, given by Eq. (2-42), the partial pressure of water =

$x_W P_W^s = 0.945(2.89) = 2.73$ psia

Assuming that Na_2SO_4 has no vapor pressure in solution, crystallizer pressure = 2.73 psia.

Exercise 4.71

Subject: Bubble, secondary dew, and primary dew points of a three-component mixture assuming immiscibility of water and hydrocarbons.

Given: (a) 50 mol% benzene (B), 50 mol% water (W).
(b) 50 mol% toluene (T), 50 mol% water (W).
(c) 40 mol% benzene (B), 40 mol% toluene (T), and 20 mol% water (W)

Assumptions: Ideal hydrocarbon solutions and immiscibility with water.

Find: Bubble, secondary dew, and primary dew point pressures at 50°C.

Analysis: From the CHEMCAD program, vapor pressures at 50°C are:
benzene 5.22 psia, toluene 1.78 psia, water 1.79 psia
(a) At the bubble point, both pure liquid phases are present. Therefore, P = sum of the vapor pressures = 5.22 + 1.79 = 7.01 psia. This is also the secondary dew-point pressure.
For a binary mixture, the primary dew point occurs when the pressure is increased to the point where the partial pressure of one component equals it vapor pressure. Since we have a 50-50 molar mixture, this occurs for the component with the lowest vapor pressure, water. Thus, water will condense first, with $P = p_W + p_B = 1.79 + 1.79 = 3.58$ psia.

(b) Calculations for toluene and water are made in an identical manner to part (a). The results are: Bubble-point pressure = 1.79 + 1.78 = 3.57 psia. This is also the secondary dew point. The primary dew point is controlled by the toluene. Thus, the primary dew point pressure = 1.78 +1.78 = 3.56 psia.

(c) Assuming Raoult's law from Eq. (2-42) to hold for the hydrocarbon phase, which is equimolar in B and T, and the water phase exerting its full vapor pressure, we have for the bubble point pressure from Eq. (4-34):

$$P = P_W^s + x_B P_B^s + x_T P_T^s = 1.79 + 0.5(5.22) + 0.5(1.78) = 5.29 \text{ psia for the bubble point.}$$

For the primary dew point, assume first that the water condenses first. Then, using Dalton's law:

$$P = \frac{p_W}{y_W} = \frac{P_W^s}{y_W} = \frac{1.79}{0.2} = 8.95 \text{ psia}$$

But this higher than the bubble point pressure. So, instead, assume that the hydrocarbon phase condenses first. Apply the dew point equation, Eq. (4-13) to just the hydrocarbon phase:

$$\sum_{HCs} x_i = 1 = \sum_{HCs} \frac{z_i}{K_i} = \sum_{HCs} \frac{z_i P}{P_i^s} \qquad (1)$$

Therefore, solving Eq. (1) for P,

$$P = \frac{1}{\sum_{HCs} \frac{z_i}{K_i}} = \frac{1}{\left(\frac{0.4}{5.22} + \frac{0.4}{1.78}\right)} = 3.32 \text{ psia for the primary dew point.}$$

Exercise 4.71 (continued)

Analysis: (c) (continued)

For this condition, the partial pressure of water is 0.2(3.32) = 0.664 psia (less than 1.79 psia).

The secondary dew point is much more difficult to determine. We now know that as the pressure is increased, the hydrocarbons condense first. At the primary dew point, the partial pressure of W is 0.664 psia. W will not condense until its partial pressure increases to its vapor pressure of 1.79 psia. As the pressure is increased above the primary dew point pressure of 3.32 psia, the hydrocarbons will condense, reducing their mole fractions in the vapor phase and causing the mole fraction of water to increase in the vapor phase. This plus the increased total pressure will eventually cause the water partial pressure to reach its vapor pressure and begin condensing. We know the secondary dew point pressure must lie between the bubble point pressure of 5.29 psia and the primary dew point pressure of 3.32 psia.

The equations that apply at the secondary dew point, where all pressures are in psia, are:

Dalton's law: $P = p_B + p_T + 1.79 = y_B P + y_T P + 1.79$ (2)

Raoult's law:

$p_B = x_B P_B^s = x_B(5.22)$ (3)

$p_T = x_T P_T^s = x_T(1.78)$ (4)

Substituting Eqs. (3) and (4) into (2),

$P = 5.22x_B + 1.78x_T + 1.79$ (5)

But in the hydrocarbon-rich liquid phase, $x_T = 1 - x_B$. Therefore, Eq. (5) becomes:

$P = 5.22x_B + 1.78(1 - x_B) + 1.79 = 3.44\, x_B + 3.57$ (6)

Material balance equations for a basis of 100 moles, with 40 moles of B, 40 moles of T, and 20 moles of W:

At the secondary dew point, only HCs have condensed. Therefore, the total moles of vapor is:

$V = 20P/1.79 = 11.17P$ (7)

The moles of liquid is: $L = 100 - V$ (8)

A benzene material balance is: $40 = y_B V + x_B L$ (9)

Substituting Eqs. (7) and (8) into (9),

$40 = 11.17\, y_B P + 100x_B - 11.17x_B P$ (10)

We can also write from Eq. (3), $y_B = 5.22x_B/P$ (11)

Combining Eqs. (6), (10), and (11) to eliminate x_B and y_B,

$3.247P^2 - 57.61P + 204.29 = 0$ (12)

Solving for the root between the bubble point and the primary dew point, the secondary dew point pressure = P = 4.90 psia.

Exercise 4.72

Subject: Bubble and dew points of a mixture of benzene, toluene, and water.

Given: Pressure of 2 atm.
(a) 50 mol% benzene and 50 mol% water.
(b) 50 mol% toluene and 50 mol% water.
(c) 40 mol% benzene, 40 mol% toluene, and 20 mol% water.

Assumptions: hydrocarbons and water immiscible.

Find: For each mixture, bubble-point, primary dew-point, and secondary dew-point temperatures.

Analysis: Use the CHEMCAD simulator with API-SRK for *K*-values, with the immiscible option and the three-phase flash model. The following results are obtained:

	T **for Case (a),** ^{o}**C**	***T*** **for Case (b),** ^{o}**C**	***T*** **for Case (c),** ^{o}**C**
Bubble point	89.4	104.3	93.9
Secondary dew point	89.4	104.3	98.0
Primary dew point	100.0	110.3	99.7

Exercise 4.73

Subject: Bubble-point of a mixture of toluene, ethyl benzene, and water.

Given: Mixture of 30 mol% toluene, 40 mol% ethylbenzene, and 30 mol% water at 0.5 atm.

Assumptions: Hydrocarbons and water are immiscible.

Find: Bubble-point temperature and vapor composition.

Analysis: : Use the CHEMCAD simulator with API-SRK for *K*-values, with the immiscible option and the three-phase flash model. The following results are obtained:

$T = 70.8^{o}$C Vapor mole fractions are toluene 0.23, ethyl benzene 0.13, water 0.64

Exercise 4.74

Subject: Bubble, dew, and 50 mol% flash conditions for water-n butanol mixture.

Given: Mixture of 60 mol% water (W) and 40 mol% n-butanol (B) at 101 kPa

Find: (a) Dew-point temperature and liquid composition.
(b) Bubble-point temperature and vapor composition.
(c) Temperature and phase compositions for 50 mol% vaporization.

Analysis: Use the CHEMCAD simulator with UNIFAC LLE for *K*-values, with the three-phase flash model. The following results are obtained:
(a) 100.1°C with liquid mole fractions of 0.242 for W and 0.758 for B.

(b) 93.5°C with vapor mole fractions of 0.773 for W and 0.227 for B. Note that the liquid consists of two phases, with the water-rich phase containing mole fractions of 0.969 for W and 0.031 for B. The less W-rich phase contains mole fractions of 0.564 for W and 0.436 for B.

(c) 94.5°C with vapor mole fractions of 0.742 for W and 0.258 for B and a single liquid-phase mole fractions of 0.458 for W and 0.542 for B.

The results deviate somewhat from Fig. 4.8.

Exercise 4.75

Subject: Isothermal three-phase flash of 6-component mixture.

Given: Feed mixture with composition given below.

Find: Flow rates and compositions for 25°C and 300 kPa.

Analysis: Use the CHEMCAD simulator with UNIFAC LLE for *K*-values, with the three-phase flash model. The following results are obtained:

	kmol/h:			
Component:	**Feed**	**Vapor**	**Liquid I**	**Liquid II**
Hydrogen	350	349.90	0.07	0.03
Methanol	107	4.87	14.31	87.82
Water	491	3.32	3.04	484.64
Toluene	107	0.75	106.16	0.09
Ethyl benzene	141	0.37	140.59	0.04
Styrene	350	0.57	349.19	0.24
Total:	1,546	359.78	613.36	572.86

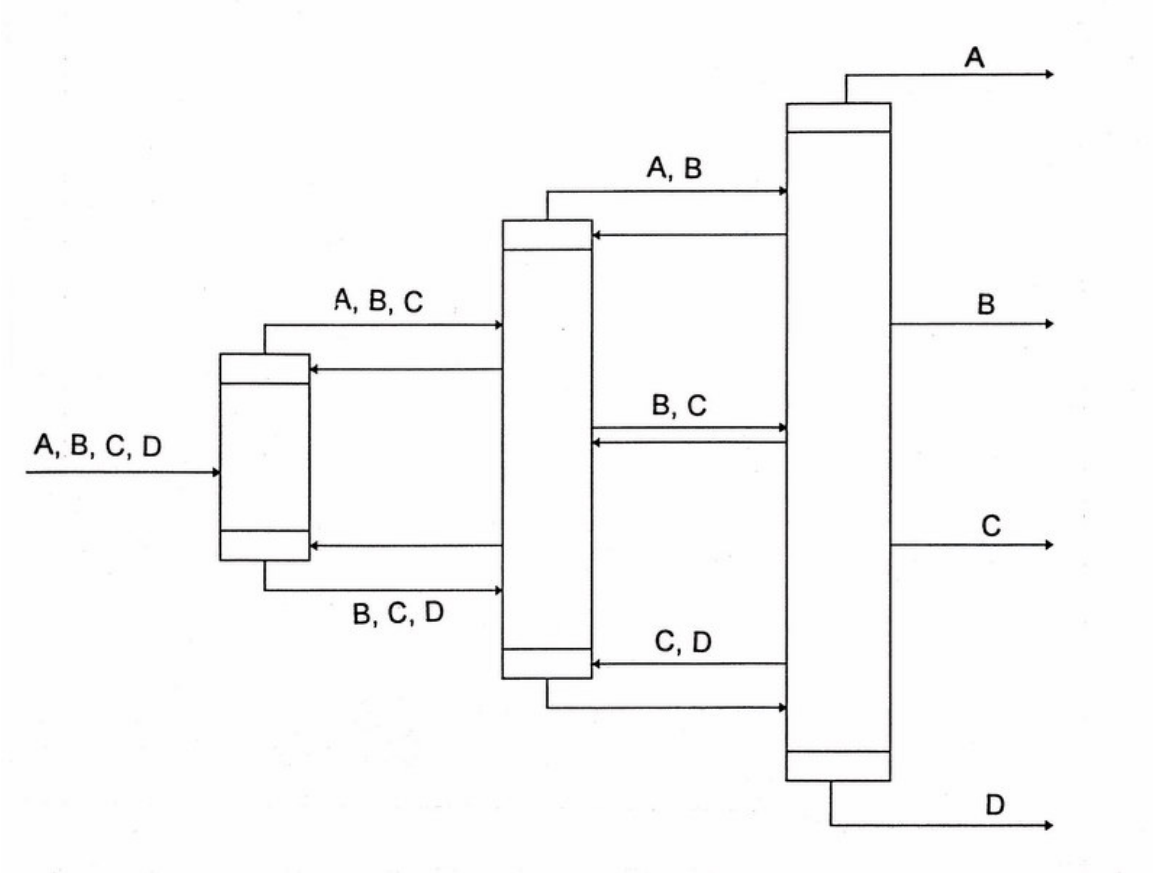
Exercise 5.1

Subject: Three-column interlinked cascade for a four-component system.

Given: Configuration for a two-column interlinked cascade for a three-component system

Find: Devise the three-column cascade.

Analysis: The system is shown in the sketch below. Assume that the feed is comprised of components A, B, C, and D in the order of decreasing volatility. Starting from the feed end at the left-hand side, Column 1 performs a sloppy split to separate the feed into an overhead of A, part of B, and part of C; and a bottoms of part of B, part of C, and D. In the second column, the overhead is A and part of B, the middle sidestream is part of B and part of C, while the bottoms is D and part of C. In the third column, the four products are removed in nearly pure states.



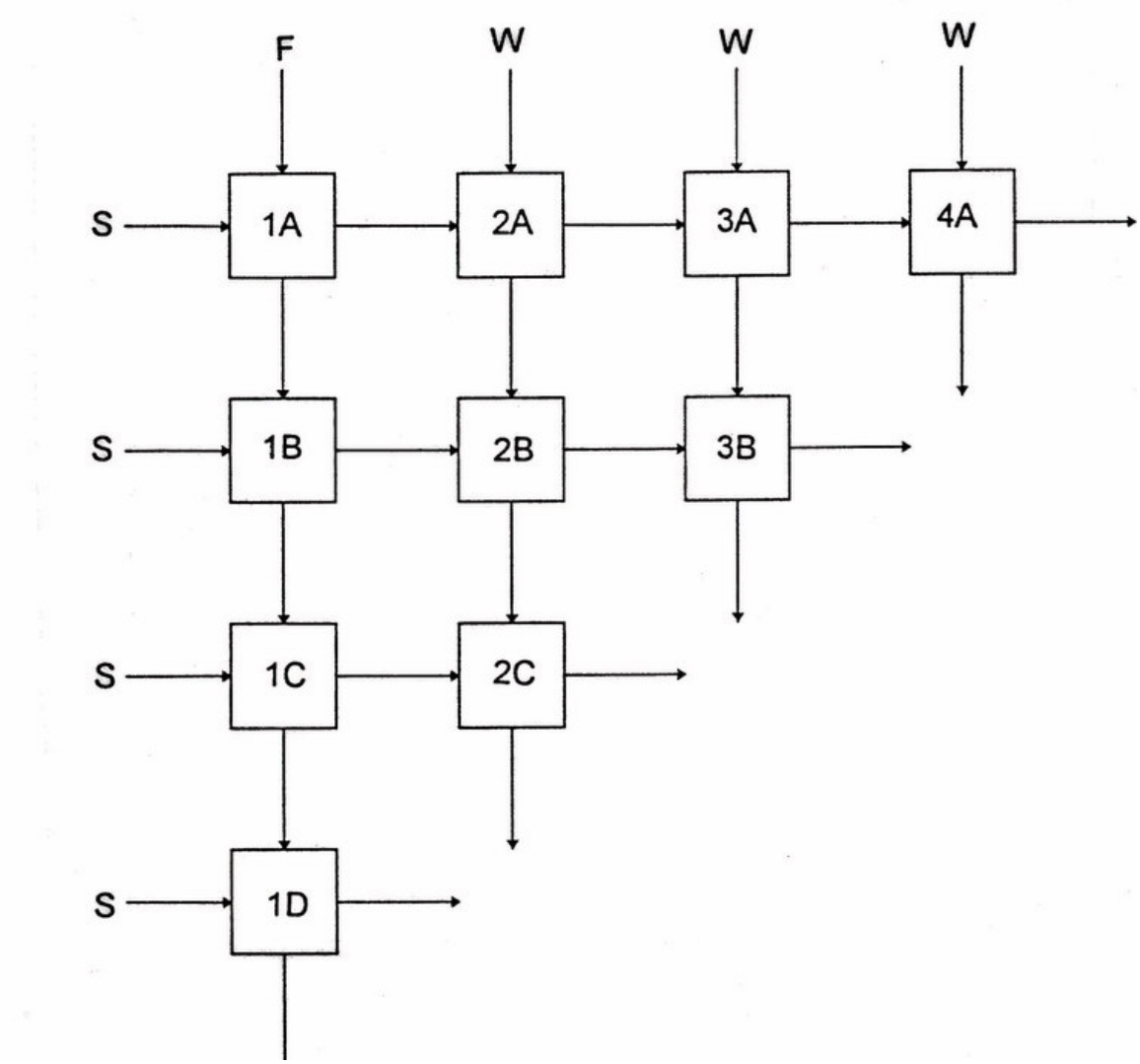
Exercise 5.2

Subject: Batch cascades for liquid-liquid extraction

Given: Batch process in Fig. 5.19

Find: (a) Cascade diagram for Fig. 5.19.
(b) Type of cascade in Part (a).
(c) Comparison of process in Fig. 5.19 to a single stage process.
(d) Modification to achieve a countercurrent cascade.

Analysis: (a) A cascade diagram representing Fig. 5.19 is the following:



Exercise 5.2 (continued)

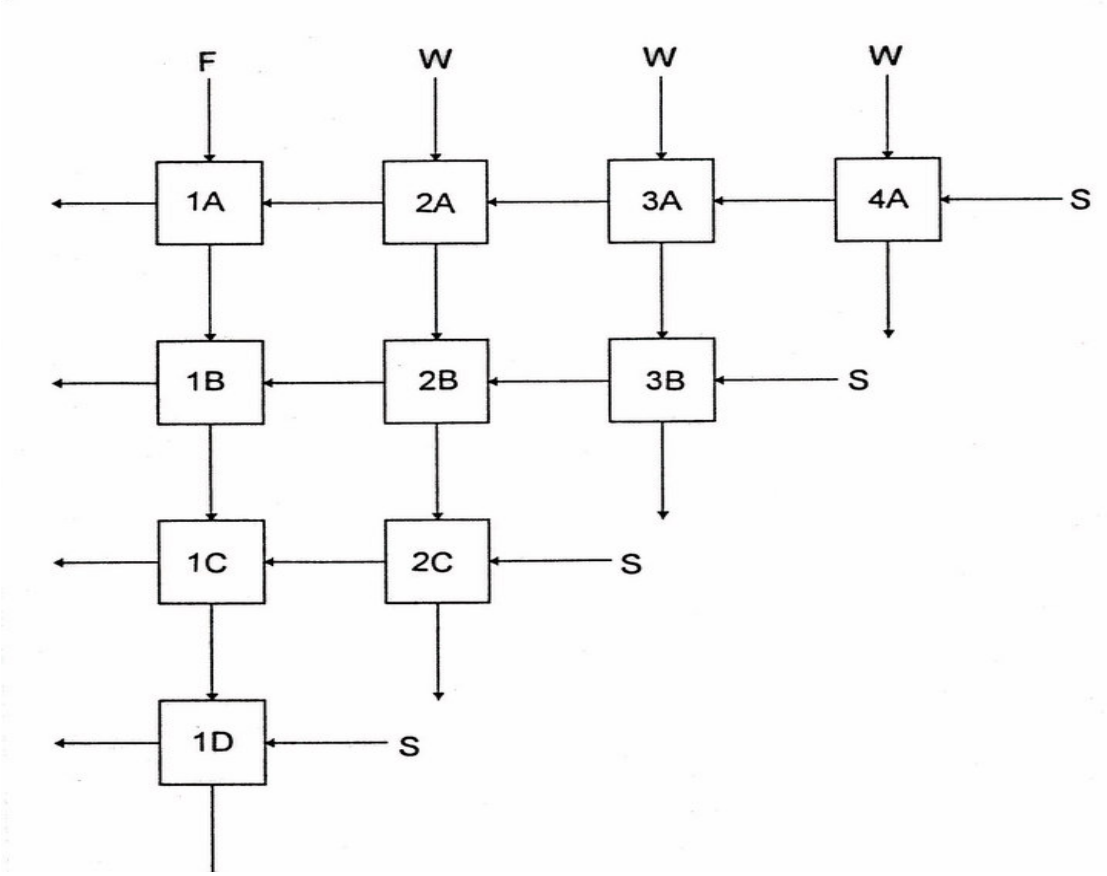
(b) The above cascade is a two-dimensional triangular cascade of the crosscurrent type.

(c) For a single batch extraction using just the feed and one portion of the solvent, i.e. 100 ml of organic solvent and 100 ml of water containing 100 mg each of A and B, the resulting products are: Extract containing 100 ml solvent, 66.7 mg A, and 33.3 mg B.
Raffinate containing 100 ml water, 33.3 mg A, and 66.7 mg B.

If all 4 extracts and all 4 raffinates for the Fig. 5.19 are combined, we find:
Extract containing 400 ml solvent, 66.7 mg A, and 33.3 mg B.
Raffinate containing 400 ml water, 33.3 mg A, and 66.7 mg B.

The process in Fig. 5.19 does produce extracts of varying purity, but overall, it is not effective.

(d) The cascade above in Part (a) can be modified to give a more countercurrent process by reversing the flows of the solvents as shown in the following diagram. However, it is not possible to carry this out batchwise.



Exercise 5.3

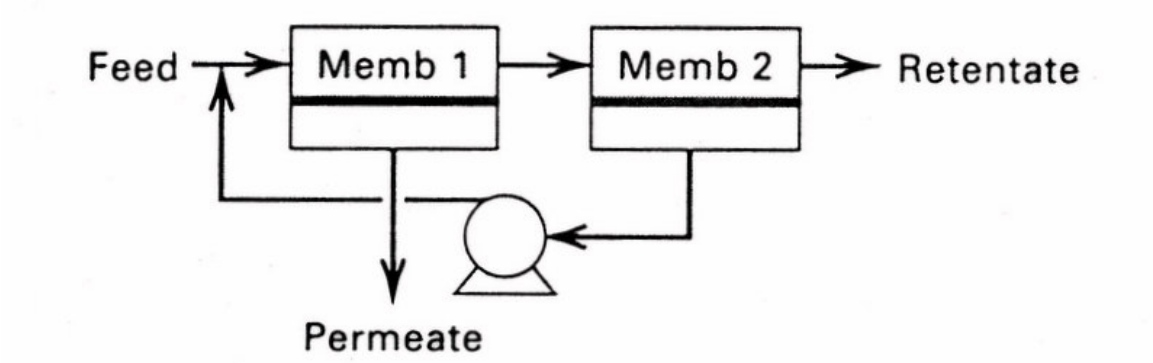
Subject: Two-stage membrane cascades for removal of nitrogen from methane by gas permeation.

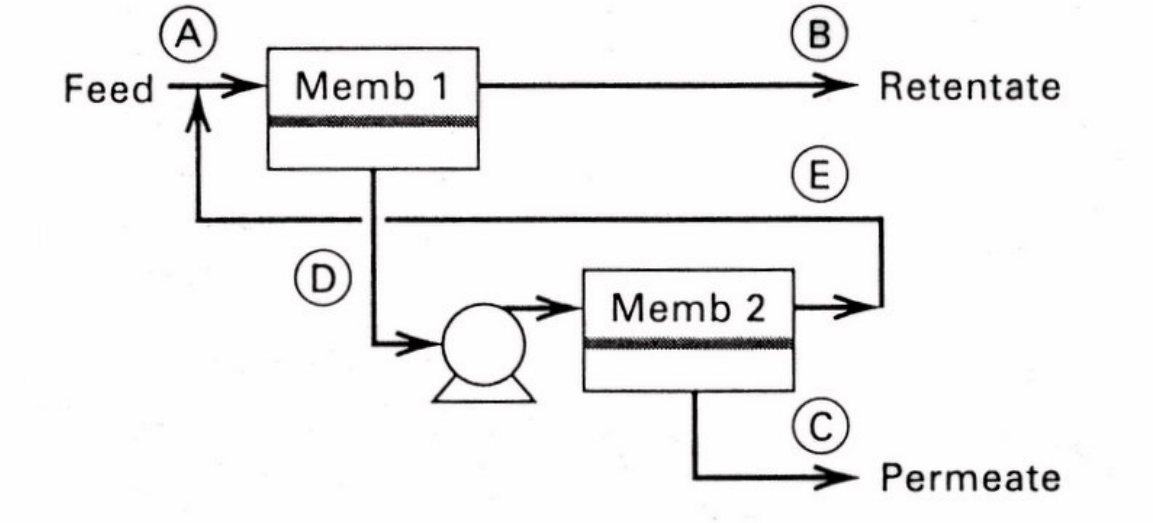
Given: Glassy polymer membrane that is selective for nitrogen.

Assumptions: Desired degree of separation can not be achieved with one stage.

Find: Two different two-stage cascades.

Analysis: The two cascades are shown below. In both cases, the retentate is methane-rich and the permeate is nitrogen-rich. In the first cascade, the permeate from Stage 2 is recycled to the feed to obtain a more pure methane retentate. In the second cascade, the retentate from Stage 2 is recycled to the feed to obtain a more pure nitrogen permeate.





Exercise 5. 4

Subject: Leaching of oil from soybeans with benzene using countercurrent-flow cascades.

Given: Soybean meal containing 2,500 kg/h of oil = L_0 and 2,500 kg/h of insoluble solids. Benzene solvent as in Example 4.9.

Assumptions: Equilibrium leaching stages where, for each stage, the weight fraction of oil in the overflow equals that in the underflow liquid. No solids in the overflows. Underflows contain 65 wt% solids.

Find: Percent extraction of oil if:

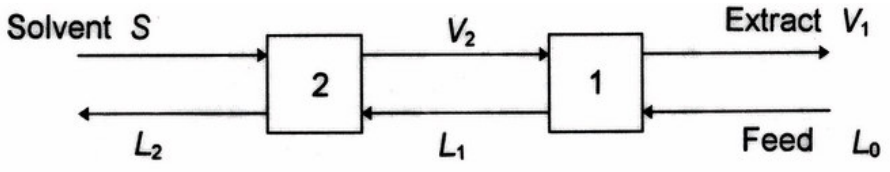
(a) Two stages are used with 5,000 kg/h of benzene = S.

(b) Three stages are used with 5,000 kg/h of benzene = S.

and (c) Number of stages to extract 98% of the oil with two times the min. benzene rate.

Analysis: Let x_i = mass fraction of oil in the underflow liquid from Stage i and y_i = mass fraction of oil in the overflow liquid from Stage i. Let L_i = underflow liquid leaving Stage i and V_i = overflow liquid leaving Stage i. At any stage, $y_i = x_i$. Since all solids entering a stage leave in the underflow from that stage and the total underflow is 65 wt% solids with 2,500 kg/h of solids, $L_i = (35/65)2{,}500 = 1{,}346$ kg/h

(a) The two-section cascade is shown below. Soybean meal enters Stage 1 at 5,000 kg/h and the benzene solvent enters Stage 2 at 5,000 kg/h. Underflow liquids are $L_1 = L_2 = 1{,}346$ kg/h.



Total liquid material balance around Stage 2:

$S + L_1 = V_2 + L_2$ or $5{,}000 + 1{,}346 = V_2 + 1{,}346$. Therefore, $V_2 = 5{,}000$ kg/h.

Total liquid material balance around Stage 1:

$V_2 + L_0 = V_1 + L_1$ or $5{,}000 + 2{,}500 = V_1 + 1{,}346$. Therefore, $V_1 = 6{,}154$ kg/h.

Oil material balance around Stage 1:

$$L_0 + V_2y_2 = L_1x_1 + V_1y_1 \quad \text{or} \quad 2{,}500 + 5{,}000y_2 = 1{,}346x_1 + 6{,}154y_1 \qquad (1)$$

Oil material balance around Stage 2:

$$L_1x_1 = L_2x_2 + V_2y_2 \quad \text{or} \quad 1{,}346x_1 = 1{,}346x_2 + 5{,}000y_2 \qquad (2)$$

From equilibrium at each stage for the leaving liquids,

$$y_1 = x_1 \quad \text{and} \quad y_2 = x_2 \qquad (3, 4)$$

Solving the four linear equations, (1), (2), (3), and (4), we obtain:

$y_1 = 0.3882$ $x_1 = 0.3882$ $y_2 = 0.08234$ $x_2 = 0.08234$

Exercise 5. 4 (continued)

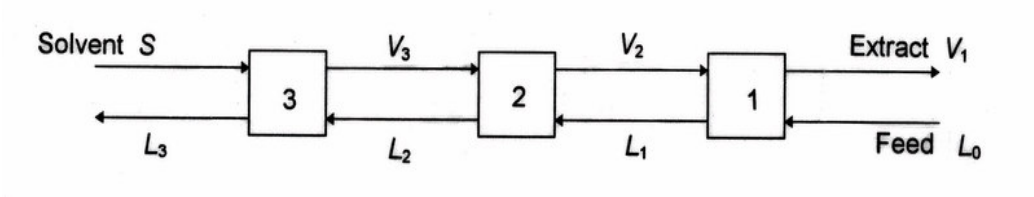
Analysis: (continued)

Oil in the final extract = V_1y_1 = 6,154(0.3882) = 2,389 kg/h

Percent extraction of oil = (2,389/2,500) x 100% = 95.6%

This compares to 83.3% for one stage.

(b)) The three-section cascade is shown below. Soybean meal enters Stage 1 at 5,000 kg/h and the benzene solvent enters Stage 3 at 5,000 kg/h. Underflow liquids are $L_1 = L_2 = L_3 =$ 1,346 kg/h.



Total liquid material balances around Stages 3, 2, and 1, respectively, similar to those in Part (a), give: $V_3 = V_2 = 5{,}000$ kg/h and $V_1 = 6{,}154$ kg/h.

Oil material balances around Stages 1, 2, and 3, respectively, similar to those in Part (a) give:

$$2{,}500 + 5{,}000y_2 = 1{,}346x_1 + 6{,}154y_1 \qquad (5)$$

$$1{,}346x_1 + 5{,}000y_3 = 1{,}346x_2 + 5{,}000y_2 \qquad (6)$$

$$1{,}346x_2 = 1{,}346x_3 + 5{,}000y_3 \qquad (7)$$

From equilibrium at each stage for the leaving liquids,

$$y_1 = x_1 \qquad y_2 = x_2 \qquad y_3 = x_3 \qquad (8, 9, 10)$$

Solving the six linear equations, (5) through (10), we obtain:

$$y_1 = x_1 = 0.4015 \qquad y_2 = x_2 = 0.1023 \qquad y_3 = x_3 = 0.02169$$

Oil in the final extract = V_1y_1 = 6,154(0.4015) = 2,471 kg/h

Percent extraction of oil = (2,471/2,500) x 100% = 98.8%

This compares to 83.3% for one stage and 95.6% for two stages.

(c) From Eq. (5-12), the minimum solvent rate corresponds to zero overflow, with all liquid going to the underflow. Liquid in the underflow = 1,346 kg/h. Can not apply the minimum solvent rate concept here because the liquid in the underflow is not stated as just solvent, but as total liquid including the oil. The total liquid in the underflow is less than the oil in the feed. However, note that for the given solvent rate, somewhat more than the desired 98% extraction is achieved with three stages.

Exercise 5.5

Subject: Leaching of sodium carbonate from an insoluble oxide with water in a countercurrent-flow cascade.

Given: From Example 5.1, entering flow rates are: $Na_2CO_3 = F_B = 1{,}350$ kg/h, insoluble oxide = $F_A = 2{,}400$ kg/h, and water = $S = 4{,}000$ kg/h. Underflow from each stage = 40 wt% on a solute (Na_2CO_3)-free basis.

Assumptions: Equilibrium leaching stages where, for each stage, the weight fraction of carbonate in the overflow equals that in the underflow liquid. No solids in the overflows.

Find: Minimum solvent water rate in lb/h. Ratio of solvent rate to minimum solvent rate. Percent recovery of carbonate with five stages and solvent rates from 1.5 to 7.5 times the minimum solvent rate.

Analysis: R = mass of solvent/mass of insoluble solids = 40/60 = 0.667.

Therefore solvent rate in the underflow = 2,400(0.667) = 1,600 kg/h.
From Eq. (5-12), $S_{min} = RF_A = 0.667(2{,}400) = 1{,}600$ kg/h or 3,630 lb/h
Therefore, the ratio of solvent to minimum solvent = 2,400/1,600 = 2.5
To determine percent recoveries (extraction) of carbonate for 5 stages and various S/S_{min}, apply Eq. (5-10) to determine the mass ratio of carbonate to solvent in the final underflow leaving the

last Stage N:
$$X_N = \frac{F_B}{S}\left(\frac{1}{W^{N-1}}\right) \qquad (1)$$

where, from Eq. (5-5), $W = S/RF_A = S/S_{min}$ (2)
Combining Eqs. (1) and (2), noting that $F_B = 1{,}350$ kg/h, $F_A = 2{,}400$ kg/h, $R = 0.667$, and $N = 5$,

$$X_N = \frac{F_B}{F_A R}\left(\frac{1}{W^N}\right) \quad \text{or} \quad X_5 = \frac{1{,}350}{(2{,}400)(0.667)}\left[\frac{1}{\left(\frac{S}{S_{min}}\right)^5}\right] = \frac{0.84375}{\left(\frac{S}{S_{min}}\right)^5} \qquad (3)$$

With a solvent rate in the underflow of 1,600 kg/h, the carbonate leaving in the underflow is 1,600 X_5. Therefore, the carbonate leaving in the final overflow (extract) = F_B - 1,600 X_5 = 1,350 - 1,600 X_5.

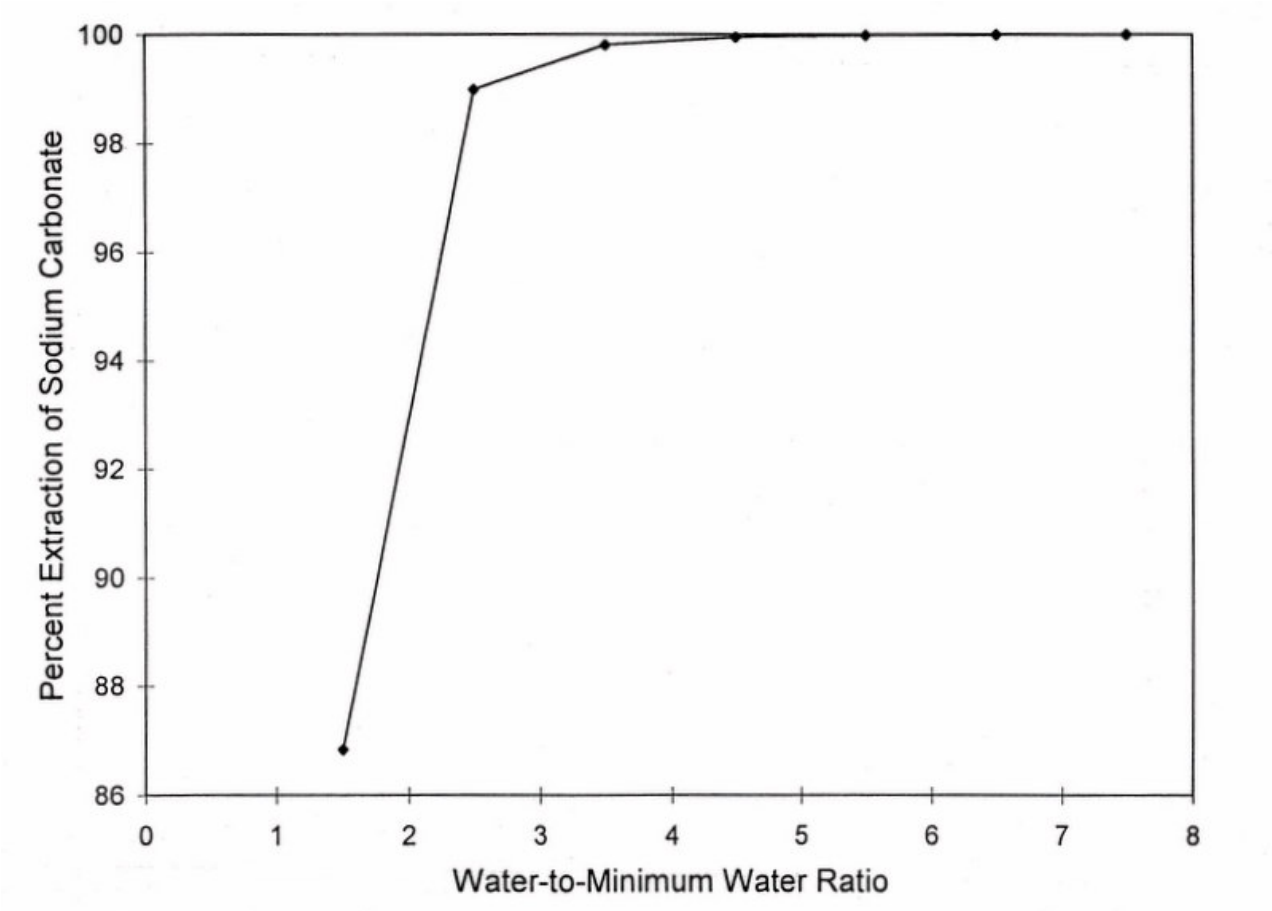
The percent extraction = $$\left(\frac{1{,}350 - 1{,}600X_5}{1{,}350}\right) \times 100\% \qquad (4)$$

Exercise 5.5 (continued)

Analysis: (continued)

Solving Eqs. (3) and (4), the following results are obtained:

S/S_{min}	X_5	% Recovery
1.5	0.1111	86.83
2.5	0.00864	98.98
3.5	0.001607	99.81
4.5	0.0004573	99.95
5.5	0.0001676	99.98
6.5	0.00007272	99.99
7.5	0.00003556	99.996



Exercise 5.6

Subject: Recovery of $Al_2(SO_4)_3$ from bauxite ore by reaction of Al_2O_3 with sulfuric acid followed by three-stage countercurrent washing with water, with the flowsheet below

Given: 40,000 kg/day of bauxite ore containing 50 wt% Al_2O_3 and 50 wt% inert.Stoichiometric amount of 50 wt% aqueous H_2SO_4 to convert the Al_2O_3 to $Al_2(SO_4)$

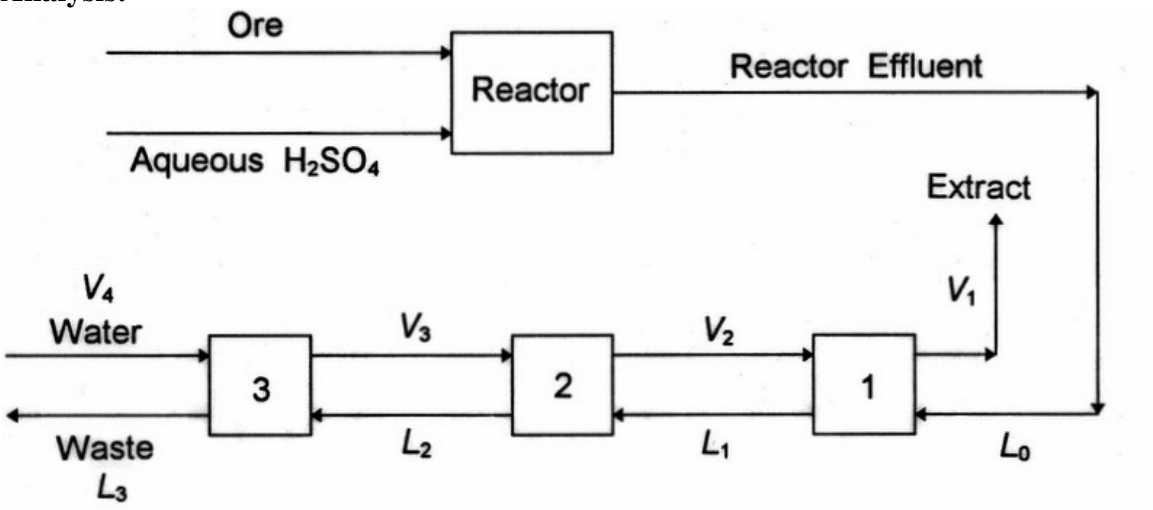
by the reaction: $Al_2O_3 + 3\ H_2SO_4 = Al_2(SO_4)_3 + 3H_2O$ (1)

S = 240,000 kg/day of water to extract the sulfate in three countercurrent washing stages. Underflow from each washing stage contains 1 kg of water/kg of insoluble inert.

Assumptions: Equilibrium washing stages where, for each stage, the weight fraction of sulfate in the overflow equals that in the underflow liquid. No solids in the overflows. Reaction of oxide with sulfuric acid is complete.

Find: Flow rates in kg/day of sulfate, water, and inert solid in each product stream. Percent recovery of sulfate. Effect of adding one more stage.

Analysis:



In Eq. (1), the molecular weights from left to right are 101.96, 98.082, 342.158, and 18.016.
Therefore, the yield of sulfate = 0.50(40,000)(342.158)/101.96 = 67,116 kg/day.
Water leaving the reactor = water entering with the sulfuric acid + water from the reaction.
Sulfuric acid entering the reactor = 0.50(40,000)(3)(98.082)/101.96 = 57,718 kg/day.
Same amount of water, 57,718 kg/day, enters the reactor.

Exercise 5.6 (continued)

Analysis: (continued)

Water from the reaction = 0.50(40,000)(3)(18.016)/101.96 = 10,602 kg/day.
Total water leaving reactor and entering Stage 1 = 57,718 + 10,602 = 68,320 kg/day = L_0

Inert solid leaving reactor = 0.5(40,000) = 20,000 kg/day.

For the three-section washing cascade shown above, reactor effluent enters Stage 1 at a liquid rate of 68,320 + 67,116 = 135,436 kg/day and an inert solids rate of 20,000 kg/day.

Water solvent enters Stage 3 at a rate, S, of 240,000 kg/day. Let $L_1 = L_2 = L_3$ = water leaving in each underflow, which equals the inert solids rate or 20,000 kg/day. Let V_i = water rate in overflow from Stage i. Water material balances around Stages 2 and 3 give, respectively, $V_3 = V_2$ =240,000 kg/day. The water balance around Stage 1 is:

$$L_0 + V_2 = L_1 + V_1 \quad \text{or} \quad 68{,}320 + 240{,}000 = 20{,}000 + V_1$$

Solving, V_1 = 288,320 kg/day

Because the underflow liquid rates are constant in water, rather than water plus dissolved sulfate, it is preferable to work with mass ratios of sulfate to water, instead of sulfate mass fractions.

Sulfate material balances around Stages 1, 2, and 3, respectively, in terms of mass ratios,

Y_i = kg dissolved $Al_2(SO_4)_3$ / kg H_2O in overflow from Stage i

X_i = kg dissolved $Al_2(SO_4)_3$ / kg H_2O in underflow from Stage i

are:

$$67{,}116 + 240{,}000Y_2 = 20{,}000X_1 + 288{,}320Y_1 \qquad (2)$$

$$20{,}000X_1 + 240{,}000Y_3 = 20{,}000X_2 + 240{,}000Y_2 \qquad (3)$$

$$20{,}000X_2 = 20{,}000X_3 + 240{,}000Y_3 \qquad (4)$$

From equilibrium at each stage for the leaving liquids,

$$Y_1 = X_1 \qquad Y_2 = X_2 \qquad Y_3 = X_3 \qquad (5, 6, 7)$$

Solving the six linear equations, (2) through (7), we obtain:

$$Y_1 = X_1 = 0.2327 \qquad Y_2 = X_2 = 0.01927 \qquad Y_3 = X_3 = 0.001482$$

Sulfate in the final extract = V_1Y_1 = 288,320(0.2327) = 67,092 kg/day

The overall material balance for flow rates in kg/day is:

Component	Bauxite ore	Acid	Reactor effluent	Solvent	Final Extract	Waste
Al_2O_3 solid	20,000					
Inert solid	20,000		20,000			20,000
H_2SO_4		57,718				
Dissolved $Al_2(SO_4)_3$			67,116		67,092	24
H_2O		57,718	68,320	240,000	288,320	20,000
Total:	40,000	115,436	155,436	240,000	355,412	40,024

Percent extraction of sulfate = (67,092/67,116) x 100% = 99.96%

Exercise 5.6 (continued)

Analysis: (continued)

If an additional stage is added, a sulfate material balance for Stage 4 is needed and eight equations in eight unknowns are solved to give $Y_1 = X_1 = 0.23277$.

The percent extraction of sulfate now = (288,320)(0.23277)/67,116 x 100% = 99.996%.

For the small additional recovery of sulfate (only 20 kg/day out of 67,116 kg/day), it is doubtful that an additional stage could be justified.

Exercise 5.7

Subject: Efficient rinsing of clothes in a washing machine

Given: Fixed amount of rinse water.

Assumptions: Perfect mixing such that the concentration of soluble dirt in water adhering to the clothes (underflow) is equal to that in the discharged water (overflow).

Find: (a) Whether the rinse water should be divided into two rinses.
(b) Devise an efficient machine cycle.

Analysis: Use the nomenclature of Section 5.2, letting:

F_A = mass of dry insoluble clothing
F_B = mass of soluble dirt.
S = mass of rinse water
Y = mass of soluble dirt/mass of overflow water
X = mass of soluble dirt/mass of underflow water
R = mass of water/mass of insoluble clothing in the underflow

(a) For one rinsing stage, a material balance on soluble dirt gives,

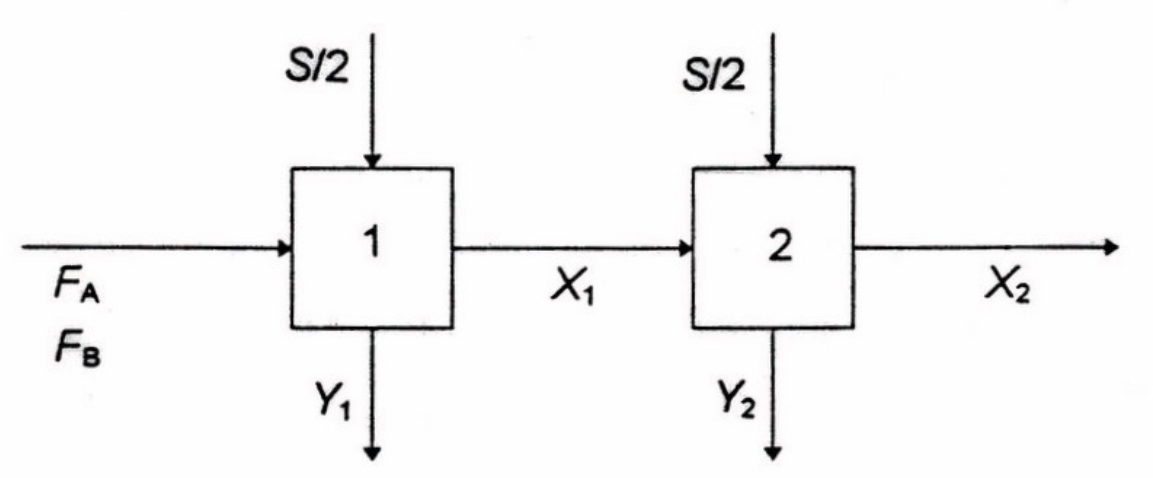
$$F_B = XRF_A + Y(S - RF_A) \quad (1)$$

For equilibrium between overflow and underflow liquids, $Y = X$ (2)

Combining Eqs. (1) and (2), $X = Y = F_B/S$ (3)

Mass of solids still left in liquid adhering to the clothes = $XRF_A = F_BRF_B/S$

Consider two crossflow rinsing stages, as shown in the diagram below, where the rinse water to each stage is 50% of the total rinse water of $S/2$.



A soluble dirt material balance around Stage 1, with $X_1 = Y_1$ gives,

$$F_B = X_1RF_A + Y_1(S/2 - RF_A) = Y_1S/2 \quad (4)$$

Solving, $$Y_1 = X_1 = 2F_B/S \quad (5)$$

Exercise 5.7 (continued)

Analysis: (a) (continued)

The underflow sent to Stage 2 is $X_1RF_A = 2F_BRF_A/S$
A similar material balance around Stage 2, with $X_2 = Y_2$, gives,

$$2F_BRF_A/S = Y_2(S/2 - RF_A) + X_2RF_A = X_2S/2 \qquad (6)$$

Solving, $Y_2 = X_2 = 4F_BRF_A/S^2$

The mass of solubles still left in the underflow from Stage 2 = $X_2RF_A = 4F_B(RF_A)^2/S^2$
The ratio of the mass of soluble dirt in the final underflow for two stages to that for one stage is,

$$\frac{\dfrac{4F_B\left(RF_A\right)^2}{S^2}}{\dfrac{F_BRF_A}{S}} = \frac{4RF_A}{S}$$

It is highly likely that the rinsing will be such that the amount of rinse water used, S, will be much greater than the amount of water, RF_A, that adheres to the clothing leaving in the underflow.
Therefore, $S >> 4\ RF_A$ and two stages of rinsing is much better than one stage.

(b) A possible clothes washing cycle for efficient use of rinse water might be as follows:

Put clothes and detergent in tub..
Fill tub with water.
Agitate.
Spin to small value of R.

Fill tub with half of the rinse water.
Agitate.
Spin to small value of R.

Fill tub with other half of the rinse water.
Agitate.
Spin to small value of R.

Remove damp clothes and put into dryer.

Exercise 5.8

Subject: Liquid-liquid extraction of acetic acid (B) from water (A) using chloroform (C).

Given: Q = 10 liters of aqueous solution with 6 moles of acetic acid per liter. S = 10 liters of chloroform solvent. Extraction at 25°C with a distribution coefficient,

$$K''_{D_B} = \frac{(c_B)_C}{(c_B)_A} = 2.8 \qquad (1)$$

where concentrations are in moles/liter.

Assumptions: Water is insoluble in chloroform. Chloroform is insoluble in water. Equilibrium is achieved in each stage. No change in volumes of feed and solvent as acid transfers from feed to the solvent.

Find: Percent extraction of acid for:

(a) One stage.

(b) Three stages (crosscurrent) with one-third of solvent to each stage.

(c) Three stages (crosscurrent) with 5 liters of solvent to Stage 1, 3 liters to Stage 2, and 2 liters to Stage 3.

Analysis: To simplify the nomenclature, let:

$K = K''_{D_B}$ $\quad y = (c_B)_C$ $\quad x = (c_B)_A$

Thus, from Eq. (1) $y = Kx = 2.8x$ (2)

(a) For one stage, the acid material balance is,

$$x_F Q = y_1 S + x_1 Q \quad \text{or} \quad (6)(10) = 60 = y_1 10 + x_1 10 \qquad (3)$$

Combining Eqs. (2) and (3), y_1 = 4.42 mol/L, x_1 = 1.58 mol/L

% extracted = $y_1 S / x_F Q$ x 100% = (4.42)(10)/(6)(10) x 100% = 73.7%

(b) For three crosscurrent stages, can use Eq. (5-21) in the following form,

$$\frac{x_3}{x_F} = \frac{1}{(1 + E/N)^3} \qquad (4)$$

where from Eq. (5-14), $E = KS/Q$ = (2.8)(10)/10 = 2.8 and N = 3.

Therefore, from Eq. (4),

$$\text{Percent extraction} = \left(1 - \frac{x_3}{x_F}\right) \times 100\% = \left(1 - \frac{1}{(1 + 2.8/3)^3}\right) \times 100\% = 86.2\%$$

Exercise 5.8 (continued)

(c) Use Eq. (5-13) one stage at a time,

where from Eq. (5-14), $E_i = KS_i/Q = (2.8)S_i/10 = 0.28\ S_i$

For Stage 1, $S_1 = 5$ L, $E_1 = 1.4$, and $x_1 = x_F[1/(1+E_1)] = 6[1/(1+1.4)] = 2.5$ mol/L

For Stage 2, $S_2 = 3$ L, $E_2 = 0.84$, and $x_2 = x_1[1/(1+E_2)] = 2.5[1/(1+0.84)] = 1.36$ mol/L

For Stage 3, $S_3 = 2$ L, $E_3 = 0.56$, and $x_3 = x_2[1/(1+E_3)] = 1.36[1/(1+0.56)] = 0.872$ mol/L

Percent extraction = (6 - 0.872)/6 x 100% = 85.5%, just slightly lower than in Part (b).

Exercise 5.9

Subject: Liquid-liquid extraction of uranyl nitrate (UN) from water (W) with tributyl phosphate (TBP)

Given: 100 grams of 20 wt% UN in water. Thus, $F_W = 80$ g .

Assumptions: Equilibrium batch contacts. W and TBP are mutually insoluble.

Distribution coefficient is given in the form of Eq. (5-15): $K'_{D_{UN}} = \dfrac{Y_{UN}}{X_{UN}} = 5.5$ (1)

Find: Grams of TBP solvent needed to extract 90% of the UN by the following schemes:

(a) One stage
(b) Two crosscurrent stages with 50% of solvent to each stage.
(c) Two countercurrent stages.
(d) Infinite number of crosscurrent stages.
(e) Infinite number of countercurrent stages.

Analysis: Let: $K = K'_{D_{UN}}$ $X^{(i)} = X_{UN}$ in aqueous liquid leaving Stage i

$Y^{(i)} = Y_{UN}$ in TBP liquid leaving Stage i

From Eq. (5-14), the extraction factor = $E = KS/F_W = 5.5S/80 = 0.0688S$

For 90% extraction, $X^{(N)}/X^{(F)} = 1 - 0.90 = 0.10$.

(a) For a single stage, using Eq. (5-13),

$$\frac{X^{(1)}}{X^{(F)}} = 0.10 = \frac{1}{1+E} = \frac{1}{1+0.0688S} \qquad (2)$$

Solving Eq. (2), $S = 130.8$ g of TBP.

(b) For two crosscurrent stages with equal solvent additions, where S = total solvent, Eq. (5-21) applies:

$$\frac{X^{(2)}}{X^{(F)}} = 0.10 = \frac{1}{(1+E/2)^2} = \frac{1}{(1+0.0688S/2)^2} \qquad (3)$$

Solving Eq. (3), $S = 62.9$ g of TBP.

Exercise 5.9 (continued)

Analysis (continued):

(c) For two countercurrent stages, Eq. (5-28) applies:

$$\frac{X^{(2)}}{X^{(F)}} = 0.10 = \frac{1}{\left(1 + E + E^2\right)} = \frac{1}{\left[1 + 0.0688S + \left(0.0688S\right)^2\right]} \qquad (4)$$

Solving Eq. (4), S = 36.9 g of TBP.

(d) For an infinite number of crosscurrent stages, Eq. (5-23) applies:

$$\frac{X^{(\infty)}}{X^{(F)}} = 0.10 = \frac{1}{\exp E} = \frac{1}{\exp(0.0688S)} \qquad (5)$$

Solving Eq. (5), S = 33.5 g of TBP.

(e) For an infinite number of countercurrent stages, if $E < 1$, Eq. (5-32) applies:

$$X^{(\infty)} / X^{(F)} = 0.10 = 1 - E = 1 - 0.0688S$$

Solving, S = 13.1 g of TBP

Exercise 5.10

Subject: Liquid-liquid extraction of uranyl nitrate (UN) from water (W) with tributyl phosphate (TBP)

Given: 2 kg of 20 wt% UN in water. Thus, F_W =1.6 kg. S = 0.5 kg of TBP.

Assumptions: Equilibrium batch contacts. W and TBP are mutually insoluble.

Distribution coefficient is given in the form of Eq. (5-15): $K'_{D_{UN}} = \dfrac{Y_{UN}}{X_{UN}} = 5.5$ (1)

Find: Percent recovery of UN for:

(a) Two-stage batch extraction.
(b) Three batch extractions.
(c) Two-stage cocurrent extraction.
(d) Three-stage countercurrent extraction.
(e) Infinite-stage countercurrent extraction.
(f) Infinite-stage crosscurrent extraction.

Analysis: Let: $K = K'_{D_{UN}}$ $X^{(i)} = X_{UN}$ in aqueous liquid leaving Stage i

$Y^{(i)} = Y_{UN}$ in TBP liquid leaving Stage i

From Eq. (5-14), the extraction factor = $E = KS/F_W$ = 5.5(0.5)/1.6 = 1.72

(a) For a single stage, using Eq. (5-13),

$$\frac{X^{(1)}}{X^{(F)}} = \frac{1}{1+E} = \frac{1}{1+1.72} = 0.368 \qquad (2)$$

% extraction = (1 - 0.368) x 100% = 63.2%

(b) Three batch extractions is equivalent to a crosscurrent arrangement with equal solvent additions, where S = total solvent. Eq. (5-21) applies:

$$\frac{X^{(3)}}{X^{(F)}} = \frac{1}{\left(1+E/3\right)^3} = \frac{1}{\left(1+1.72/3\right)^3} = 0.257 \qquad (3)$$

% extraction = (1 - 0.257) x 100% = 74.3%

(c) Two-stage cocurrent is same as one stage. Therefore, % extraction = 63.2%.

Exercise 5.10 (continued)

Analysis (continued):

(d) For three-stage countercurrent extraction, Eq. (5-28) applies:

$$\frac{X^{(3)}}{X^{(F)}} = \frac{1}{\left(1 + E + E^2 + E^3\right)} = \frac{1}{\left[1 + 1.72 + 1.72^2 + 1.72^3\right]} = 0.093 \qquad (4)$$

% extraction = (1 - 0.093) x 100% = 90.7%

(e) For infinite-stage countercurrent extraction, because $E > 1$, Eq. (5-31) applies.

Therefore, $X^{(\infty)} / X^{(F)} = 0.0$ and % extraction = 100%

(f) For infinite-stage crosscurrent extraction, Eq. (5-23) applies:

$$\frac{X^{(\infty)}}{X^{(F)}} = \frac{1}{\exp E} = \frac{1}{\exp(1.72)} = 0.179 \qquad (5)$$

% extraction = (1 - 0.179) x 100% = 82.1%

Exercise 5.11

Subject: Liquid-liquid extraction of dioxane (B) from water (A) with benzene (C).

Given: 1,000 kg of 30 wt% B in A. Thus, F_A = 700 kg .

Assumptions: Equilibrium batch contacts. A and C are mutually insoluble.
Distribution coefficient from Example 5.2, in the form of Eq. (5-15) is:

$$K'_{D_B} = \frac{Y_B}{X_B} = 1.2 \qquad (1)$$

Find: S = kg of C needed to extract 95% of the dioxane by the following schemes:
(a) One stage
(b) Two crosscurrent stages with 50% of solvent to each stage.
(c) Two countercurrent stages.
(d) Infinite number of crosscurrent stages.
(e) Infinite number of countercurrent stages.

Analysis: Let: $K = K'_{D_B}$ $X^{(i)} = X_B$ in aqueous liquid leaving Stage i
$Y^{(i)} = Y_B$ in benzene liquid leaving Stage i

From Eq. (5-14), the extraction factor = $E = KS/F_A = 1.2S/700 = 0.001714S$

For 95% extraction, $X^{(N)}/X^{(F)} = 1 - 0.95 = 0.05$.

(a) For a single stage, using Eq. (5-13),

$$\frac{X^{(1)}}{X^{(F)}} = 0.05 = \frac{1}{1+E} = \frac{1}{1+0.001714S} \qquad (2)$$

Solving Eq. (2), S = 11,090 kg of benzene.

(b) For two crosscurrent stages with equal solvent additions, where S = total solvent, Eq. (5-21) applies:

$$\frac{X^{(2)}}{X^{(F)}} = 0.05 = \frac{1}{(1+E/2)^2} = \frac{1}{(1+0.001714S/2)^2} \qquad (3)$$

Solving Eq. (3), S = 4,050 kg of benzene.

Exercise 5.11 (continued)

Analysis (continued):

(c) For two countercurrent stages, Eq. (5-28) applies:

$$\frac{X^{(2)}}{X^{(F)}} = 0.05 = \frac{1}{\left(1 + E + E^2\right)} = \frac{1}{\left[1 + 0.001714S + \left(0.001714S\right)^2\right]} \qquad (4)$$

Solving Eq. (4), S = 2,270 kg of benzene.

(d) For an infinite number of crosscurrent stages, Eq. (5-23) applies:

$$\frac{X^{(\infty)}}{X^{(F)}} = 0.05 = \frac{1}{\exp E} = \frac{1}{\exp(0.001714S)} \qquad (5)$$

Solving Eq. (5), S = 1,748 kg of benzene

(e) For an infinite number of countercurrent stages, if $E < 1$, Eq. (5-32) applies:

$$X^{(\infty)} / X^{(F)} = 0.05 = 1 - E = 1 - 0.001714S$$

Solving, S = 554 kg of benzene

Exercise 5.12

Subject: Liquid-liquid extraction of benzoic acid (B) from water (A) using chloroform (C).

Given: Q = 1,000 L/h of aqueous waste containing 0.05 mol/L of B. S = 500 L/h of chloroform solvent. Extraction with a distribution coefficient,

$$K''_{D_B} = \frac{(c_B)_C}{(c_B)_A} = 4.2 \qquad (1)$$

where concentrations are in mol/L.

Assumptions: Water is insoluble in chloroform. Chloroform is insoluble in water. Equilibrium is achieved in each stage. No change in volumes of feed and solvent as acid transfers from feed to the solvent.

Find: Percent extraction of acid for:

(a) One stage.
(b) Three crosscurrent stages with one-third of solvent to each stage.
(c) Three countercurrent stages.

Analysis: To simplify the nomenclature, let:

$K = K''_{D_B}$ $\quad y = (c_B)_C$ $\quad x = (c_B)_A$

Thus, from Eq. (1) $y = Kx = 4.2x$ (2)

(a) For one stage, the acid material balance is,

$x_F Q = y_1 S + x_1 Q$ or $(0.05)(1{,}000) = 50 = y_1 500 + x_1 1{,}000$ (3)

Combining Eqs. (2) and (3), y_1 = 0.0672 mol/L, x_1 = 0.016 mol/L

% extracted = $y_1 S / x_F Q$ x 100% = (0.0672)(500)/(0.05)(1,000) x 100% = 67.2%

(b) For three crosscurrent stages, can use Eq. (5-21) in the following form,

$$\frac{x_3}{x_F} = \frac{1}{(1 + E/N)^3} \qquad (4)$$

where from Eq. (5-14), $E = KS/Q$ = (4.2)(500)/1,000 = 2.1 and N = 3. Frm Eq. (4),

$$\text{Percent extraction} = \left(1 - \frac{x_3}{x_F}\right) \times 100\% = \left(1 - \frac{1}{(1 + 2.1/3)^3}\right) \times 100\% = 79.6\%$$

(c)) For three-stage countercurrent extraction, Eq. (5-28) applies in the form,

$$\frac{x_3}{x_F} = \frac{1}{(1 + E + E^2 + E^3)} = \frac{1}{[1 + 2.1 + 2.1^2 + 2.1^3]} = 0.058 \qquad (5)$$

% extraction = (1 - 0.058) x 100% = 94.2%

Exercise 5.13

Subject: Extraction of p-dioxane (B) from water (A) with solvent (C).

Given: Extraction factor, $E = 0.9$ compared to 2.4 in Example 5.2.

Assumptions: Water and solvent are mutually insoluble. Equilibrium stages.

Find: The effect on % extraction of the number and configuration of stages.

Analysis: For a single stage and the cocurrent arrangement with any number of stages, N, Eq. (5-13) applies, where the B subscript has been dropped:

$$\frac{X^{(N)}}{X^{(F)}} = \frac{1}{1+E} = \frac{1}{1+0.9} = 0.526$$

Therefore, the % extraction = (1 - 0.526) x 100% = 47.4% for any number of cocurrent stages.

For a crosscurrent cascade, Eq. (5-21) applies:

$$\frac{X^{(N)}}{X^{(F)}} = \frac{1}{(1+E/N)^N} = \frac{1}{(1+0.9/N)^N} \qquad (1)$$

For a countercurrent cascade, Eq. (5-29) applies:

$$\frac{X^{(N)}}{X^{(F)}} = \frac{1}{\sum_{n=0}^{N} E^n} = \frac{1}{\sum_{n=0}^{N} 0.9^n} \qquad (2)$$

Results from Eqs. (1) and (2) are used to calculate % extraction from:

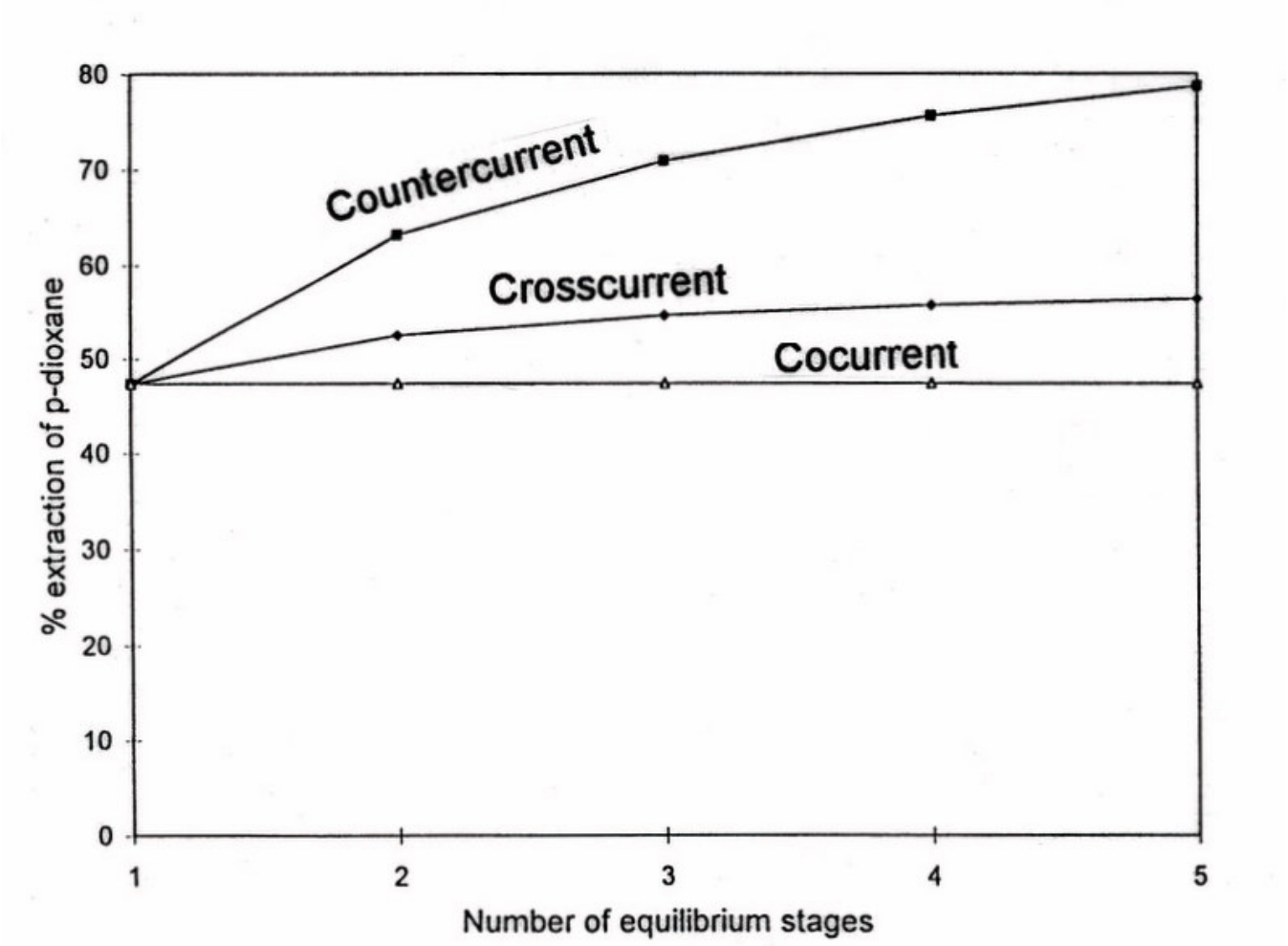
$$\%\ \text{extraction} = \left(1 - \frac{X^{(N)}}{X^{(F)}}\right) \times 100\% \qquad (3)$$

Using Eqs. (1) to (3), the following results are obtained:

N	% extraction, crosscurrent	% extraction, countercurrent
2	52.4	63.1
3	54.5	70.9
4	55.6	75.6
5	56.3	78.7

Exercise 5.13 (continued)

We see that for $E < 1$, the % extraction increases only slowly with increasing number of stages. It is desirable to have the situation where $E > 1$.



Exercise 5.14

Subject: Multistage absorption of a hydrocarbon gas with a high-molecular-weight oil.

Given: Hydrocarbon feed gas and absorbent oil of Example 5.3 in Fig. 5.11. Absorber pressure of 400 psia and average temperature of 97.5°F, with *K*-values at these conditions.

Assumptions: Applicability of Kremser's method.

Find: % absorption of components and total gas and % stripping of oil for N = 1, 3, 10, and 30 equilibrium stages. Effect of N on each component.

Analysis: The same values of the absorption factors, A, and stripping factors, S, apply. Also Eqs. (5-48) and (5-50) are used to compute the fractions not absorbed, ϕ_A, and not stripped, ϕ_B, respectively. Then Eq. (5-54) is used to compute the component flow rates in the exit vapor. Then an overall material balance is used to compute the component flow rates in the exit liquid:

$$l_N = l_0 + v_{N+1} - v_1$$

Let the % absorption of a component in the entering gas = $\left[l_N / \left(l_0 + v_{N+1}\right)\right] \times 100\%$

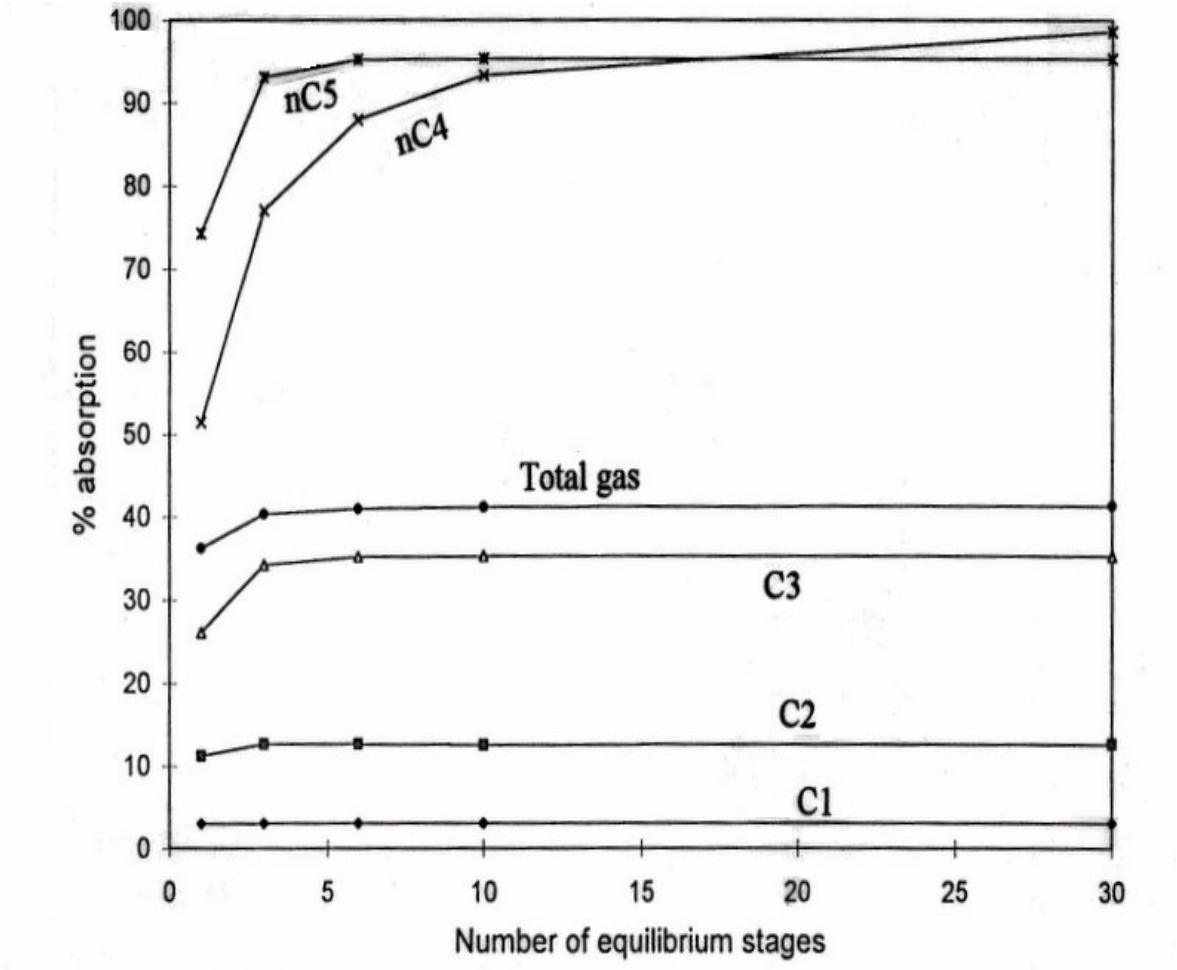
The % stripping of the oil in the absorbent = $\left[\left(v_1\right)_{\text{oil}} / \left(l_0\right)_{\text{oil}}\right] \times 100\%$

Using a spreadsheet, the following results are obtained for the % absorption of C_1, C_2, C_3, nC_4, and nC_5, the total % absorption of these light hydrocarbons, and % stripping of oil.

N	C_1	C_2	C_3	nC_4	nC_5	Total Gas	oil
1	3.01	11.19	26.09	51.46	74.29	36.26	0.05
3	3.10	12.58	34.28	77.04	93.08	40.32	0.05
6	3.10	12.60	35.26	87.94	95.24	40.98	0.05
10	3.10	12.50	35.30	93.34	95.33	41.15	0.05
30	3.10	12.60	35.30	98.64	95.33	41.33	0.05

Additional stages have little effect on the absorption of C_1, C_2, and C_3 because their absorption factors are less than one.

Exercise 5.14 (continued)



Exercise 5.15

Subject: Multistage absorption of a hydrocarbon gas with a high-molecular-weight oil.

Given: Hydrocarbon feed gas and absorbent oil of Example 5.3 in Fig. 5.11. Absorber pressure of 400 psia and average temperature of 97.5°F, with *K*-values at these conditions.

Find: Material balance for absorbent rate of 330 lbmol/h instead of the 165 lbmol/h and 3 stages instead of the 6 in Example 5.3. Compare results with Example 5.3 and discuss effect of trading stages for absorbent flow rate.

Analysis: With two times the absorbent rate of Example 5.3, double the absorption factors and halve the stripping factors given in Example 5.3. Then, using the same procedure as in that example, the following results are obtained and compared.

	$N = 3$ and $L_0 = 330$ lbmol/h:		$N = 6$ and $L_0 = 165$ lbmol/h:	
Component	v_1 **, lbmol/h**	l_3 **, lbmol/h**	v_1 **, lbmol/h**	l_6 **, lbmol/h**
C_1	150.1	9.9	155.0	5.0
C_2	278.1	91.9	323.5	46.5
C_3	93.8	146.2	155.4	84.6
nC_4	1.5	23.6	3.0	22.0
nC_5	0.3	6.3	0.3	5.5
Oil	0.1	328.3	0.1	164.1
Total	523.9	606.2	637.3	327.7

The results show that considerably more absorption takes place when the absorbent rate is doubled and the number of stages is halved.

Exercise 5.16

Subject: Multistage absorption of a hydrocarbon gas with a high-molecular-weight oil.

Given: Hydrocarbon feed gas and absorbent oil of Example 5.3 in Fig. 5.11. Absorber pressure of 400 psia and average temperature of 97.5°F, with *K*-values at these conditions.

Find: Minimum absorbent rate to reduce the propane flow rate to 155.4 lbmol/h in exit vapor.

Analysis: The minimum absorbent rate corresponds to $N = \infty$. Use Eq. (5-48) to obtain the absorption factor, $A = L/KV$, needed for propane. Because A for propane < 1 for $N = 6$, it will be < 1 for $N = \infty$, since the absorbent rate, L, will be lower. From Eq. (5-48),

Fraction of propane not absorbed = 155.4/240 = 0.648 = $\phi_A = (A - 1)/(A^{N+1} - 1)$

When $A < 1$, $A^{N+1} = 0$, therefore, Eq. (5-48) reduces to:

$$A = 1 - \phi_A = 1 - 0.648 = 0.352$$

From Eq. (5-38), $L = AKV = 0.352(0.584)(800) =$ 165 lbmol/h = minimum rate

This is the same L as in Example 5.3 because for $\phi_A >$ about 0.5, N above 5 has no effect on A.

Exercise 5.17

Subject: Multistage absorption of a hydrocarbon gas with a high-molecular-weight oil.

Given: Hydrocarbon feed gas and absorbent oil of Example 5.3 in Fig. 5.11. Absorber pressure of 400 psia and isothermal operation with $N = 6$ equilibrium stages at:

(a) 125°F.
(b) 150°F.

Assumptions: Applicability of Kremser's method.

Find: % absorption of components and % stripping of oil.

Analysis: From Fig. 2.8, the following *K*-values are obtained, where for methane, the oil is assumed to have a MW of 300. The *K*-values for the absorbent oil are rough guesses. The values are compared to those in Example 5.3.

***K*-values at 400 psia:**

Component	T = 97.5F	T = 125°F	T = 150°F
C_1	6.65	8.0	8.8
C_2	1.64	2.0	2.4
C_3	0.584	0.73	0.90
nC_4	0.195	0.26	0.34
nC_5	0.0713	0.098	0.135
Oil	0.0001	0.0002	0.0003

Absorption and stripping factors are obtained with Eqs. (5-38) and (5-51), respectively, using the above *K*-values with the entering vapor and liquid flow rates.
Using the same procedure as in Example 5.3 and letting:

The % absorption of a component in the entering gas = $\left[l_N / (l_0 + v_{N+1})\right] \times 100\%$

The % stripping of the oil in the absorbent = $\left[(v_1)_{\text{oil}} / (l_0)_{\text{oil}}\right] \times 100\%$

The following results are obtained and compared with those of Example 5.3.

% absorption for $N = 6$ stages at 400 psia:

Component	T = 97.5F	T = 125°F	T = 150°F
C_1	3.10	2.58	2.34
C_2	12.60	10.31	8.59
C_3	35.26	28.24	22.91
nC_4	87.94	74.09	59.32
nC_5	95.24	93.08	88.93
Oil	0.05	0.10	0.15

These results show that increasing temperature decreases the % absorption of gaseous components and increases the % stripping of the absorbent.

Exercise 5.18

Subject: Multistage absorption of a light-hydrocarbon gas mixture with n-heptane.

Given: V_{N+1} = 1,000,000 lbmol/day of feed gas containing in mole %, C_1 94.9, C_2 4.2, C_3 0.7, nC_4 0.1, nC_5 0.1. Absorption at 550 psia and -30°F with N = 10 equilibrium stages and K-values below.

Assumptions: Applicability of Kremser's method.

Find: Absorbent flow rate, L_0 , and component distribution for 50% absorption of C_2.

Analysis: From Eq. (5-48), $\phi_{A_{C_2}}$ = fraction of C_2 not absorbed = 0.50 = $\dfrac{A_{C_2}-1}{A_{C_2}^{N+1}-1}$

Solving and using Eq. (5-38), $A_{C_2} = 0.50 = \dfrac{L_0}{K_{C_2}V_{N+1}} = \dfrac{L_0}{(0.36)(1{,}000{,}000)}$

Therefore, L_0 = 0.50(0.36)(1,000,000) = 180,000 lbmol/day

To compute the distribution of the other components,i, between products V_1 and L_{10} , compute $A_i = L_0/K_iV_{N+1}$ and ϕ_A for i from Eq. (5-48). Then Eq. (5-54) is used to compute the component flow rates in the exit vapor. Then an overall material balance is used to compute the component flow rates in the exit liquid:

$$l_N = l_0 + v_{N+1} - v_1$$

The results are as follows, using a spreadsheet:

				Flow rates, lbmol/day:		
Component	***K*-value**	***A***	**ϕ_A**	**$v_{n+1} = v_{11}$**	**v_1**	**l_{10}**
C_1	2.85	0.063	0.937	949,000	889,200	59,800
C_2	0.36	0.50	0.500	42,000	21,000	21,000
C_3	0.066	2.73	0.0000276	7,000	0.2	6,999.8
nC_4	0.017	10.59	0	1,000	0	1,000
nC_5	0.004	45.0	0	1,000	0	1,000

Exercise 5.19

Subject: Stripping of a hydrocarbon liquid with steam at 50 psia and 300°F.

Given: In Fig. 5.8(b), L_{N+1} = 1,000 kmol/h of 0.03% C_1, 0.22% C_2, 1.82% C_3, 4.47% nC_4, 8.59 nC_5, and 84.87% nC_{10}, in mol%. V_0 = 1,000 kmol/h of superheated steam. Stripper with N = 3 equilibrium stages. K-value for nC_{10} = 0.20. Other K-values from Fig. 2.8.

Assumptions: Applicability of Kremser's equation. Negligible absorption of steam.

Find: Compositions and flow rates of exiting stripped liquid and rich gas. Dew point.

Analysis: For a stripper, Eq. (5-55) applies, which for no hydrocarbons in the entering steam simplifies to:

$$l_1 = l_{N+1}\,\phi_S \qquad (1)$$

where, from Eq. (5-50),

$$\phi_S = \frac{S-1}{S^{N+1}-1} = \frac{S-1}{S^4-1} \qquad (2)$$

where, from Eq. (5-53),

$$S = KV/L = KV_0/L_{N+1} = K(1{,}000)/(1{,}000) = K \qquad (3)$$

By overall material balance,

$$v_N = l_{N+1} + v_0 - l_1 \qquad (4)$$

The results from applying the above equations with a spreadsheet are as follows:

			Flow rates, kmol/h:		
Component	$K_i = S$	ϕ_S	$l_{N+1} = l$ in	$l_i = l$ out	$v_N = v$ out
C_1	60	0	0.3	0.0	0.3
C_2	28	0	2.2	0.0	2.2
C_3	14	0	18.2	0.0	18.2
nC_4	6.5	0.003	44.7	0.1	44.6
nC_5	3.5	0.0168	85.9	1.4	84.5
nC_{10}	0.20	0.8013	848.7	680.0	168.7
Steam					1,000.0
Total			1,000.0	681.5	1,318.5

Now check the primary dew point. Partial pressure of steam in the exit vapor = $y_i P$ = (1,000)/(1,318.5) x 50 = 37.9 psia. Vapor pressure of water at 300°F = 67 psia. Therefore, steam will not condense. Now check the possibility of the HCs condensing.

No condensation if, for the HCs, from Eq. (4-13), $\sum_{HCs} \frac{y_i}{K_i} = \frac{1}{V}\sum_{HCs} \frac{v_i}{K_i} < 1.0$

Using the above table, this sum is:

$$\frac{1}{1{,}318.5}\left[\frac{0.3}{60}+\frac{2.2}{28}+\frac{18.2}{14}+\frac{44.6}{6.5}+\frac{84.5}{3.5}+\frac{168.7}{0.2}\right] = 0.0+0.0+0.001+0.005+0.018+0.640 = 0.664$$

Therefore, no condensation occurs. CHEMCAD computes a primary dew point of 287°F.

Exercise 5.20

Subject: Successive flash distillation as in Fig. 5.12

Given: Two multiple flash arrangements, one with no recycle and one with recycle.

Assumptions: Equilibrium at each flash stage.

Find: Cooling requirements if heaters in Stages 2 and 3 are removed, and if so whether system will produce the same products.

Analysis: Nothing is gained by totally condensing the vapor leaving each stage, followed by partial vaporization in the stage because equilibrium compositions depend only on the temperature and pressure. Therefore, remove a heater at a stage (2 or 3) and reduce the condenser duty on the vapor feed to that stage by the amount of the heater. Product compositions will be the same.

In Fig. 12(a), new duty of condenser feeding stage 2 = 734 - 487 = 247 MBH.
New duty of condenser feeding stage 3 = 483 - 376 = 107 MBH.

Save two heat exchangers and reduce the size of the two condensers.
Save total heating and cooling duties of 247 + 107 = 364 MBH.

In Fig. 12(b), new duty of condenser feeding stage 2 = 883 - 665 = 218 MBH.
New duty of condenser feeding stage 3 = 646 - 503 = 143 MBH.

Save two heat exchangers and reduce the size of the two condensers.
Save total heating and cooling duties of 218 + 143 = 361 MBH.

Exercise 5.21

Subject: Effect of reflux rate on key-component distribution in multicomponent distillation by the group method.

Given: Results in Example 5.4 for distillation at 400 psia of a superheated vapor feed at 105°F and containing, lbmol/h of 160 C_1, 370 C_2, 240 C_3, 25 nC_4, and 5 nC_5 in a column with a partial condenser, 5 equilibrium rectification stages, equilibrium feed stage, 5 equilibrium stripping stages, and a partial reboiler, for an external reflux rate of 1,000 lbmol/h.

Assumptions: No changes in stage temperatures when reflux rate is changed.

Find: Molar ratio of C_3 flow rate in the distillate to that in the bottoms, with a plot, for reflux rates of (a) 1,500, (b) 2,000, and (c) 2,500 lbmol/h.

Analysis: Using the Edmister group method, the ratio of *d* to *b* for any component is given by a rearrangement of Eq. (5-66),

$$\frac{d}{b} = \frac{1}{A_F} \frac{\left[\left(S_B \phi_{AX} + 1\right) / \phi_{SX}\right]}{\left[\left(A_C \phi_{SE} + 1\right) / \phi_{AE}\right]} \tag{1}$$

From Eq. (5-65),

$$A_F = L_F / K_F V_F \tag{2}$$

From Eq. (5-59),

$$A_C = L_C / K_C V_C = L_C / K_C D \tag{3}$$

From just below Eq. (5-64),

$$S_B = K_B V_B / L_B = K_B V_B / B \tag{4}$$

where values of K are assumed to be the same as for Example 5.4 because of the assumption of no change in stage temperatures. Thus, A_F, A_C, and S_B change only by changes in the reflux rate, which changes stagewise vapor and liquid rates as given below.

From Eqs. (5-48) and (5-50),

$$\phi_A = \frac{A - 1}{A^{N+1} - 1} \tag{5}$$

$$\phi_S = \frac{S - 1}{S^{N+1} - 1} \tag{6}$$

where $A = L/KV$ and $S = KV/L$.

Exercise 5.21 (continued)

Analysis: (continued)

In Eq. (1), ϕ_{AX} and ϕ_{SX} pertain to the stripping (exhauster)section,
ϕ_{AE} and ϕ_{SE} pertain to the rectifying (enricher) section,
Because the temperatures change over the stripping and rectifying sections, average absorption and stripping factors are used.

For all three cases, the new flow rates needed in the absorption and stripping factors are determined from the assumption of constant molar overflow, with the following results:

Flow rates, lbmol/h:

	L_0 = 1,000		(a) L_0 = 1,500		(b) L_0 = 2,000		(c) L_0 = 2,500	
Section	Vapor	Liquid	Vapor	Liquid	Vapor	Liquid	Vapor	Liquid
Condenser	530	1,000	530	1,500	530	2,000	530	2,500
Enricher	1,530	1,000	2,030	1,500	2,530	2,000	3,030	2,500
Feed	1,530	1,000	2,030	1,500	2,530	2,000	3,030	2,500
Exhauster	730	1,000	1,230	1,500	1,730	2,000	2,230	2,500
Reboiler	730	270	1,230	270	1,730	270	2,230	270

Assume that as with Example 5.4 and at higher reflux rates, components C_1, C_2, and nC_5 will not distribute to any extent. Therefore, make distribution calculations only for the component of interest, propane. Using the above flow rates for Cases (a), (b), and (c) , the absorption and stripping factors for C_3 with L_0 = 1,000 lbmol/h become as follows, where, for example, A_C for Case (a) is given from Eq. (3) by:

$$\left(A_C\right)_{\text{Case (a)}} = \frac{L_0}{DK_C} = \frac{L_0}{D\left[\dfrac{L_0}{A_C D}\right]_{\text{Example 5.4}}} = \frac{1{,}500}{530\left[\dfrac{1{,}000}{10.48(530)}\right]} = 15.72$$

Factor	L_0 = 1,000	(a) L_0 = 1,500	(b) L_0 = 2,000	(c) L_0 = 2,500
A_C	10.48	15.72	20.96	26.20
A_E	1.72	1.94	2.08	2.17
$S_E = 1/A_E$	0.581	0.515	0.481	0.461
A_F	1.108	1.250	1.340	1.397
A_X	1.73	1.54	1.46	1.416
$S_X = 1/A_X$	0.577	0.649	0.685	0.706
S_B	2.78	4.68	6.59	8.49

Exercise 5.21 (continued)

Analysis: (continued)

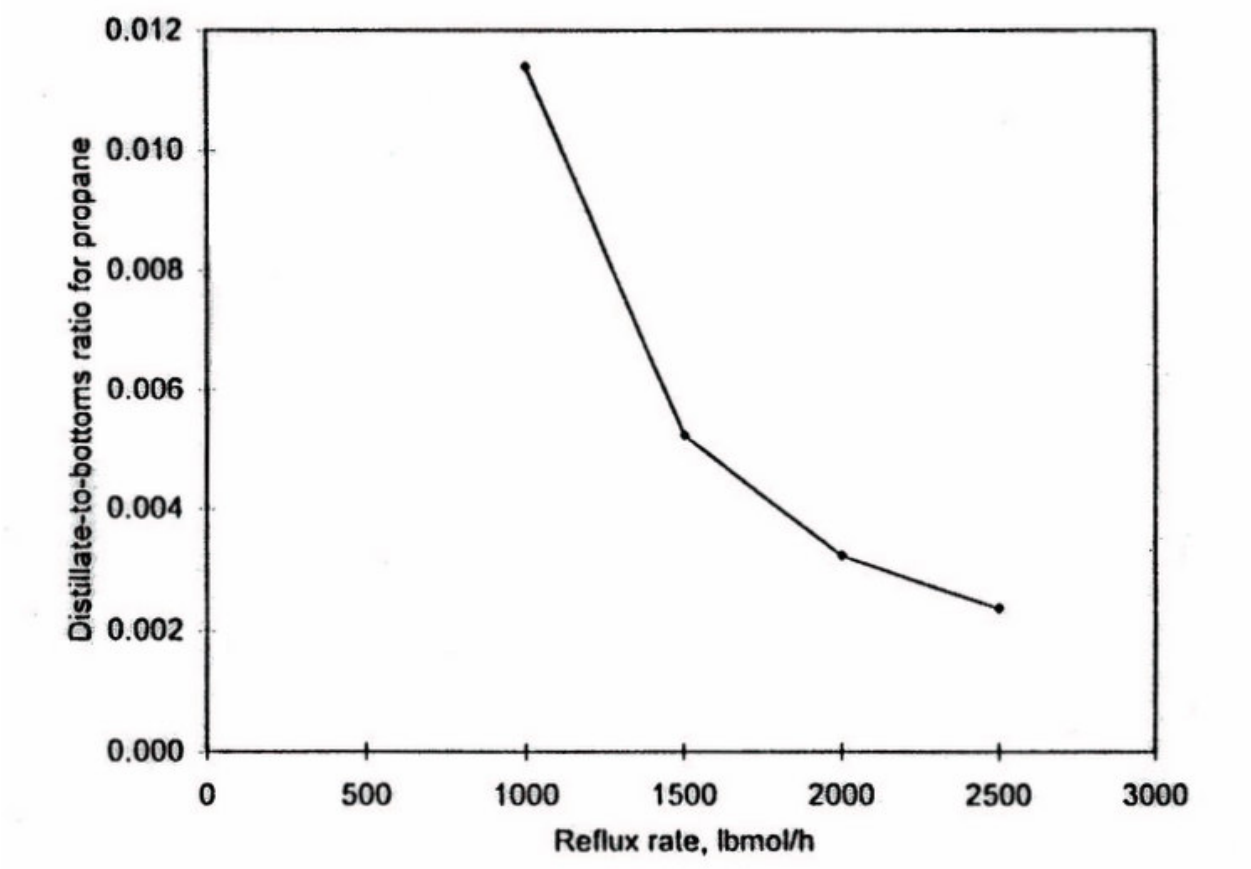
Using Eqs. (5) and (6), the following ϕ factors are determined for the enricher and exhauster from the above values of A_E, S_E, A_X, and S_X:

Factor	L_0 = 1,000	(a) L_0 = 1,500	(b) L_0 = 2,000	(c) L_0 = 2,500
ϕ_{AE}	0.0289	0.0180	0.0135	0.0113
ϕ_{AX}	0.028	0.0438	0.0530	0.0589
ϕ_{SE}	0.435	0.494	0.526	0.544
ϕ_{SX}	0.439	0.379	0.351	0.336

Using Eq. (1) with the above factors, the following *d/b* ratios for C_3 are obtained:

Case	***d/b* for C_3**
Example5.4	0.0114
(a)	0.00522
(b)	0.00322
(c)	0.00237

As the reflux rate increases, the separation is enhanced.



Exercise 5.22

Subject: Effect of numbers of rectification and stripping equilibrium stages on key-component distribution in multicomponent distillation by the group method.

Given: Results in Example 5.4 for distillation at 400 psia of a superheated vapor feed at 105°F and containing, lbmol/h of 160 C_1, 370 C_2, 240 C_3, 25 nC_4, and 5 nC_5 in a column with a partial condenser, 5 equilibrium rectification stages, equilibrium feed stage, 5 equilibrium stripping stages, and a partial reboiler, for an external reflux rate of 1,000 lbmol/h.

Assumptions: No changes in absorption and stripping factors when numbers of equilibrium stages are changed.

Find: Molar ratio of C_3 flow rate in the distillate to that in the bottoms, with a plot, for (a) 10 rectification and 10 stripping stages, and (b) 15 rectification and 15 stripping stages.

Analysis: Using the Edmister group method, the ratio of *d* to *b* for any component is given by a rearrangement of Eq. (5-66),

$$\frac{d}{b} = \frac{1}{A_F} \frac{\left[\left(S_B \phi_{AX} + 1\right)/\phi_{SX}\right]}{\left[\left(A_C \phi_{SE} + 1\right)/\phi_{AE}\right]} \qquad (1)$$

From Eqs. (5-48) and (5-50),

$$\phi_A = \frac{A-1}{A^{N+1}-1} \qquad (2)$$

$$\phi_S = \frac{S-1}{S^{N+1}-1} \qquad (3)$$

where $A = L/KV$ and $S = KV/L$.

In Eq. (1), ϕ_{AX} and ϕ_{SX} pertain to the stripping (exhauster)section,
ϕ_{AE} and ϕ_{SE} pertain to the rectifying (enricher) section.

Assume that all absorption and stripping factors are unchanged from the values given for Example 5.4. Recalculate the ϕ factors from Eqs. (2) and (3) for Case (a), where $N = 10$ for each section and Case (b), where $N = 15$ for each section.

Exercise 5.22 (continued)

Analysis: (continued)

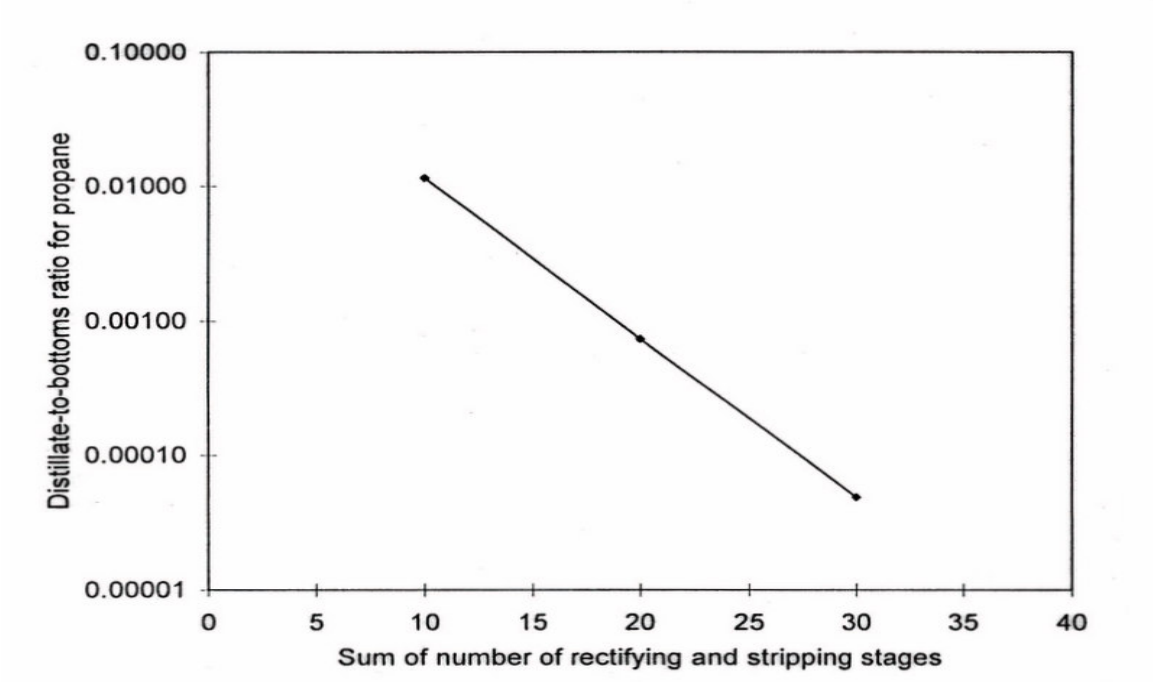
Factor	$N = 5$	$N = 10$	$N = 15$
ϕ_{AE}	0.0289	0.00185	0.000123
ϕ_{AX}	0.028	0.00176	0.000113
ϕ_{SE}	0.435	0.420	0.419
ϕ_{SX}	0.439	0.424	0.423

Using Eq. (1) with the above phi factors and the absorption and stripping factors from Example 5.4, as given below, the following *d/b* ratios for C_3 are obtained:

Factor	Example 5.4
A_C	10.48
A_E	1.72
$S_E = 1/A_E$	0.581
A_F	1.108
A_X	1.73
$S_X = 1/A_X$	0.577
S_B	2.78

Case	***d/b* for C_3**
Example 5.4	0.0114
(a)	0.000733
(b)	0.0000487

As the number of stages increases, the separation is greatly enhanced.



Exercise 5.23

Subject: Light hydrocarbon distillation by the Edmister group method.

Given: Column feed at 225°F and 250 psia, corresponding to approximately 23 mol% vapor, with component flow rates below. Distillate rate is 230 kmol/h to give a separation between C_3 and nC_4. Column operates at 250 psia with a partial condenser and a reflux ratio of 5.0. Column contains 14 theoretical stages, with feed to stage 8, counting up from the bottom.

Find: Compositions of the distillate and bottoms.

Analysis: Using the DISTL (Edmister method) model of ASPEN PLUS with the Chao-Seader method for *K*-values, the results, with a computed 25.4 mol% vaporization, are:

kmol/h:

Component	Feed	Distillate	Bottoms
C_2	30	29.999	0.001
C_3	200	192.663	7.337
nC_4	370	7.325	362.674
nC_5	350	0.012	349.988
nC_6	50	0	50.000
Total	1,000	229.999	770.000

Exercise 5.24

Subject: Light hydrocarbon distillation by the Edmister group method.

Given: Bubble-point column feed at 120 psia, with component flow rates below. Distillate rate is 45 kmol/h to give a separation between nC_4 and iC_5. Column operates at 120 psia with a partial condenser and a boilup of 200 kmol/h Column contains 20 theoretical stages, with feed to stage 10, counting up from the bottom.

Find: Compositions of the distillate and bottoms.

Analysis: Using the DISTL (Edmister method) model of ASPEN PLUS with the Chao-Seader method for *K*-values, and a reflux rate of 200 - 45 = 155 kmol/h (reflux ratio = 155/45), gives:

kmol/h:

Component	Feed	Distillate	Bottoms
C_3	5	4.996	0.004
iC_4	15	14.987	0.013
nC_4	25	24.587	0.413
iC_5	20	0.354	19.646
nC_5	35	0.077	34.923
Total	100	45.001	54.999

Exercise 5.25

Subject: Degrees of freedom analyses for a partial reboiler and a total condenser.

Given: A partial reboiler with exiting vapor and liquid in equilibrium. A total condenser.

Find: Number of variables, number of independent equations, and degrees of freedom.

Analysis:

Partial reboiler:

Have 3 streams with $C + 3$ variables each, plus the heat transfer rate.

Therefore, $N_V = 3(C + 3) + 1 = 3C + 10$

The independent relationships are:

C	Component material balances
1	Enthalpy balance
1	Equality of temperatures of exiting vapor and liquid
1	Equality of pressures of exiting vapor and liquid
C	Component phase equilibrium between exiting vapor and liquid
3	Mole fraction summations for 3 streams

Therefore, $N_E = 2C + 6$

From Eq. (5-67), $N_D = N_V - N_E = (3C + 10) - (2C + 6) = C + 4$

Total condenser:

Have 2 streams with $C + 3$ variables each, plus the heat transfer rate.

Therefore, $N_V = 2(C + 3) + 1 = 2C + 7$

The independent relationships are:

C	Component material balances
1	Enthalpy balance
2	Mole fraction summations for 2 streams Therefore,

$N_E = C + 3$

From Eq. (5-67), $N_D = N_V - N_E = (2C + 7) - (C + 3) = C + 4$

Exercise 5.26

Subject: Degrees of freedom analyses for a stream mixer and a stream divider.

Given: A steam mixer and a stream divider, each with heat transfer.

Find: Number of variables, number of independent equations, and degrees of freedom.

Analysis:

Stream mixer with two inlet streams:

Have 3 streams with $C + 3$ variables each, plus the heat transfer rate.

Therefore, $N_V = 3(C + 3) + 1 = 3C + 10$

The independent relationships are:

C	Component material balances
1	Enthalpy balance
3	Mole fraction summations for 3 streams

Therefore, $N_E = C + 4$

From Eq. (5-67), $N_D = N_V - N_E = (3C + 10) - (C + 4) = 2C + 6$

Stream divider with two exiting streams:

Have 3 streams with $C + 3$ variables each, plus the heat transfer rate.

Therefore, $N_V = 3(C + 3) + 1 = 3C + 10$

The independent relationships are:

1	Total material balance
$2(C - 1)$	Component mole fraction equalities for exiting streams relative to the feed
1	Enthalpy balance
1	Equality of temperatures of exiting streams
1	Equality of pressures of exiting streams
3	Mole fraction summations for 3 streams

Therefore, $N_E = 2C + 5$

From Eq. (5-67), $N_D = N_V - N_E = (3C + 10) - (2C + 5) = C + 5$

Exercise 5.27

Subject: Degrees of freedom analysis for the specifications of a distillation column.

Given: Feed of 10 mol% benzoic acid and 90 mol% maleic anhydride. Column has a total condenser and a partial reboiler. Operation is at 100 torr with a reflux ratio of 1.2 times minimum. Desired products are a distillate of 99.5 mol% maleic anhydride and a bottoms of 0.5 mol% anhydride.

Find: Whether problem is completely specified.

Analysis: From operation (b) in Table 5.4,

$N_D = 2N + C + 9 = 2N + 11$

The given specifications are equivalent to:

Pressure at each stage, including partial reboiler	N
Pressure at reflux divider outlet	1
Pressure at total condenser outlet	1
Heat transfer rate for each stage, except reboiler	N - 1
Heat transfer rate for divider	1
Feed mole fractions (only count C - 1)	1
Reflux rate	1
Mole fraction of component in distillate	1
Mole fraction of component in bottoms	1
Total	$2N + 6$

Need 5 more specifications, which might be:

Feed rate
Feed temperature
Feed pressure
Optimal feed location
Saturated liquid leaving condenser

Exercise 5.28

Subject: Verification of numbers of degrees of freedom for 3 operations, and effect of adding another feed.

Given: Degrees of freedom for operations (b), (c), and (g) in Table 5.4.

Find: Verify values of N_D and determine effect of adding another feed.

Analysis: Operation (b), distillation with total condenser and partial reboiler:

From Eq. (5-70),

$$\left(N_D\right)_{\text{unit}} = \sum_{\text{all elements}} \left(N_D\right)_e - N_R\left(C+2\right) + N_A \qquad (1)$$

$N_R = 9$ and $N_A = 0$

Therefore, Eq. (1) becomes,

$$\left(N_D\right)_{\text{unit}} = \sum_{\text{all elements}} \left(N_D\right)_e - 9\left(C+2\right) \qquad (2)$$

Let N_1 = number of rectifying stages and N_2 = number of stripping stages.

Using the values of N_D for the elements in Table 5.3:

Total condenser	$C + 4$
Reflux divider	$C + 5$
Rectifying section	$2N_1 + 2C + 5$
Feed stage with heat transfer	$3C + 8$
Stripping section	$2N_2 + 2C + 5$
Partial reboiler	$\underline{C + 4}$

$$\sum_{\text{all elements}} \left(N_D\right)_e = 2(N_1 + N_2) + 10C + 31 \qquad (3)$$

Substituting Eq. (3) into (2),

$$\left(N_D\right)_{\text{unit}} = 2\left(N_1 + N_2\right) + 10C + 31 - 9\left(C+2\right) = 2\left(N_1 + N_2\right) + C + 13 \qquad (4)$$

However, in Operation (b) of Table 5.4, the feed stage and the partial reboiler are counted in N.

Therefore, $N_1 + N_2 = N - 1 - 1 = N - 2$. Substituting this into Eq. (4), gives

$$\left(N_D\right)_{\text{unit}} = 2(N-2) + C + 13 = 2N + C - 9 \qquad (5)$$

which verifies the result given in Table 5.4.

Exercise 5.28 (continued)

If a second feed is added, we add $C + 2$ degrees of freedom for the feed variables and for feed location.
Then,

$$(N_D)_{2\text{ feeds}} = (N_D)_{1\text{ feed}} + C + 3 = 2N + 2C + 12$$

Operation (c), distillation with a partial condenser and partial reboiler:

With a partial condenser instead of a total condenser, there are only 8 redundant streams and no reflux divider. Therefore, Eq. (4) becomes:

$$(N_D)_{\text{unit}} = 2N + C + 9 + (C + 2) - (C + 5) = 2N + C + 6 \qquad (6)$$

which verifies the result given in Table 5.4. With two feeds,

$$(N_D)_{2\text{ feeds}} = (N_D)_{1\text{ feed}} + C + 3 = 2N + 2C + 9$$

Operation (g), distillation with a partial reboiler and a mixed condenser that produces both vapor distillate and liquid distillate:

With a mixed condenser, we can modify Operation (c), by adding a reflux divider and one redundant stream. Therefore, Eq. (6) becomes:

$$(N_D)_{\text{unit}} = 2N + C + 6 + (C + 5) - (C + 2) = 2N + C + 9$$

which verifies the result given in Table 5.4.

With two feeds, $(N_D)_{2\text{ feeds}} = (N_D)_{1\text{ feed}} + C + 3 = 2N + 2C + 12$

Exercise 5.29

Subject: Verification of numbers of degrees of freedom for 2 operations, and effect of adding a vapor sidestream..

Given: Degrees of freedom for operations (e) and (f) in Table 5.4.

Find: Verify values of N_D and determine effect of adding a vapor stream

Analysis: Operation (e), reboiled absorber:

From Eq. (5-70),

$$\left(N_D\right)_{\text{unit}} = \sum_{\text{all elements}} \left(N_D\right)_e - N_R\left(C+2\right) + N_A \qquad (1)$$

$N_R = 6$ and $N_A = 0$

Therefore, Eq. (1) becomes,

$$\left(N_D\right)_{\text{unit}} = \sum_{\text{all elements}} \left(N_D\right)_e - 6(C+2) \qquad (2)$$

Let N_1 = number of rectifying stages and N_2 = number of stripping stages.

Using the values of N_D for the elements in Table 5.3:

Rectifying section	$2N_1 + 2C + 5$
Feed stage with heat transfer	$3C + 8$
Stripping section	$2N_2 + 2C + 5$
Partial reboiler	$\underline{C + 4}$

$$\sum_{\text{all elements}} \left(N_D\right)_e = 2(N_1 + N_2) + 8C + 22 \qquad (3)$$

Substituting Eq. (3) into (2),

$$\left(N_D\right)_{\text{unit}} = 2\left(N_1 + N_2\right) + 8C + 22 - 6\left(C+2\right) = 2\left(N_1 + N_2\right) + 2C + 10 \qquad (4)$$

However, in Operation (e) of Table 5.4, the feed stage and the partial reboiler are counted in N.

Therefore, $N_1 + N_2 = N - 1 - 1 = N - 2$. Substituting this into Eq. (4), gives

$$\left(N_D\right)_{\text{unit}} = 2(N-2) + 2C + 10 = 2N + 2C + 6 \qquad (5$$

which verifies the result given in Table 5.4.

Exercise 5.29 (continued)

Analysis: (continued)

If a vapor sidestream is added, we add 2 degrees of freedom, one for the location and one for the sidestream flow rate.

$$\text{Then, } (N_D)_{\text{unit with sidestream}} = 2N + 2C + 6 + (2) = 2N + 2C + 8$$

Operation (f), reboiled stripper:

Using the values of N_D for the elements in Table 5.3:

Section of N - 1 stages	$2(N - 1) + 2C + 5$
Partial reboiler	$\underline{C + 4}$
$\sum_{\text{all elements}} (N_D)_e =$	$2N + 3C + 7$ (6)

Substituting Eq. (3) into (2), with $N_R = 2$ and $N_A = 0$,

$$(N_D)_{\text{unit}} = 2N + 3C + 7 - 2(C + 2) = 2N + C + 3 \qquad (7)$$

If a vapor sidestream is added, we add 2 degrees of freedom, then,

$$(N_D)_{\text{unit with sidestream}} = 2N + C + 3 + (2) = 2N + C + 5$$

Exercise 5.30

Subject: Verification of numbers of degrees of freedom for one operation, and effect of adding a liquid sidestream..

Given: Degrees of freedom for operation (h) in Table 5.4.

Find: Verify value of N_D and determine effect of adding a liquid sidestream

Analysis: Operation (h), extractive distillation:

From Eq. (5-70),

$$\left(N_D\right)_{\text{unit}} = \sum_{\text{all elements}} \left(N_D\right)_{\text{e}} - N_R\left(C+2\right) + N_A \qquad (1)$$

$N_R = 13$ and $N_A = 0$

Therefore, Eq. (1) becomes,

$$\left(N_D\right)_{\text{unit}} = \sum_{\text{all elements}} \left(N_D\right)_{\text{e}} - 13(C+2) \qquad (2)$$

Let N_1 = number of rectifying stages above the MSA feed,

N_2 = number of intermediate stages between the MSA feed and the feed,

N_3 = number of stripping stages.

Using the values of N_D for the elements in Table 5.3:

Total condenser	$C + 4$
Reflux divider	$C + 5$
Rectifying section	$2N_1 + 2C + 5$
MSA Feed stage with heat transfer	$3C + 8$
Intermediate section	$2N_2 + 2C + 5$
Feed stage with heat transfer	$3C + 8$
Stripping section	$2N_2 + 2C + 5$
Partial reboiler	$\underline{C + 4}$

$$\sum_{\text{all elements}} \left(N_D\right)_{\text{e}} = 2(N_1 + N_2 + N_3) + 15C + 44 \qquad (3)$$

Substituting Eq. (3) into (2),

$$\left(N_D\right)_{\text{unit}} = 2\left(N_1 + N_2 + N_3\right) + 15C + 44 - 13\left(C+2\right) = 2\left(N_1 + N_2 + N_3\right) + 2C + 18 \qquad (4)$$

However, in Operation (h) of Table 5.4, the two feed stages and the partial reboiler are counted in N. Therefore, $N_1 + N_2 + N_3 = N - 3$. Substituting this into Eq. (4), gives

$$\left(N_D\right)_{\text{unit}} = 2(N-3) + 2C + 18 = 2N + 2C + 12 \qquad (5)$$

which verifies the result in Table 5.4.

If a liquid sidestream is added, we add 2 degrees of freedom, then,

$$\left(N_D\right)_{\text{unit with sidestream}} = 2N + 2C + 12 + (2) = 2N + 2C + 14$$

Exercise 5.31

Subject: Alternative design variables for distillation

Given: Distillation design variables in Table 5.4

Find: Conditions under which the alternative variables below could be specified.

Analysis: (a) Condenser heat duty might be substituted for the reflux ratio if the maximum heat duty of the condenser in an existing tower were known.

(b) Stage temperature might be substituted for the recovery of a light or heavy component if there was a limit on the temperature of the cooling or heating medium in the condenser or reboiler.

(c) Intermediate stage vapor rate might be substituted for reflux ratio for an existing tower diameter with a limiting vapor velocity to prevent flooding.

(d) Reboiler heat load might be substituted for reflux ratio in the case of an existing reboiler area to prevent transition to film boiling.

Exercise 5.32

Subject: Difference in degrees of freedom between a distillation column with a total condenser and one with a partial condenser.

Given: A difference of 3 provided that only a vapor distillate leaves the partial condenser.

Find: The difference in degrees of freedom

Analysis: From Eq. (5-70),

$$\left(N_D\right)_{\text{unit}} = \sum_{\text{all elements}} \left(N_D\right)_e - N_R\left(C+2\right) + N_A \qquad (1)$$

For a total condenser plus reflux divider, $N_R = 1$ and $N_A = 0$

Therefore, Eq. (1) becomes,

$$\left(N_D\right)_{\text{unit}} = \sum_{\text{all elements}} \left(N_D\right)_e - (C+2) \qquad (2)$$

Using the values of N_D for the elements in Table 5.3:

Total condenser	$C + 4$
Reflux divider	$C + 5$

Therefore, $\left(N_D\right)_{\text{unit}} = (C+4) + (C+5) - (C+2) = C+7$

For a partial condenser, $N_R = 0$ and $N_A = 0$, and using Table 5.3,

$\left(N_D\right)_{\text{unit}} = (C+4)$

Therefore, the difference = $(C + 7)$ - $(C + 4)$ = 3 degrees of freedom

Exercise 5.33

Subject: Replacement of a partial reboiler with live steam injection.

Given: Operation (b) in Table 5.4 for distillation with a total condenser and partial reboiler. A column without the reboiler, but with steam injection and design variables listed below.
Assumptions: Injection of steam will not cause the formation of a second liquid phase.

Find: (a) The number of degrees of freedom = number of design variables.
(b) The additional design specifications needed.

Analysis: (a) Table 5.4, Operation (b), $N_D = 2N + C + 9$.
If the partial reboiler is eliminated, then from Eq. (5-70),

$$(N_D)_{\text{unit}} = \sum_{\text{all elements}} (N_D)_e - N_R(C+2) + N_A \qquad (1)$$

$N_R = 7$ and $N_A = 0$
Therefore, Eq. (1) becomes,

$$(N_D)_{\text{unit}} = \sum_{\text{all elements}} (N_D)_e - 7(C+2) \qquad (2)$$

Let N_1 = number of rectifying stages
N_2 = number of stripping stages
Using the values of N_D for the elements in Table 5.1:

Total condenser	$C + 4$
Reflux divider	$C + 5$
Rectifying section	$2N_1 + 2C + 5$
Feed stage with heat transfer	$3C + 8$
Stripping section	$2N_2 + 2C + 5$

$$\sum_{\text{all elements}} (N_D)_e = 2(N_1 + N_2) + 9C + 27 \qquad (3)$$

Substituting Eq. (3) into (2),

$$(N_D)_{\text{unit}} = 2(N_1 + N_2) + 9C + 27 - 7(C+2) = 2(N_1 + N_2) + 2C + 13 \qquad (4)$$

However, if the feed stage is counted in the total N stages, then $N_1 + N_2 = N - 1$.
Substituting this into Eq. (4), gives

$$(N_D)_{\text{unit}} = 2(N-1) + 2C + 13 = 2N + 2C + 11 \qquad (5)$$

(b) The specifications are: Pressures at all stages + condenser + divider = $N + 3$
Heat transfer rate for all stages + divider = $N + 1$
Feed conditions = $C + 2$
Alcohol concentration in distillate = 1
Stripping steam composition = $C - 1$
This totals $2N + 2C + 6$. Therefore, 5 additional specifications are needed.
Might also specify: Temperature and pressure of stripping steam, saturated liquid reflux, alcohol concentration in bottoms, and optimal feed-stage location.

Exercise 5.34

Subject: Degrees of freedom and specs for distillation column with a boilup divider.

Given: Column flow diagram in Fig. 5.26 and specifications listed below.

Find: (a) Number of degrees of freedom.
(b) The reason why a feed rate cannot be specified.

Analysis: (a) From Eq. (5-70),

$$\left(N_D\right)_{\text{unit}} = \sum_{\text{all elements}} \left(N_D\right)_e - N_R\left(C+2\right) + N_A \qquad (1)$$

N_R =10 and $N_A = 0$

Therefore, Eq. (1) becomes,

$$\left(N_D\right)_{\text{unit}} = \sum_{\text{all elements}} \left(N_D\right)_e - 10\left(C+2\right) \qquad (2)$$

Let N_1 = number of rectifying stages and N_2 = number of stripping stages.
Using the values of N_D for the elements in Table 5.3:

Total condenser	$C + 4$
Reflux divider	$C + 5$
Rectifying section	$2N_1 + 2C + 5$
Feed stage with heat transfer	$3C + 8$
Stripping section	$2N_2 + 2C + 5$
Boilup divider	$C + 5$
Total reboiler	$\underline{C + 4}$

$$\sum_{\text{all elements}} \left(N_D\right)_e = 2(N_1 + N_2) + 11C + 36 \qquad (3)$$

Substituting Eq. (3) into (2),

$$\left(N_D\right)_{\text{unit}} = 2\left(N_1 + N_2\right) + 11C + 36 - 10\left(C+2\right) = 2\left(N_1 + N_2\right) + C + 16 \qquad (4)$$

However, the feed stage is counted in N.
Therefore, $N_1 + N_2 = N - 1$. Substituting this into Eq. (4), gives

$$\left(N_D\right)_{\text{unit}} = 2(N-1) + C + 16 = 2N + C + 14 \qquad (5)$$

(b) The specified variables are:

Number of stages and feed stage	2	
Pressures of all stages, condenser, reboiler, and 2 dividers	$N + 4$	
Adiabatic for all stages and 2 dividers		$N + 2$
Feed composition , temperature, and pressure	$C + 1$	
Reflux rate set by L/V = 1.2 and vapor rate by velocity	2	
Condensate temperature set by water temperature	1	
Concentrations of A in distillate and C in bottoms	2	
Total	$2N + C + 14$	

Thus, all of degrees of freedom are utilized and the column feed rate can not be specified.

Exercise 5.35

Subject: Degrees of freedom and specifications for a mixed-feed, triple-effect evaporation system to concentrate an aqueous solution of an organic acid.

Given: Flow diagram of system in Fig. 5.27, and design specifications listed below

Assumptions: Organic acid is non-volatile. No heat losses from evaporator effects.

Find: Number of degrees of freedom. Any additional specifications needed.

Analysis: The system in Fig. 5.27 consists of 3 evaporator effects, a total condenser, and a pump. Number of interconnecting streams = $N_R = 6$, and $N_A = 0$. First determine the number of degrees of freedom for one evaporator effect.

Let: V = vapor mass rate leaving an effect.
L = aqueous solution mass rate leaving an effect.
F = aqueous solution mass feed rate to an effect.
S (= D) = heating steam mass rate to and from an effect.
w_F = weight fraction of organic acid in feed.
w_L = weight fraction of organic acid in aqueous solution leaving effect.
T_F and P_F be temperature and pressure of feed.
T and P be temperature and pressure of leaving vapor and liquid.
T_S and P_S be temperature and pressure of steam to effect.
T_C and P_C be temperature and pressure of condensate from effect.

Therefore, $N_V = 14$.

The relationships among the variables are:
Total material balance: $F = V + L$
Acid material balance: $Fw_F = Lw_L$
Equilibrium temperature: $T = f\{P, w_L\}$, i.e. a modified Raoult's law
Energy balance: $LH_L + VH_V - FH_F = S(H_S - H_C)$

Therefore, $N_E = 4$

From Eq. (5-67), $N_D = N_V - N_E = 14 - 4 = 10$.
A typical specification for a single evaporator effect might be F, w_F, T_F, P_F, w_L, P, T_S, P_S, T_C, and P_C.
For the total condenser, the variables are: (Into) V, T, P; (out of) V, P_T, T_T; Q
Therefore, $N_V = 6$.
The relationships among the variables are:

Energy balance: $Q = V(H_V \text{ in} - H_V \text{ out})$

Exercise 5.35 (continued)

Analysis: (continued)

Therefore, N_E =1 and N_D = 6 - 1 = 5.
Typical specs might be V, T, P, P_T, T_T
For the pump, the variables are L, w_L, T_L, P_L, P_P with no equations and 5 degrees of freedom.

Now analyze the system. From Eq. (5-70),

$$(N_D)_{\text{system}} = \sum_{\text{all units}} (N_D)_{\text{u}} - \text{interconnecting redundant variables} \qquad (1)$$

$$\sum_{\text{all units}} (N_D)_{\text{u}} = 3(10) + 5 + 5 = 40$$

The number of interconnecting redundant variables are 4 (L, w_L, T, P) for each of 3 liquid streams and 3 (V, T, P) for each of 3 vapor streams, or 4(3) + 3(3) = 21

Therefore, from Eq. (1), $(N_D)_{\text{system}}$ = 40 - 21 = 19

The given specifications are as follows, where effects are numbered 1, 2, 3 from left to right in Fig. 5.23: $w_{F_1}, w_{L_3}, P_{S_1}, T_{S_1}$. Therefore, additional specifications needed = 19 - 4 = 15,

which might be:

Feed rate to Effect 1 = F_1
Temperature and pressure of feed to Effect 1 = T_{F_1}, P_{F_1}
Pressure in each effect = P_1, P_2, P_3
Temperature and pressure leaving condenser = T_T, P_T
Pressure leaving the pump = P_P

Pressure of condensed steam leaving each effect = pressure of steam entering the effect

Temperature of condensed steam leaving each effect = saturation for the exit pressure

Exercise 5.36

Subject: Degrees of freedom and additional specifications for a reboiled stripper.

Given: Reboiled stripper with specifications in Fig. 5.28.

Find: (a) Number of variables
(b) Number of relationships.
(c) Number of degrees of freedom.
(d) Additional specifications, if any.

Analysis: (a) and (b) For an N -1 cascade and a partial reboiler from Table 5.3

Element	N_V	N_E
N -1 cascade	$7(N\text{-}1)+2C(N\text{-}1)+2C+7$	$5(N\text{-}1)+2C(N\text{-}1)+2$
Partial reboiler	$3C+10$	$2C+6$
Total	$7N+2NC+3C+10$	$5N+2NC+3$

From Eq. (5-68), $$(N_V)_{\text{unit}} = \sum_{\text{all elements}} (N_V)_e - N_R(C+3) + N_A \qquad (1)$$

From Eq. (5-69), $$(N_E)_{\text{unit}} = \sum_{\text{all elements}} (N_E)_e - N_R \qquad (2)$$

Since $N_R = 2$ and $N_A = 0$, Eqs. (1) and (2) become,

$$(N_V)_{\text{unit}} = (7N+2NC+3C+10) - 2(C+3) = 7N + 2NC + C + 4$$

$$(N_E)_{\text{unit}} = 5N+2NC+3-2 = 5N+2NC+1$$

(c) From Eq. (5-67), $N_D = N_V - N_E = (7N+2NC+C+4) - (5N+2NC+1) = 2N + C + 3$

(d) Specifications are:

All feed conditions		$C + 2$
Number of stages		1
	Total	$C + 3$

Therefore, can make $2N$ additional specifications, which might be:

All stage and reboiler pressures	N
Adiabatic stages	N - 1

Have one specification left. Make it the bottoms rate, distillate rate, or boilup rate or ratio.

Exercise 5.37

Subject: Degrees of freedom and specifications for thermally coupled distillation.

Given: Distillation system in Fig. 5.29.

Find: (a) Number of variables
(b) Number of relationships.
(c) Number of degrees of freedom.
(d) Reasonable set of specifications.

Analysis: Treat the system as one of two units with $N_R = 4$ interconnecting streams and $N_A = 0$.

(a) and (b) The feed unit is like an absorber with an additional intermediate feed. Therefore, from Table 5.3 for an N-stage cascade,

$$N_V = (7N + 2NC + 2C + 7) + (C + 3) \text{ for extra feed } +1 \text{ for extra feed location}$$
$$= 7N + 2NC + 3C + 11$$
$$N_E = (5N + 2NC + 2) + 1 \text{ for extra feed}$$
$$= 5N + 2NC + 3$$

The second unit is a distillation column like that in Example 5.5, except with an additional feed and two more sidestreams that are located at the two feed stages. Therefore, from Example 5.5, using M for the number of stages, including the reboiler,

$$N_V = (7M + 2MC + 5C + 20) +$$
$$3(C + 3) \text{ for extra feed and 2 extra sidestreams } +1 \text{ for extra feed location}$$
$$= 7M + 2MC + 8C + 30$$
$$N_E = (5M + 2MC + 4C + 9) + 2(C + 2) \text{ for 2 extra sidestreams } + \text{ 1 for extra feed}$$
$$= 5M + 2MC + 6C + 14$$

From Eq. (5-68), $$\left(N_V\right)_{\text{system}} = \sum_{\text{all units}} \left(N_V\right)_{\text{u}} - N_R\left(C + 3\right) + N_A \qquad (1)$$

From Eq. (5-69), $$\left(N_E\right)_{\text{system}} = \sum_{\text{all units}} \left(N_E\right)_{\text{u}} - N_R \qquad (2)$$

Therefore, since $N_R = 4$ and $N_A = 0$, Eqs. (1) and (2) become,

$$\left(N_V\right)_{\text{system}} = (7N + 2NC + 3C + 11) + \left(7M + 2MC + 8C + 30\right) - 4\left(C + 3\right)$$
$$= 7(N + M) + 2C(N + M) + 7C + 29$$
$$\left(N_E\right)_{\text{system}} = (5N + 2NC + 3) + (5M + 2MC + 6C + 14) - 4$$
$$= 5(N + M) + 2C(N + M) + 6C + 13$$

Exercise 5.37 (continued)

Analysis: (d)

(c) From Eq. (5-71),

$$(N_D)_{\text{system}} = (N_V)_{\text{system}} - (N_E)_{\text{system}}$$

$$= [7(N+M)+2C(N+M)+7C+29]-[5(N+M)+2C(N+M)+6C+13]$$

$$= 2(N+M)+C+16$$

A reasonable set of specifications is as follows:

Pressure at each stage, reboiler, condenser, reflux divider	$N + M + 2$
Heat transfer at each stage and, divider	$N + M$
Complete feed specification	$C + 2$
Number of stages, N	1
Number of stages, M	1
Feed stage location	1
Locations of 3 sidestreams	3
Flow rates of 3 sidestreams	3
Reflux ratio	1
Distillate rate	1
Saturated liquid reflux or reflux temperature if subcooled	1
Total	$2(N + M) + C + 16$

Exercise 5.38

Subject: Degrees of freedom and specs for a column with a liquid sidestream.

Given: Column in Fig. 5.30.

Find: (a) Number of degrees of freedom.
(b) Reasonable set of design variables.

Analysis: (a) The column in Fig. 5.30 has a partial condenser. A similar column with total condenser is analyzed in Example 5.5, giving $N_D = 2N + C + 11$. In Table 5.2, in operations (b) and (c), it is seen that a column with a partial condenser has 3 less degrees of freedom than a column with a total condenser. Therefore, here,
$N_D = (2N + C + 11) - 3 = 2N + C + 8$.

(b) A reasonable set of specifications is:

Pressures of stages, reboiler, condenser	$N + 1$
Heat transfer for stages	$N - 1$
Feed completely specified	$C + 2$
Feed stage and sidestream stage locations	2
Distillate (volatile impurities) rate	1
Reflux ratio	1
Number of stages	1
Sidestream rate	1
Total	$2N + C + 8$

Exercise 5.39

Subject: Degrees of freedom analysis for distillation with a sidecut reboiled stripper.

Given: Distillation system in Fig. 5.31.

Find: (a) Number of variables.
(b) Number of equations.
(c) Number of degrees of freedom.
(d) Reasonable set of design variables.

Analysis: The system consists of (1) distillation column with 2 feeds and a sidestream, (2) reboiled stripper, (3) cooler, and (4) valve, with $N_R = 4$ and $N_A = 0$.

(a) and (b)

From Eq. (5-68), $$\left(N_V\right)_{\text{system}} = \sum_{\text{all units}} \left(N_V\right)_{\text{u}} - N_R\left(C+3\right) + N_A \qquad (1)$$

From Eq. (5-69), $$\left(N_E\right)_{\text{system}} = \sum_{\text{all units}} \left(N_E\right)_{\text{u}} - N_R \qquad (2)$$

For the distillation column, N_V and N_E can be obtained by adding a second feed to the results given in Example 5.5. This adds $C + 3$ to N_V and 1 to N_E. Therefore,

$N_V = (7N+2NC+5C+20) + (C+3) = 7N+2NC+6C+23$

and $N_E = (5N+2NC+4C+9) + 1 = 5N+2NC+4C+10$

For the reboiled stripper, the determination of N_V and N_E is given in Exercise 5.36.

For the cooler, use the total condenser in Table 5.1.

For the valve, use the total condenser in Table 5.1, less one variable for no heat transfer.

Unit (or element)	N_V	N_E
Distillation column	$7N+2NC+6C+23$	$5N+2NC+4C+10$
Reboiled stripper	$7M+2MC+C+4$	$5M+2MC+1$
Cooler	$2C+7$	$C+3$
Valve (no heat transfer)	$2C+6$	$C+3$
Total	$7(N+M)+2(N+M)C+11C+40$	$5(N+M)+2(N+M)C+6C+17$

Using Eqs. (1) and (2),

$$\left(N_V\right)_{\text{system}} = 7(N+M)+2(N+M)C+11C+40-4\left(C+3\right)$$
$$= 7(N+M)+2(N+M)C+7C+28$$
$$\left(N_E\right)_{\text{system}} = 5(N+M)+2(N+M)C+6C+17-4$$
$$= 5(N+M)+2(N+M)C+6C+13$$

(c) From Eq. (5-71),

$$\left(N_D\right)_{\text{system}} = \left(N_V\right)_{\text{system}} - \left(N_E\right)_{\text{system}}$$
$$= \left[7(N+M)+2(N+M)C+7C+28\right] - \left[5(N+M)+2(N+M)C+6C+13\right]$$
$$= 2(N+M)+C+15$$

Exercise 5.39 (continued)

Analysis:. (d)

A reasonable set of specifications is:

Pressures of stages, 2 reboilers, condenser	$N + M + 1$
Pressures of cooler, reflux divider, valve	3
Heat transfer for stages and divider	$N + M - 1$
Feed completely specified	$C + 2$
Feed stage and sidestream stage locations	2
Distillate rate	1
Reflux ratio	1
Number of stages for N and M	2
Sidestream rate	1
Boilup ratio in stripper	1
Saturated liquid reflux	1
Exit temperature from cooler	1
Total	$2(N + M) + C + 15$

Exercise 5.40

Subject: Allowable specifications for system of extractive distillation and distillation

Given: System in Fig. 5.32

Find: If given specifications are sufficient. If not, give additional specifications.

Analysis: System consists of a distillation column with 2 feeds (Case h in Table 5.4), a distillation column (Case b in Table 5.4), a cooler (use total condenser in Table 5.3), and a mixer (Table 5.4). From these sources, the degrees of freedom areas follows:

Unit	N_D
Extractive distillation	$2N_1+2C+12$
Distillation	$2N_2+C+9$
Cooler	$C+4$
Mixer	$2C+6$
Total	$2(N_1+N_2)+6C+31$

From Eq. (5-70),

$$(N_D)_{\text{unit}} = \sum_{\text{all elements}} (N_D)_e - N_R(C+2) + N_A \qquad (1)$$

$N_R = 4$ and $N_A = 0$

Therefore, Eq. (1) becomes,

$$(N_D)_{\text{unit}} = 2(N_1+N_2)+6C+31-4(C+2) = 2(N_1+N_2)+2C+23$$

A reasonable set of specifications is:

Pressures of stages, 2 reboilers, 2 condensers	$N_1 + N_2 + 2$
Pressures of cooler, 2 reflux dividers, mixers	4
Heat transfer for stages, 2 dividers, mixer	$N_1 + M_2 + 1$
Feed completely specified	$C + 2$
Makeup specified except flow rate	$C + 1$
Two feed stage locations	2
Distillate rate	1
Two reflux rates	2
Number of stages for N_1 and N_2	2
Phenol recycle rate	1
Total	$2(N_1 + N_2) + 2C + 18$

Therefore, 5 more specifications are needed. They might be the following:

Saturated liquid reflux from 2 condensers	2
Feed stage location for extractive distillation	1
Temperature leaving cooler	1
Makeup phenol rate	1

Exercise 5.41

Subject: Specifications for a distillation column with sidestream

Given: Distillation column in Fig. 5.33 with specifications.

Find: If given specifications are sufficient. If not, give additional specifications.

Analysis: For a distillation column with a total condenser and sidestream, Example 5.5 applies, giving $N_D = 2N + C + 11$.

The following specifications are given:

Pressures of stages, reboiler, condenser, divider	$N + 2$
Heat transfer for stages and divider	N
Feed completely specified	$C + 2$
Feed stage and sidestream stage locations	2
Distillate purity	1
Sidestream rate and purity	2
Number of stages	1
Total	$2N + C + 10$

Therefore, one more specification is needed. It might be saturated liquid leaving condenser or temperature of reflux if subcooled.

Exercise 6.1

Subject: Simultaneous absorption and stripping.

Given: Fig. 6.1 in which simultaneous absorption and stripping occur.

Find: Whether absorption and stripping is more important.

Analysis: Stripping of water = 22 kmol/h
Absorption of acetone = 10.35 kmol/h
Therefore, more stripping than absorption occurs.
However, the operation is primarily absorption because a very large percentage, 99.5%, of the acetone is absorbed. Only a very small fraction of the water is stripped.

Exercise 6.2

Subject: Column packings since 1950.

Given: History of the development of column packings.

Find: Advantages of new packings. Advances in packing design and fabrication. Need for structured packings.

Analysis: The newer packings provide more surface area for mass transfer, a higher flow capacity, and a lower pressure drop. They provide more effective through flow. Many are plastics made from molds or thin metal strips that can be inexpensively fabricated into intricate shapes. Structured packings largely eliminate the problems of channeling and at the same time give improvement in efficiency, capacity, and pressure drop.

Exercise 6.3

Subject: Advantages of bubble-cap trays

Given: Characteristics and performance of bubble-cap trays

Find: Characteristics that give bubble-cap trays a very high turndown ratio.

Analysis: Unlike sieve and valve trays, bubble-cap trays do not allow liquid to weep. Therefore, bubble-cap trays can be operated at very low liquid flow rates. Also, bubble caps force the vapor to flow out sideways, rather than vertically up, thus allowing a relatively high vapor rate.

Exercise 6.4

Subject: Selection of alternative absorbent for Example 6.3

Given: Flow rate, density, and MW of three potential absorbents listed below.

Find: Select the best absorbent with reasons why. Are any of the absorbents unacceptable?

Analysis: In Example 6.3, the rich gas contains C_1 to nC_6 hydrocarbons, with mostly C_3. Object of absorber is to absorb most of the nC_4. The absorbent is an oil of 250 MW and 21°API, at a flow rate, *L*, of 368 lbmol/h. An alternative absorbent must also be of higher molecular weight than nC_4 and must have a flow rate of at least 368 lbmol/h. If its molecular weight is too low, a significant amount of it will be stripped. This can be judged by its *K*-value and stripping factor, *S=KV/L*. The entering gas rate, *V*, is 946 lbmol/h. Column operating conditions are about 94 psia and a maximum temperature of 126°F.

Pertinent properties and factors for the three potential absorbents are:

Absorbent	gpm	ρ, lb/gal	lb/h	MW	lbmol/h	*K*-value	*S=KV/L*
C_5s	115	5.24	36,200	72	500	0.9	2.3
light oil	36	6.0	13,000	130	100	0.005	0.013
medium oil	215	6.2	80,000	180	440	0.0005	0.0013

The light oil can not be used because its flow rate of 100 lbmol/h is much lower than the necessary 368 lbmol/h. The C_5s can not be used because their stripping factor is very high. The only possible alternative is the medium oil.

Exercise 6.5

Subject: Stripping of VOCs from water effluents by air and water

Given: Packed tower for stripping

Find: Advantages and disadvantages of air over steam

Analysis: Advantages: Air is available anywhere.
Air is inexpensive.
Disadvantages: Air can form a flammable or explosive mixture with the VOC.
With steam, the exit gas can be condensed and the VOC recovered as a liquid.

Exercise 6.6

Subject: Preferred operating conditions for absorbers and strippers.

Find: Best conditions of temperature and pressure, and the trade-off between number of stages and flow rate of separating agent, using equations.

Analysis: Absorbers:

For high performance, want a large absorption factor, ***A = L/KV***

Therefore, want a small *K*-value.

Assume that:

$$K_i = \frac{\gamma_{iL} P_i^s}{P}$$

P_i^s = vapor pressure, which increases with increasing temperature

Therefore, operate at a high pressure and a low temperature.

Strippers:

For high performance, want a large stripping factor, $S = KV/L$

Therefore, want a large *K*-value.

Therefore, operate at low pressure and a high temperature.

For the tradeoff between number of equilibrium stages, *N*, and flow rate of mass separating agent, *L* or *V*. Consider absorption. The fraction of a component absorbed is given from a modification of Eq. (5-48),

$$1-\phi_A = 1-\frac{A-1}{A^{N+1}-1} = \frac{A^{N+1}-A}{A^{N+1}-1}$$

Thus, a large fraction absorbed can be achieved with either *N* or $A = L/KV$. The tradeoff is most clearly shown in Fig. 5.9. For low fractions absorbed (i.e. high ϕ_A), *N* has little effect and $(1 - \phi_A)$ is approximately equal to *A*. But for high fractions absorbed, the larger the value of *N*, the smaller the required value of *A*, and, thus, the smaller the required value of the flow rate of the liquid separating agent, *L*.

The tradeoff for stripping is similar. The fraction of a component stripped is given by a modification of Eq. (5-51),

$$1-\phi_S = 1-\frac{S-1}{S^{N+1}-1} = \frac{S^{N+1}-S}{S^{N+1}-1}$$

Thus, a large fraction stripped can be achieved with either *N* or $S = KV/L$. The tradeoff is most clearly shown in Fig. 5.9. For low fractions stripped (i.e. high ϕ_S), *N* has little effect and $(1 - \phi_S)$ is approximately equal to *S*. But for high fractions absorbed, the larger the value of *N*, the smaller the required value of *S*, and, thus, the smaller the required value of the flow rate of the vapor separating agent, *V*.

xercise 6.7

Subject: Absorption of CO_2 from air at 25°C by 5-N aqueous triethanolamine

Given: Feed gas containing 10 mol% CO_2 and 90 mol% air. Absorbent of 5N aqueous triethanolamine containing 0.04 moles of CO_2 per mole of amine solution. Column with 6 equilibrium stages. Exit liquid to contain 78.4% of the CO_2 in the feed gas. Therefore, exit gas contains 21.6% of the CO_2 in the entering gas. Equilibrium data for CO_2 at 25°C in terms of mole ratios.

Assumptions: Negligible absorption of air and stripping of amine and water.

Find: (a) Moles of amine solution required per mole of feed gas.
(b) Exit gas composition.

Analysis: Use the nomenclature and type of plot shown in Fig. 6.11(a). Therefore, for CO_2,

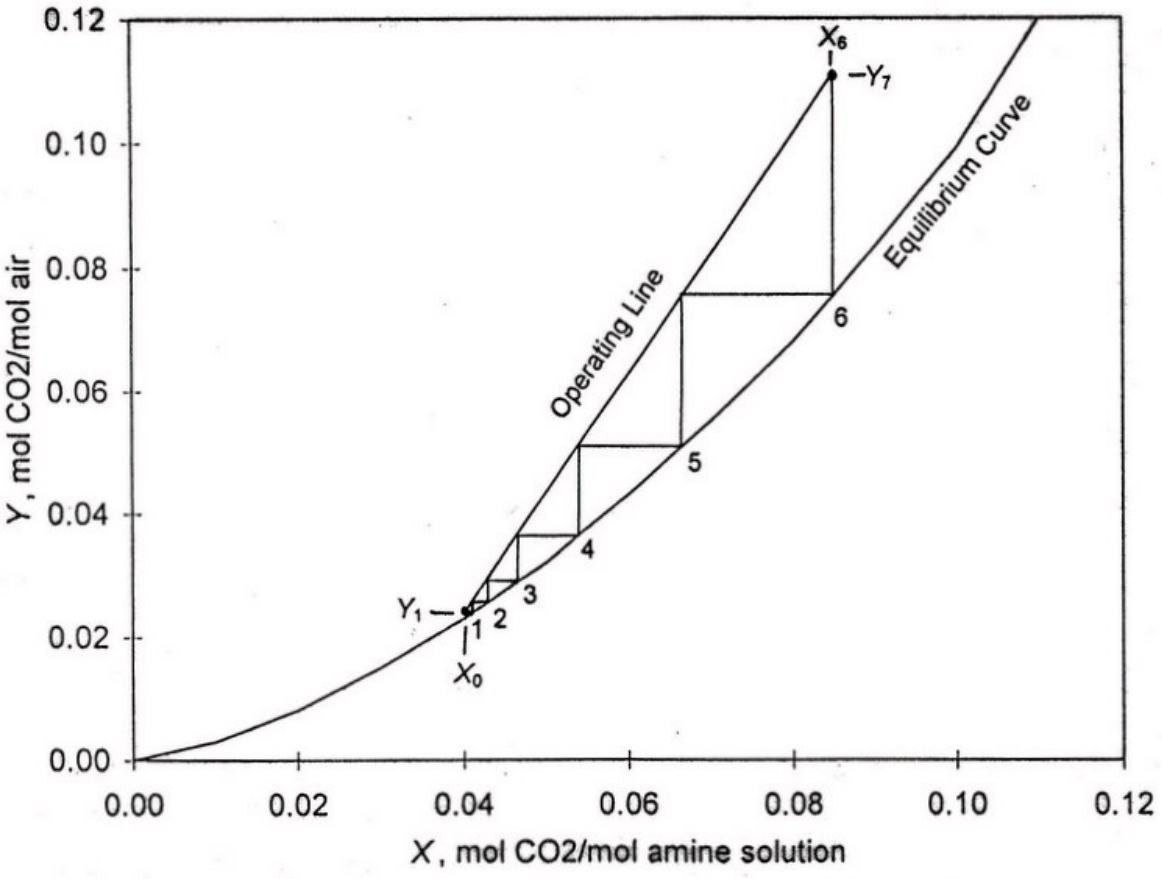
X_0 = 0.04 mol CO_2/mol amine solution
$Y_{N+1} = Y_7$ = 10/90 = 0.1111 mol CO_2/mol air
Y_1 = 0.216(10)/90 = 0.024 mol CO_2/mol air

(b) Therefore, the exit gas composition is 0.024 mol CO_2/mol air or 0.024/(1 + 0.024) x 100% = 2.34 mol% CO_2 and 97.66 mol% air.

(a) A plot of the equilibrium data as Y vs. X is given below. The operating point (X_0, Y_1) at the top of the column is included. A straight operating line through this point is found by trial and error to give 6 equilibrium stages, when using Y_7 = 0.1111. The resulting $X_N = X_6$ = 0.085. From Eq. (6-3), the slope of the operating line = L'/V' = (0.1111 - 0.024)/(0.085 - 0.04) = 1.936 mol triethanolamine solution/mol air. The feed gas contains 9 mol air/10 mol feed gas. Therefore, mols of amine solution/mol feed gas = 1.936(0.9) = 1.74.

See plot on next page.

Exercise 6.7 (continued)



Exercise 6.8

Subject: Absorption of acetone from air by water at 20°C and 101 kPa (760 torr) in a valve-tray column.

Given: 100 kmol/h of feed gas containing 85 mol% air and 15 mol% acetone. Pure water is the absorbent. Overall tray efficiency is 50%. Absorb 95% of the acetone. Equilibrium *p*-*x* data for acetone are given as listed below.

Assumptions: Negligible absorption of air and stripping of water.

Find: (a) Minimum ratio, L'/V' of moles of water/mole of air.
(b) Number of equilibrium stages for L'/V' = 1.25 times minimum.
(c) Concentration of acetone in the exit water.

Analysis: Use the nomenclature and type of plot shown in Fig. 6.11(a). Then, the operating line will be straight. For acetone,

X_0 = 0.0 mol acetone/mol entering water

Y_{N+1} = 0.15/0.85 = 0.1765 mol acetone/mol air in entering gas

Flow rate of acetone in exit gas = (1 - 0.95)(15) = 0.75 kmol/h. With 85 kmol/h of air,

Y_1 = 0.75/85 = 0.00882 mol acetone/mol air

Convert the *p*-*x* equilibrium data to mole ratio, *Y*-*X* data, using $y = p/P$, $Y = y/(1- y)$, $X = x/(1-x)$

p, torr	*x*	*y*	*X*	*Y*
30.0	0.033	0.0395	0.0341	0.0411
62.8	0.072	0.0826	0.0776	0.0901
85.4	0.117	0.1124	0.1325	0.1266
103.0	0.171	0.1355	0.2063	0.1568

(a) With the type of curvature in the *Y*-*X* equilibrium curve, shown below, the minimum absorbent rate is determined by a straight operating line that passes through the point (Y_1 , X_0) and is drawn tangent to the equilibrium curve, as shown. From Eq. (6-3), the slope of the operating line = L'/V' = 1.06 mol water/mol of air on an acetone-free basis = minimum ratio.

(b) For 1.25 times minimum, L'/V' = 1.25(1.06) = 1.325. Now a straight operating line that passes through the point (Y_1 = 0.00882 and X_0 = 0.0) is drawn as shown below, where equilibrium stages are stepped off, as in Figs. 6.11(a) and 6.12, until the steps reach or exceed the required value of Y_{N+1} = 0.1765. As seen, in the figure below, the determined number of equilibrium stages is approximately 9.

(c) The concentration of acetone in the exit liquid, X_N is the point on the operating line for Part (b), where Y_{N+1} = 0.1765. From Eq. (6-3), for the operating line for an absorber,

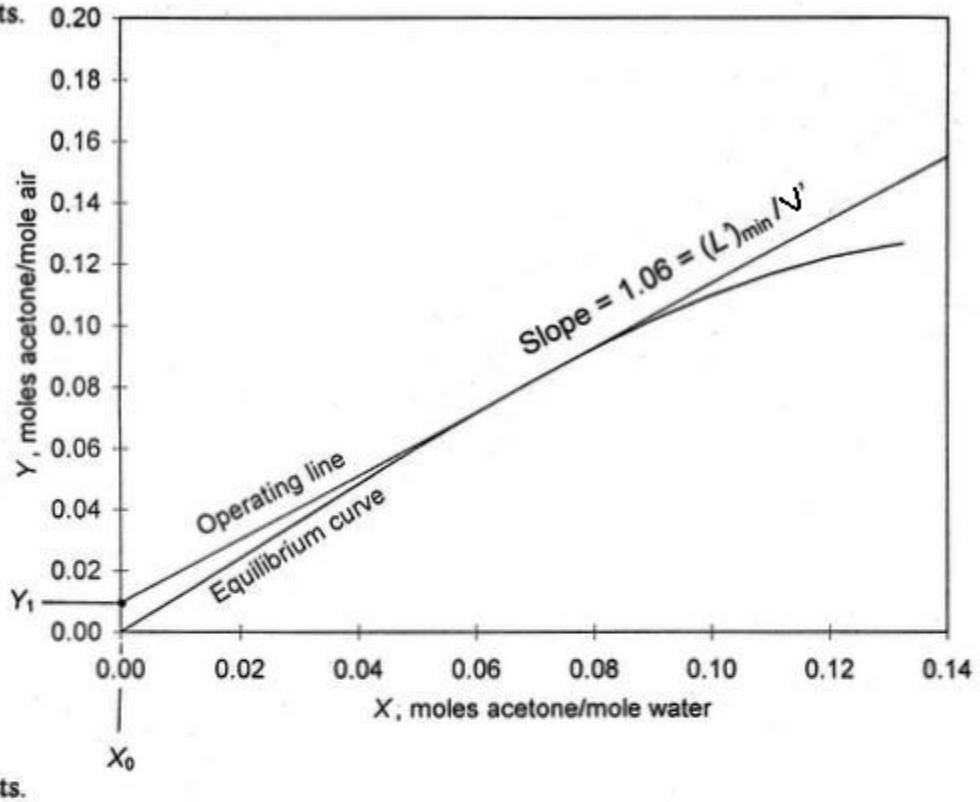
$$X_N = \frac{Y_{N+1} - Y_1}{\left(\frac{L'}{V'}\right)} + X_0 = \frac{0.1765 - 0.00882}{1.325} + 0.0 = 0.127 \text{ mol acetone/mol water}$$

or an exit mole fraction of acetone in the water of 0.127/(1.127) = 0.113

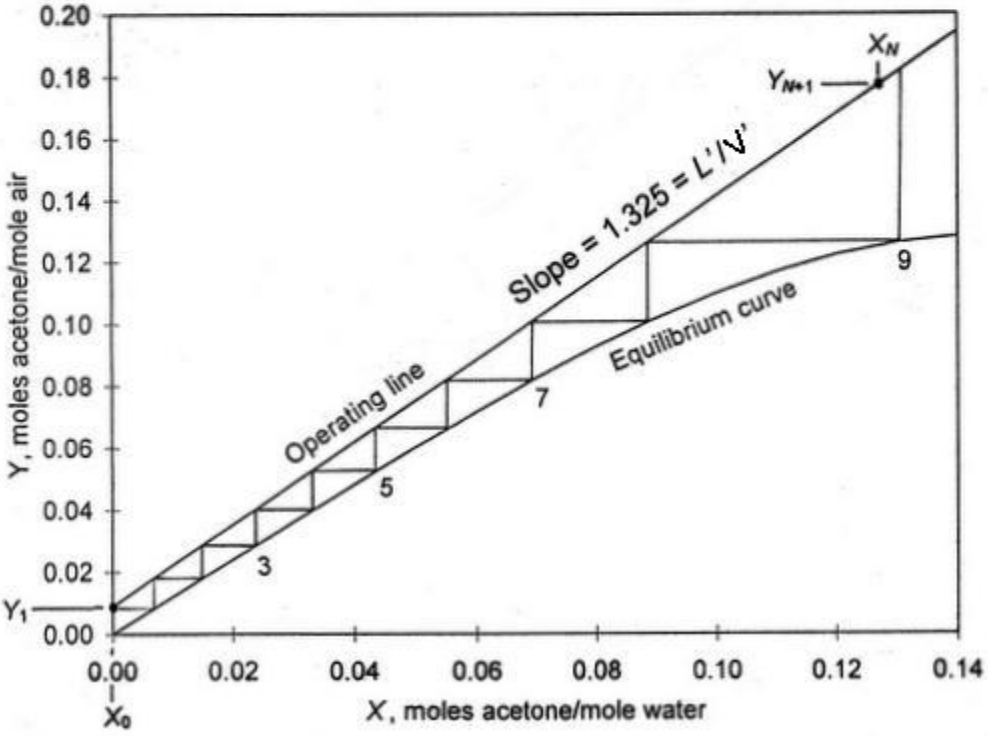
Exercise 6.8 (continued)

Analysis: (continued)

(a) Plot of results.



(b) Plot of results.



Exercise 6.9

Subject: Absorption-stripping system for benzene (B) removal from gas by oil and subsequent stripping of benzene from oil by steam.

Given: Plate column absorber and stripper. Feed gas containing 0.06 mol B/mol B-free gas. Absorbent oil containing 0.01 mol B/mol B-free oil. Liquid leaving absorber contains 0.19 mol B/mol B-free oil. 90% of B in the gas stream is absorbed. Liquid leaving stripper contains 0.01 mol B/mol oil. Flow ratio of B-free oil-to-B-free steam = 2.0. Molecular weights are 200, 78, and 32 for oil, benzene, and gas, respectively. Equilibrium X-Y data given for absorber (25°C) and stripper (110°C).

Assumptions: Gas is not soluble in oil and oil is not volatile.

Find: (a) Molar flow rate ratio of B-free oil to B-free gas in the absorber.
(b) Number of equilibrium stages in the absorber.
(c) Minimum steam flow rate in the stripper per mol of B-free oil.

Analysis: A flow diagram of the absorber-stripper system is shown in Fig. 5.10(a), except that there is no makeup absorbent oil because the oil is assumed to be non-volatile.

(a) Consider just the absorber. Take a basis of V' = 1 mol/h of B-free gas entering the absorber. Because Y_{N+1} = 0.06 mol B/mol B-free gas, we have 0.06 mol/h of B in entering gas. With 90% absorption, 0.06(0.9) = 0.054 mol/h of B absorbed, leaving 0.006 mol/h of B in the exiting gas. In the entering absorbent oil, X_0 = 0.01 mol B/mol B-free oil. In the liquid leaving the absorber, X_N = 0.19 mol B/mol B-free oil. A material balance around the absorber on the benzene gives:

$$Y_{N+1}V' + X_0L' = Y_1V' + X_NL' \qquad \text{Therefore,}$$
$$0.06(1.0) + 0.01L' = 0.006 + 0.19L' \qquad (1)$$

Solving Eq. (1), L' = 0.30 mol/h of B-free oil, giving L'/V'' = 0.30 mol B-free oil to B-free gas.

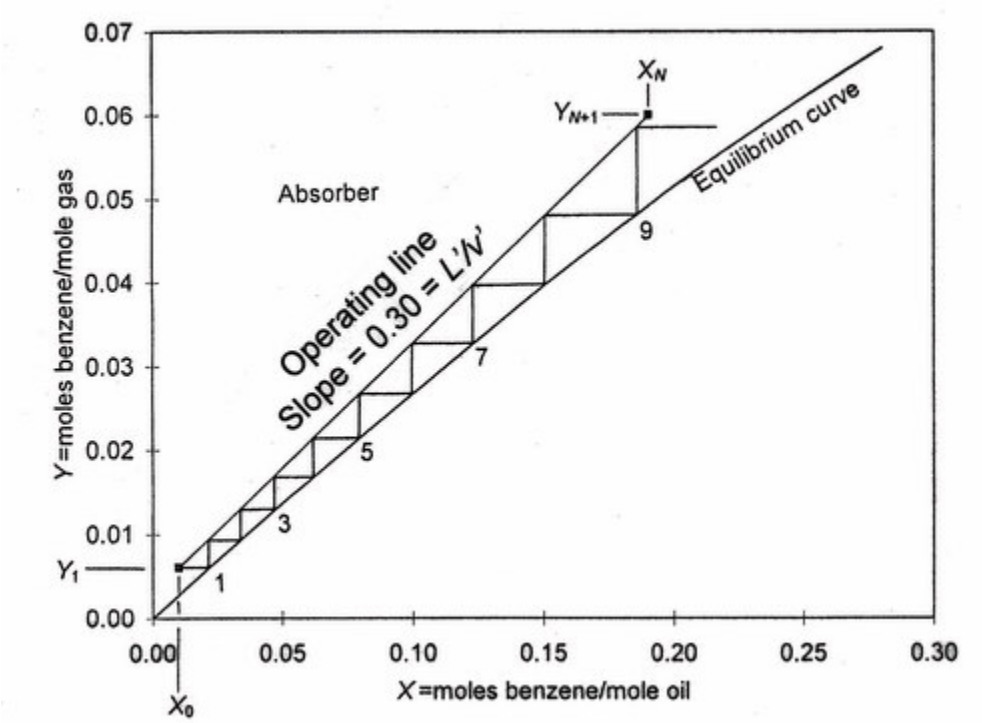
(b) Use a graphical method to determine the number of equilibrium stages in the absorber, using Y-X coordinates to give a straight operating line. Data for the equilibrium curve of the absorber are given and the operating line is obtained from terminal values of Y and X. The results are given in the plot below. As seen, between 9 and 10 equilibrium stages are needed.

(c) The equilibrium curve for the stripper is shown in the plot below. With the type of curvature in the Y-X equilibrium curve the minimum stripping gas rate is determined by a straight operating line that passes through the operating point (Y_0 = 0 , X_1 = 0.01) at the bottom of the column, as shown in Fig. 6.11(b) and is drawn tangent to the equilibrium curve, as shown. From Eq. (6-5), the slope of the operating line = L'/V' = 3.0 mol B/mol of steam on a B-free basis. Therefore,
$(V'')_{min}/L'$ = 0.33. This is compared to the given operating value of L'/V' = 2.0 or V'/L' = 0.5.

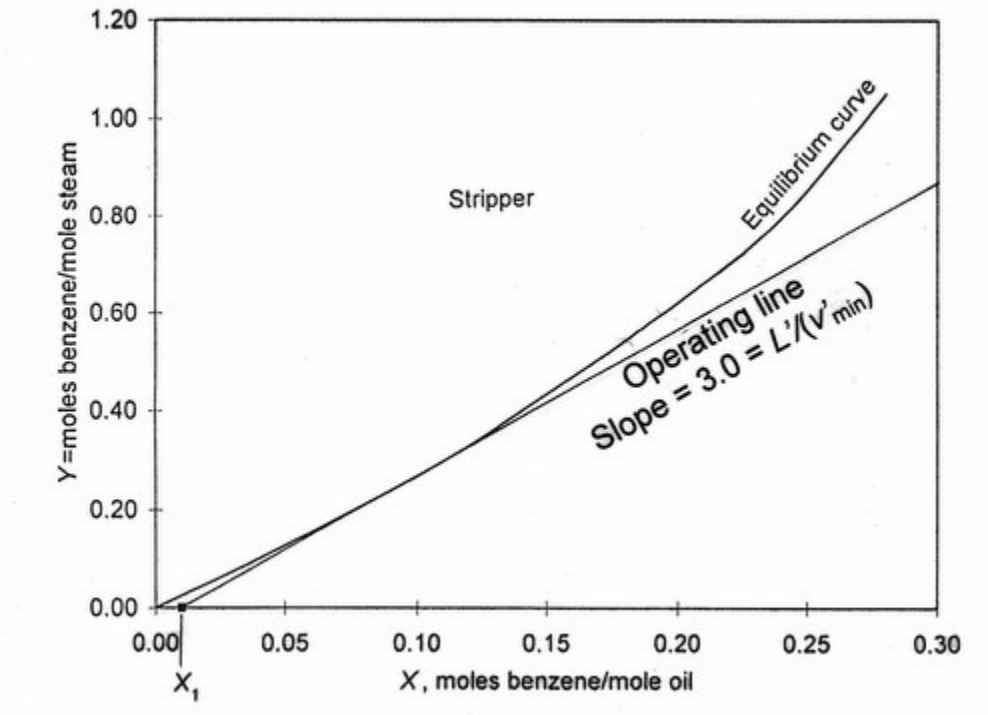
Exercise 6.9 (continued)

Analysis: (continued)

(a) Plot of results:



(b) Plot of results:



Exercise 6.10

Subject: Stripping of benzene (B) from straw oil by steam at 1 atm (101.3 kPa).

Given: Oil enters stripper with 8 mol% benzene. 75% of B is stripped. Pure steam enters. Steam exits with 3 mol% B. Sieve-plate column. Henry's law holds with a B partial pressure of 5.07 kPa when benzene mole fraction in the oil is 10 mol%.

Assumptions: Straw oil is not volatile and steam does not condense. Dalton's law.

Find: (a) Number of equilibrium stages required.
(b) Moles of steam required per 100 moles of benzene-oil feed to stripper.
(c) Number of equilibrium stages needed if 85% of B is stripped with same amount of steam as in Part (b).

Analysis: With reference to the stripper in Fig. 6.11(b),
X_{N+1} = 8/92 = 0.087 mol B/mol B-free oil
Y_0 = 0.0 mol B/mol B-free steam
Y_N = 3/97 = 0.0309 mol B/mol B-free steam
(b) For 100 moles of benzene-oil feed mixture, have 8 moles of benzene. Amount of benzene stripped = 0.75(8) = 6 moles. Because the exit gas contains 0.0309 mol B/mol B-free steam, the steam rate = 6/0.0309 = 194 moles.
Therefore, moles of steam/100 moles of benzene-oil feed = 194
Also, X_1 = (8 - 6)/92 = 0.0217 mol B/mol B-free oil

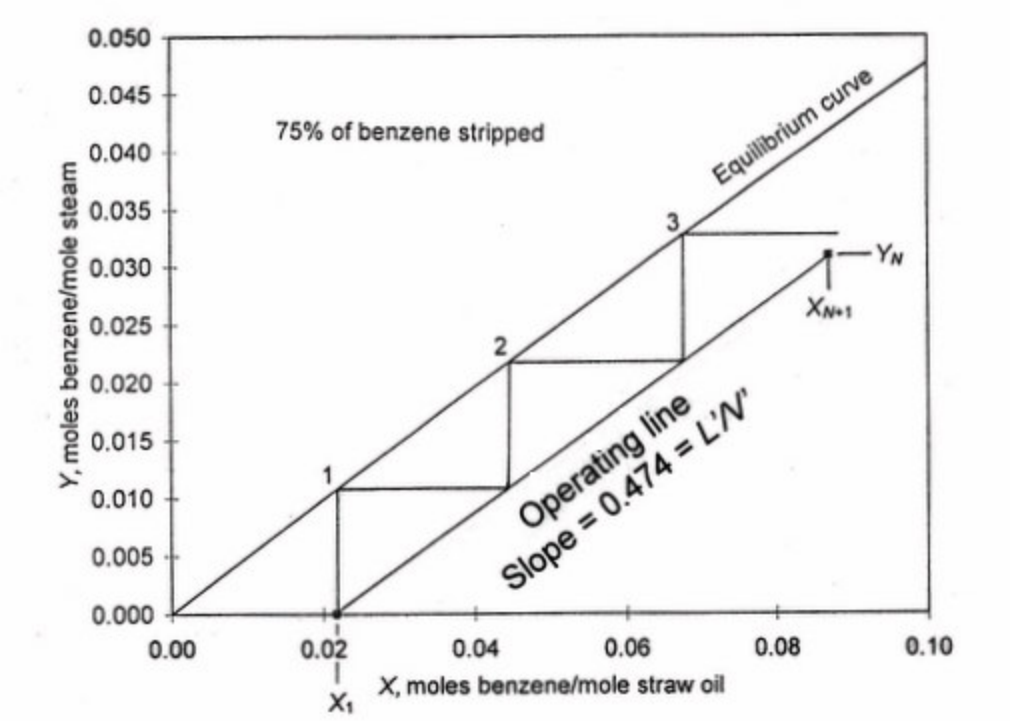
(a) Assume Henry's law is given by Eq. (4-32), $p_B = Hx_B$. Because p_B = 5.07 kPa when x_B = 0.10, H = 5.07/0.1 = 50.7 kPa. Convert this to an Y-X equilibrium equation. For a pressure of 101.3 kPa, assuming Dalton's law, $y_B = p_B/P = 50.7x_B/101.3 = 0.5x_B$. From Eq. (6-1), dropping the benzene subscript, B, and noting that K_B = 0.5,

$$K_B = 0.5 = \frac{Y/(1+Y)}{X/(1+X)} \qquad \text{Solving, } Y = \frac{0.5X}{1+0.5X} \qquad (1)$$

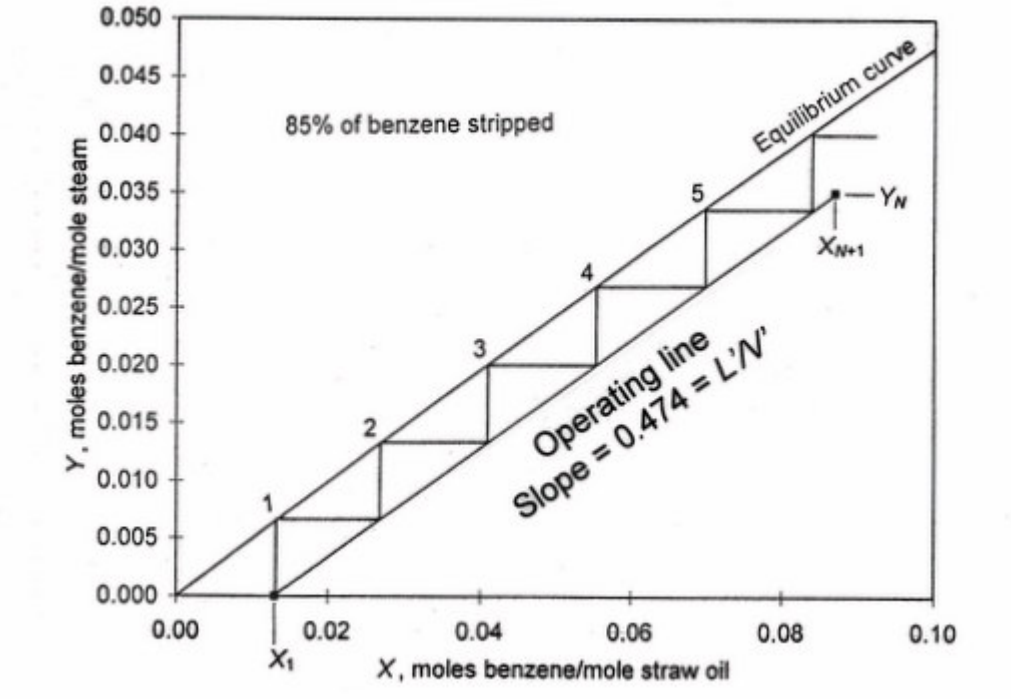
The Y-X plot includes the equilibrium curve given by Eq. (1), and a straight operating line that connects the column terminal points (Y_0 = 0.0, X_1 = 0.0217) and (Y_N = 0.0309, X_{N+1} = 0.087). The corresponding slope of the operating line is (0.0309 - 0.0)/(0.087 - 0.0217) = L'/G' = 0.474. From the plot below, stepping off stages as in Fig. 6.11(b), required N = approximately 3 stages.
(c) For 85% stripping of B, amount of B stripped = 0.85(8) = 6.8 moles B. Not stripped is1.2 moles B. Therefore, for the same B-oil and steam feeds, X_1 = 1.2/92 = 0.01304 mol B/mol oil and Y_N =6.8/194 = 0.03505 mol B/mol steam. The Y-X plot for this case is also given below, where the equilibrium curve is the same as in Part (a), and a straight operating line connects the column terminal points (Y_0 = 0.0, X_1 = 0.01304) and (Y_N = 0.03505, X_{N+1} = 0.087). The corresponding slope of the operating line is (0.03505 - 0.0)/(0.087 - 0.01304) = L'/G' = 0.474 (same as in Part (a)). From the plot below, stepping off stages as in Fig. 6.11(b), required N = between 5 and 6 stages.

Exercise 6.10 (continued)

Analysis: (continued)
(a) Plot of results:



(b) Plot of results:



Exercise 6.11

Subject: Stripping of VOCs from water by air in a trayed tower to produce drinking water.

Given: 1,500 gpm of groundwater containing ppm amounts of DCA, TCE, and TCA given below. Stripping at 1 atm and 25°C to reduce the ppm amounts to the very low levels below. *K*-values of VOCs given below.

Assumptions: No stripping of water and no absorption of air. System is dilute with respect to the VOCs.

Find: Minimum air flow rate in scfm (60°F and 1 atm).
Number of equilibrium stages for 2 times the minimum air flow.
Composition in ppm for each VOC in the resulting drinking water.

Analysis: Flow rate of water = L = (1,500 gpm)(8.33 lb/gal)/18.02 lb/lbmol = 693 lbmol/min
% stripping of a VOC = (inlet ppm - outlet ppm)/inlet ppm)

VOC	K-value	Inlet ppm	Outlet ppm	% stripping
DCA	60	85	0.005	99.994
TCE	650	120	0.005	99.996
TCA	275	145	0.200	99.862

Because of its high % stripping and a *K*-value that is much lower than for the other two VOCs, the stripper is likely to be controlled by DCA. So base the calculations on DCA and then check to see that the % stripping for TCE and TCA exceed the above requirements. Because of the dilute conditions, use Kremser's method.

From Eq. (6-12), $$V_{\min} = \frac{L}{K}(\text{fraction stripped}) = \frac{693}{60}(0.99994) = 11.55 \text{ lbmol./min}$$

or minimum air flow rate = 11.55 (379 scf/lbmol) = 4,377 scfm at 60°F and 1 atm
For 2 times the minimum value, V = 2(11.55) = 23.1 lbmol/min.

The stripping factor, given by Eq. (6-16), is for DCA, $$S_{DCA} = \frac{K_{DCA}V}{L} = \frac{60(23.1)}{693} = 2.0$$

From Eq. (6-14), Fraction stripped $$= 0.99994 = \frac{S^{N+1} - S}{S^{N+1} - 1} = \frac{2^{N+1} - 2}{2^{N+1} - 1} \qquad (1)$$

Solving Eq. (1), N = 13 stages.
Now, for V = 11.55 lbmol/min and N = 13 stages, compute the fraction stripped for TCE and TCA from Eq. (6-14) with the stripping factor from Eq. (6-16). The results are:

VOC	S	Fraction stripped
DCA	2.0	0.99994
TCE	21.6	1.00000
TCA	9.17	1.00000

The drinking water contains 0.005 ppm of DCA and essentially zero ppm of TCE and TCA.

Exercise 6.12

Subject: Stripping of a solution of SO_2, butadienes, and butadiene sulfone with nitrogen.

Given: 120 lbmol/h of liquid containing in lbmol/h,10.0 SO_2, 8.0 1,3-butadiene (B3), 2.0 1,2-butadiene (B2), and 100.0 butadiene sulfone (BS). Liquid effluent to contain < 0.05 mol% SO_2 and < 0.5 mol% (B3 + B2). Stripping agent is pure nitrogen. Stripping at 70°C and 30 psia. *K*-values are 6.95 for SO_2, 3.01 for B2, 4.53 for B3, and 0.016 BS.

Assumptions: Negligible stripping of BS because of its low *K*-value. No absorption of N_2.

Find: Flow rate of nitrogen. Number of equilibrium stages.

Analysis: Assuming no stripping of BS, the exiting liquid will contain 0.05 mol% SO_2, 0.50 mol% (B3 + B2), and 99.45 mol% BS, or in lbmol/h, 100.0 BS, 0.0503 SO_2, and 0.503 (B3 + B2). Therefore, % stripping of SO_2 = (10.0 - 0.0503)/10.0 = 0.99497 and % stripping of (B3 + B2) = (8.0 + 2.0 - 0.503)/(8.0 + 2.0) = 0.9497.
The minimum stripping agent flow rate is given by Eq. (6-12). Assume that because the *K*-value of B2 is the lowest of SO_2, B2, and B3, that B2 controls. Further assume that essentially all of the B3 is stripped so that the 0.5 mol% of (B2 + B3) is entirely B2. The solute-free liquid rate = flow rate of BS = L' = 100 lbmol/h and the fraction of B2 stripped = (2.0 - 0.503)/2.0 = 0.748

$$V'_{\min} = \frac{L'}{K_{SO_2}}(\text{fraction stripped}) = \frac{100}{3.01}(0.748) = 24.9 \text{ lbmol/h}$$

Now use this value to compute the values of fraction stripped of SO_2 and B3.

$$\text{Fraction stripped of } SO_2 = \frac{KV'}{L'} = \frac{6.95(24.9)}{100} > 1.0$$

$$\text{Fraction stripped of B3} = \frac{KV'}{L'} = \frac{4.53(24.9)}{100} > 1.0$$

Therefore, the assumption that B2 controls is correct at the minimum stripping gas rate.
Assume an operational nitrogen flow rate of 1.5 times minimum. Therefore V' =1.5(24.9) = 37.4 lbmol./h. The stripping factor, given by Eq. (6-16), is for B2,

$$S_{B2} = \frac{K_{B2}V'}{L'} = \frac{3.01(37.4)}{100} = 1.13$$

Using Eq. (6-14), Fraction B2 stripped $= 0.748 = \dfrac{S^{N+1} - S}{S^{N+1} - 1} = \dfrac{1.13^{N+1} - 1.13}{1.13^{N+1} - 1}$

Solving, N = 2.4 equilibrium stages.

Exercise 6.12 (continued)

Analysis: (continued)

$$\text{Fraction B3 stripped} = \frac{S^{N+1} - S}{S^{N+1} - 1} = \frac{1.7^{2.4+1} - 1.7}{1.7^{2.4+1} - 1} = 0.863$$

$$\text{Fraction } SO_2 \text{ stripped} = \frac{S^{N+1} - S}{S^{N+1} - 1} = \frac{2.61^{2.4+1} - 2.61}{2.61^{2.4+1} - 1} = 0.936$$

These fractions do not meet specifications. Therefore, the number of stages and/or the nitrogen flow rate must be increased.

First try increasing the number of stages.

	SO_2	B2	B3
$S = KV/L$	2.61	1.13	1.7
Fraction stripped:			
$N = 5$	0.995	0.880	0.970
$N = 7$	0.9993	0.922	0.990
$N = 10$	0.99996	0.954	0.998

For $N = 5$ stages, have in the exit liquid in lbmol/h, 0.05 SO_2, 0.24 B2, and 0.24 B3. These values correspond to a total of 100.53 lbmol/h of exit liquid. This results in 0.05 mol% SO_2 and 0.48% (B2 + B3). Therefore, $N =$ 5 stages is sufficient with a feed gas rate, V' , of 37.4 lbmol/h. Other combinations of N and V' could be used..

Exercise 6.13

Subject: Absorption of a light hydrocarbon gas mixture by n-decane as a function of pressure and number of equilibrium stages at 90°F.

Given: Light hydrocarbon gas containing in lbmol/h, 1,660 C_1, 168 C_2, 96 C_3, 52 nC_4, and 24 nC_5 for a total of 2,000 lbmol/h = V. Absorbent of L = 500 lbmol/h of nC_{10}. K-value of nC_{10} = 0.0011.

Find: Component flow rates in the lean gas and rich oil for:
(a) N = 6 and P = 75 psia.
(b) N = 3 and P = 150 psia.
(c) N = 6 and P = 150 psia.

Analysis: Use the Kremser method with Eqs. (5-48) for fraction not absorbed, ϕ_A, (5-50 for fraction not stripped, ϕ_A ,(5-38) for absorption factor, A, (5-51) for stripping factor, S , (5-45) and (5-53) for component flow rates in the exit gas, v_1 , and (5-44) and (5-52) for component flow rates in the exit liquid, l_N, since no light hydrocarbons enter with the absorbent. Use Fig. 2.8 or other source for K-values of C_1 through nC_5. For nC_{10} , assume the K-value is inversely proportional to pressure.

(a) N = 6 and P = 75 psia:

Component	K-value	A	S	ϕ_A	ϕ_S	v_1 lbmol/h	l_6 lbmol/h
C_1	2.9	0.0086		0.9914		1,646.0	14.0
C_2	6.5	0.0385		0.9615		161.5	6.5
C_3	1.95	0.1282		0.8718		83.7	12.3
nC_4	0.61	0.4098		0.5916		30.8	21.2
nC_5	0.19	1.3160		0.0541		1.3	22.7
nC_{10}	0.0011		0.0044		0.9956	2.2	497.8
Total						1,925.5	574.5

(b) N = 3 and P = 150 psia:

Component	K-value	A	S	ϕ_A	ϕ_S	v_1 lbmol/h	l_3 lbmol/h
C_1	14.0	0.0179		0.9821		1,630.0	30.0
C_2	3.5	0.0714		0.9284		156.0	12.0
C_3	1.05	0.2381		0.7644		73.4	22.6
nC_4	0.33	0.7576		0.3615		18.8	33.2
nC_5	0.105	2.3810		0.0443		1.1	22.9
nC_{10}	0.00055		0.0022		0.9978	1.1	498.9
Total						1,880.4	619.6

Exercise 6.13 (continued)

Analysis: (continued)

(c) $N = 6$ and $P = 150$ psia:

Component	K-value	A	S	ϕ_A	ϕ_S	v_1 lbmol/h	l_6 lbmol/h
C_1	14.0	0.0179		0.9821		1,630.0	30.0
C_2	3.5	0.0714		0.9284		156.0	12.0
C_3	1.05	0.2381		0.7619		73.1	22.9
nC_4	0.33	0.7576		0.2829		14.7	37.3
nC_5	0.105	2.3810		0.0032		0.1	23.9
nC_{10}	0.00055		0.0022		0.9978	1.1	498.9
Total						1,875.0	625.0

Exercise 6.14

Subject: Absorption of a light hydrocarbon gas by nC_{10}.

Given: 1,000 kmol/h of rich gas at 70°F with, in kmol/h, 250 C_1, 150 C_2, 200 C_3, 200 nC_4, and 150 nC_5. 500 kmol/h of nC_{10} at 90°F. Absorber operates at 4 atm. *K*-value of nC_{10} at 80°F and 4 atm = 0.0014.

Assumptions: Using the Kremser method, use V = 1,000 kmol/h and L = 500 kmol/h, with an average temperature of 80°F for *K*-values from Fig. 2.8 or other source.

Find: Percent absorption of each component for 4, 10, and 30 equilibrium stages.

Analysis: The *K*-values and absorption factors, from Eq. (6-15), $A = L/KV$, are:

Component	*K*-value	*A*
C_1	38	0.0132
C_2	7.6	0.0658
C_3	2.25	0.2222
nC_4	0.64	0.7813
nC_5	0.195	2.564

For each component in the feed gas, the percent absorption is given by Eq. (6-13) x 100%,

$$\text{Percent absorbed} = \frac{A^{N+1} - A}{A^{N+1} - 1} \times 100\% \qquad (1)$$

Using Eq. (1) with the values of *A* from the above table, the results are:

	Percent absorbed:		
Component	for $N = 4$	for $N = 10$	for $N = 30$
C_1	1.32	1.32	1.32
C_2	6.58	6.58	6.58
C_3	22.03	22.22	22.22
nC_4	65.14	76.58	78.12
nC_5	96.30	99.995	100.00

The number of stages affects only the heavier hydrocarbons that are absorbed to the greatest extent.

Exercise 6.15

Subject: Back calculation of tray efficiency from performance data on absorption of propane.

Given: Large commercial absorber with N_a = 16 actual plates. From Example 6.3, average total liquid rate, L, is 446.7 lbmol/h, average total gas rate, V, is 866.5 lbmol/h. Propane in gas feed = 213.8 lbmol/h. Propane in exit liquid = 43 lbmol/h. P = 93.7 psia. Average T = 111°F.

Find: Tray efficiency from performance data. Estimated tray efficiency from Drickamer-Bradford and O'Connell correlations.

Analysis: Fraction of propane absorbed = 43/213.8 = 0.20

From Fig. 2.8, for propane, K-value = 2.0

From Eq. (6-15), $A = L/KV = 446.7/(2.0)(866.5) = 0.258$

From Eq. (6-13),

$$\text{Fraction absorbed} = 0.20 = \frac{A^{N+1} - A}{A^{N+1} - 1} = \frac{0.258^{N+1} - 0.258}{0.258^{N+1} - 1} \qquad (1)$$

Solving Eq. (1), $N = N_t = 0.93$

From Eq. (6-1), $E_o = N_t / N_a = 0.93/16 = 0.058$ or 5.8%

From Drickamer-Bradford correlation, Eq. (6-22), with μ_L = 1.4 cP from Example 6.3,

$$E_o\,,\ \% = 19.2 - 57.8 \log \mu_L = 19.2 - 57.8 \log(1.4) = 10.8\ \%$$

From O'Connell correlation, Eq. (6-23), with M_L = 250, ρ_L = 57.9 lb/ft^3 from Example 6.3,

$$\log E_o = 1.587 - 0.199 \log C - 0.0896 [\log C]^2 \qquad (2)$$

$$\text{where, } C = \left(\frac{K M_L \mu_L}{\rho_L} \right) = \left[\frac{(2.0)(250)(1.4)}{57.9} \right] = 12.1$$

Therefore, from Eq. (2),

$$\log E_o = 1.587 - 0.199 \log 12.1 - 0.0896 [\log 12.1]^2 = 1.277$$

which gives E_o = 18.9%

The propane tray efficiency is lower than predicted.

Exercise 6.16

Subject: Oil absorption of a gas to produce 95% hydrogen

Given: 800,000 scfm (0°C, 1 atm) of fuel gas containing 72.5% H_2, 25% CH_4, and 2.5% C_2H_6. Absorbent of nC_8. Absorber operates at 400 psia and 100°F. Exiting gas is to contain at least 80% of the entering H_2 at a H_2 purity of 95 mol%.

Assumptions: Ideal gas law.

Find: (a) Minimum absorbent rate in gpm.
(b) Actual absorbent rate at 1.5 times minimum.
(c) Number of theoretical stages.
(d) Stage efficiency of each component from O'Connell correlation.
(e) Number of actual trays needed.
(f) Composition of exit gas, accounting for stripping of octane.
(g) Annual cost of lost octane.

Analysis: At 0°C and 1 atm, have 359 scf/lbmol. Therefore, entering V = 800,000/359 = 2,230 lbmol/min, with 0.725(2,230) = 1,616 lbmol/min H_2, 558 lbmol/min CH_4, 56 lbmol/min C_2H_6 . From Fig. 2.8, at 400 psia, 100°F, K-values are: 30 for H_2 , 7 for CH_4 , and 1.75 for C_2H_6 .

(a) Assume the key component is CH_4. If we neglect stripping of octane and assume complete absorption of C_2H_6, with 20% absorption of H_2, then exit gas will be 0.8(1,616) = 1,293 lbmol/min H_2 and the exit liquid will contain 1,616 - 1,293 = 323 lbmol/min H_2. For a purity of 95 mol% H_2, then will have 5 mol% CH_4 or 1,293(5/95) = 68 lbmol/min of CH_4 in the exit gas and 558 - 68 = 490 lbmol/min of CH_4 in exit liquid. Can not use Eq. (6-11) to compute the minimum absorbent rate because we do not have a dilute system. Instead, for infinite stages, assume the exiting rich oil is in equilibrium with the inlet gas. Then, for CH_4, $K = 7 = y/x$. But y for the inlet gas = 0.25. Therefore, x in the exiting oil = 0.25/7= 0.0357. Therefore, with 490 lbmol/min of CH_4 in this oil, the total exiting oil = 490/0.0357 = 13,700 lbmol/min. Therefore, the entering oil is 13,700 - 323 - 490 - 56 = 12,831 lbmol/min of $nC_8 = L_{min}$. For nC_8 , MW = 114 and from Perry's Handbook, SG = 0.703. Therefore, liquid density = 0.703(8.33) = 5.86 lb/gal. Therefore, L_{min} = 12,831(114)/5.86 = 250,000 gpm.

(b) For 1.5 times minimum, inlet absorbent rate = 19,200 lbmol/min = 375,000 gpm.

(c) Calculate the number of equilibrium stages from the Kremser equation based on CH_4 absorption, inlet vapor and liquid flow rates. From Eq. (6-15),

$$A_{CH_4} = L / KV = 19{,}200 / (7)(2{,}230) = 1.23$$

From Eq. (6-13), for CH_4, with a fraction absorbed = 490/558 = 0.878,

$$\text{fraction of } CH_4 \text{ absorbed} = 0.878 = \frac{A_{CH_4}^{N+1} - A_{CH_4}}{A_{CH_4}^{N+1} - 1} = \frac{1.23^{N+1} - 1.23}{1.23^{N+1} - 1} \qquad (1)$$

Exercise 6.16 (continued)

Analysis: (c) (continued)

Solving Eq. (1), N =4.1 stages.
Check absorption of H_2. Absorption factor = A = 19,200/(30)(2,230) =0.287

From Eq. (6-13, fraction of H_2 absorbed = $\dfrac{A_{H_2}^{N+1} - A_{H_2}}{A_{H_2}^{N+1} - 1} = \dfrac{0.287^{4.1+1} - 0.287}{0.287^{4.1+1} - 1} = 0.286$

This exceeds the minimum 20% specified. Actually, this problem is overspecified. The absorber can be designed for 95 mol% purity of H_2 in the exit gas or 20% absorption of H_2. In this problem, we can not achieve both specifications, unless the plate efficiency for H_2 is much less than that for CH_4. Check this next.

(d) From the O'Connell correlation, Eq. (6-23), with M_L = 114, ρ_L = 44 lb/ft^3, and μ_L= 0.47 cP from Perry's Handbook,

$$\log E_o = 1.587 - 0.199 \log C - 0.0896 [\log C]^2 \qquad (2)$$

where, for H_2, $C = \left(\dfrac{K M_L \mu_L}{\rho_L} \right) = \left[\dfrac{(30)(114)(0.47)}{44} \right] = 36.5$

Therefore, from Eq. (2),

$$\log E_o = 1.587 - 0.199 \log 36.5 - 0.0896 [\log 36.5]^2 = 1.057$$

which gives E_o = 11.4 % for H_2. Similarly, E_o = 21.1 % for CH_4, and E_o = 32.5 % for C_2H_6.

(e) From Eq. (6-21), using CH_4, $N_a = N_t / E_o$ = 4.1/0.211 = 19.4 or say 20 trays.
(f) For the stripping of nC_8, from Fig. 2.8 by extrapolation, K = 0.003. From Eq. (2), E_o = 0.35. Therefore, if 20 trays, have 20(0.35) = 7 equilibrium stages. From Eq. (6-16), $S = KV/L$ =0.003(2,230)/19,200 = 0.00035. From Eq. (6-14) for 7 stages,

$$\text{fraction stripped} = \frac{S^{N+1} - S}{S^{N+1} - 1} = \frac{0.00035^{7+1} - 0.00035}{0.00035^{7+1} - 1} = 0.00035$$

Therefore, 0.00035(19,200) = 7 lbmol/h of nC_8 leaves in the exit gas.
For H_2, with 20 trays and E_o = 0.114, we have (0.114)(20) = 2.3 equilibrium stages. From Eq. (6-13), with A = 0.287, fraction H_2 absorbed = $\dfrac{A_{H_2}^{N+1} - A_{H_2}}{A_{H_2}^{N+1} - 1} = \dfrac{0.287^{2.3+1} - 0.287}{0.287^{2.3+1} - 1} = 0.275$

Therefore, we can not meet the specification of less than 20% absorbed.
For C_2H_6, with 20 trays and E_o = 0.325, we have (0.325)(20) = 6.5 equilibrium stages.
From Eq. (6-13), with A = (19,200)/(1.75)(2,230) = 4.92,

$$\text{fraction } C_2H_6 \text{ absorbed} = \frac{A^{N+1} - A}{A^{N+1} - 1} = \frac{4.92^{6.5+1} - 4.92}{4.92^{6.5+1} - 1} = 0.999975$$

Composition of exit gas in lbmol/min is 1,172 H_2, 68 CH_4, and 7 nC_8. H_2 purity = 94%
(g) Cost of lost oil = 7(114)(60)(7,900)($1.00)/(5.86 lb/gal) = 64.6 million $/year.

Exercise 6.17

Subject: Scale-up of absorber using Oldershaw column efficiency.

Given: Absorption operation of Examples 6.1 and 6.4 with a column diameter of 3 ft. New column with 11.5 ft diameter. New tray with Oldershaw-column efficiency of 55% ($E_{OV} = 0.55$). Liquid flow path length from Fig. 6.16. Value of $u/D_E = 6$ ft^{-1}. From Example 6.4, $\lambda = 0.68$.

Assumptions: Straight operating line and equilibrium line as stated in Example 6.4

Find: Efficiencies E_{MV} and E_o .

Analysis: Consider three cases: (a) complete mixing, (b) plug flow, and (c) partial mixing.

(a) From Eq. (6-31), $E_{MV} = E_{OV} = 0.55$. From Eq. (6-37),

$$E_o = \frac{\log\left[1 + E_{MV}(\lambda - 1)\right]}{\log \lambda} = \frac{\log\left[1 + 0.55(0.68 - 1)\right]}{\log 0.68} = 0.50$$

(b) From Eq. (6-32),

$$E_{MV} = \frac{1}{\lambda}\left(e^{\lambda E_{OV}} - 1\right) = \frac{1}{0.68}\left(e^{(0.68)(0.55)} - 1\right) = 0.67$$

From Eq. (6-37),

$$E_o = \frac{\log\left[1 + E_{MV}(\lambda - 1)\right]}{\log \lambda} = \frac{\log\left[1 + 0.67(0.68 - 1)\right]}{\log 0.68} = 0.63$$

(c) To use Fig. 6.16, we need an estimate of the liquid flow rate. For the 3 ft diameter column of Examples 6.1 and 6.4, liquid rate = 151.5 kmol/h of water. Assume the liquid rate is proportional to the column cross-sectional area. Thus, for the 11 ft diameter, the liquid rate = $151.5(11/3)^2 = 2{,}037$ kmol/h = 162 gpm. From Fig. 6.16, a single-pass tower is adequate. Assume liquid flow path = $Z_L = 7$ ft. Eq. (6-34) is used to compute E_{MV}, which requires the Peclet number, given by Eq. (6-36),

$$N_{Pe} = \frac{Z_L u}{D_E} = 7(6) = 42$$

From Eq. (6-35), $\eta = \frac{N_{Pe}}{2}\left[\left(1 + \frac{4\lambda E_{OV}}{N_{Pe}}\right)^{1/2} - 1\right] = \frac{42}{2}\left[\left(1 + \frac{4(0.68)(0.55)}{42}\right)^{1/2} - 1\right] = 0.37$

From Eq. (6-34), $E_{MV}/E_{OV} = 1.20$. Therefore, $E_{MV} = 1.20(0.55) = 0.66$

From Eq. (6-37),

$$E_o = \frac{\log\left[1 + E_{MV}(\lambda - 1)\right]}{\log \lambda} = \frac{\log\left[1 + 0.66(0.68 - 1)\right]}{\log 0.68} = 0.62$$

From these results, we see that the column is operating closely to plug flow for the liquid.

Exercise 6.18

Subject: Estimation of column diameter based on conditions at bottom tray of a reboiled stripper.

Given: Vapor and liquid conditions at bottom tray given in Fig. 6.48. Valve trays with 24-inch spacing.

Find: Column diameter for 80% of flooding.

Analysis: Use entrainment flooding correlation of Fig. 6.24, where the abscissa is,

$$F_{LV} = \frac{LM_L}{VM_G}\left(\frac{\rho_G}{\rho_L}\right)^{1/2} \qquad (1)$$

From Fig. 6.48, V = 546.2 lbmol/h and L = 621.3 lbmol/h

Average molecular weights of the gas and liquid are computed from $M = \sum_{i=1}^{C} z_i M_i$,

Component	M	y	My	x	Mx
Ethane	30.07	0.000006	0.0	0.000010	0.0
Propane	44.10	0.004817	0.2	0.001448	0.1
n-Butane	58.12	0.602573	35.0	0.391389	22.7
n-Pentane	72.15	0.325874	23.5	0.430599	31.1
n-Hexane	86.18	0.066730	5.8	0.176563	15.2
Total			64.5		69.1

Therefore, M_V = 64.5 and M_L = 69.1

Gas volumetric flow rate = Q_V = 6.192 ft^3/s.

Therefore, $\rho_V = VM_V/Q_V$ = (546.2)(64.5)/(6.192)(3,600) = 1.58 lb/ft^3

Liquid volumetric flow rate = 171.1 gpm = (171.1)(60)/7.48 = 1,372 ft^3/h

Therefore, $\rho_L = LM_L/Q_L$ = (621.3)(69.1)/1,372 = 31.3 lb/ft^3

From Eq. (1), $F_{LV} = \frac{621.3(69.1)}{546.2(64.5)}\left(\frac{1.58}{31.3}\right)^{1/2} = 0.274$

Assume 24-inch tray spacing. From Fig. 6.24, C_F = 0.24 ft/s

From relations below Eq. (6-44), since F_{LV} is between 0.1 and 1.0,

$$\frac{A_d}{A} = 0.1 + \frac{(F_{LV} - 0.1)}{9} = 0.1 + \frac{(0.274 - 0.1)}{9} = 0.119$$

From Perry's Handbook, surface tension = σ = 7 dyne/cm

From relation below Eq. (6-42), $F_{ST} = (\sigma/20)^{0.2} = (7/20)^{0.2} = 0.8$. F_F = 1.0 , F_{HA} = 1.0

From Eq. (6-42), $C = F_{ST}F_F F_{HA}C_F$ = (0.8)(1.0)(1.0)(0.24) = 0.192 ft/s

From Eq. (6-40), $U_f = C\left[(\rho_L - \rho_V)/\rho_V\right]^{1/2} = 0.192\left[(31.3 - 1.58)/1.58\right]^{1/2} = 0.833$ ft/s

Exercise 6.18 (continued)

From Eq. (6-44),

$$D_T = \left[\frac{4VM_V}{fU_f\pi(1-A_d/A)\rho_V}\right]^{1/2} = \left[\frac{4(546.2/3,600)(64.5)}{0.80(0.833)(3.14)(1-0.119)(1.58)}\right]^{1/2} = 3.\ 56\,\text{ft}$$

Exercise 6.19

Subject: Estimation of column diameter based on conditions at the top tray of an absorber.

Given: Vapor and liquid conditions at the top tray. Valve trays with 24-inch spacing.

Find: Flooding velocity and column diameter for 85% of flooding ($f = 0.85$)

Analysis: Use entrainment flooding correlation of Fig. 6.24, where the abscissa is,

$$F_{LV} = \frac{LM_L}{VM_V}\left(\frac{\rho_V}{\rho_L}\right)^{1/2} = \frac{889(109)}{530(26.6)}\left(\frac{1.924}{41.1}\right)^{1/2} = 1.487 \qquad (1)$$

For 24-inch tray spacing, from Fig. 6.24, $C_F = 0.082$ ft/s

From relations below Eq. (6-44), since F_{LV} is < 0.1, $A_d/A = 0.1$

From relation below Eq. (6-42), $F_{ST} = (\sigma/20)^{0.2} = (18.4/20)^{0.2} = 0.98$. $F_F = 0.75$, $F_{HA} = 1.0$

From Eq. (6-42), $C = F_{ST}F_F F_{HA}C_F = (0.98)(0.75)(1.0)(0.082) = 0.0603$ ft/s

From Eq. (6-40), $U_f = C\left[\left(\rho_L - \rho_V\right)/\rho_V\right]^{1/2} = 0.0603\left[\left(41.1 - 1.924\right)/1.924\right]^{1/2} = 0.272$ ft/s

From Eq. (6-44), $D_T = \left[\frac{4VM_V}{fU_f\pi\left(1 - A_d/A\right)\rho_V}\right]^{1/2} = \left[\frac{4(530/3,600)(26.6)}{0.85(0.272)(3.14)(1-0.1)(1.924)}\right]^{1/2} = 3.53$ ft

Exercise 6.20

Subject: Hydraulic calculations for bottom tray of a sieve-tray column

Given: Absorber of Exercise 6.16 with an absorbent flow rate of 40,000 gpm of nC_8. Sieve trays on 24-inch spacing , with a weir height of 2.5 inches and 1/4-inch holes. Foaming factor = 0.80 and fraction flooding = 0.70.

Find: (a) Column diameter at bottom.
(b) Vapor pressure drop/tray.
(c) Whether weeping will occur.
(d) Entrainment rate.
(e) Fractional decrease in Murphree efficiency due to entrainment.
(f) Froth height in downcomer.

Analysis: From Exercise 6.16, V = 800,000/359 = 2,230 lbmol/min of entering gas.
Average MW of gas = 0.725(2.016) + 0.25(16.04) + 0.025(30.05) = 6.22
Assuming ideal gas law for gas at 400 psia and 100°F,

$\rho_V = PM/RT$ = (400)(6.22)/(10.73)(560) = 0.414 lb/ft^3

For the liquid, neglect absorbed components. ρ_L = 43.9 lb/ft^3 = 5.86 lb/gal
MW of nC_8 = 114. Therefore, L = 40,000(5.86)/114 = 2,056 lbmol/min

(a) Use entrainment flooding correlation of Fig. 6.24, where the abscissa is,

$$F_{LV} = \frac{LM_L}{VM_V}\left(\frac{\rho_V}{\rho_L}\right)^{1/2} = \frac{2,056(114)}{2,230(6.22)}\left(\frac{0.414}{43.9}\right)^{1/2} = 1.64 \qquad (1)$$

From Fig. 6.24, for 24-inch tray spacing, C_F = 0.08. Because $F_{LV} > 1$, A_d/A = 0.2.
F_{HA} = 1.0, F_F = 0.8, and since σ = 20 dynes/cm, F_{ST} = 1.0.
From Eq. (6-24), $C = F_{ST}F_FF_{HA}C_F$ = (1)(0.8)(1)(0.08) = 0.064 ft/s

From Eq. (6-40), $U_f = C\left[(\rho_L - \rho_V)/\rho_V\right]^{1/2} = 0.064\left[(43.9 - 0.414)/0.414\right]^{1/2} = 0.66$ ft/s

From Eq. (6-44), $D_T = \left[\frac{4VM_V}{fU_f\pi(1 - A_d/A)\rho_V}\right]^{1/2} = \left[\frac{4(2,230/60)(6.22)}{0.70(0.66)(3.14)(1-0.2)(0.414)}\right]^{1/2} = 44$ ft

This is a very large diameter. Would probably use two parallel columns of 31 ft each, but continue with 44 ft diameter.

(b) Vapor pressure drop per tray is given by Eq. (6-49), $h_t = h_d + h_l + h_\sigma$ (2)
From the continuity equation, $m = uA\rho$, hole velocity for 10% hole area =
u_o = (2,230/60)(6.22)/(3.14/4)(44)^2(0.414)(0.1) = 3.68 ft/s and superficial velocity = 0.368 ft/s

From Eq. (6-50), $h_d = 0.186\left(\frac{u_o^2}{C_o^2}\right)\left(\frac{\rho_V}{\rho_L}\right) = 0.186\left(\frac{3.68^2}{0.73^2}\right)\left(\frac{0.414}{43.9}\right) = 0.045$ in. of nC_8

Exercise 6.20 (continued)

Analysis: (continued)

Active bubbling area for $A_d/A = 0.2$ is $A_a = A - 2A_d = 0.6\,A$. So, $U_a = 0.368/0.6 = 0.61$ ft/s

From Eq. (6-53), $K_s = U_a\left(\frac{\rho_V}{\rho_L - \rho_V}\right)^{1/2} = 0.61\left(\frac{0.414}{43.9 - 0.414}\right)^{1/2} = 0.06$ ft/s

From Eq. (6-52), $\phi_e = \exp(-4.257K_s^{0.91}) = \exp[-4.257(0.06)^{0.91}] = 0.72$
From Eq. (6-54), $C = 0.362 + 0.317\exp(-3.5h_w) = 0.362 + 0.317\exp[-3.5(2.5)] = 0.362$
Take weir length, $L_w = 0.73D_T = 0.73(44) = 32.1$ ft = 385 in.

From Eq. (6-51), $h_l = \phi_e\left[h_w + C\left(\frac{q_L}{L_w\phi_e}\right)^{2/3}\right] = 0.72\left[2.5 + 0.362\left(\frac{40{,}000}{(385)0.72}\right)^{2/3}\right] = 9.0$ in. of nC_8

From Eq. (6-55), with maximum bubble size of 1/4 inch = 0.00635 m,
$h_\sigma = 6\sigma / g\rho_L D_{B_{max}} = 6(20/1000)/(9.8)(703)(0.00635) = 0.00274$ m = 0.11 in. nC_8

From Eq. (2), $h_t = h_d + h_l + h_\sigma = 0.045 + 9.0 + 0.11 = 9.2$ in. nC_8 = 0.23 psi/tray. Excessive!

(c) Apply criterion of Eq. (6-64). $h_d + h_\sigma = 0.045 + 0.11 = 0.155$ in. < h_l = 9.0 in.
Therefore, weeping will occur.

(d) From Fig. 6.28, since $F_{LV} = 1.64$, entrainment will be very low.

(e) Because entrainment is very low, E_{MV} will not decrease.

(f) From Eqs. (6-70) and (6-72), $h_{df} = (h_t + h_l + h_{da})/2$ (3)

Area of downcomer opening = $A_{da} = L_w h_a$ Take $h_a = 2$ in., $A_{da} = (32.1)(2/12) = 5.4$ ft^2

From Eq. (6-71), $h_{da} = 0.03\left(\frac{q_L}{100A_{da}}\right)^2 = 0.03\left(\frac{40{,}000}{100(5.4)}\right)^2$ =164 in. Very excessive

Exercise 6.21

Subject: Column performance for 40% of flooding.

Given: Data in Examples 6.5, 6.6, and 6.7.

Find: (a) Column diameter in Example 6.5 for $f = 0.4$.
(b) Vapor pressure drop in Example 6.6 for $f = 0.4$.
(c) Murphree vapor-point efficiency in Example 6.7 for $f = 0.4$

Analysis: (a) Example 6.5:

In this example, a value of $f = 0.80$ was used, giving $D_T = 2.65$ ft

From Eq. (6-44), by ratioing values of f,

$$D_T = 2.65\left(\frac{0.80}{0.40}\right)^{1/2} = 3.75 \text{ ft} = 1.15 \text{ m}$$

(b) Example 6.6:

In this example, a tower diameter of 1 m gives a vapor pressure drop = 0.093 psi/tray, with a vapor hole velocity of 47.9 ft/s, a weir length of 0.73 m, an active area vapor velocity of 5.99 ft/s, and $K_s = 0.265$ ft/s.

Vapor hole velocity varies inversely with the square of the column diameter. Therefore,

$u_o = 14.6(1/1.15)^2 = 11.0$ m/s = 36 ft/s

From Eq. (6-50), h_d is directly proportional to hole velocity squared. Therefore,

$h_d = 1.56(36/47.9)^2 = 0.88$ in. of liquid

Weir length is proportional to column diameter. So, $L_w = 0.73(1.15/1) = 0.84$ m = 0.33 in.

Vapor velocity based on active area varies inversely with the square of column diameter. Therefore, $U_a = 5.99(1/1.15)^2 = 4.53$ ft/s.

From Eq. (6-53), K_s is proportional to U_a. Thus, $K_s = 0.265(4.53/5.99) = 0.20$ ft/s

From Eq. (6-52), $\phi_e = \exp(-4.257K_s^{0.91}) = \exp[-4.257(0.20)^{0.91}] = 0.37$

The value of C in Eq. (6-51) remains at 0.362.

From Eq. (6-51),

$$h_l = \phi_e\left[h_w + C\left(\frac{q_L}{L_w\phi_e}\right)^{2/3}\right] = 0.37\left[2 + 0.362\left(\frac{12.9}{(33)0.37}\right)^{2/3}\right] = 0.88 \text{ in.}$$

$h_\sigma = 0.36$ in. (no change from Example 6.6)

From Eq. (6-49), $h_t = h_d + h_l + h_\sigma = 0{,}88 + 0.88 + 0.36 = 2.12$ in.

Tray pressure drop = $h_t\rho_L = 2.12(0.0356) = 0.076$ psi/tray

(c) Example 6.7:

In this example, a tower diameter of 1 m gives a $E_{OV} = 0.77$. Must redo all calculations.

$D_T = 1.15$ m, $A = 1.038$ m^2 = 10,380 cm^2, $A_a = 0.8(1.038) = 0.83$ m^2 = 8,300 cm^2

$L_w = 33$ in. = 0.84 m, $\phi_e = 0.37$, $h_l = 0.88$ in. = 2.24 cm

$U_a = 4.53$ ft/s = 137 cm/s, $U_f = 10.2$ ft/s, $f = U_a/U_f = 4.53/10.2 = 0.44$

Exercise 6.21 (continued)

Analysis: (c) (continued)

$F = U_a \rho_V^{0..5} = 1.37(1.92)^{0.5} = 1.90\ (\text{kg/m})^{0.5}/\text{s}$, $q_L = 812\ \text{cm}^3/\text{s}$

From Eq. (6-64), $\overline{t_L} = \dfrac{h_l A_a}{q_L} = \dfrac{2.24(10{,}380)}{812} = 28.6\ \text{s}$

From Eq. (6-65), $\overline{t_G} = \dfrac{(1-\phi_e)h_l}{\phi_e U_a} = \dfrac{(1-0.37)2.24}{0.37(137)} = 0.028\,\text{s}$

From Eq. (6-67), $k_L \overline{a} = 78.8 D_L^{0.5}(F + 0.425) = 78.8(1.81\times10^{-5})(1.90+0.425) = 0.78\,\text{s}^{-1}$

From Eq. (6-66),

$$k_G \overline{a} = \frac{1{,}030 D_V^{0.5}\left(f - 0.842 f^2\right)}{h_l^{0.5}} = \frac{1{,}030(7.86\times10^{-2})^{0.5}\left[0.44 - 0.842(0.44)^2\right]}{2.24^{0.5}} = 53.4\ \text{s}^{-1}$$

From Eq. (6-63), $N_L = k_L \overline{a}\,\overline{t_L} = 0.78(28.6) = 22.3$

From Eq. (6-62), $N_G = k_G \overline{a}\,\overline{t_G} = 53.4(0.28) = 1.5$

From Example 6.7, $KV/L = 0.662$

From Eq. (6-61), $N_{OG} = \dfrac{1}{\dfrac{1}{N_G} + \dfrac{KV/L}{N_L}} = \dfrac{1}{\dfrac{1}{1.5} + \dfrac{0.662}{22.3}} = \dfrac{1}{0.667 + 0.030} = 1.44$

Mass transfer is controlled by the vapor phase.

From a rearrangement of Eq. (6-52), $E_{OV} = 1 - \exp(-N_{OG}) = 1 - \exp(-1.44) = 0.76$ or 76%.

Exercise 6.22

Subject: Sizing, hydraulics, and mass transfer for an acetone absorber

Given: Acetone absorber of Fig. 6.1, using sieve trays with 10% hole area, 3/16-inch holes, and an 18-inch tray spacing. Foaming factor = 0.85.

Find: (a) Column diameter for 75% of flooding.
(b) Vapor pressure drop per tray.
(c) Number of transfer units.
(d) Number of overall transfer units.
(e) Controlling resistance to mass transfer.
(f) Murphree point vapor efficiency
If 30 trays are adequate.

Analysis: (a) Base column diameter on the top tray, where pressure is the lowest and gas flow rate is the highest. Use data in Fig. 6.1. L = 1,943 kmol/h, M_L = 18, ρ_L = 1,000 kg/m^3
V = 6.9 + 144.3 + 536.0 + 22.0 + 0.1 = 709.3 kmol/h, M_V = 28.8, P = 90 kPa, T = 25°C
From the ideal gas law, $\rho_V = PM/RT$ = (90)(28.8)/(8.314)(298) = 1.05 kg/m^3
Use entrainment flooding correlation of Fig. 6.24, where the abscissa is,

$$F_{LV} = \frac{LM_L}{VM_V}\left(\frac{\rho_V}{\rho_L}\right)^{1/2} = \frac{1{,}943(18)}{709.2(28.8)}\left(\frac{1.05}{1{,}000}\right)^{1/2} = 0.056$$

From Fig. 6.24, for 18-inch tray spacing, C_F = 0.28 ft/s. Because $F_{LV} < 1$, A_d/A = 0.1.
F_{HA} = 1.0, F_F = 0.85, and since σ = 70 dynes/cm, $F_{ST} = (70/20)^{0.2}$ = 1.285
From Eq. (6-24), $C = F_{ST}F_FF_{HA}C_F$ = (1.285)(0.85)(1)(0.28) = 0.306 ft/s
From Eq. (6-40), $U_f = C\left[(\rho_L - \rho_V)/\rho_V\right]^{1/2} = 0.306\left[(1{,}000 - 1.05)/1.05\right]^{1/2} = 9.44$ ft / s
From Eq. (6-44),

$$D_T = \left[\frac{4VM_V}{fU_f\pi(1 - A_d/A)\rho_V}\right]^{1/2} = \left[\frac{4(709.2/3{,}600)(28.8)}{0.75(9.44/3.28)(3.14)(1-0.1)(1.05)}\right]^{1/2} = 1.89 \text{ m} = 6.2 \text{ ft}$$

(b) Vapor pressure drop per tray is given by Eq. (6-49), $h_t = h_d + h_l + h_\sigma$ (1)
From the continuity equation, $m = uA\rho$, hole velocity for 10% hole area =
u_o = (709.2/3,600)(28.8)/(3.14/4)(1.9)^2(1.05)(0.1) = 19.0 m/s =62.3 ft/s
Superficial velocity = (0.1)(19.0) = 1.90 m/s = 6.23 ft/s
From Eq. (6-50), $h_d = 0.186\left(\frac{u_o^2}{C_o^2}\right)\left(\frac{\rho_V}{\rho_L}\right) = 0.186\left(\frac{62.3^2}{0.73^2}\right)\left(\frac{1.05}{1{,}000}\right) = 1.42$ in. of liquid
Active bubbling area for A_d/A = 0.1 is $A_a = A - 2A_d = 0.8\,A$. So, U_a = 6.23/0.8 = 7.8 ft/s
From Eq. (6-53), $K_s = U_a\left(\frac{\rho_V}{\rho_L - \rho_V}\right)^{1/2} = 7.8\left(\frac{1.05}{1{,}000 - 1.05}\right)^{1/2} = 0.253$ ft/s
From Eq. (6-52), $\phi_e = \exp(-4.257K_s^{0.91}) = \exp[-4.257(0.253)^{0.91}] = 0.30$
Assume a 2-inch weir height = h_w

Exercise 6.22 (continued)

Analysis: (b) (continued)

From Eq. (6-54), $C = 0.362 + 0.317\exp(-3.5h_w) = 0.362 + 0.317\exp[-3.5(2.0)] = 0.362$

Take weir length, $L_w = 0.73D_T = 0.73(6.2) = 4.52$ ft = 54.3 in.

Volumetric liquid rate = $q_L = m/\rho_L = (1{,}943/60)(18)/(1{,}000)(0.003785\ \text{m}^3/\text{gal}) = 154$ gpm

From Eq. (6-51), $h_l = \phi_e\left[h_w + C\left(\frac{q_L}{L_w\phi_e}\right)^{2/3}\right] = 0.30\left[2 + 0.362\left(\frac{154}{(54.3)0.30}\right)^{2/3}\right] = 1.09$ in. of liquid

From Eq. (6-55), with maximum bubble size of 3/16 inch = 0.00476 m,

$h_\sigma = 6\sigma / g\rho_L D_{B_{\max}} = 6(70/1000)/(9.8)(1{,}000)(0.00476) = 0.009\,\text{m} = 0.35$ in. of liquid

From Eq. (2), $h_t = h_d + h_l + h_\sigma = 1.42 + 1.09 + 0.35 = 2.86$ in. liquid = 0.103 psi/tray = 0.7 kPa/tray

(c) $D_T = 1.89$ m, $A = 2.804\ \text{m}^2 = 28{,}040\ \text{cm}^2$, $A_a = 0.8(2.804) = 2.24\ \text{m}^2 = 22{,}400\ \text{cm}^2$

$\phi_e = 0.30$, $h_l = 1.09$ in. = 2.77 cm

$U_a = 7.8$ ft/s = 238 cm/s, $U_f = 9.44$ ft/s, $f = U_a/U_f = 7.8/9.44 = 0.826$

$F = U_a\rho_V^{0..5} = 2.38(1.05)^{0.5} = 2.44\ (\text{kg/m})^{0.5}/\text{s}$, $q_L = 154$ gpm = $9{,}716\ \text{cm}^3/\text{s}$

From Eq. (6-64), $\bar{t}_L = \frac{h_l A_a}{q_L} = \frac{2.77(22{,}400)}{9{,}716} = 6.39$ s

From Eq. (6-65), $\bar{t}_G = \frac{(1-\phi_e)h_l}{\phi_e U_a} = \frac{(1-0.30)2.77}{0.30(238)} = 0.027$ s

From the Wilke-Chang Eq. (3-39), $D_L = 1.12 \times 10^{-5}\ \text{cm}^2/\text{s}$

From Eq. (6-67), $k_L\bar{a} = 78.8D_L^{0.5}(F + 0.425) = 78.8(1.12\times10^{-5})(2.44 + 0.425) = 0.756\ \text{s}^{-1}$

From Perry's Handbook, with a temperature correction based on Eq. (3-36), $D_V = 0.127\ \text{cm}^2/\text{s}$

From Eq. (6-66),

$$k_G\bar{a} = \frac{1{,}030D_V^{0.5}\left(f - 0.842f^2\right)}{h_l^{0.5}} = \frac{1{,}030(0.127)^{0.5}\left[0.826 - 0.842(0.826)^2\right]}{2.77^{0.5}} = 55.4\ \text{s}^{-1}$$

From Eq. (6-63), $N_L = k_L\bar{a}\bar{t}_L = 0.756(6.39) = 4.83$

From Eq. (6-62), $N_G = k_G\bar{a}\bar{t}_G = 55.4(0.027) = 1.5$

(d) From p. 271, for acetone, $A = L/KV = 1.38$. Therefore, $KV/L = 1/1.38 = 0.725$

From Eq. (6-61), $N_{OG} = \frac{1}{\frac{1}{N_G} + \frac{KV/L}{N_L}} = \frac{1}{\frac{1}{1.5} + \frac{0.725}{4.83}} = \frac{1}{0.667 + 0.150} = 1.22$

(e) Mass transfer is controlled by the vapor phase.

(f) From a rearrangement of Eq. (6-56), $E_{OV} = 1 - \exp(-N_{OG}) = 1 - \exp(-1.22) = 0.705$ or 70 %

Now, the separation requires 10 equilibrium stages. Assume the liquid on a tray is well mixed. Then, from Eq. (6-31), $E_{MV} = E_{OV} = 0.70$. From below Eq. (6-33), take $\lambda = KV/L = 0.725$.

From Eq. (6-37), $E_o = \frac{\log[1 + E_{MV}(\lambda - 1)]}{\log\lambda} = \frac{\log[1 + 0.70(0.725 - 1)]}{\log 0.725} = 0.66$ (worst case)

Therefore, at most, we need from Eq. (6-21), $N_a = N_t/E_o = 10/0.66 = 15$. Therefore, 30 okay.

Exercise 6.23

Subject: Design of a column to strip VOCs from water by air at 15 psia and 70°F.

Given: Conditions in Example 6.2 except that entering flow rates are twice as much.

Assumptions: Dilute system such that changes in vapor and liquid rates in the column are negligible. Sieve trays on 24-inch spacing, with 10 % hole area of 3/16-inch holes, $F_F = 0.9$, $F_{HA} = 1.0$ and $f = 0.80$.

Find: (a) Number of equilibrium stages required.
(b) Column diameter for sieve trays.
(c) Vapor pressure drop per tray.
(d) Murphree vapor-point efficiency from Chan-Fair method.
(e) Number of actual trays.

Analysis: (a) Need 3 equilibrium stages, as determined in Example 6.2 and which is unchanged when flow rates are doubled.

(b) liquid rate = 2(500) = 1,000 gpm or 1,000(60)(8.33)/18.02 = 27,800 lbmol/h = L
vapor rate = 2(3,400) = 6,800 scfm or 6,800(60)/379 = 1,077 lbmol/h = V

$\rho_L = 62.4$ lb/ft^3. From ideal gas law, $\rho_V = PM/RT = (15)(29)/(10.73)(530) = 0.0765$ lb/ft^3
Use entrainment flooding correlation of Fig. 6.24, where the abscissa is,

$$F_{LV} = \frac{LM_L}{VM_V}\left(\frac{\rho_V}{\rho_L}\right)^{1/2} = \frac{27{,}800(18)}{1{,}077(29)}\left(\frac{0.0765}{62.4}\right)^{1/2} = 0.56$$

From Fig. 6.24, for 24-inch tray spacing, $C_F = 0.18$ ft/s.
Because $0.1 < F_{LV} > 1$, from below Eq. (6-44), $A_d/A = 0.1 + (F_{LV} - 0.1)/9 = 0.15$
$F_{HA} = 1.0$, $F_F = 0.9$, and since $\sigma = 80$ dynes/cm, $F_{ST} = (80/20)^{0.2} = 1.32$
From Eq. (6-24), $C = F_{ST}F_F F_{HA} C_F = (1.32)(0.9)(1)(0.18) = 0.21$ ft/s
From Eq. (6-40), $U_f = C\left[(\rho_L - \rho_V)/\rho_V\right]^{1/2} = 0.21\left[(62.4 - 0.0765)/0.0765\right]^{1/2} = 6.0$ ft/s
From Eq. (6-44), for $f = 0.80$,

$$D_T = \left[\frac{4VM_V}{fU_f\pi(1 - A_d/A)\rho_V}\right]^{1/2} = \left[\frac{4(1{,}077/3{,}600)(29)}{0.80(6.0)(3.14)(1-0.15)(0.0765)}\right]^{1/2} = 6.0 \text{ ft}$$

(c) Vapor pressure drop per tray is given by Eq. (6-49), $h_t = h_d + h_l + h_\sigma$ (1)
From the continuity equation, $m = uA\rho$. Hole velocity for 10% hole area =
$u_o = (1{,}077/3{,}600)(29)/(3.14/4)(6)^2(0.0765)(0.1) = 40$ ft/s

Superficial velocity = (0.1)(40) = 4 ft/s

Exercise 6.23 (continued)

Analysis: (c) (continued)

From Eq. (6-50), $h_d = 0.186\left(\frac{u_o^2}{C_o^2}\right)\left(\frac{\rho_V}{\rho_L}\right) = 0.186\left(\frac{40^2}{0.73^2}\right)\left(\frac{0.0765}{62.4}\right) = 0.68$ in. of liquid

Active bubbling area for $A_d/A = 0.15$ is $A_a = A - 2A_d = 0.7\,A$. Therefore, $U_a = 4/0.7 = 5.7$ ft/s

From Eq. (6-53), $K_s = U_a\left(\frac{\rho_V}{\rho_L - \rho_V}\right)^{1/2} = 5.7\left(\frac{0.0765}{62.4 - 0.0765}\right)^{1/2} = 0.20$ ft/s

From Eq. (6-52), $\phi_e = \exp(-4.257K_s^{0.91}) = \exp[-4.257(0.20)^{0.91}] = 0.37$
Assume a 2-inch weir height = h_w
From Eq. (6-54), $C = 0.362 + 0.317\exp(-3.5h_w) = 0.362 + 0.317\exp[-3.5(2.0)] = 0.362$
Take weir length, $L_w = 0.73D_T = 0.73(6)(12) = 53$ in.

From Eq. (6-51), $h_l = \phi_e\left[h_w + C\left(\frac{q_L}{L_w\phi_e}\right)^{2/3}\right] = 0.37\left[2 + 0.362\left(\frac{1,000}{(53)0.37}\right)^{2/3}\right] = 2.58$ in. of liquid

From Eq. (6-55), with maximum bubble size of 3/16 inch = 0.00476 m,
$h_\sigma = 6\sigma / g\rho_L D_{B_{max}} = 6(80/1,000)/(9.8)(1,000)(0.00476) = 0.0103$ m = 0.40 in. of liquid
From Eq. (2), $h_t = h_d + h_l + h_\sigma = 0.68 + 2.58 + 0.40 = 3.66$ in. liquid = 0.13 psi/tray

(d) $D_T = 6$ ft, $A = 28.3$ ft^2, $A_a = 0.7(28.3) = 19.8$ ft^2 = 18,390 cm^2
$\phi_e = 0.37$, $h_l = 2.58$ in. = 6.55 cm, $\rho_G = 0.0765$ lb/ft^3 = 1.23 kg/m^3
$U_a = 5.7$ ft/s = 1.74 m/s, $U_f = 6.0$ ft/s, $f = U_a/U_f = 5.7/6.0 = 0.95$
$F = U_a\rho_V^{0..5} = 1.74(1.23)^{0.5} = 1.93$ (kg/m)$^{0.5}$/s, $q_L = 1,000$ gpm = 63,100 cm^3/s
From Eq. (6-64), $\overline{t_L} = \frac{h_l A_a}{q_L} = \frac{6.55(18,390)}{63,100} = 1.9$ s
From Eq. (6-65), $\overline{t_G} = \frac{(1-\phi_e)h_l}{\phi_e U_a} = \frac{(1-0.37)6.55}{0.37(174)} = 0.064$ s
From the Wilke-Chang Eq. (3-39), $D_L = 0.96 \times 10^{-5}$ cm^2/s
From Eq. (6-67), $k_L\overline{a} = 78.8D_L^{0.5}(F + 0.425) = 78.8(0.96\times10^{-5})(1.93 + 0.425) = 0.58$ s^{-1}
From Perry's Handbook, with T and P corrections based on Eq. (3-36), $D_V = 0.086$ cm^2/s

From Eq. (6-66),

$$k_G\overline{a} = \frac{1,030D_V^{0.5}\left(f - 0.842f^2\right)}{h_l^{0.5}} = \frac{1,030(0.086)^{0.5}\left[0.95 - 0.842(0.95)^2\right]}{6.55^{0.5}} = 2.56\ \text{s}^{-1}$$

From Eq. (6-63), $N_L = k_L\overline{a}\,\overline{t_L} = 0.58(1.9) = 1.1$

Exercise 6.23 (continued)

Analysis: (continued)

From Eq. (6-62), $N_G = k_G \overline{\overline{at}}_G = 2.56(0.064) = 0.16$

(d) From Example 6.2, for benzene, $S = KV/L = 9.89$

From Eq. (6-61), $N_{OG} = \dfrac{1}{\dfrac{1}{N_G} + \dfrac{KV/L}{N_L}} = \dfrac{1}{\dfrac{1}{0.16} + \dfrac{9.89}{1.1}} = \dfrac{1}{6.25 + 8.99} = 0.066$

From a rearrangement of Eq. (6-52), $E_{OV} = 1 - \exp(-N_{OG}) = 1 - \exp(-0.066) = 0.064$ or 6.4%

(e) From Example 6.2, the separation requires 3 equilibrium stages.
If we assume the liquid on a tray is well mixed. Then, from Eq. (6-31), $E_{MV} = E_{OV} = 0.064$.

From Eq. (6-21), $N_a = N_t / E_o = 3/0.064 = 47$ trays.

If we assume plug flow of liquid on a tray, then, if we take, below Eq. (6.33), $\lambda = KV/L = 9.89$,

from Eq. (6-37),

$$E_o = \frac{\log[1 + E_{MV}(\lambda - 1)]}{\log \lambda} = \frac{\log[1 + 0.064(9.89 - 1)]}{\log 9.89} = 0.197$$

Then we need from Eq. (6-21), $N_a = N_t / E_o = 3/0.197 = 15$ trays. Sufficient information is not given to establish the partial mixing prediction. Therefore, the number of trays required ranges widely from 15 to 47.

Exercise 6.24

Subject: Absorption of SO_2 from air into water in an existing packed column.

Given: Feed gas flow rate of 0.062 kmol/s containing 1.6 mol% SO_2. Absorbent is 2.2 kmol/s of pure water. Packed column is 1.5 m^2 in cross sectional area and packed with No. 2 plastic super Intalox saddles to a 3.5-m height. Exit gas contains an SO_2 mole fraction of 0.004. Operating pressure is 1 atm. At operating temperature, equilibrium curve for SO_2 is $y = Kx = 40x$

Assumptions: No stripping of water. No absorption of air.

Find: (a) L/L_{min}
(b) N_{OG} and N_t
(c) H_{OG} and HETP
(d) K_Ga

Analysis: Compute material balance. SO_2-free inlet air rate = 0.062(1-0.016) = 0.061 kmol/s
SO_2 inlet rate in feed gas = 0.062(0.016) = 0.001 kmol/s = V'
SO_2 outlet rate in gas = 0.061(0.004/0.996) = 0.00025 kmol/s
SO_2 rate in outlet water = 0.001 - 0.00025 = 0.00075 kmol/s
Fraction absorbed = 0.00075/0.001 = 0.75 or 75%

(a) From Eq. (6-11), $L'_{min} = V'K$(fraction absorbed) = 0.061(40)(0.75) = 1.83 kmol/s
Therefore, L/L'_{min} = 2.2/1.83 = 1.20

(b) Take $A = L/KV$ = 2.2/[(40)(0.062)] = 0.887, From Eq. (6-13), $0.75 = \dfrac{0.887^{N+1} - 0.887}{0.887^{N+1} - 1}$

Solving, $N_t = 4$. For N_{OG}, use Eq. (6-89) with $y_{in} = 0.016$, $y_{out} = 0.004$, x_{in} =0.0,

$$N_{OG} = \frac{\ln\left\{\left[\dfrac{0.887-1}{0.887}\right]\left[\dfrac{0.016}{0.004}\right] + \dfrac{1}{0.887}\right\}}{(0.887-1)/0.887} = 3.78$$

(c) Given height of packing = 3.5 m = l_T
From Eq. (6-73), HETP = l_T/N_t = 3.5/4 = 0.875 m
From Eq. (6-89), $H_{OG} = l_T/N_{OG}$ = 3.5/3.78 = 0.926 m

(d) From Table 6.7, $H_{OG} = \dfrac{V}{K_GaPS}$ Therefore, $K_Ga = \dfrac{V}{H_{OG}PS} = \dfrac{0.062}{(0.926)(1)(1.5)}$
= 0.045 kmol/s-m^3-atm

Exercise 6.25

Subject: Operating data for absorption of SO_2 from air into water in a packed column.

Given: Column operates at 1 atm (760 torr) and 20°C. Solute-free water enters at 1,000 lb/h. Mole ratio of water to air is 25. Liquid leaves with 0.6 lb SO_2/100 lb of solute-free water. Partial pressure of SO_2 in exit gas is 23 torr (0.0303 atm). Equilibrium data are given as partial pressures of SO_2 in air as a function of lb SO_2 dissolved/ 100 lb H_2O.

Assumptions: No stripping of water. No absorption of air. Density of liquid taken as water.

Find: (a) % of SO_2 absorbed.
(b) Concentration of SO_2 in the liquid at the gas-liquid interface in lbmol/ft^3 at a point where the bulk liquid concentration is 0.001 lbmol SO_2/lbmol of water and:
k_L = 1.3 ft/h k_p = 0.195 lbmol/h-ft^2-atm

Analysis: (a) Inlet water rate = 1,000/18.02 = 55.5 lbmol/h
Inlet air rate = water rate/25 = 55.5/25 = 2.22 lbmol/h
Partial pressure of air in exit gas = 760 - 23 = 737 torr
By partial pressure ratio, SO_2 flow rate in exit gas = 2.22(23/737) = 0.0693 lbmol/h
Molecular weight of SO_2 = 64.06
SO_2 flow rate in exit liquid = 0.6(1,000/(100)(64.06) = 0.0937 lbmol/h
By material balance, SO_2 flow rate in entering air = 0.0693 + 0.0937 = 0.1630 lbmol/h
Partial pressure of SO_2 in entering gas = 0.1630/(0.1630 + 2.22) = 0.0690 atm
% of SO_2 absorbed = 0.0937/0.1630 x 100% = 57.5%

(b) At the point, the rate of mass transfer for SO_2 as a flux across the gas-liquid interface, can be written by the two-film theory as,

$$k_p(p_b - p_i) = k_L(c_i - c_b) \qquad (1)$$

As shown in Fig. 6.31, the equilibrium interface composition can be determined in terms of the ratio of mass-transfer coefficients. However, here, instead of compositions in mole fractions, the gas composition is in partial pressure and the liquid is in concentration. From Eq. (1),

$$\frac{k_L}{k_p} = \frac{1.3}{0.195} = 6.67 = \frac{p_b - p_i}{c_i - c_b} \qquad (2)$$

At the point (column height location), bulk liquid concentration = 0.001 lbmol SO_2/lbmol H_2O and the flow rate is 0.001(55.5) = 0.0555 lbmol/h for SO_2 in the liquid phase. The flow of SO_2 in the gas phase at that location is obtained by a material balance around the top of the column:
SO_2 in entering liquid + SO_2 in gas at the point = SO_2 in liquid at the point + SO_2 in exit gas
Therefore, 0 + SO_2 flow rate in gas at the point = 0.0693 + 0.0555

Exercise 6.25 (continued)

Analysis: (b) (continued)

SO_2 flow rate in gas at the point = 0.1248 lbmol/h. Therefore, the partial pressure of SO_2 in the bulk gas at the point = 0.1248/(0.1248 + 2.22) x 1 atm = 0.0532 atm = p_b .
The density of water is 62.4 lb/ft^3 or 62.4/18.02 = 3.46 lbmol/ft^3. Therefore,
the concentration of SO_2 in the bulk liquid at the point = 0.001(3.46) = 0.00346 lbmol/ft$_3$ = c_b .

We now need an algebraic equilibrium relationship between p_i and c_i .
Convert the given equilibrium data to partial pressures and concentrations in the vicinity of the values at the point:
The SO_2 concentration in the liquid is obtained from,

$$c, \ \frac{\text{lbmol } SO_2}{\text{ft}^3} = \left(\frac{\text{lb } SO_2}{100 \text{ lb } H_2O}\right)\left(\frac{62.4}{64.06}\right)\left(\frac{1}{100}\right)$$

lb SO_2 / 100 lb H_2O	c_i , lbmol SO_2 / ft^3	Partial pressure SO_2 , torr	p_i of SO_2 , atm
0.30	0.00292	14.1	0.01855
0.50	0.00487	26.0	0.03421
0.70	0.00682	39.0	0.05132
1.00	0.00974	59.0	0.07763

These equilibrium data fit the curve, $p_i = 5.04536c_i + 511.783c_i^2 - 21714.4c_i^3$ (3)

From Eq. (2), $0.0532 - p_i = 6.67(c_i - 0.00346)$ (4)

Solving Eqs. (3) and (4), $c_i = 0.00550$ lbmol/ft^3 and $p_i = 0.0396$ atm

The same result can be obtained by constructing a plot of SO_2 partial pressure versus SO_2 concentration in the liquid, similar to Fig. 6.31. First, the operating line is drawn as a straight line connecting the column end points (0.0303, 0.0) and (0.0690, 0.00584), as (p , c). Then the equilibrium curve is drawn, using Eq. (3). Then the point (p_b , c_b) is marked on the operating line. A straight line is extended from this point, with a slope of ($-k_L/k_p$) = -6.67, to the point of intersection on the equilibrium line, giving the same result as above

Exercise 6.26

Subject: Stripping of benzene from wastewater with air in a packed column.

Given: Column operation at 2 atm (1,520 torr) and 25°C. Wastewater enters at 600 gpm containing 10 ppm by weight of benzene. Suggested air rate is 1,000 scfm (60°F and 1 atm). Exit water to contain just 0.005 ppm benzene. Vapor pressure of benzene = 95.2 torr at 25°C. Solubility of benzene in water = 0.180 g/100 g water at 25°C. Packing is 2-inch polypropylene Flexirings. Mass transfer coefficients are: $k_La = 0.067$ s^{-1} and $k_Ga = 0.80$ s^{-1} (both driving forces are in concentration units).

Assumptions: No stripping of water. No absorption of air.

Find: (a) Minimum air stripping rate. Is it less than suggested? If not, use 1.4 times minimum rate.
(b) Stripping factor
(c) N_{OG}
(d) K_Ga in units of s^{-1} and mol/m^3-s-kPa, and which phase controls mass transfer
(e) Volume of packing in m^3

Analysis: Water flow rate = 600(8.33)(60)/18.02 = 16,640 lbmol/h
For benzene, x_{in} = (10/1,000,000)(18.02/78) = 2.31 x 10^{-6}
x_{out} = (0.005/1,000,000)(18.02/78) = 1.16 x 10^{-9}
Fraction of benzene stripped = 1 - (2.31 x 10^{-6}/1.16 x 10^{-9}) = 0.9995

(a) System is very dilute with respect to benzene, therefore use Kremser equation to determine the minimum gas rate. From Eq. (6-12), $V_{min} = L$ (fraction stripped)/ K (1)
For the K-value, use Eq. (4) in Table 2.3, a modified Raoult's law, $K = \gamma_L P^s/P$ (2)
To obtain the liquid-phase activity coefficient, use the given benzene solubility data. For liquid-liquid equilibrium with respect to benzene, which is distributed between a water-rich phase (2) and a benzene-rich phase (1), using Eq. (2-30), $\gamma^{(2)} = \left(x^{(1)} / x^{(2)}\right)\gamma^{(1)}$. But if the benzene-rich phase is nearly pure benzene, $\gamma^{(1)} = 1$ and $x^{(1)} = 1$. Therefore, $\gamma^{(2)} = 1/x^{(2)}$ (3)
From the given benzene solubility in water, $x = \dfrac{0.18(18.02)}{100(78)} = 4.2\times10^{-4}$

Therefore from Eq. (3), $\gamma_L = \dfrac{1}{4.2\times10-4} = 2{,}380$

From Eq. (2), K = (2,380)(95.2)/1,520 = 149
From Eq. (1), V_{min} = 16,640(0.9995)/150 = 111.6 lbmol/h
At 60°F and 1 atm, there are 379 scf/lbmol. Therefore, V_{min} = 111(379)/60 = 705 scfm.
This is less than the 1,000 scfm suggested by the expert. Therefore, use the value suggested by the expert, rather than revise it.

Exercise 6.26 (continued)

Analysis: (continued)

(b) Operating V = 111.6(1,000/705) = 158.3 lbmol/h
From Eq. (5-51), $S = KV/L$ = 149(158.3)/16,640 = 1.417 (a good value)

(c) For N_{OG}, use Eq. (6-93), with $A = 1/S = 1/1.417 = 0.7057$
Benzene stripped = $L_{in}x_{in}$(fraction stripped) = 16,640(2.31 x 10^{-6})(0.9995) = 0.0384 lbmol/h
Therefore, y_{out} = 0.0384/158.3 = 0.0002427. Also, x_{in} = 2.31 x 10^{-6} and y_{in} = 0.0. Therefore,

$$N_{OG} = \frac{\ln\left\{\left[\frac{0.7057-1}{0.7057}\right]\left[\frac{0.0-149(2.31\times10^{-6})}{0.0002427-149(2.31\times10^{-6})}\right]+\frac{1}{0.7057}\right\}}{(0.7057-1)/0.7057} = 14.2$$

(d) Note that both k_L and k_G are given for concentration driving forces. Therefore, we write the rate of mass transfer of benzene as:

$$r = k_G a c_G (y_b - y_i) = k_L a c_L (x_i - x_b) = K_G a c_G (y_b - y^*) \qquad (4)$$

where c_G and c_L are total gas and liquid concentrations, respectively, and y^* is the vapor mole fraction in equilibrium with the bulk liquid mole fraction, as given by $y^* = Kx_b$.
Solving Eq. (4) for the driving vapor and liquid phase driving forces,

Adding Eqs. (5) and (6) to eliminate y_i and solving for r and equating to the last term in Eq. (4),

$$r = \frac{y_b - y^*}{\left[\frac{1}{k_G a c_G} + \frac{K}{k_L a c_L}\right]} = \frac{y_b - y^*}{\frac{1}{K_G a c_G}} \qquad (7)$$

Solving Eq. (7) for $K_G a$,

$$K_G a = \frac{1}{\frac{1}{k_G a} + \frac{Kc_G}{k_L a c_L}} \qquad (8)$$

The total gas concentration is obtained from the ideal gas law,

xercise 6.26 (continued)

Analysis: (d) continued)

$$c_G = \frac{P}{RT} = \frac{2(101.3)}{8.314\times10^{-3}(298)} = 81.8 \text{ mol/m}^3$$

$$c_L = \frac{\rho_L}{M_L} = \frac{10^6 \text{ g/m}^3}{18.02} = 55{,}500 \text{ mol/m}^3$$

$$K_G a = \frac{1}{\frac{1}{0.80} + \frac{150(81.8)}{0.067(55{,}500)}} = \frac{1}{1.25 + 3.29} = 0.22 \text{ s}^{-1}$$

This is with a concentration driving force.

The liquid phase controls with a relative resistance of 3.29 compared to 1.25 for the gas phase.

To obtain $K_G a$ with a partial pressure driving force, we write the rate of mass transfer as,

$$r = K_G a c_G (y_b - y^*) = (K_G)_p \, aP(y_b - y^*) \qquad (9)$$

where $K_G a$ is with the concentration driving force = 0.22 s^{-1} and $(K_G)_p a$ is with the partial pressure driving force. Solving Eq. (9), and applying the ideal gas law in the form, $c_G = P/RT$,

$$(K_G)_p a = K_G a \frac{c_G}{P} = \frac{K_G a}{RT} = \frac{0.22}{(8.314\times10^{-3})(298)} = 0.089 \text{ mol/kPa-m}^3\text{-s}$$

(e) From Table 6.7, with a partial pressure driving force,

$$H_{OG} = \frac{G}{(K_G)_p aPS}$$

However, the cross sectional area of the tower, S, is not known. Therefore, can not compute H_{OG}

From Eq. (6-89), $l_T = H_{OG} N_{OG}$. Therefore, can not compute the height because H_{OG} is unknown. However, we can compute the packed volume.

$$\text{Packed volume} = l_T S = N_{OG} H_{OG} S = N_{OG} \frac{G}{(K_G)_p aP} = (14.2)\frac{(149)(454)}{0.089(3{,}600)(2)(101.3)} = 14.8 \text{ m}^3$$

Exercise 6.27

Subject: Absorption of $GeCl_4$ from air into dilute caustic solution in an existing packed column.

Given: Column operates at 25°C (77°F) and 1 atm. Gas enters at 23,850 kg/day containing 288 kg/day of $GeCl_4$ and 540 kg/day of Cl_2. Dissolved $GeCl_4$ and Cl_2 react with the caustic so that neither has a vapor pressure. Packed tower is 2-ft diameter with 10 ft of 1/2-inch ceramic Raschig ring packing of given characteristics. Liquid rate is to give 75% of flooding. Equation is given for estimating $K_y a$.

Assumptions: No stripping of water. No absorption of air.

Find: (a) Entering dilute caustic flow rate.
(b) Required packed height. Which controls, $GeCl_4$ or Cl_2? Is 10-ft height adequate?
(c) % absorption of $GeCl_4$ and of Cl_2 for 10 ft of packing. If necessary, select an alternative packing.

Analysis: (a) Determine entering dilute caustic flow rate from the 75% of flooding specification, using the flooding curve of Fig. 6.36(a), with the correction factors of Figs. 6.36(b,c). The air rate in the entering gas = 23,850 - 288 - 540 = 23,022 kg/day.
MW of Cl_2 = 71. MW of $GeCl_4$ = 214.6. MW of air = 29.

Molar gas rate = $V = \dfrac{23{,}022}{29} + \dfrac{288}{214.6} + \dfrac{540}{71} = 803$ kmol/day or 73.7 lbmol/h or 2189 lb/h

Average molecular weight of gas = 23,850/803 = 29.7
Tower cross sectional area for 2-ft diameter = $3.14(2)^2/4 = 3.14$ ft^2
The continuity equation for flow through the tower based on the gas superficial velocity is, $m = u_o S\rho$. Therefore, the superficial velocity is, $u_o = m/S\rho$ (1)
From the ideal gas law, $\rho = PM/RT = (1)(29.7)/(0.7302)(460+77) = 0.076$ lb/ft^3
Therefore, from Eq. (1), $u_o = (2189)/(3.14)(0.076) = 9{,}170$ ft/h or 2.55 ft/s.
From Eq. (6-102), noting that for the dilute caustic solution at 25°F, $f\{\rho_L\} = 1$ and $f\{\mu_L\} = 0.98$ for a liquid viscosity of 0.95 cP at 25°C,

$$Y = \frac{u_o^2 F_P}{g}\left(\frac{\rho_V}{\rho_{H_2O}}\right) f\{\rho_L\} f\{\mu_L\} = \frac{(2.55)^2(580)}{32.2}\left(\frac{0.076}{62.4}\right)(1.0)(0.98) = 0.14$$

$(u_o)_{flood} = u_o/0.75 = 2.55/0.75 = 3.40$ ft/s. Therefore, $Y_{flood} = 0.14/(0.75)^2 = 0.25$

From Fig. 6.36, $\left(\dfrac{LM_L}{VM_V}\right)\left(\dfrac{\rho_V}{\rho_L}\right)^{1/2} = 0.009$

$$LM_L = X(GM_G)\left(\frac{\rho_L}{\rho_G}\right)^{1/2} = 0.009(2{,}191)\left(\frac{62.4}{0.076}\right)^{1/2} = 565 \text{ lb/h or } 0.071 \text{ kg/s of entering liquid}$$

Exercise 6.27 (continued)

Analysis:

(b) Assume that $GeCl_4$ is the controlling species, with mass transfer controlled in the gas phase.
From Table 6.7, column height = $l_T = H_G N_G$ where, $H_G = V/k_y aS$ (1)

$$\text{and, } N_G = \int \frac{(1-y)_{LM}\, dy}{(1-y)(y-y_I)} \qquad (2)$$

At the interface, $y_I = 0$ because it is given that dissolved $GeCl_4$ has no vapor pressure
In entering gas, $y = (288/214.6)/803 = 0.00162$. Therefore $(1 - y)_{bottom} = (1 - 0.00162) = 0.9984$
In exiting gas, $y = 0.01$ of y in entering gas $= 0.0000162$. Therefore $(1 - y)_{top} = 1.0000$
Therefore, $(1 - y)_{LM} = 0.9992$. Also, on the average, $(1 - y)$ is approximately 0.9992.
Therefore, Eq. (2) for N_G simplifies to,

$$N_G = \int_{0.0000162}^{0.00162} \frac{dy}{y} = \ln\left(\frac{0.00162}{0.0000162}\right) = 4.61$$

Equation given for k_y is, $k_y = \left(\frac{V}{S}\right) 1.195 \left[\frac{D_P V'}{\mu(1-\varepsilon_o)}\right]^{-0.36} (N_{Sc})^{-2/3}$ (3)

$V = 803/24(3{,}600) = 0.0093$ kmol/s $S = 3.14$ ft^2 or 0.292 m^2
$D_P = 0.01774$ m $V' = (V/S)M_G = (0.0093/0.292)(29.7) = 0.944$ kg/s-m^2
At 25°C, from Perry's Handbook, for air, $\mu = 0.018$ cP or 1.8×10^{-5} kg/m-s
$\varepsilon_o = \varepsilon - h_L$ $\varepsilon = 0.63$ $h_L = 0.03591(L')^{0.331}$ (4)
$L' = (LM_L)/S = 0.071/0.292 = 0.243$ kg/s-m^2 From Eq. (4), $h_L = 0.0359(0.243)^{0.331} = 0.0225$
Therefore, $\varepsilon_o = 0.63 - 0.0225 = 0.608$ $N_{Sc} = \mu/\rho D_{GeCl4}$ (5)
From above, ρ of the gas = 0.076 lb/ft^3 = 1.21 kg/m^3 $D_{GeCl4} = 6 \times 10^{-6}$ m^2/s
From Eq. (5), $N_{Sc} = (1.8 \times 10^{-5})/(1.21)(6 \times 10^{-6}) = 2.48$

From Eq. (3), $k_y = \left(\frac{0.0093}{0.292}\right) 1.195 \left[\frac{(0.01774)(0.944)}{(1.8\times10^{-5})(1-0.608)}\right]^{-0.36} (2.48)^{-2/3} = 1.26\times10^{-3}$ kmol/s-m^2

Equation given for interfacial area is, $a = \frac{14.69(808\ V'/\rho^{1/2})^n}{(L')^{0.111}}$ (6)

Equation given for exponent, $n = 0.01114\ L' + 0.148 = 0.01114(0.243) + 0.148 = 0.151$

Therefore, from Eq. (6), $a = \frac{14.69\left[\frac{(808)(0.944)}{(1.21)^{1/2}}\right]^{0.151}}{(0.243)^{0.111}} = 46.2$ m^2/m^3

Exercise 6.27 (continued)

Analysis: (b) (continued)

$K_y a = k_y a = (1.26 \times 10^{-3})(46.2) = 0.058$ kmol/s-m^3
From Eq. (1), $H_G = H_{OG} = (V/S)/k_y a = (0.0093/0.292)/0.058 = 0.55$ m or 1.8 ft
Packed height = $H_G N_G = 0.55(4.61) = 2.53$ m or 8.3 ft.
Therefore, a 10 foot height is sufficient.

Now check the assumption that $GeCl_4$ controls. Because gas is dilute in Cl_2 and 99% of it is absorbed, N_G is the same as for $GeCl_4$. Note that in Eq. (3),
k_y is proportional to $(N_{Sc})^{-2/3}$ or $D_i^{2/3}$. Since the given gas diffusivity of Cl_2 is about twice that of $GeCl_4$, the mass transfer coefficient for Cl_2 is higher and the corresponding H_G is lower.
Therefore, the assumption that $GeCl_4$ controls is correct.

(c) If a packed height of 10 ft rather than the computed 8.3 ft is used, then for $GeCl_4$,
$N_G = l_T / H_G = 10/1.8 = 5.55$ rather than 4.61.

From above, $N_G = \ln \dfrac{y_{in}}{y_{out}} = 5.55$

Solving, $\dfrac{y_{in}}{y_{out}} = 258$ Therefore, $y_{out} = 0.00162/258 = 0.0000063$

% absorption of $GeCl_4$ = (1 - 0.0000063/0.00162) = 0.996 or 99.6% compared to 99% specified

For Cl_2, from above, $H_G = H_G$ of $GeCl_4$ $(D_{GeCl4}/D_{Cl2})^{2/3} = 1.8(0.000006/0.000013)^{2/3} = 1.08$

Therefore, $N_G = 10/1.08 = 9.26 = = \ln \dfrac{y_{in}}{y_{out}}$ Solving, $\dfrac{y_{in}}{y_{out}} = 10{,}500$

% absorption of Cl_2 = (1 - 1/10,500) = 0.9999 or 99.99% compared to 99% specified

Exercise 6.28

Subject: Packed tower diameter and pressure drop for conditions of Exercise 6.26.

Given: Suggested tower diameter of 0.80 m and pressure drop of 500 N/m^2-m of packed height (0.612 in. H_2O/ft).

Find: (a) Fraction of flooding if F_P = 24 ft^2/ft^3.
(b) Pressure drop at flooding.
(c) Pressure drop at operating conditions using GPDC chart.
(d) Pressure drop at operating conditions using Billet-Schultes correlation.

Analysis: (a) Using data from Exercise 6.26 and Fig. 6.36,

LM_L = 600(8.33) = 5,000 lb/min

VM_V = (1,000/379)(29) = 76.5 lb/min

From ideal gas law, $\rho_V = PM/RT$ = (2)(29)/(0.7302)(460+77) = 0.148 lb/ft^3

ρ_L =62.3 lb/ft^3

From Fig. 6.36, $X = \left(\frac{LM_L}{VM_V}\right)\left(\frac{\rho_V}{\rho_L}\right)^{1/2} = \left(\frac{5{,}000}{76.5}\right)\left(\frac{0.148}{62.3}\right)^{1/2} = 3.19$

From Fig. 6.36, at flooding, Y = 0.0053

For the actual operation, by the continuity equation, $m = u_o S\rho$

Area for flow = $S = \pi D^2/4$ = (3.14)(0.8/0.3048)^2/4 = 5.41 ft^2

Superficial velocity = $u_o = m/S\rho$ = (76.5/60)/(5.41)(0.148) = 1.59 ft/s

From Eq. (6-102), noting that for the dilute aqueous solution at 25°F, $f\{\rho_L\} = 1$ and $f\{\mu_L\} = 0.98$ for a liquid viscosity of 0.95 cP at 25°C,

$$Y = \frac{u_o^2 F_P}{g}\left(\frac{\rho_V}{\rho_{H_2O}}\right) f\{\rho_L\} f\{\mu_L\} = \frac{(1.59)^2(24)}{32.2}\left(\frac{0.148}{62.3}\right)(1.0)(0.98) = 0.0044$$

$$\text{Fraction of flooding} = \frac{u_o}{u_{flood}} = \left(\frac{Y}{Y_{flood}}\right)^{1/2} = \left(\frac{0.0044}{0.0053}\right)^{1/2} = 0.91 \text{ or } 91\%$$

This is too high. Should increase tower diameter.

(b) From Eq. (6-104), $\Delta P_{flood} = 0.115 F_P^{0.7} = 0.115(24)^{0.7} = 1.06$ in. H_2O/ft of packed height

(c) From Fig. 6.36, ΔP at design = 1.50 in. H_2O/ ft of packed height (seems high)

(d) From Table 6.8, for 2-inch (50-mm) plastic Pall rings, the packing characteristics are:
a = 111.1 m^2/m^3 or 33.9 ft^2/ft^3, ε = 0.919 m^3/m^3, C_h = 0.593, C_p = 0.698, C_s = 2.816

The pressure drop per unit height of packed bed is given by Eq. (6-115),

$$\frac{\Delta P}{\Delta P_o} = \left(\frac{\varepsilon}{\varepsilon - h_L}\right)^{3/2} \exp\left[\frac{13300}{a^{3/2}}\left(N_{Fr_L}\right)^{1/2}\right] \qquad (1)$$

Exercise 6.28 (continued)

Analysis: (d) (continued)

where, h_L is given by (6-97) and is in m^2/m^3 and N_{Fr_L} is given by (6-99).

From Eq. (6-110), $$\frac{\Delta P_o}{l_T} = \Psi_o \frac{a}{\varepsilon^3}\frac{u_V^2 \rho_V}{2}\frac{1}{K_W} \qquad (2)$$

From Eq. (6-112), $D_P = 6\left(\frac{1-\varepsilon}{a}\right) = 6\left(\frac{1-0.919}{33.9}\right) = 0.0143$ ft

From Eq. (6-111), $\frac{1}{K_W} = 1+\frac{2}{3}\left(\frac{1}{1-\varepsilon}\right)\frac{D_P}{D_T} = 1+\frac{2}{3}\left(\frac{1}{1-0.919}\right)\frac{0.0143}{2.62} = 1.045$

Therefore, $K_W = 0.957$.

From Perry's Handbook, μ for air at 25°C = 0.018 cP, and $u_o = u_V$ = 1.59 ft/s

From Eq. (6-114), $N_{Re_V} = \frac{u_V D_P \rho_V}{(1-\varepsilon)\mu_V} K_W = \frac{(1.59)(0.0143)(0.148)(0.957)}{(1-0.919)[(0.018)(0.000672)]} = 3,287$

From Eq. (6-113), $\Psi_o = C_p\left(\frac{64}{N_{Re_V}} + \frac{1.8}{N_{Re_V}^{0.08}}\right) = 0.698\left(\frac{64}{3,287} + \frac{1.8}{3,287^{0.08}}\right) = 0.671$

From Eq. (2), with the introduction of g_c because of the use of American Engineering units,

$$\frac{\Delta P_o}{l_T} = \Psi_o \frac{a}{\varepsilon^3}\frac{u_V^2 \rho_V}{2g_c}\frac{1}{K_W} = 0.671\frac{33.9}{0.919^3}\left[\frac{1.59^2(0.148)}{2(32.2)}\right]\frac{1}{0.957} = 0.164 \text{ lbf/ft}^3 \text{ or } 0.00114 \text{ psi/ft}$$

From Eq. (6-97), $$h_L = \left(12\frac{N_{Fr_L}}{N_{Re_L}}\right)^{1/3}\left(\frac{a_h}{a}\right)^{2/3} \qquad (3)$$

Superficial liquid velocity = $u_L = m/S\rho_L = (5{,}000/60)/(5.41)(62.4) = 0.247$ ft/s
From Perry's Handbook, liquid viscosity = 0.95 cP

From Eq. (6-99), $N_{Fr_L} = \frac{u_L^2 a}{g} = \frac{(0.247)^2(33.9)}{32.2} = 0.064$

From Eq. (6-98), $N_{Re_L} = \frac{u_L \rho_L}{a\mu_L} = \frac{(0.247)(62.4)}{(33.9)(0.95)(0.000672)} = 712$

From Eq. (6-101), $\frac{a_h}{a} = 0.85 C_h N_{Re_L}^{0.25} N_{Fr_L}^{0.1} = 0.85(0.593)(712)^{0.25}(0.247)^{0.1} = 2.27$

Exercise 6.28 (continued)

Analysis: (d) (continued)

From Eq. (3), $h_L = \left(12\frac{0.064}{712}\right)^{1/3} 2.27^{2/3} = 0.177$ m^3/m^3 or ft^3/ft^3

From Eq. (1),

$$\frac{\Delta P}{\Delta P_o} = \left(\frac{\varepsilon}{\varepsilon - h_L}\right)^{3/2} \exp\left[\frac{13300}{a^{3/2}}\left(N_{\mathrm{Fr}_L}\right)^{1/2}\right]$$

$$\frac{\Delta P}{l_T} = (0.00114)\left(\frac{0.919}{0.919-0.103}\right)^{3/2} \exp\left[\frac{13300}{111.1^{3/2}}(0.064)^{1/2}\right] = 0.0241 \text{ psi/ft or } 0.669 \text{ in. } H_2O/\text{ft}$$

This is only 10% higher than the suggested value of 0.612 in. H_2O/ft

Exercise 6.29

Subject: Mass-transfer coefficients for conditions of Exercise 6.26.

Given: Suggested mass-transfer coefficients in Exercise 6.26.

Find: Mass-transfer coefficients k_La and k_Ga from Billet-Schultes correlation.

Analysis: Coefficient k_La is obtained from a rearrangement of the left-most part of Eq. (6-131),

$$k_L a = \frac{u_L}{H_L\left(a_{Ph}/a\right)} \tag{1}$$

with H_L from Eq. (6-132) and (a_{Ph}/a) from (6-136).

From Table 6.8, C_L = 1.239 , ε = 0.919, and a = 111.1 m^2/m^3. From the results of Exercise 6.28, come the following parameters and properties:

h_L = 0.177 ft^2/ft^3, u_L = 0.247 ft/s, ρ_L = 62.4 lb/ft^3, μ_L = 0.95 cP

Take the surface tension, σ = 0.005 lb_f/ft or 0.005(32.2) = 0.161 lb/s^2

To compute (a_{Ph}/a), we need for the liquid phase, the Reynolds, Weber, and Froude numbers from equations (6-138), (6-139), and (6-140), respectively, based on the packing hydraulic diameter from (6-137).

d_h = packing hydraulic diameter = $4\dfrac{\varepsilon}{a} = 4\dfrac{0.919}{111.1} = 0.0331$ m = 0.108 ft

From Exercise 6.28,

Reynolds number = $N_{\mathrm{Re}_L,h} = \dfrac{u_L d_h \rho_L}{\mu_L} = \dfrac{(0.247)(0.108)(62.4)}{[(0.95)(0.000672)]} = 2,607$

Weber number = $N_{\mathrm{We}_L,h} = \dfrac{u_L^2 \rho_L d_h}{\sigma} = \dfrac{(0.247)^2\,(62.4)(0.108)}{0.161} = 2.55$

Froude number = $N_{\mathrm{Fr}_L,h} = \dfrac{u_L^2}{g d_h} = \dfrac{(0.247)^2}{32.2(0.108)} = 0.0175$

From (6-136), $\dfrac{a_{Ph}}{a} = 1.5\left(a d_h\right)^{-1/2}\left(N_{\mathrm{Re}_L,h}\right)^{-0.2}\left(N_{\mathrm{We}_L,h}\right)^{0.75}\left(N_{\mathrm{Fr}_L,h}\right)^{-0.45}$

$$= 1.5\left[(111.1)(0.0331)\right]^{-1/2}\left(2607\right)^{-0.2}\left(2.55\right)^{0.75}\left(0.0175\right)^{-0.45} = 2.02$$

Exercise 6.29 (continued)

Analysis: (continued)

From Exercise 6.23, correcting for temperature, D_L = 9.6 x 10^{-6}(298/294) = 9.73 x 10^{-6} cm^2/s or 1.05 x 10^{-8} ft^2/s

From (6-132), using American Engineering Units,

$$H_L = \frac{1}{C_L}\left(\frac{1}{12}\right)^{1/6}\left(\frac{4h_L\varepsilon}{D_L a u_L}\right)^{1/2}\frac{u_L}{a}\left(\frac{a}{a_{ph}}\right)$$

$$= \frac{1}{1.239}\left(\frac{1}{12}\right)^{1/6}\left[\frac{4(0.177)(0.919)}{(1.05\times10^{-8})(33.9)(0.247)}\right]^{1/2}\frac{0.247}{33.9}\left(\frac{1}{2.02}\right) = 5.23 \text{ ft}$$

From (1), $k_L a = \dfrac{u_L}{H_L\left(a_{Ph}/a\right)} = \dfrac{0.247}{5.23(2.02)} = 0.0234 \text{ s}^{-1}$

This is 35% of the suggested value of 0.067 s^{-1}

Coefficient $k_G a$ is obtained from the gas-phase analog of (1), $k_G a = \dfrac{u_V}{H_G\left(a_{Ph}/a\right)}$ (2)

with H_G obtained from (6-133), using dimensionless groups from (6-134) and (6-135).

From Exercise 6.28, u_V = 1.59 ft/s, ρ_V = 0.148 lb/ft^3, μ_V = 0.018 cP = 1.21 x 10^{-5} lb/ft-s

From Eq. (6-134), $N_{Re_V} = \dfrac{u_V\rho_V}{a\mu_V} = \dfrac{(1.59)(0.148)}{(33.9)(1.21\times10^{-5})} = 574$

From Exercise 6.23, the diffusivity of benzene in air = D_V = 0.086 cm^2/s at 70°F and 15 psia. Using Eq. (3-36) to correct for temperature and pressure,

$$D_V = 0.086\left[\frac{15}{(2)(14.7)}\right]\left(\frac{77+460}{70+460}\right)^{1.75} = 0.045 \text{ cm}^2/\text{s} = 4.84 \text{ x } 10^{-5} \text{ ft}^2/\text{s}$$

From Eq. (6-135), $N_{Sc_V} = \dfrac{\mu_V}{\rho_V D_V} = \dfrac{1.21\times10^{-5}}{(0.148)(4.84\times10^{-5})} = 1.69$

Exercise 6.29 (continued)

Analysis: (continued)

From Eq. (6-133) $H_G = \frac{1}{C_V}(\varepsilon - h_L)^{1/2}\left(\frac{4\varepsilon}{a^4}\right)^{1/2}\left(N_{\mathrm{Re}_V}\right)^{-3/4}\left(N_{\mathrm{Sc}_V}\right)^{-1/3}\left(\frac{u_V}{D_V}\right)\left(\frac{a}{a_{Ph}}\right) =$

$$\frac{1}{0.368}(0.919-0.177)^{1/2}\left[\frac{4(0.919)}{33.9^4}\right]^{1/2}(574)^{-3/4}(1.69)^{-1/3}\left(\frac{1.59}{4.84\times10^{-5}}\right)\left(\frac{1}{2.02}\right)=0.455 \text{ ft}$$

From (2), $k_G a = \frac{1.59}{0.455(2.02)} = 1.73 \text{ s}^{-1}$

This is approximately twice the suggested value of 0.80 s^{-1}.

Exercise 6.30

Subject: Absorption of NH_3 from air into water in a packed tower.

Given: Column operation at 68°F and 1 atm. Inlet gas mass velocity = 240 lb/h-ft^2. Inlet water mass velocity = 2,400 lb/h-ft^2. Tower packed with 1.5-inch ceramic Berl saddles. Henry's law applies for NH_3 with p (atm) = 2.7x.

Assumptions: No stripping of water. No absorption of air. Dilute system.

Find: (a) Packed height for 90% absorption of NH_3.
(b) Minimum water mass velocity for 98% absorption of NH_3.
(c) K_Ga, pressure drop, maximum liquid rate, K_La, packed height, column diameter, H_{OG}, and N_{OG} for 1.5-inch ceramic Hiflow rings.

Analysis: (a) Assuming Dalton's law, the equilibrium equation for 1 atm is,

$$p = yP = 2.7x \text{ atm or with } P = 1 \text{ atm}, \; y = Kx = 2.7x \qquad (1)$$

Because the system is dilute, Eq. (6-89) can be used to compute N_{OG}.
Then the packed height is given by Eq. (6-85),

$$l_T = N_{OG}H_{OG} \quad (2)$$

The absorption factor from Eq. (6-15) is, $A = L/KV = (2{,}400/18)/2.7(240/29) = 6.0$
Entering and exiting ammonia mole fractions are: $y_{in} = 0.02$, $y_{out} = 0.002$, $x_{in} = 0.0$
The ammonia mole fraction in the exiting liquid is obtained by an overall ammonia balance:

$$\frac{240}{29}y_{in} + \frac{2{,}400}{18}x_{in} = \frac{240}{29}y_{out} + \frac{2{,}400}{18}x_{out} \qquad (3)$$

Solving Eq. (3), $x_{out} = 0.00112$.
From Eq. (6-89),

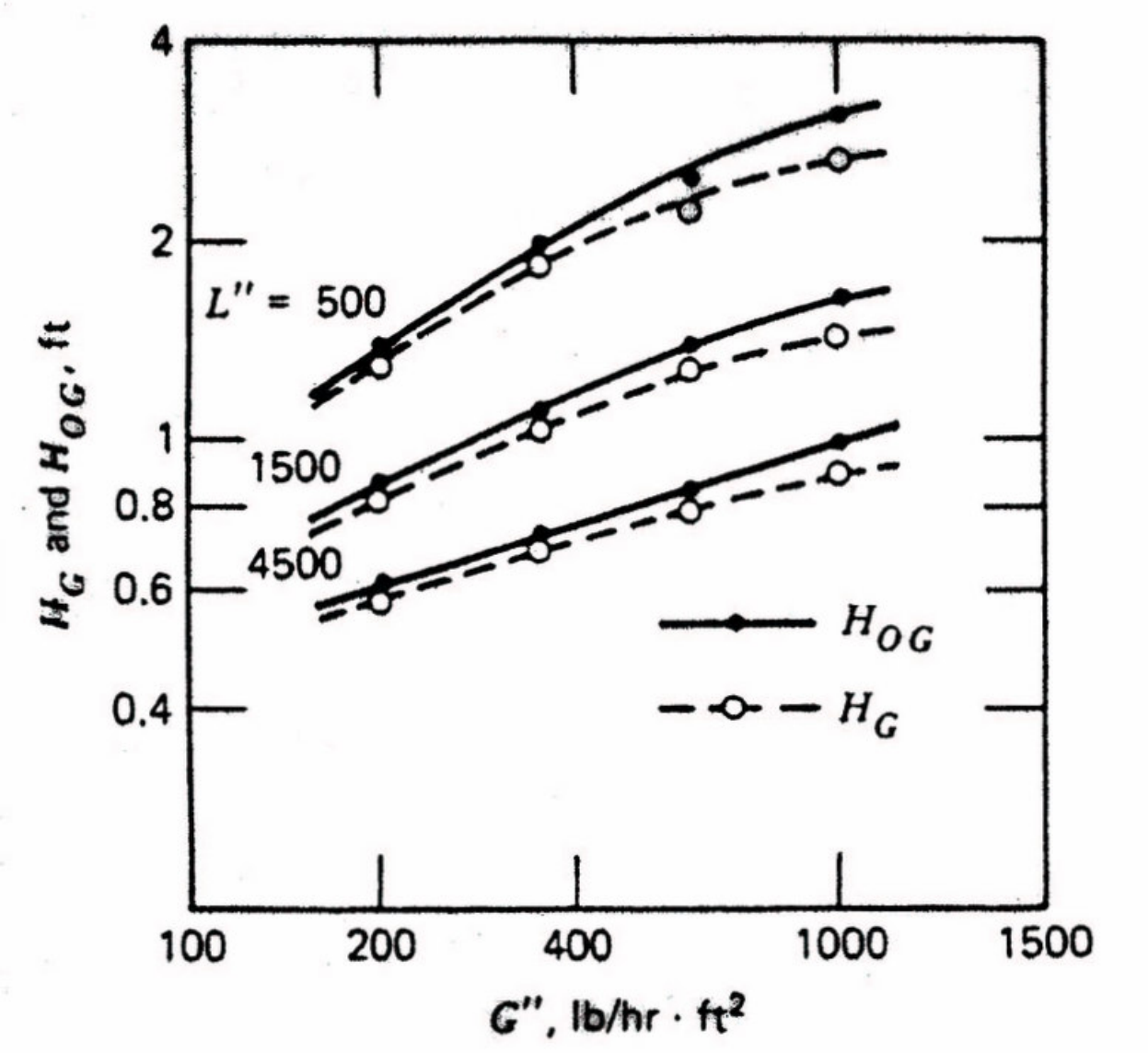
$$N_{OG} = \frac{\ln\left\{\left[(A-1)/A\right]\left[(y_{in} - Kx_{in})/(y_{out} - Kx_{in})\right] + (1/A)\right\}}{(A-1)/A} = \frac{\ln\left\{\left[(6-1)/6\right]\left[0.02/0.002\right] + (1/6)\right\}}{(6-1)/6} = 2.57$$

To obtain an estimate of H_{OG}, the correlations of Billet and Schultes in Chapter 6 or literature data can be used. The latter is found on page 16-38 of Perry's Chemical Engineers' Handbook, 6th edition or on page 663 of "Equilibrium-Stage Separation Operations in Chemical Engineering" by Henley and Seader, as shown below.

Exercise 6.30 (continued)

Analysis: (a) (continued)

Air-Ammonia-Water system with 1.5-inch Berl Saddles, AE units



From the above figure, H_{OG} = 0.85 ft. From Eq. (2), l_T = 2.57(0.85) = 2.2 ft

(b) From Eq. (6-11), $(L/S)_{min}$ = (V/S) K (fraction absorbed) = 240(2.7)(0.98) = 635 lb/h-ft^2

(c) Consider the differences between 1.5-inch ceramic Berl saddles (Saddles) and 1.5-inch ceramic Hiflow rings (Rings). In Table 6.8, data are given for the rings, but not for the saddles of the 1.5-inch size. To make the comparison, take the near-1 inch size. Then, the following parameters apply:

Packings	F_P	a	ε	C_h	C_p	C_L	C_V
Saddles	110	260	0.68	0.62		1.246	0.387
Rings		261.2	0.779	1.167	0.628	1.744	0.465

Exercise 6.30 (continued)

Analysis: (c) (continued)

Note that for the NH_3-air-water system, the above plot shows that H_{OG} is approximately equal to H_G. Therefore, the liquid-phase resistance is small and $K_L a$ need not be considered.

Consider $K_G a$ and H_{OG}:

In the above table, values of a are essentially the same. From Eqs. (6-136) and (6-140), a_{Ph}/a is proportional to $\varepsilon^{1/2}/a$. Therefore, $\dfrac{a_{Ph}/a \text{ for Rings}}{a_{Ph}/a \text{ for Saddles}} = \left(\dfrac{0.779}{0.68}\right)^{1/2} = 1.07$

From Eq. (6-133), if we ignore holdup, h_L, in the term ($\varepsilon - h_L$), and differences in a, then,

$$H_G \text{ is proportional to } \frac{1}{C_V}\varepsilon^4\left(\frac{a}{a_{Ph}}\right)$$

Therefore,
$$\frac{H_G \text{ for Rings}}{H_G \text{ for Saddles}} = \frac{\dfrac{1}{0.465}(0.779)^4}{\dfrac{1}{0.387}(0.680)^4}(1.07) = 1.53$$

This ratio should be about the same for H_{OG} .

From Table 6.7, K_G is inversely proportional to H_G. Therefore, $\dfrac{K_G a \text{ for Rings}}{K_G a \text{ for Saddles}} = \dfrac{1}{1.53} = 0.653$

Consider pressure drop:

The pressure drop is given by Eq. (6-106). If we ignore holdup, h_L, in the term ($\varepsilon - h_L$), and differences in a, and combine Eqs. (6-99) and (6-110) to (6-115), then,

$$\Delta P \text{ is approximately proportional to } \frac{C_p}{\varepsilon^3}$$

However, Table 6.8 does not contain C_p for Berl saddles, so no comparison can be made.

Consider Column N_{OG} and height:

The value of N_{OG} is independent on packing material. Therefore, the height is shorter for the saddle packing because the H_{OG} is smaller.

Consider column diameter:

The column diameter is related to the flooding velocity, as given in Fig. 6.36(a). For a given value X, the value of Y is fixed and the product $(u_o)^2 F_P$ is a constant. The packing factor for the ceramic Hiflow rings is not given in Table 6.8. However, if a value is extrapolated from data for larger rings, the packing factor for the Rings is much less than for the Saddles. Therefore, the flooding velocity for the Rings will be higher and the column diameter smaller.

Consider maximum liquid rate:

For a fixed gas velocity, the value of Y in Fig. 6.36(a) is smaller for the Rings because the packing factor is less. Therefore, as shown in the same figure, the value of X is greater for flooding, which gives a larger maximum liquid rate.

Exercise 6.31

Subject: Absorption of CO_2 from air into a dilute caustic solution with a packed column.

Given: 5,000 ft^3/min at 60°F and 1 atm, containing 3 mol% CO_2. Recovery of 97% of CO_2. Equilibrium curve is $Y = KX = 1.75X$ (i.e. mole ratios) at column operating conditions.

Assumptions: No stripping of water. No absorption of air. Caustic solution has properties of water. Initial estimate of column diameter is 30 inches. Try 2-inch Intalox saddles packing.

Find: (a) Minimum caustic solution-to-air molar flow-rate ratio.
(b) Maximum possible concentration of CO_2 in caustic solution.
(c) N_t at L/V = 1.4 times minimum.
(d) Caustic solution rate.
(e) Pressure drop per ft of column packed height.
(f) N_{OG}
(g) Packed height for K_Ga = 2.5 lbmol/h-ft^3-atm.

Analysis: Gas flow rate = 5,000(60)/379 = 792 lbmol/h.
Therefore, air in entering gas = V' = 0.97(792) = 768 lbmol/h
The CO_2 in the entering gas = 0.03(792) = 24 lbmol/h
The CO_2 in the exiting gas = 0.03(24) = 0.72 lbmol/h
The CO_2 absorbed in the leaving liquid = 24 - 0.72 = 23.28 lbmol/h
The mole ratios are Y_{in} = 24/768 = 0.03125, Y_{out} = 0.72/768 = 0.0009375, X_{in} = 0.0

(a) From Eq. (6-11), $L'_{min} = V'K$(fraction absorbed) = 768(1.75)(0.97) = 1,304 lbmol/h

(b) The maximum possible CO_2 concentration in the caustic solution occurs at infinite stages with the minimum liquid rate. The leaving liquid is in equilibrium with the entering gas. Therefore,

$X_{out} = Y_{in}/K$ = 0.03125/1.75 = 0.0179 mol CO_2 / mol caustic solution.

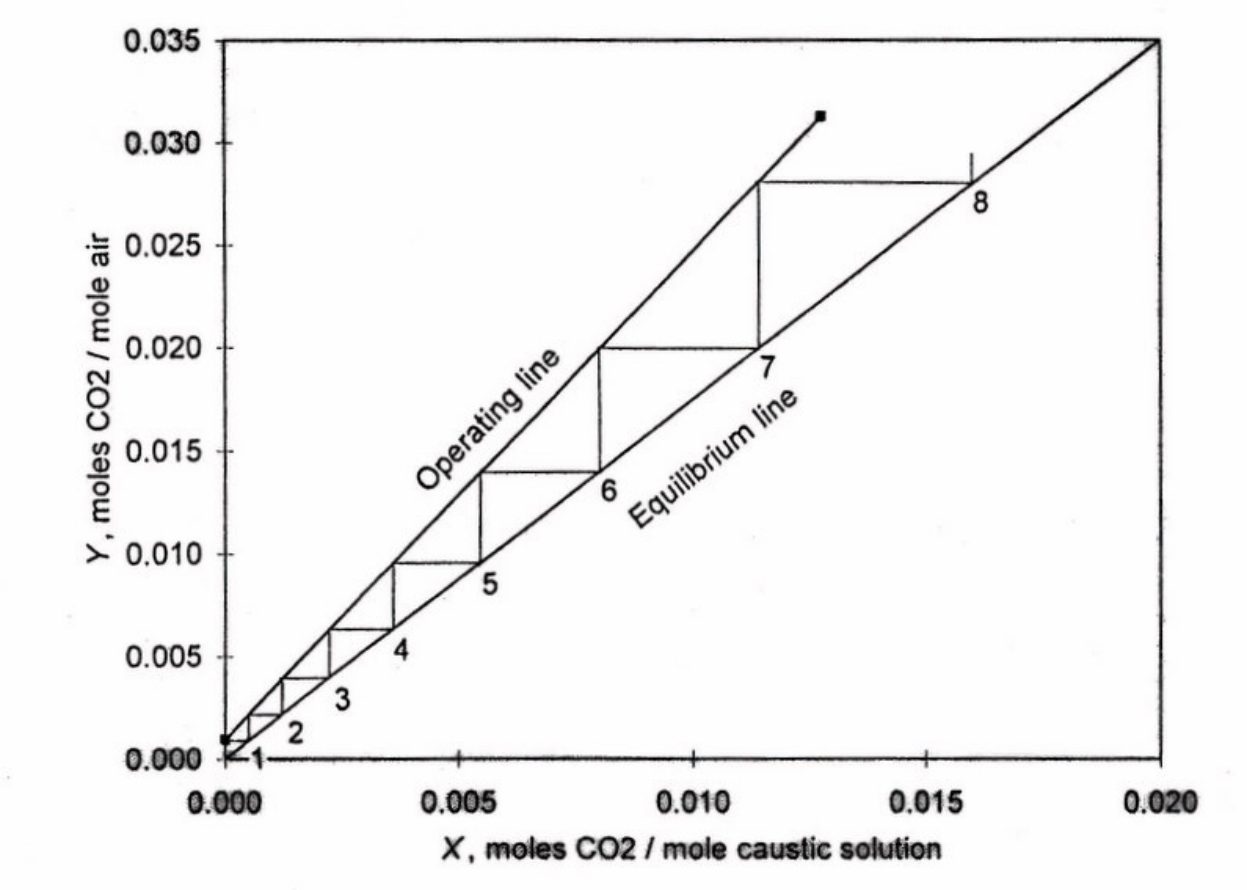
(c) Let $L/V = L'/V'$. Then, L = 1.4 (1,304) = 1,826 lbmol/h and L/G = 1,826/768 = 2.38.
For this liquid flow rate, a material balance for CO_2 is,
768(0.03125 - 0.0009375) = 23.28 = 1,826(X_{out} - 0.0). Solving, X_{out} = 0.01275
In the Y-X plot on the next page, the equilibrium line, $Y = 1.75X$, and the straight operating line, passing through the column Y-X end points {Y_{in} = 0.03125, X_{out} = 0.01275} and {Y_{out} = 0.0009375, X_{in} = 0.0} are shown, with the equilibrium stages stepped off, giving N_t = 7.3.

(d) From Part (c), caustic rate = 1,826 lbmol/h.

(e) Assume the use of 2-inch of ceramic Intalox saddles. From Table 6.8, F_P = 40 ft^2/ft^3.
Use Fig. 6.36(a). Assume for the dilute caustic solution, $f\{\rho_L\} = 1.0$ and $f\{\mu_L\} = 1.0$.
Take M_V = 29, M_L = 18, ρ_L = 62.4 lb/ft^3, ρ_V = 29/379 = 0.0765 lb/ft^3
Using conditions at the bottom of the column,

Exercise 6.31 (conditions)

Analysis: (d) and (e) (continued)



$$X = \frac{LM_L}{VM_V}\left(\frac{\rho_V}{\rho_L}\right)^{1/2} = \frac{(1{,}849)(18)}{(792)(29)}\left(\frac{0.0765}{62.4}\right)^{1/2} = 0.051$$

From Fig. 6.36(a), at flooding, $Y = 0.18$
Now compute Y for the suggested column diameter of 30 inches = 2.5 ft.
From the continuity equation, $u_o = m/S\rho_V = [(792)(29)/3600]/[3.14(2.5)^2/4](0.0765) = 17$ ft/s
From Table 6.8, the packing factor, $F_P = 40$ ft^2/ft^3.

$$Y = \frac{u_o^2 F_P}{g}\left(\frac{\rho_V}{\rho_{H_2O}}\right) = \frac{17^2(40)}{32.2}\left(\frac{0.0765}{62.4}\right) = 0.440\text{, which is much greater than } 0.18$$

Therefore, a diameter of 30 inches places the operation badly into the flooding region and a pressure drop calculation is meaningless. A larger diameter is necessary.

Exercise 6.31 (continued)

(f) From Eq. (6-95), with $A = L/KV = (1{,}826)/1.75(768) = 1.36$,

$$N_{OG} = N_t = A \ln(1/A)/(1- A) = 7.3(1.36) \ln (1/1.36)/(1 - 1.36) = 8.5$$

(g) From Table 6.7, $H_{OG} = V/K_G aPS$, with $V = 792$ lbmol/h,
$K_G a = 2.5$ lbmol/h-ft^3-atm, $P = 1$ atm

For column cross sectional area, S, assume 50% of flooding. At flooding, with $Y = 0.18$,
by ratio with the Y of 0.440 for a 2.5 ft diameter, need u_o at flooding $= 17(0.18/0.44)^{0.5} = 10.9$ ft/s

At 50% of flooding, $u = 5.45$ ft/s. By ratio, column diameter $= 2.5(17/5.45)^{0.5} = 4.4$ ft
Column cross sectional area $= S = 3.14(4.4)^2/4 = 15.2$ ft^2.

Therefore, $H_{OG} = (792)/(2.5)(1)(15.2) = 20.8$ ft, which is very high.

From Eq. (6-89), $l_T = H_{OG} N_{OG} = 20.8(8.5) = 177$ ft. Given value of $K_G a$ seems very low.

Exercise 6.32

Subject: Absorption of NH_3 from air into water with a packed column.

Given: Conditions at a point in the column where P = 101.3 kPa, T = 20°C, 10 mol% NH_3 in bulk gas, 1 wt NH_3 in bulk liquid, NH_3 partial pressure of 2.26 kPa at the interface, and ammonia absorption rate of 0.05 kmol/h-m^2.

Find: (a) X, Y, Y_i, X_i, X^*, Y^*, K_Y, K_X, k_Y, *and* k_X in Fig. 6.49.
(b) % of mass transfer resistance in each phase.
(c) Verify that $\dfrac{1}{K_Y} = \dfrac{1}{k_Y} + \dfrac{H'}{k_X}$

Analysis: (a) At the point, as shown in Fig. 6.49, the mole ratios in the bulk are
X = (1/17)/(99/18) = 0.0107 and Y = 0.1/0.9 = 0.111.
At the interface, Y_i = 2.26/(101.3 - 2.26) = 0.0229.
Then, using the equilibrium curve in Fig. 6.49, X_i = 0.028
The values of the mole fractions in equilibrium with the bulk values are obtained from the equilibrium curve in Fig. 6.49. Thus, in equilibrium with Y = 0.111 is X^* = 0.114.
In equilibrium with X = 0.0107 is Y^* = 0.007
The given NH_3 mass-transfer flux can be written with the following combinations of mass-transfer coefficients and driving forces, using Table 6.7 as a guide:

$$N = 0.05 = K_Y\left(Y - Y^*\right) = K_X\left(X^* - X\right) = k_Y\left(Y - Y_i\right) = k_X\left(X_i - X\right) \qquad (1)$$

From Eq. (1), $K_Y = 0.05/(Y - Y^*) = 0.05/(0.111 - 0.007)$ = 0.480 kmol/h-ft^2-mole ratio
From Eq. (1), $K_X = 0.05/(X^* - X) = 0.05/(0.114 - 0.0107)$ = 0.484 kmol/h-ft^2-mole ratio
From Eq. (1), $k_Y = 0.05/(Y - Y_i) = 0.05/(0.111 - 0.0229)$ = 0.568 kmol/h-ft^2-mole ratio
From Eq. (1), $k_X = 0.05/(X_i - X) = 0.05/(0.028 - 0.0107)$ = 2.89 kmol/h-ft^2-mole ratio

(b) To determine the relative mass-transfer resistances in each phase, Eq. (1) can be rearranged as in Eq. (6-78):

$$\frac{k_X}{k_Y} = -\frac{(Y - Y_i)}{(X - X_i)} = -\frac{2.89}{0.568} = -5.08$$

Thus, the lowest coefficient and the highest driving force is that associated with the gas phase. From the ratio of 5.08, the largest mass-transfer resistance is in the gas phase. That resistance is about five times the resistance in the liquid phase, with 84% in the gas phase, 16% in the liquid.

(c) From a mole ratio form of Eq. (6-80),

$$\frac{1}{K_Y} = \frac{1}{k_Y} + \frac{1}{k_X}\left(\frac{Y_i - Y^*}{X_i - X}\right) \qquad (2)$$

Therefore, $$H' = \left(\frac{Y_i - Y^*}{X_i - X}\right) = \left(\frac{0.0229 - 0.007}{0.028 - 0.0107}\right) = 0.919$$

Therefore, $\dfrac{1}{k_Y} + \dfrac{H'}{k_X} = \dfrac{1}{0.568} + \dfrac{0.919}{2.89} = 2.08$ compared to $\dfrac{1}{K_Y} = \dfrac{1}{0.480} = 2.08$

Exercise 6.33

Subject: Stripping of ammonia from an aqueous solution with air in a packed column.

Given: Aqueous solution of 20 wt% NH_3. Exit liquid to contain no more than 1 wt% NH_3. Exit gas to be 1,000 ft^3/h of a 10 mol% NH_3 in air. Equilibrium data in Fig. 6.49. Temperature = 20°C = 68°F.

Assumptions: No stripping of water. No absorption of air. Operation at 1 atm.

Find: Volume of packing for $K_G a$ = 4 lbmol/h-ft^3-atm.

Analysis: First, determine the molar flow rates of components in the exit gas.
From the ideal gas law applied to the exiting gas at 1 atm and 68°F,
$\rho = P / RT = 1/(0.7302)(68+460) = 0.00259$ lbmol/ft^3
Flow rate of exit gas = 1,000(0.00259) = 2.59 lbmol/h
Gas contains 0.10(2.59) = 0.259 lbmol/h of NH_3 and 0.90(2.59) = 2.331 lbmol/h of air.
Next, determine the mole fractions in the inlet and exit liquid streams.
Take as a basis, 100 lb of inlet liquid.

	Inlet liquid:			Outlet liquid:		
Component	lb	lbmol	mole fraction	lb	lbmol	mole fraction
H_2O	80	4.44	0.79	80.000	4.4400	0.9894
NH_3	20	1.18	0.21	0.808	0.0475	0.0106
Total	100	5.62	1.00	80.808	4.4875	1.0000

Determine the water flow rate, L', in and out by an ammonia balance:

$$\left(\frac{0.21}{0.79}\right)L' + 0 = \left(\frac{0.0106}{0.9894}\right)L' + 0.259 \qquad (1)$$

Solving Eq. (1), L' = 1.015 lbmol/h of H_2O.
NH_3 in entering liquid = (0.21/0.79)1.015 = 0.270 lbmol/h
NH_3 in leaving liquid = 0.270 - 0.259 = 0.011 lbmol/h
Because of the concentrated solution, take into account the bulk-flow effect.
For a partial pressure driving force, can write the rate of mass transfer, V for volume, as,

$$n_{NH_3} = 0.259 = \frac{K_G a V}{(y_{air})_{avg}}\left(p^*_{NH_3} - p_{NH_3}\right)_{LM} \qquad (2)$$

Rearranging Eq. (1), $$V = \frac{0.259(y_{air})_{avg}}{\left(p^*_{NH_3} - p_{NH_3}\right)_{LM} K_G a} \qquad (3)$$

Exercise 6.33 (continued)

Analysis: (continued)

First consider the bulk-flow effect.
At the top of the column, in the bulk exiting air, $y_{air} = 0.90$
To obtain the corresponding value of y in the vapor in equilibrium with the entering liquid at the top of the column, use Fig. 6.49. In entering bulk liquid, moles NH_3/moleH_2O =1.18/4.44=0.266.
From Fig. 6.49, by a rough extrapolation, moles NH_3/mole H_2O in equilibrium gas = 0.266.
Therefore, $y^*_{air} = 1 - 0.266/1.266 = 1 - 0.210 = 0.79$. The average $y_{air} = (0.90 + 0.79)/2 = 0.845$.

At the bottom of the column, in the bulk entering air, $y_{air} = 1.00$
To obtain the corresponding value of y^* in the vapor in equilibrium with the leaving liquid at the column bottom, use Fig. 6.49.
In leaving bulk liquid, moles NH_3/mol $H_2O = 0.0475/4.4 = 0.0108$.
From Fig. 6.49, moles NH_3/mole H_2O in equilibrium gas = 0.007 = mole fraction of NH_3
Therefore, $y^*_{air} = 1 - 0.007 = 0.993$. The average $y_{air} = (1.000 + 0.993)/2 = 0.997$
The $(y_{air})_{avg} = (0.845 + 0.997)/2 = 0.921$

Now, determine the log mean partial pressure driving force for ammonia, using Dalton's law with the above mole fractions.
At the top of the column, for ammonia, $(p^* - p)_{top} = P\,(y^* - y)_{top} = (1.0)(0.210 - 0.10) = 0.11$ atm
At the column bottom, for ammonia, $(p^* - p)_{bottom} = P\,(y^* - y)_{bottom} = (1.0)(0.007 - 0.0) = 0.007$ atm
Therefore, for ammonia, $(p^* - p)_{LM} = 0.037$ atm

$$\text{From Eq. (3), packed volume} = V = \frac{0.259(0.921)}{(0.037)(4)} = 1.61 \text{ ft}^3$$

Exercise 6.34

Subject: Absorption of NH_3 from air into water in a packed column.

Given: Entering gas is 2,000 lb/h of air (dry basis) containing NH_3 with a partial pressure of 12 torr and saturated with water vapor at 68°F and 1 atm. Equilibrium data in Fig. 6.49. Absorb 99.6% of the NH_3.

Assumptions: No absorption of air. No stripping of water.

Find: (a) Minimum water rate.
(b) Column diameter and height for water rate of 2 times minimum and 50% of flooding gas velocity if 38-mm ceramic Berl saddles are used.
(c) Same as Part (b) for 50-mm Pall rings.
(d) Packing recommendation.

Analysis: First compute the ammonia material balance.
Flow rate of NH_3-free air = 2,000/29 = 69 lbmol/h
Flow rate of NH_3 in the entering gas = 12(69)/(760-12) = 1.107 lbmol/h
Flow rate of NH_3 in the exiting liquid = 0.996(1.107) = 1.1026 lbmol/h
Flow rate of NH_3 in the leaving gas = 1.107 - 1.1026 = 0.0044 lbmol/h
(a) Operation in dilute region, where we can apply Henry's law. From Fig. 6.49, using results from Exercise 6.33, when x=0.0108, y=0.007. Therefore, the equilibrium equation is $y = 0.65x$.
Therefore, $K = 0.65$. Entering gas rate = V = 69 + 1.107 = 70.1 lbmol/h
From Eq. (6-11), $L_{min} = VK$(fraction absorbed) = 45.4 lbmol/h
(b) $L = 2L_{min} = 2(45.4) = 90.8$ lbmol/h
Compute column diameter for 50% of flooding, using Fig. 6.36.
Take properties of gas and liquid as those of air and water, respectively.
From the ideal gas law, $\rho_G = PM/RT = (1)(29)/(0.7302)(528) = 0.0752$ lb/ft^3

In Fig. 6.36(a), $X = \dfrac{LM_L}{VM_V}\left(\dfrac{\rho_V}{\rho_L}\right)^{1/2} = \dfrac{(45.4)(18)}{(70.1)(29)}\left(\dfrac{0.0752}{62.4}\right)^{1/2} = 0.014$

Take $f\{\rho_L\}$ and $f\{\mu_L\}$ =1.0. From Fig. 6.36(a), at flooding, $Y = \dfrac{u_o^2 F_P}{g}\left(\dfrac{\rho_V}{\rho_{H_2O}}\right) = 0.22$ (1)

For 38-mm Berl saddles, the packing factor, F_P, is not included in Table 6.8. However, it can be found in Perry's Chemical Engineers' Handbook, which gives F_P = 65 ft^2/ft^3.

Solving Eq. (1), $u_o^2 = \dfrac{Yg}{F_P}\left(\dfrac{\rho_{H_2O}}{\rho_V}\right) = \dfrac{(0.22)(32.2)}{65}\left(\dfrac{62.4}{0.0752}\right) = 90.4$

Therefore, u_o = 9.5 ft/s. The fraction of flooding = f = 0.5.
From Eq. (6-103), the column diameter is,

$$D_T = \left(\frac{4VM_V}{fu_o\pi\rho_V}\right)^{1/2} = \left[\frac{4(70.1/3,600)(29)}{(0.5)(9.5)(3.14)(0.0752)}\right]^{1/2} = 1.42 \text{ ft}$$ and $S=\pi D_T^2/4 = 3.14(1.42)^2/4 = 1.58$ ft^2

Exercise 6.34 (continued)

Analysis: (b) (continued)

For column height, use Eq. (6-89), because mass-transfer is controlled by the gas phase.

For N_{OG} , use Eq. (6-88) with $x_{in} = 0$. Absorption factor = $A = L/KV = (90.8)/(0.65)(70.1) = 2$

From Eq. (6-93), using $y_{in} = 1.107/70.1 = 0.0158$, $y_{out} = 0.0044/69 = 0.0000638$

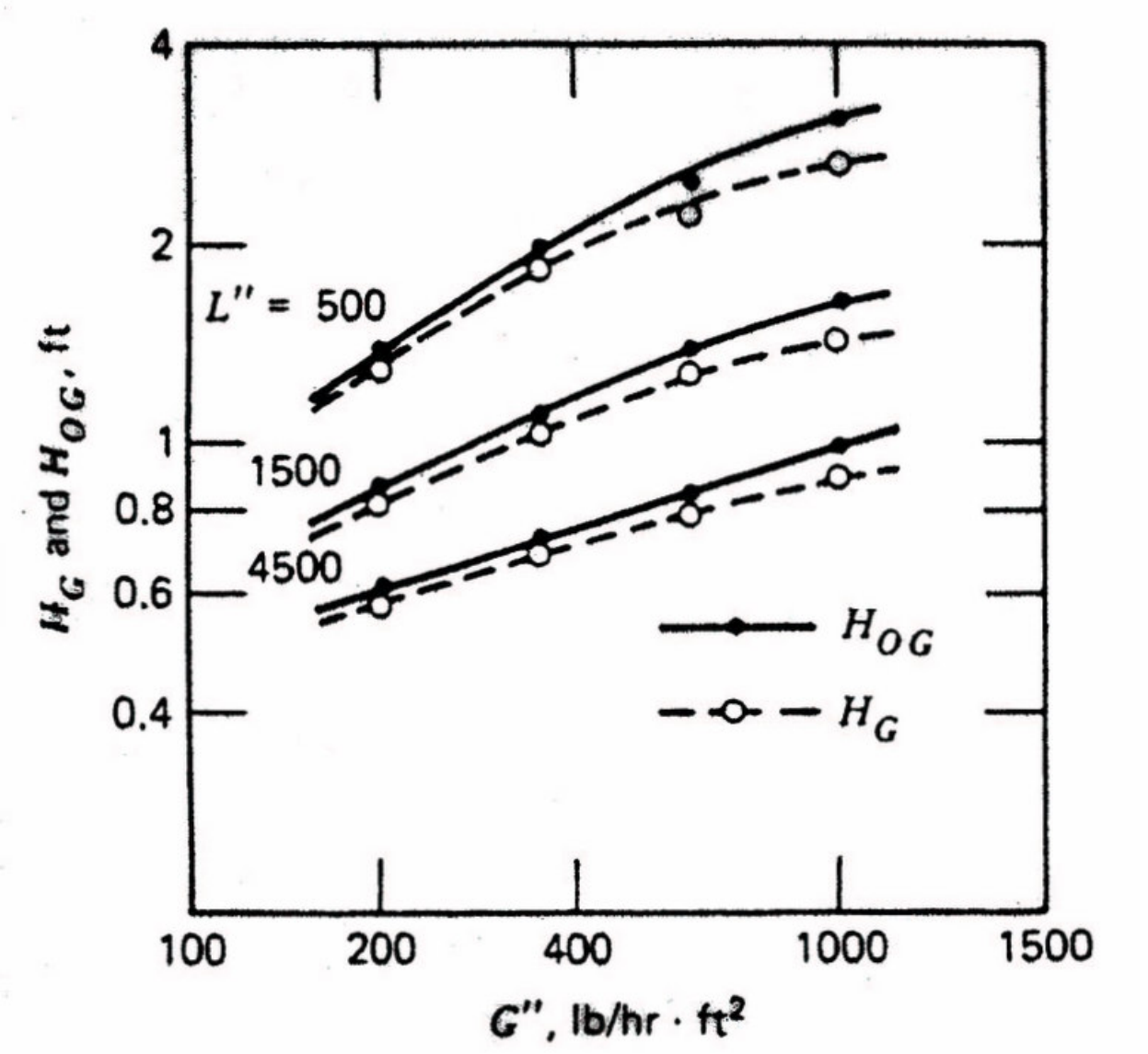
$$N_{OG} = \frac{\ln\left\{\left[(A-1)/A\right]\left[(y_{in})/(y_{out})\right]+(1/A)\right\}}{(A-1)/A} = \frac{\ln\left\{\left[(2-1)/2\right]\left[0.0158/0.0000638\right]+(1/2)\right\}}{(2-1)/2} = 9.65$$

For H_{OG}, literature data can be used, as found on page 16-38 of Perry's Chemical Engineers' Handbook, 6th edition or on page 663 of "Equilibrium-Stage Separation Operations in Chemical Engineering" by Henley and Seader, as shown below.

To use this plot, $L'' = 90.9(18)/1.58 = 1{,}040$ lb/h-ft^2 and $V''=G'' = 70.1(29)/1.58 = 1{,}290$ lb/h-ft^2

Then, $H_{OG} = 1.9$ ft and column height = $l_T = N_{OG}H_{OG} = (9.65)(1.9) = 18.3$ ft.

Air-Ammonia-Water system with 1.5-inch Berl Saddles, AE units



Exercise 6.34 (continued)

Analysis: (c) (continued)

(c) Assume the 50-mm Pall rings are metal. From Table 6.8, $F_P = 27$ ft^2/ft^3.

Solving Eq. (1), $u_o^2 = \dfrac{Yg}{F_P}\left(\dfrac{\rho_{H_2O}}{\rho_V}\right) = \dfrac{(0.22)(32.2)}{27}\left(\dfrac{62.4}{0.0752}\right) = 235$

Therefore, $u_o = 15.3$ ft/s. The fraction of flooding = $f = 0.5$.
From Eq. (6-103), the column diameter is,

$$D_T = \left(\frac{4VM_V}{fu_o\pi\rho_V}\right)^{1/2} = \left[\frac{4(70.1/3,600)(29)}{(0.5)(15.3)(3.14)(0.0752)}\right]^{1/2} = 1.12 \text{ ft}$$ and $S = 3.14(1.12)^2/4 = 0.985$ ft^2

The value of $N_{OG} = 9.65$, the same as in Part (b)

For H_{OG}, can use Figs. 6.42 and 6.43 for 50 mm Pall rings.
Gas capacity factor = $F = u_G(\rho_V)^{0.5} = f\,u_o(\rho_V)^{0.5} = (0.5)(15.3)(0.0752)^{0.5} = 2.1$ lb$^{1/2}$-s^{-1}-ft$^{-1/2}$
or 5.12 kg$^{1/2}$-s^{-1}-m$^{-1/2}$

By the continuity equation, liquid load = $Q_L/S = u_L = m/S\rho_L$ =
(90.8/3600)(18)/(0.985)(62.4) =0.0074 ft/s or 0.00225 m/s or 2.25 x 10^{-3} m^3/m^2-s

In Fig. 6.42, from the slope of the correlating line, k_Ga is proportional to $F^{0.7}$
In Fig. 6.43, from the slope of the correlating line, k_Ga is proportional to $u_L^{0.45}$

Using the value of $k_Ga = 3.1$ s^{-1} at $u_L = 2.25$ x 10^{-3} m^3/m^2-s and $F = 1.16$, then the two plots are represented by the equation, $k_Ga = 43.4\,F^{0.7}\,u_L^{0.45}$

For our case, $k_Ga = 43.4\,(5.12^{0.7})(0.00225^{0.45}) = 8.8$ s^{-1}
Note that this k_Ga is in concentration units for the driving force.

Therefore, from Table 6.7 by analogy to the liquid phase case,

$$H_G = VM_V/k_GaS\rho_V = (70.1/3,600)(29)/(8.8)(0.985)(0.0752) = 0.87 \text{ ft}$$

The column height is $l_T = 9.65(0.87) = 8.4$ ft.

Exercise 6.34 (continued)

Analysis:

(d) Now compare the two packings on the basis of flooding and mass transfer:

Packing	Column diameter, ft	Column height, ft
38-mm ceramic Berl saddles	1.42	18.3
50-mm metal Pall rings	1.12	8.4

Clearly the 50-mm metal Pall rings are superior in performance. However, the selection would have to be made on the basis of cost. Because of the much smaller column and volume of packing, it is likely that the 50-mm Pall rings would be favored.

From page 14-59 of Perry's Chemical Engineers' Handbook, 7th edition (1997), the cost of 38-mm ceramic Berl saddles is approximately $\$21/ft^3$. The cost of 50-mm Pall rings depends on whether they can be made of carbon steel or must be made of stainless steel, with the former $\$19.9/ft^3$ and the latter $\$99.0/ft^3$. So the material of construction is a very important factor.

Exercise 6.35

Subject: Absorption of Cl_2 from air with water in a packed column.

Given: 100 kmol/h of feed gas containing 20 mol% Cl_2. Column operation at 20°C and 1 atm. Table of *y*-*x* data for Cl_2. Exit gas to contain 1 mol% Cl_2.

Assumptions: No stripping of water. No absorption of air.

Find: (a) Minimum water rate in kg/h.
(b) N_{OG} for a water rate of 2 times minimum.

Analysis: Solve this problem using mole ratios. Feed gas is 80 kmol/h of air = G' , and 20 kmol/h of Cl_2 with $Y_{in} = 20/80 = 0.25$. Exit gas has $Y_{out} = 1/99 = 0.0101$. $X_{in} = 0.0$. Highest value of Y in the table of equilibrium data is 0.06/0.94 = 0.0638. Therefore, data for higher values of Y are needed. Can obtain this from Perry's Handbook, page 3-102 in the 6th edition and page 2-126 in the 7th edition. The expanded table of equilibrium data with conversion to mole ratios includes the following values added from Perry's Handbook, using the conversions:

$y = p_{Cl2}$, torr/760 torr

x = [(grams Cl_2/L)/71]/[1,000/18 + (grams Cl_2/L/71)]

p_{Cl2}, torr	grams Cl_2/L	y	x
100	1.773	0.132	0.000450
150	2.27	0.197	0.000576
200	2.74	0.263	0.000695

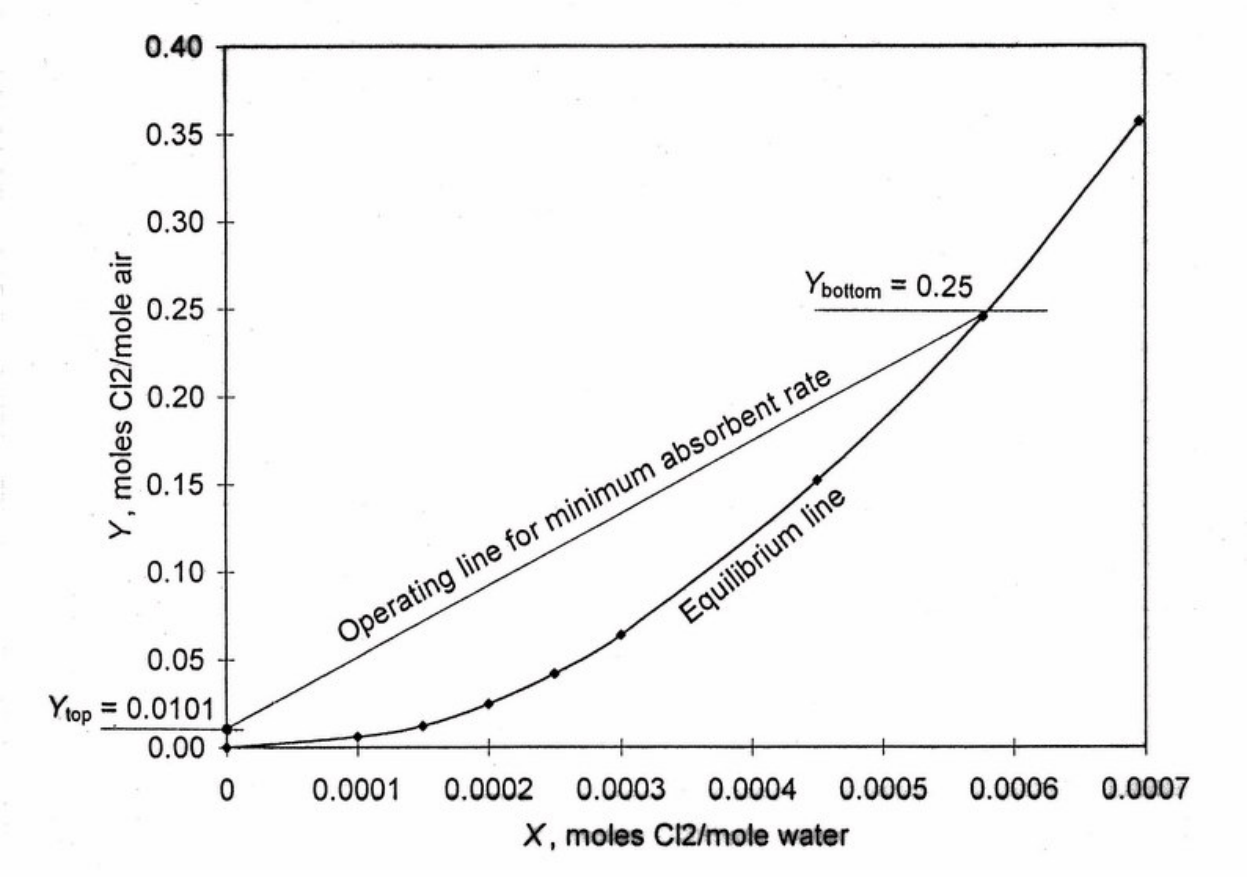
These equilibrium data and those given in the exercise are now converted to mole ratios using, $Y = y/(1 - y)$ and $X = x/(1 - x)$

y	x	Y	X
0.006	0.000100	0.00604	0.000100
0.012	0.000150	0.01215	0.000150
0.024	0.000200	0.02459	0.000200
0.040	0.000250	0.04167	0.000250
0.060	0.000300	0.06383	0.000300
0.132	0.000450	0.15207	0.000450
0.197	0.000576	0.24533	0.000576
0.263	0.000695	0.35685	0.000695

(a) To determine the minimum water rate, it is best to do this graphically because of the high degree of curvature of the equilibrium curve. The pinch region of infinite stages at minimum absorbent rate occurs at the bottom of the column, such that the leaving liquid is in equilibrium with the entering gas, with a $Y = 0.25$. With mole-ratio coordinates, the operating line is straight and passes through the following point at the top of the column {$X = 0.0$, $Y = 0.0101$}.

Exercise 6.35 (continued)

Analysis: (a) (continued)
The point at the bottom of the column must pass through the point {X^* in equilibrium with $Y = 0.25$}. This is shown in the following plot, which is similar to Fig. 6.9.

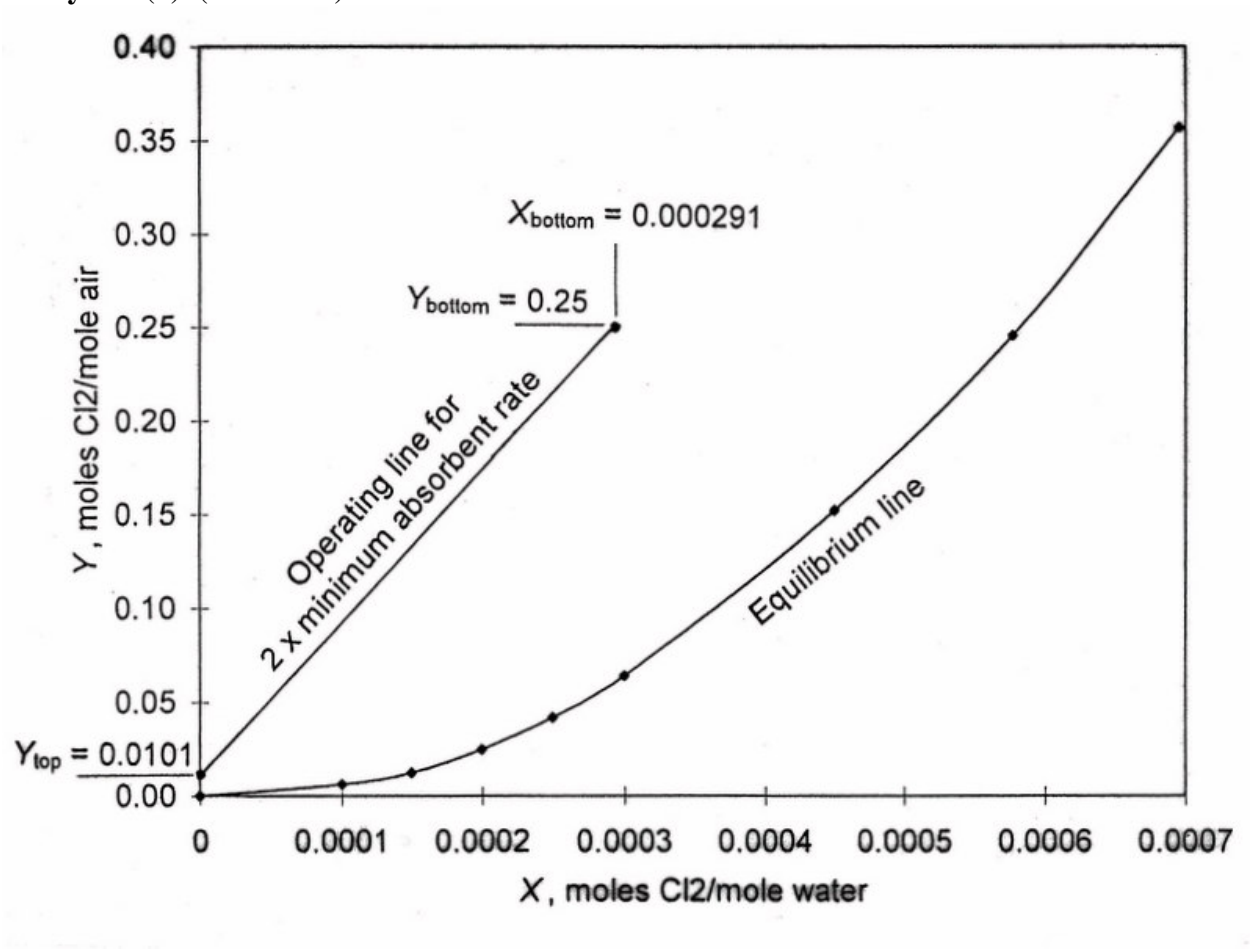


From the solute material balance, Eq. (6-6), the slope of the operating line is given by L'/V'. From the above plot, X_{bottom} = 0.000581, and, thus, the slope of that line is, $L'/V' = (0.25 - 0.0101)/(0.000581 - 0.0) = 413$. Since $V' = 80$ kmol/h, $L' = 80(413) = 33{,}000$ kmol/h. Alternatively, since the Cl_2 absorption rate = $V'(Y_{bottom} - Y_{top}) = 80(0.25 - 0.0101) =$ 19.19 kmol/h, then $L' = 19.19/ X_{bottom} = 19.19/0.000581 = 33{,}000$ kmol/h. Take the result as 33,000 kmol/h or 33,000 (18) = 594,000 kg/h.

(b) Twice the minimum water rate = 2(33,000) = 66,000 kmol/h. This gives a mole ratio of chlorine in the leaving water of X_{bottom} =19.19/66,000 = 0.000291 moles Cl_2 / mole water. This operating line is shown in the plot below. To obtain N_{OG} , using mole ratios, the integral in Eq. (6-138) or Table 6.7 can be used,

Exercise 6.35 (continued)

Analysis: (b) (continued)



$$N_{OG} = \int_{Y=0.0101}^{Y=0.25} \frac{dY}{(Y - Y^*)} \qquad (1)$$

Eq. (1) can be solved graphically or numerically. Both require a table of values of $\frac{1}{(Y - Y^*)}$ as a function of Y, where for a given value of X, the value of Y is obtained from the operating line and Y^* is obtained from the equilibrium curve, with values as follows. The values of X are taken from the above table, where the values of Y are the corresponding values of Y^*. For given values of X, values of Y for the operating line are obtained from the following equation of the straight operating line passing through the points $\{ X = 0.0,\ Y = 0.0101\}$ and $\{ X = 0.000291,\ Y = 0.25\}$,

$$Y = 0.0101 + \frac{L'}{V'} X = 0.0101 + \frac{66,000}{80} X = 0.0101 + 825X$$

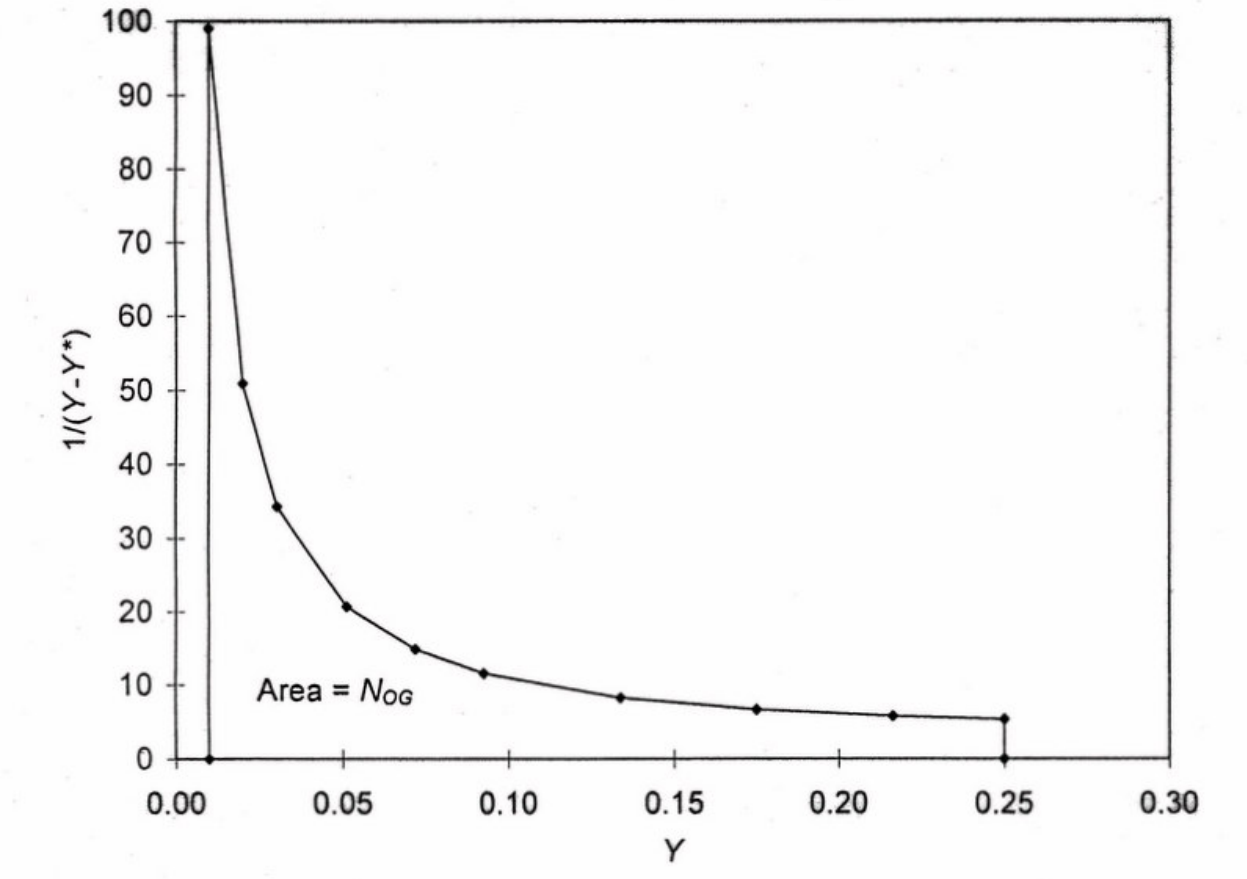
Note that several values of X are added by interpolation to increase the accuracy.

Exercise 6.35 (continued)

Analysis: (b) (continued)

X	Y^*	Y	$1/(Y-Y^*)$	ΔY	Avg $1/(Y-Y^*)$	Area
0.000000	0.00000	0.0101	99.01			
0.0000125	0.00075	0.0204	50.86	0.0103	74.9	0.772
0.000025	0.00150	0.0307	34.22	0.0103	42.5	0.438
0.000050	0.00301	0.0514	20.69	0.0207	27.5	0.569
0.000075	0.00452	0.0720	14.82	0.0206	17.8	0.367
0.000100	0.00604	0.0926	11.55	0.0206	13.2	0.272
0.000150	0.01215	0.1339	8.22	0.0413	9.88	0.408
0.000200	0.02459	0.1751	6.64	0.0412	7.43	0.306
0.000250	0.04167	0.2164	5.72	0.0413	6.18	0.256
0.000291	0.06030	0.2500	5.27	0.0336	5.50	0.185

The following is a plot of $\dfrac{1}{(Y-Y^*)}$ versus Y. The area under the curve is the value of the integral for N_{OG}. In the above table, the trapezoidal method is used to break the curve into 9 segments of ΔY each, varying in width from 0.0103 to 0.0413. For each segment (width), the average value of $1/(Y-Y^*)$ is listed and the product = Area = ΔY times $1/(Y-Y^*)$ is given in the last column. The sum of these areas is $N_{OG} = 3.573$.



Exercise 6.36

Subject: Absorption of ammonia from air into water with a packed column.

Given: Operating conditions in Example 6.15. Entering gas is 100 lbmol/h containing 40 mol% NH_3. Absorbent is 488 lbmol/h of water. Absorb 95% of the NH_3. Equilibrium data in Fig. 6.44. Column operates at 1 atm and 25°C.

Assumptions: No stripping of water. No absorption of air. Liquid has properties of water.

Find: Column diameter and height if packing is 1.5-inch metal Pall rings, using conditions at bottom of tower.

Analysis: From Example 6.15, the conditions at the bottom of the tower are:

Entering gas: 60 lbmol/h of air and 40 lbmol/h of NH_3
Exiting liquid: 488 lbmol/h of water and 38 lbmol/h of NH_3
Operating temperature is 298 K (536°F) and pressure is 1 atm

To compute column diameter use Fig. 6.36 to obtain flooding gas velocity, assume operation at 50% of flooding to obtain operating gas velocity, and use continuity equation to obtain column cross sectional area and column diameter.

Average gas molecular weight = [(60)(29) + (40)(17)]/100 = 24.2
Gas density = $\rho_V = PM/RT$ = (1)(24.2)/(0.7302)(536) = 0.0618 lb/ft^3
From the abscissa of Fig. 6.36(a),

$$X = \frac{LM_L}{VM_V}\left(\frac{\rho_V}{\rho_L}\right)^{1/2} = \frac{(526)(17.9)}{(100)(24.2)}\left(\frac{0.0618}{62.4}\right)^{1/2} = 0.123$$

From Fig. 6.36(a), $Y = 0.105 = \dfrac{u_o^2 F_P}{g}\left(\dfrac{\rho_V}{\rho_{H_2O}}\right) f\{\rho_L\} f\{\mu_L\}$ (1)

For 1.5-inch (35 mm) metal Pall rings, from Table 6.8, F_P = 40 ft^2/ft^3
At 25°C, from Figs. 6.36(b) and (c), $f\{\rho_L\}$ = 1.0 and $f\{\mu_L\}$ = 0.98
From a rearrangement of Eq. (1),

$$u_o^2 = \frac{Yg}{F_P}\left(\frac{\rho_{H_2O}}{\rho_V}\right)\frac{1}{f\{\rho_L\}f\{\mu_L\}} = \frac{(0.105)(32.2)}{40}\left(\frac{62.4}{0.0618}\right)\frac{1}{(1)(0.98)} = 87 \text{ ft}^2/\text{s}^2$$

Then, u_o = 9.3 ft/s
Take the operating superficial velocity = $u_V = fu_o = 0.5\ u_o = 0.5(9.3) = 4.65$ ft/s
From Eq. (6-99),

$$D_T = \left(\frac{4GM_G}{fu_o\pi\rho_G}\right)^{1/2} = \left[\frac{4(100/3{,}600)(24.2)}{(0.5)(9.3)(3.14)(0.0618)}\right]^{1/2} = 1.73 \text{ ft}$$

Exercise 6.36 (continued)

Analysis: (continued)

From Eq. (6-127), column height = $l_T = H_{OG}N_{OG}$ (2)
From Example 6.15, N_{OG} = 3.46 and from above, column cross section = $S = \pi D^2/4$ = 2.35 ft^2.

Mass-transfer data for 2-inch metal Pall rings for the absorption of NH_3 from air into water are presented in Figs. 6.42 and 6.43. In the solutions to Exercise 6.34, these data are fitted to the equation, $k_G a = 43.4\, F^{0.7}\, u_L^{0.45}$, s^{-1} (3)
where the gas capacity factor = $F = u_V(\rho_V)^{0.5} = f\, u_o\, (\rho_V)^{0.5}$ in kg$^{1/2}$-s^{-1}-m$^{-1/2}$ and from the continuity equation, $u_L = m/S\rho_L$ in m/s or m^3/m^2-s

For our case, $F = (0.5)(9.3)(0.0618)^{0.5}$ = 1.16 lb$^{1/2}$-s^{-1}-ft$^{-1/2}$ or 2.83 kg$^{1/2}$-s^{-1}-m$^{-1/2}$
and u_L = [(526)(17.9)/3,600)]/(2.35)(62.4) = 0.018 ft/s = 0.00547 m^3/m^2-s
Substitution of these values into Eq. (3) gives, $k_G a = 43.4(2.83)^{0.7}(0.00547)^{0.45}$ = 8.6 s^{-1}
Note that this $k_G a$ is in concentration units for the driving force.
Therefore, from Table 6.7 by analogy to the liquid phase case,

$$H_{OG} = H_G = VM_V/k_G aS\rho_V = (100/3{,}600)(24.2)/(8.6)(2.35)(0.0618) = 0.54 \text{ ft}$$

Now, we must correct this value to 1.5-inch metal Pall rings.
From Table 6.8, using interpolation when necessary, we have the following characteristics:

Packing	a, m^2/m^3	ε	C_h	C_V
1.5-inch Pall rings	139.4	0.965	0.644	0.373
2.0-inch Pall rings	112.6	0.951	0.784	0.410

From Eqs. (6-136) to (6-140), a_{Ph}/a is proportional to $\varepsilon^{1/2}/a$. Therefore,

$$\frac{a_{Ph}/a \text{ for 1.5-inch Rings}}{a_{Ph}/a \text{ for 2.0-inch Rings}} = \left(\frac{0.965}{0.951}\right)^{1/2}\frac{112.6}{139.4} = 0.814$$

From Eq. (6-133), if we ignore holdup in the term (ε - h_L), then,

$$H_G \text{ is proportional to } \frac{1}{C_V}\frac{\varepsilon}{a^{1.25}}\left(\frac{a}{a_{Ph}}\right)$$

Therefore, $$\frac{H_G \text{ for 1.5-inch Rings}}{H_G \text{ for 2.0-inch Rings}} = \frac{\dfrac{1}{0.341}\left(\dfrac{0.965}{139.4^{1.25}}\right)}{\dfrac{1}{0.410}\left(\dfrac{0.951}{112.6^{1.25}}\right)}\left(\frac{1}{0.814}\right) = 1.15$$

This ratio should be about the same for H_{OG}.
Therefore, for the 1.5-inch rings, H_{OG} = 0.54(1.15) = 0.62 ft.
From Eq. (2), column height = 3.46(0.62) = 2.1 ft.

Exercise 6.37

Subject: Absorption of acetone from air with water in a packed column.

Given: Column operates at 60°F and 1 atm. Entering air is 50 ft^3/min at 60°F and 1 atm, containing 3 mol% acetone. 97% of the acetone is to be absorbed. Maximum allowable gas superficial velocity is 2.4 ft/s. Equilibrium equation is $Y = 1.75\,X$ (1)

Assumptions: No stripping of water. No absorption of air.

Find: (a) Minimum water-to-air ratio.
(b) Maximum acetone concentration possible in the water.
(c) N_t for absorbent flow rate equal to 1.4 times the minimum.
(d) Number of overall gas transfer units.
(e) Height of packing for $K_y a$ = 12.0 lbmol/h-ft^3-mole ratio difference.
(f) Height of packing as a function of molar flow ratio for constant V and HTU.

Analysis: First compute material balance. Total gas in = 50(60)/379 = 7.916 lbmol/h
Acetone in entering gas = 0.03(7.916) = 0.237 lbmol/h
Air in entering gas = 7.916 - 0.237 = 7.679 lbmol/h
Acetone in exiting gas = 0.03(0.237) = 0.007 lbmol/h
Acetone in entering liquid = 0.0 lbmol/h
Acetone in exiting liquid = 0.237 - 0.007 = 0.230 lbmol/h

$X_{in} = 0.0$ $Y_{in} = 0.03/0.97 = 0.03093$ $Y_{out} = 0.007/7.679 = 0.000912$

(a) For minimum water rate, the exiting liquid will be in equilibrium with the entering air. Therefore, using the equilibrium equation, Eq. (1), $X_{out} = Y_{in}/1.75 = 0.03093/1.75 = 0.01767$
Therefore, water rate out and in = 0.230/0.01767 = 13.02 lbmol/h
Minimum water-to-air molar ratio = 13.02/7.679 = 1.70

(b) Maximum possible acetone concentration in the liquid is at min. water rate, $X = 0.01767$
This corresponds to an acetone mole fraction of 0.01767/(1 + 0.01767) = 0.01736.

(c) Use $L_{in} = L' = 1.4\,L_{min} = 1.4(13.02) = 18.23$ lbmol/h
Using mole ratios with no acetone in entering liquid, and K' = constant = 1.75, can apply Eq. (5-29), which was derived for extraction but applies to absorption using:

$$\frac{Y_{out}}{Y_{in}} = \frac{1}{\sum_{n=0}^{N} E^n} \quad \text{where } E = \frac{L'}{K'G'} = \frac{18.23}{(1.75)(7.679)} = 1.356$$

Therefore, $$\frac{Y_{out}}{Y_{in}} = \frac{0.000912}{0.03093} = 0.0295 = \frac{1}{\sum_{n=0}^{N} 1.356^n}$$ Solving, N = 7.5 equilibrium stages

Exercise 6.37 (continued)

Analysis: (c) (continued)
Could also solve this using Kremser's equation or by a graphical construction like Fig. 6.12.

(d) Because operating line and equilibrium line are straight, use Eq. (6-95) with $A = E = 1.356$

$$N_{OG} = N_t \frac{\ln(1/A)}{(1-A)/A} = 7.5 \frac{\ln(1/1.356)}{(1-1.356)/1.356} = 8.7$$

(e) From Eq. (6-141), $l_T = H_{OG} N_{OG}$

From Table 6.7, $H_{OG} = \dfrac{V'}{K_Y a S} = \dfrac{7.679}{(12.0)S} = \dfrac{0.64}{S}$, where S = cross sectional area of tower in ft^2

The allowable gas superficial velocity = u_V = 2.4 ft/s. Take this at the bottom of the tower where gas rate is the highest. From the continuity equation, $Q = u_V S$ = gas volumetric rate
Therefore, $S = Q/u_V = (50/60)/2.4 = 0.347$ ft^2. Therefore, $H_{OG} = 0.64/0.347 = 1.84$ ft
Packing height = (1.84)(8.7) = 16 ft.

(f) To obtain packed height as a function of L'/V' with V' and H_{OG} constant, the only change will be the value of N_{OG} . Use Eq. (6-93), which for $x_{in} = 0$ and $y_{in}/y_{out} = 0.03/0.000911 = 32.9$, is:

$$N_{OG} = \frac{\ln\left[32.9\left(\dfrac{A-1}{A}\right)+\dfrac{1}{A}\right]}{\dfrac{A-1}{A}} \qquad (2)$$

where for a dilute system, we can take $A = L'/K'V' = (L'/V')/K' = (L'/V')/1.75$
The results obtained from Eq. (2) are as follows:

L'/V'	A	$1/A$	$N_{O'G}$	Height, ft
1.75	1.00	1.00	∞	∞
2.0	1.143	0.875	12.9	23.6
2.5	1.429	0.700	7.86	14.5
3.0	1.714	0.583	6.38	11.7
5.0	2.857	0.350	4.74	8.72
10.0	5.714	0.175	4.01	7.38

Exercise 6.38

Subject: Absorption of NH_3 from air into water with a packed column.

Given: Column operating at 68°F and 1 atm. Gas enters at 2,000 ft^3/min at 68°F and 1 atm, containing 6 mol% NH_3 in air. Entering water rate is twice the minimum. Absorb 99% of the NH_3. Gas velocity at 50% of flooding velocity.

Assumptions: No stripping of water. No absorption of air.

Find: Tower diameter and packed height.

Analysis: Entering gas rate is $\frac{2{,}000}{379}\left(\frac{60+460}{68+460}\right)60 = 312$ lbmol /h

Compute material balance. NH_3 in entering gas = 0.06(312) = 18.72 lbmol/h
NH_3 in exiting gas = 0.01(18.72) = 0.19 lbmol/h
Air in entering and exiting gas = V' = 312 - 18.72 = 293.28 lbmol/h
NH_3 in exiting water = 18.72 - 0.19 = 18.53 lbmol/h
Therefore, $X_{in} = 0.0$ $Y_{in} = 18.72/293.28 = 0.06383$ $Y_{out} = 0.19/293.28 = 0.000648$

At the minimum water rate, the exiting liquid is in equilibrium with the entering gas.
From Fig. 6.49, $X^*_{out} = 0.072$ for $Y_{in} = 0.06383$. Therefore, $L'_{min} = 18.53/0.072 = 257$ lbmol/h
Operating liquid rate = 2 times minimum = 2(257) = 514 lbmol/h

Now, compute column diameter using Fig. 6.36. Corrections for liquid density and viscosity are neglected. From the ideal gas law on the entering gas, with an average molecular weight = 28.3,

$$\rho_V = PM/RT = (1)(28.3)/(0.7302)(68+460) = 0.0734 \text{ lb/ft}^3$$

From Table 6.8, packing factor for 1-inch metal Pall rings = 56 ft^2/ft^3.

The abscissa in Fig. 6.36 is, $X = \frac{LM_L}{VM_V}\left(\frac{\rho_V}{\rho_L}\right)^{1/2} = \frac{(514+18.5)(18)}{(312)(28.3)}\left(\frac{0.0734}{62.4}\right)^{1/2} = 0.0373$

From Fig. 6.36, $Y = 0.18$. Therefore, $u_o^2 = \frac{Yg}{F_P}\left(\frac{\rho_{H_2O}}{\rho_V}\right) = \frac{(0.18)(32.2)}{56}\left(\frac{62.4}{0.0734}\right) = 88$

Therefore, flooding velocity = u_o = 9.4 ft/s
For 50% of flooding, $f = 0.5$

From Eq. (6-103), $D_T = \left[\frac{4GM_G}{fu_o\pi\rho_G}\right]^{1/2} = \left[\frac{4(312/3{,}600)(28.3)}{(0.5)(9.4)(3.14)(0.0734)}\right]^{1/2} = 3.0$ ft.

Exercise 6.38 (continued)

Analysis: (continued)

Assume gas phase controls mass transfer rate. Then, from Eq. (6-89), $l_T = H_{OG}N_{OG}$
From Eq. (6-93), for $x_{in} = 0$, $y_{in} = 0.06$, and $y_{out} = 0.00065$,

$$N_{OG} = \frac{\ln\left[92.3\left(\frac{A-1}{A}\right)+\frac{1}{A}\right]}{\frac{A-1}{A}} \qquad (1)$$

For the absorption factor, $A = L/KV$. Take $L = 514$ lbmol/h. Take $V = 312$ lbmol/h.
From Fig. 6.49, $K = 0.82$. Therefore, $A = (514)/(0.82)((312) = 2.0$
From Eq. (1),

$$N_{OG} = \frac{\ln\left[92.3\left(\frac{2-1}{2}\right)+\frac{1}{2}\right]}{\frac{2-1}{2}} = 7.7$$

Mass-transfer data for 2-inch metal Pall rings for the absorption of NH_3 from air into water are presented in Figs. 6.42 and 6.43. In the solutions to Exercise 6.34, these data are fitted to the equation,

$$k_G a = 43.4\, F^{0.7}\, u_L^{0.45}\ ,\ s^{-1} \qquad (3)$$

where the gas capacity factor = $F = u_V(\rho_V)^{0.5} = f\, u_o\, (\rho_V)^{0.5}$ in $kg^{1/2}$-s^{-1}-$m^{-1/2}$ and from the continuity equation, $u_L = m/S\rho_L$ in m/s or m^3/m^2-s. Here, $S = 3.14(3)^2/4 = 7.07$ ft^2

For our case, $F = (0.5)(9.4)(0.0734)^{0.5} = 1.27$ $lb^{1/2}$-s^{-1}-$ft^{-1/2}$ or 3.10 $kg^{1/2}$-s^{-1}-$m^{-1/2}$
and $u_L = [(532.5)(18)/3{,}600)]/(7.07)(62.4) = 0.006$ ft/s = 0.00182 m^3/m^2-s
Substitution of these values into Eq. (3) gives, $k_G a = 43.4(3.10)^{0.7}(0.00182)^{0.45} = 5.6$ s^{-1}
Note that this $k_G a$ is in concentration units for the driving force.
Therefore, from Table 6.7 by analogy to the liquid phase case,

$$H_{OG} = H_G = VM_V/k_G aS\rho_V = (312/3{,}600)(28.3)/(5.6)(7.07)(0.0734) = 0.84 \text{ ft}$$

Now, we must correct this value to 1-inch metal Pall rings.
From Table 6.8, using interpolation when necessary, we have the following characteristics:

Packing	a, m^2/m^3	ε	C_h	C_V
1.0-inch Pall rings	223.5	0.954	0.719	0.336
2.0-inch Pall rings	112.6	0.951	0.784	0.410

Exercise 6.38 (continued)

Analysis: (continued)

From Eqs. (6-136) to (6-140), a_{Ph}/a is proportional to $\varepsilon^{1/2}/a$. Therefore,

$$\frac{a_{Ph}/a \text{ for 1.0-inch Rings}}{a_{Ph}/a \text{ for 2.0-inch Rings}} = \left(\frac{0.954}{0.951}\right)^{1/2} \frac{112.6}{223.5} = 0.505$$

From Eq. (6-133), if we ignore holdup in the term (ε - h_L), then,

$$H_G \text{ is proportional to } \frac{1}{C_V}\frac{\varepsilon}{a^{1.25}}\left(\frac{a}{a_{Ph}}\right)$$

Therefore,
$$\frac{H_G \text{ for 1.0-inch Rings}}{H_G \text{ for 2.0-inch Rings}} = \frac{\dfrac{1}{0.336}\left(\dfrac{0.954}{223.5^{1.25}}\right)}{\dfrac{1}{0.410}\left(\dfrac{0.951}{112.6^{1.25}}\right)}\left(\frac{1}{0.505}\right) = 1.03$$

This ratio should be about the same for H_{OG} .
Therefore, for the 1.5-inch rings, H_{OG} = 0.84(1.03) = 0.87 ft.

From Eq. (2), column height = 7.7 (0.87) = 6.7 ft.

Exercise 6.39

Subject: Absorption of SO_2 from air by water in a packed column.

Given: Mass velocity of entering gas = 6.90 lbmol/h-ft^2 on SO_2-free basis, containing 80 mol% air and 20 mol% SO_2. Water enters at a mass velocity of 364 lbmol/h-ft^2. Gas exits with 0.5 mol% SO_2. Tower operates at 30°C and 2 atm. Equilibrium y-x equation given for SO_2. Tower is packed with Montz B1-200 metal structured packing.

Assumptions: No stripping of water. No absorption of air.

Find: (a) Molar material balance operating line.
(b) N_{OG}

Analysis: (a) A material balance for the solute, SO_2, from the top of the column to an intermediate point gives:

$$Y_{n+1}V' + X_{\text{in}}L' = Y_{\text{out}}V' + X_nL' \qquad (1)$$

Solving Eq. (1), the operating line is given by,

$$Y = \left(\frac{L'}{V'}\right)X + Y_{\text{out}} - X_{\text{in}}\left(\frac{L'}{V'}\right) \qquad (2)$$

From the given data, L'/V' = 364/6.90 = 52.75. $X_{\text{in}} = 0.0$ and Y_{out} = 0.005/0.995 = 0.005025
Rearrange Eq. (2), letting $Y = y/(1-y)$ and $X = x/(1-x)$, which is approximately x because of the dilute condition,

$$X = \frac{x}{1-x} \approx x = \frac{V'}{L'}\left(\frac{y}{1-y}\right) - \frac{V'}{L'}Y_{\text{out}} = 0.01896\left(\frac{y}{1-y}\right) - 0.000095 \qquad (3)$$

which is very close to the given operating line.

(b) From Eq. (6-138), $N_{OG} = \int_{Y=0.00503}^{Y=0.25} \frac{dY}{Y - Y^*}$ (4)

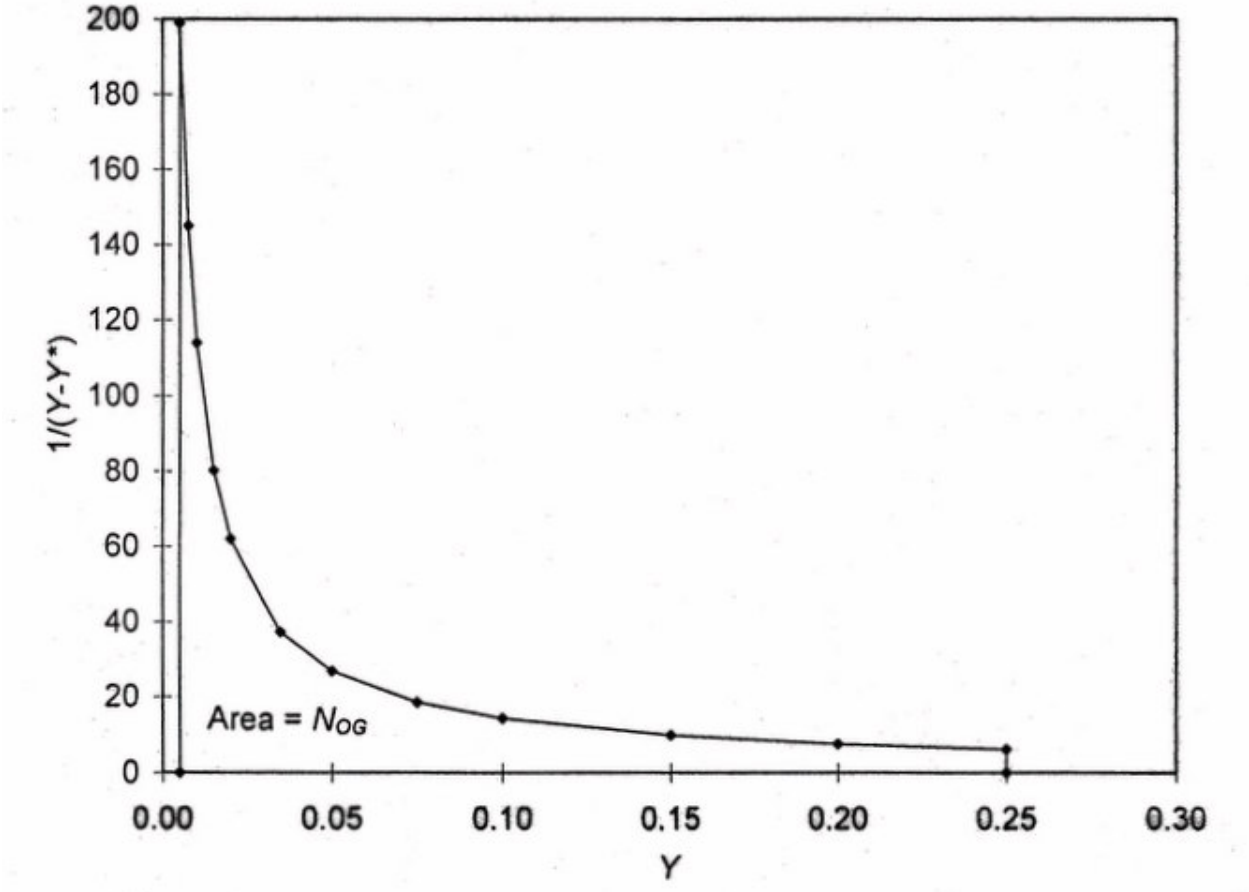
Eq. (4) can be solved graphically or numerically. Both require a table of values of $\frac{1}{(Y-Y^*)}$ as a function of Y, where for a given value of Y, the value of X is obtained from Eq. (3). Then, x is computed from X. Then, $y = y^*$ is computed from the given equilibrium equation, and Y^* is then obtained from the equilibrium curve. Below is a plot of $\frac{1}{(Y-Y^*)}$ versus Y. The area under the curve is the value of the integral for N_{OG}. In the table below, the trapezoidal method is used

Exercise 6.39 (continued)

Analysis: (b) (continued)

to break the curve into segments of ΔY. each, varying in width from 0.0103 to 0.0413. For each segment (width), the average value of $1/(Y\text{-}Y^*)$ is used to compute the product = Area = ΔY times $1/(Y\text{-}Y^*)$, which is given in the last column. The sum of these areas is $N_{OG} = 5.16$.

Y	X	x	y*	Y*	Y-Y*	1/(Y-Y*)	Area
0.00503	0.00000	0.00000	0.00000	0.00000	0.00503	198.99	
0.00750	0.00005	0.00005	0.00061	0.00061	0.00689	145.05	0.425
0.01000	0.00009	0.00009	0.00123	0.00123	0.00877	113.99	0.324
0.01500	0.00019	0.00019	0.00251	0.00251	0.01249	80.05	0.485
0.02000	0.00028	0.00028	0.00385	0.00384	0.01616	61.87	0.355
0.03500	0.00057	0.00057	0.00815	0.00808	0.02692	37.15	0.743
0.05000	0.00085	0.00085	0.01283	0.01267	0.03733	26.79	0.480
0.07500	0.00133	0.00133	0.02135	0.02090	0.05410	18.49	0.566
0.10000	0.00180	0.00180	0.03057	0.02966	0.07034	14.22	0.409
0.15000	0.00275	0.00274	0.05043	0.04801	0.10199	9.80	0.601
0.20000	0.00370	0.00368	0.07139	0.06664	0.13336	7.50	0.433
0.25000	0.00465	0.00462	0.09302	0.08511	0.16489	6.06	0.339



Exercise 7.1

Subject: Comparison of absorption, distillation, and stripping

Find: Differences between absorption and distillation, and stripping and distillation

Analysis:

Absorption	Stripping	Distillation
Feed is gas	Feed is liquid	Feed is liquid, vapor or a mixture of the two
Second phase (absorbent) is added	Second phase (stripping agent) is added	Second phase is created by heat transfer
Operation can be adiabatic	Operation can be adiabatic	Must have heat transfer at the top and bottom stages
Single-section cascade	Single-section cascade	Two-section cascade
Can be almost isothermal	Can be almost isothermal	Can have a large temperature range
Can not separate a close-boiling mixture	Can not separate a close-boiling mixture	Can separate a close-boiling mixture
Tray efficiency can be low	Tray efficiency can be moderate	Tray efficiency can be high

Exercise 7.2

Subject: Emergence of packing to replace trays.

Find: Reasons why some existing trayed towers are being retofitted with packing, and some large-diameter columns are being designed for packing.

Analysis: New random packings and structured packings have been introduced with higher capacity, lower pressure drop, and higher efficiency than trays. Also for packed columns, liquid distributors have been greatly improved. Channeling of liquid in packed columns is now much less of a problem.

Exercise 7.3

Subject: Condenser coolant for distillation of a methane-ethane mixture.

Find: Appropriate coolant.

Analysis: Assume that the distillate is nearly pure methane, the most volatile of the two components. To use cooling water, the distillate temperature would be approximately 120°F. But the critical temperature of methane is -115°F. Therefore could not condense it. The critical pressure of methane is 673 psia. Using Fig. 7.16, could consider operation at 415 psia because that is safely below the critical pressure (P/P_c = 0.62 and could operate as high as a P/P_c = 0.8). From Perry's Handbook (p. 3-203, 6th edition), at P = 415 psia (28.6 bar), the saturation temperature of methane is 176 K or -143°F. To condense at just below this temperature, could use a partial condenser with refrigerant R-14 (carbon tetrafluoride), which from Perry's Handbook (p. 12-26, 6th edition) has a saturation pressure of 70 psia at -150°F.

Exercise 7.4

Subject: Operating pressure for distillation of an ethylene-ethane mixture

Find: Suitable operating pressure.

Analysis: Assume that the distillate is nearly pure ethylene, the most volatile of the two components. To use cooling water, the distillate temperature would be approximately 120°F. But the critical temperature of ethylene is 9.7°C or 49.4°F . Therefore could not condense it. The critical pressure of ethylene is 50.5 atm or 742 psia. Using Fig. 7.16, could consider operation at 415 psia because that is safely below the critical pressure (P/P_c = 0.56 and could operate as high as a P/P_c = 0.8). From Perry's Handbook (p. 3-203, 6th edition), at P = 415 psia (28.6 bar), the saturation temperature of ethylene is 258 K or 4.7°F. To condense at just below this temperature could use a partial condenser with refrigerant R-1270 (propylene), which from Perry's Handbook (p. 12-26, 6th edition) has a saturation pressure of 35 psia at 0°F.

Exercise 7.5

Subject: Need for testing or piloting a distillation separation.

Find: Circumstances that require laboratory or pilot-plant testing of a proposed distillation.

Analysis: Laboratory and/or pilot-plant testing is recommended for:

1. A new mixture not previously separated by distillation.
2. A sharp and critical separation.
3. A mixture with uncertain vapor-liquid equilibria data.
4. A lack of experience with tray efficiency for the mixture.

Exercise 7.6

Subject: Economic tradeoff in distillation.

Find: Reasons for tradeoff between trays and reflux.

Analysis: It is well known that for a given separation, as the number of trays is increased, the reflux ratio can be decreased. Thus, as the tower height is increased, the vapor and liquid traffic up and down the column can be decreased. Therefore, the column diameter can be decreased. Also the condenser and reboiler duties and sizes, and the utility requirements can be decreased. Therefore, there is a tradeoff.

Exercise 7.7

Subject: McCabe-Thiele method for binary distillation.

Find: Reasons for the survival of the McCabe-Thiele graphical method.

Analysis: For a binary mixture, the McCabe-Thiele method shows clearly the ease or difficulty of the separation. Pinched regions are readily seen. The effect of feed location is readily seen. The method is reasonably accurate. Azeotropes are readily accommodated.

Exercise 7.8

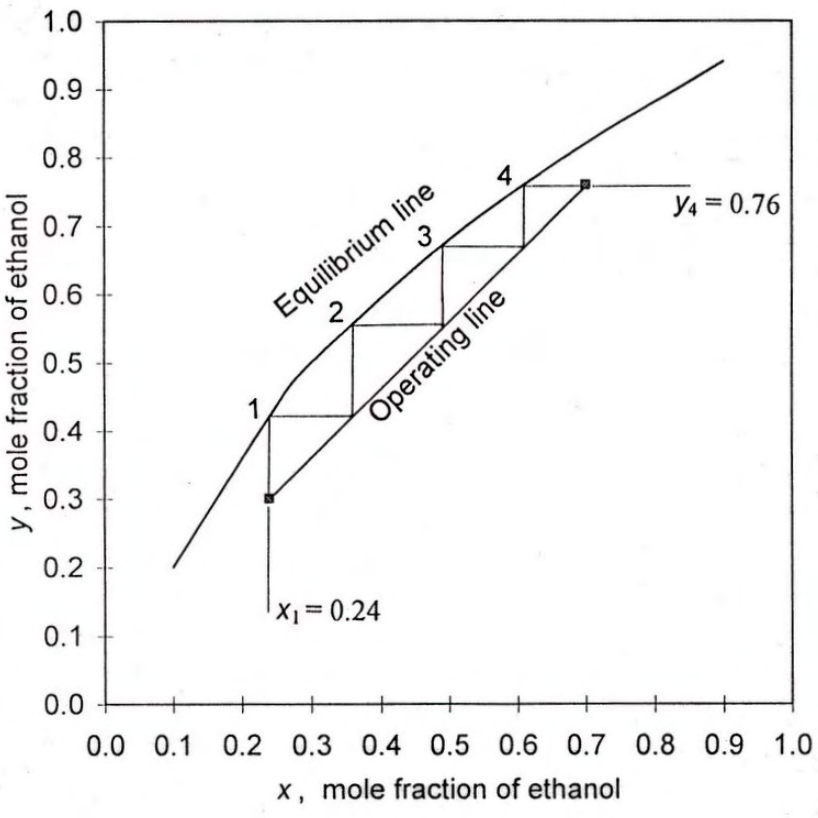
Subject: Separation of ethyl alcohol and water at 1 atm. with two countercurrent cascades.

Given: One cascade (a) with given liquid feed to top stage and given vapor feed to bottom stage. Another cascade (b) with total condenser and reflux, and given vapor feed to bottom stage. Vapor-liquid equilibrium data for 1 atm.

Assumptions: Constant molar overflow to give straight operating lines on a *y*-*x* diagram.

Find: (a) Compositions of V_4 and L_1 for 4 stages in cascade (a).
(b) Number of equilibrium stages for 85 mol% alcohol in exit vapor of cascade (a).
(c) Compositions of D and L_1 for 4 stages in cascade (b).
(d) Number of equilibrium stages for 50 mol alcohol in D of cascade (b).

Analysis: From the given vapor-liquid equilibrium data**,** in the composition range of interest, ethyl alcohol is more volatile than water. Therefore, the *y* and *x* coordinates in a *y*-*x* plot pertain to ethyl alcohol.
(a) Since $L = 100$ mol and $V = 100$ mol, the slope of the operating line from Eqs. (7-6) or (7-11) $= L/V = 100/100 = 1$. The terminal points on the operating line as (*y, x*) are: (?, 0.7) at the top and (0.3, ?) at the bottom. To determine the compositions of V_4 and L_1 for 4 stages, this operating line is located so that exactly 4 stages are stepped off in a *y*-*x* diagram, as shown below. From the diagram, the ethanol compositions are 76 mol% in V_4 and 24 mol% in L_1.



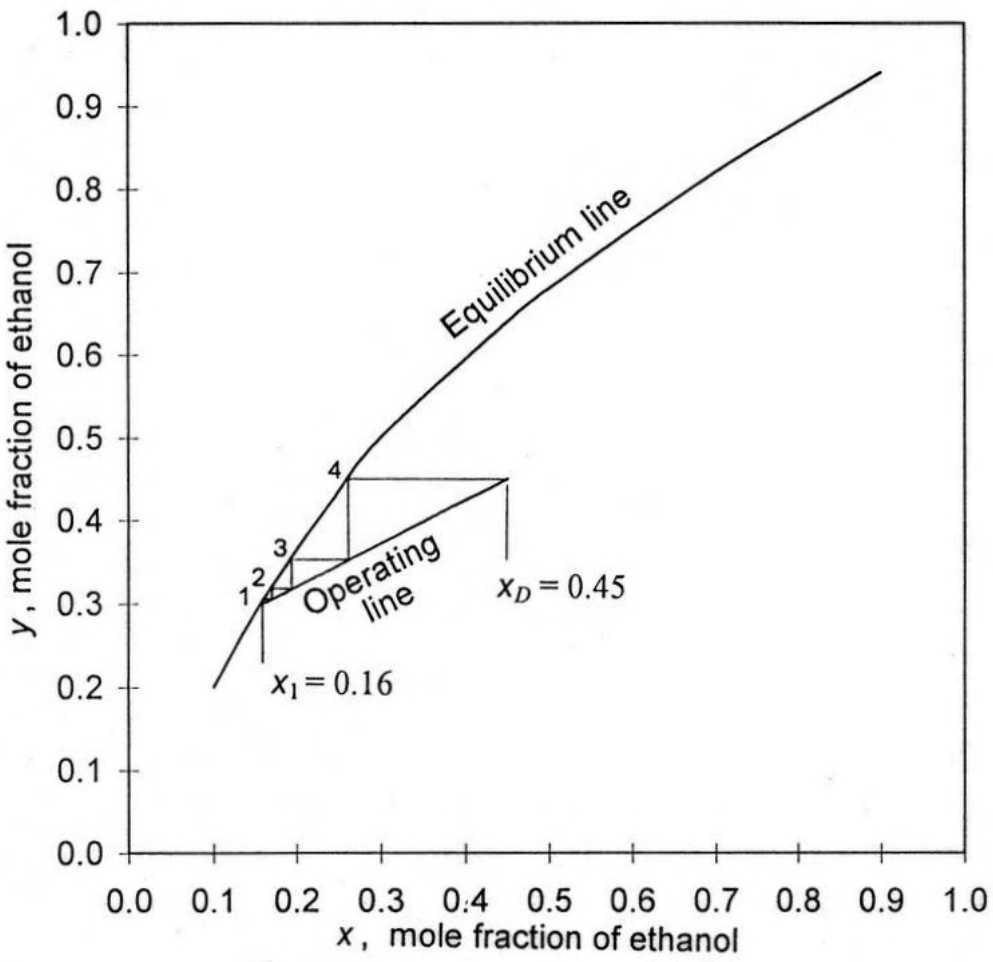
Exercise 7.8 (continued)

Analysis: (continued)

(b) It is impossible to obtain an overhead vapor with 85 mol% ethanol. With an infinite number of stages, the highest concentration of ethanol in the overhead vapor corresponds to that in equilibrium with the top liquid feed containing 70 mol% ethanol. From the given vapor-liquid equilibrium data, the highest concentration is an ethanol mole fraction of 0.82.

(c) Since the bottom vapor feed, V_0 = 100 mol and D = 50 mol, by overall material balance, $L_1 = V_0 - D = 100 - 50 = 50$ mol. Because of the assumption of constant molar overflow, $L = L_R = L_1 = 50$ mol. By material balance around the condenser or because of constant molar overflow, $V = V_4 = L_R + D = 50 + 50 = 100$ mol. The slope of the operating line from Eqs. (7-6) or (7-11) = $L/V = 50/100 = 0.5$. To determine the compositions of D and L_1 for 4 stages, an operating line of this slope is located so that exactly 4 stages are stepped off in a y-x diagram, as shown below. From the diagram, the ethanol compositions are 45 mol% in D and 16 mol% in L_1.

(d) Since the distillate is 50 mol% ethanol, 25 moles of ethanol and 25 moles of water leave in the distillate. Because the feed is 30 moles of ethanol and 70 moles of water, L_1 , the leaving liquid, contains 5 moles of ethanol and 45 moles of water. Thus, the terminal points on the operating line, because of the total condenser, as (y, x), are: (0.5, 0.5) at the top and (0.3, 0.1) at the bottom. However, point (0.3, 0.1) above the equilibrium line is impossible.


1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
y, mole fraction of ethanol
0.0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0
x, mole fraction of ethanol
Equilibrium line
Operating line
1
2
3
4
$x_D = 0.45$
$x_1 = 0.16$

Exercise 7.9

Subject: Separation of air in a reboiled stripper

Given: Reboiled stripper with total reboiler operating at 1 atm. Liquid air (79.1 mol% N_2 and 20.9 mol% O_2) fed to top stage. 60% of O_2 in the feed is drawn off in vapor product from the reboiler. Bottoms vapor product contains 0.2 mol% N_2. Vapor-liquid equilibria data are given.

Assumptions: Feed is a saturated liquid.

Find: (a) Mol% N_2 in vapor from top stage.
(b) Moles of vapor generated in reboiler per 100 moles of feed.
(c) Number of equilibrium stages required.

Analysis:

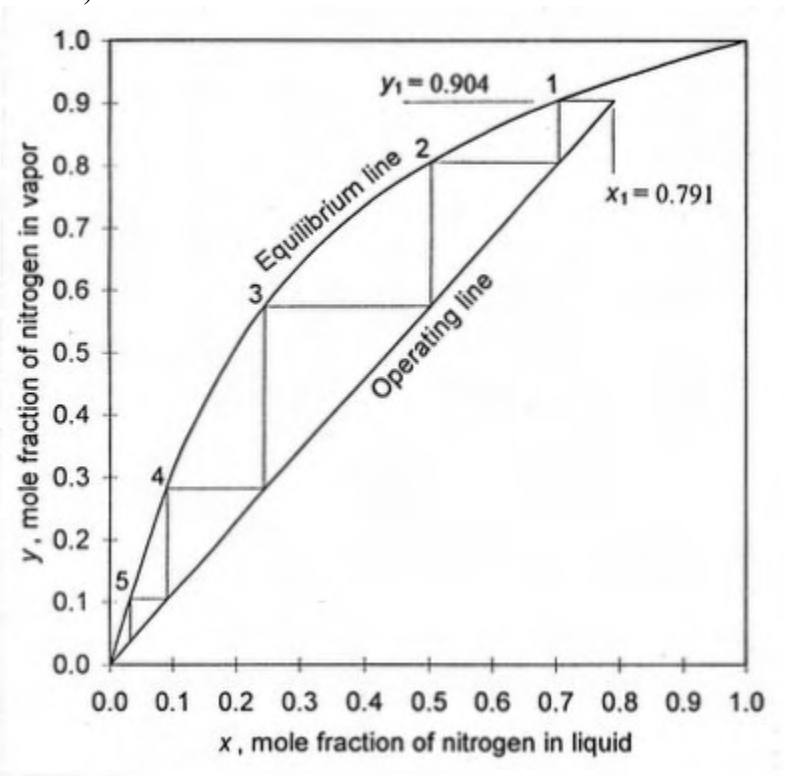
(a) Take a basis of F = 100 mol/h. Therefore, 79.1 mol/h of N_2 and 20.9 mol/h of O_2 in the feed. Bottoms product vapor contains 0.6(20.9) = 12.54 mol/h of O_2 and (0.2/99.8)(12.54) = 0.025 mol/h N_2. By material balance, the overhead vapor contains 20.9 - 12.54 = 8.36 mol/h O_2 and 79.1 - 0.025 = 79.075 mol/h of N_2. The mol% N_2 in the overhead vapor = 79.075/(8.36 + 79.075) x 100% = 90.4 %.

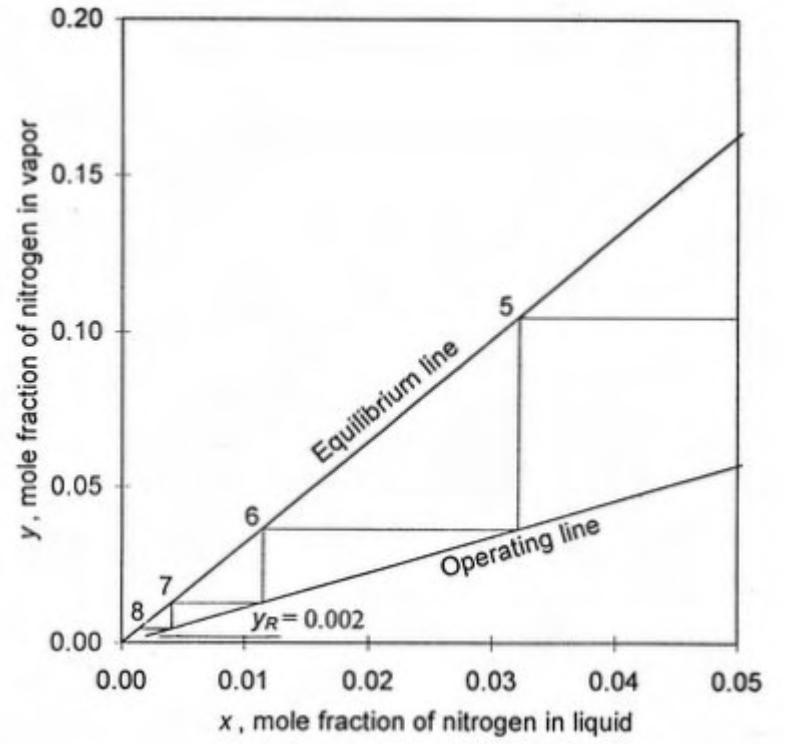
(b) Assume constant molar overflow. Then because the feed is assumed to be a saturated liquid, the moles of vapor generated in the reboiler per 100 moles of feed = mol/h of overhead vapor = 8.36 + 79.075 = 87.435 moles per 100 moles of feed.

(c) Use a y-x diagram for N_2 because it is the more volatile. The slope of the operating line is L/V = 100/87.435 = 1.14. At the top of the column, the operating line terminates at a (y-x) of (0.904, 0.791). At the bottom of the column, with a total reboiler, the operating line terminates at a (y-x) of (0.002, 0.002). To determine the number of equilibrium stages, it is convenient to use two diagrams, the usual one and a second one for just the very low mole fraction region so as to gain accuracy in the region of the lower end of the operating line. From the two diagrams, it is seen that just less than 8 equilibrium stages are required.

Exercise 7.9 (continued)

Analysis (d) (continued):





Exercise 7.10

Subject: Stage composition data for distillation of an A-B mixture.

Given: Saturated liquid feed of 40 mol% A. Test results for vapor and liquid compositioins for 3 successive stages between the feed stage and a total condenser.

	Mol % A			
	Test 1		Test 2	
Stage	Vapor	Liquid	Vapor	Liquid
M + 2	79.5	68.0	75.0	68.0
M + 1	74.0	60.0	68.0	60.5
M	67.9	51.0	60.5	53.0

Assumption: Constant molar overflow.

Find: Reflux ratio and overhead composition for each test.

Analysis:

Test 1:

By material balance for component A around stage M + 1,

$$Vy_M + Lx_{M+2} = Vy_{M+1} + Lx_{M+1} \qquad (1)$$

Solving Eq. (1) for *L/V* and substituting for *y* and *x* values from above table,

$$\frac{L}{V} = \frac{y_{M+1} - y_M}{x_{M+2} - x_{M+1}} = \frac{0.740 - 0.679}{0.680 - 0.600} = 0.763$$

From Eq. (7-7), reflux ratio = $R = L/D = (L/V)/(1 - L/V) = 0.763/(1 - 0.763) = 3.22$

$D/V = (L/V)/(L/D) = 0.763/3.22 = 0.237$. Noting that stages in the rectifying section are counted here from the bottom up instead of the top down, Eq. (7-5) becomes,

$$y_{M+1} = \frac{L}{V} x_{M+2} + \frac{D}{V} x_D \qquad (2)$$

Solving Eq. (2) for x_D ,

$$x_D = \frac{y_{M+1} - \left(\frac{L}{V}\right) x_{M+2}}{D/V} = \frac{0.740 - (0.763)(0.680)}{0.237} = 0.933$$

Therefore the composition of the distillate is 93.3 mol% A and 6.7 mol% B.

Test 2:

Because $y_{M+1} = x_{M+2}$ and $y_M = x_{M+1}$, operation is at total reflux, i.e. reflux ratio = infinity. In this case, Eq. (2) can not be solved for x_D because $D/V = 0$. We can not determine the composition of the distillate. We do know that it must at least 75 mol% A.

Exercise 7.11

Subject: Five procedures for continuous distillation of a mixture of benzene (A) and toluene (B).

Given: Operation at 1 atm to produce a distillate of 80 mol% benzene (i.e. $y_D = 0.8$) from a saturated liquid feed of 70 mol% benzene ($x_F = 0.7$). Procedures are:

1. No column. Just a partial condenser on top of a partial reboiler. Feed is to the reboiler. Reflux ratio, $L/D = 0.5$. Vapor distillate is totally condensed.
2. Same as 1 except that one equilibrium stage sits between the condenser and reboiler.
3. Same as 1 except two equilibrium stages between the condenser and reboiler.
4. Same as 3 except that reflux bypasses the top equilibrium stage.
5. Same as 2 except that feed is sent to the stage between the condenser and the reboiler.

Assumptions: Constant molar overflow. Constant relative volatility = $\alpha_{A,B} = 2.5$.

Find: For each procedure, determine:

(a) Moles of distillate per 100 moles of feed.
(b) Moles of total vapor generated per mole of distillate.
(c) Mole percent of benzene in the bottoms (residue).
(d) *y-x* diagram, indicating compositions of distillate, reflux, and residue.

Also, (e) For maximization of benzene recovery (in the distillate), which procedure is preferred.

Analysis: For each procedure, the partial condenser and the partial reboiler are equilibrium stages. Benzene is the more volatile component, so the *y-x* diagram is based on benzene. Because the relative volatility = constant = 2.5, the equilibrium relationship is given by Eq. (7-3),

$$y = \frac{\alpha x}{1 + x(\alpha - 1)} = \frac{2.5x}{1 + 1.5x} \qquad (1)$$

Take as a basis, 100 mol/s of feed. Therefore, the feed contains 70 mol/s of A and 30 mol/s of B. From the reflux ratio, $L = 0.5D$, $V = L + D = 1.5D$. Therefore, $D/V = 2/3$ and $L/V = 1/3$. Use a subscript of C for streams leaving the condenser, R for streams leaving the reboiler, 1 for the top stage when used, and 2 for the second stage when used.

Procedure 1:

Solve with material balances and Eq. (1). The liquid leaving the partial condenser is in equilibrium with the vapor distillate of $y_C = y_D = 0.8$. Solving Eq. (1),

$$x_C = \frac{y_C}{y_C + \alpha(1 - y_C)} = \frac{0.8}{0.8 + 2.5(1 - 0.8)} = 0.615 \qquad (2)$$

Benzene material balance around condenser,

$$y_R V = y_C D + x_C L \quad \text{or} \quad y_R = y_C\left(\frac{D}{V}\right) + x_C\left(\frac{L}{V}\right) = 0.80\left(\frac{2}{3}\right) + 0.615\left(\frac{1}{3}\right) = 0.738$$

Exercise 7.11 (continued)

Analysis: Procedure 1 (continued)

The vapor from the reboiler is in equilibrium with the liquid bottoms (residue). From the left-hand part of Eq. (2),

$$x_R = \frac{y_R}{y_R + \alpha(1 - y_R)} = \frac{0.738}{0.738 + 2.5(1 - 0.738)} = 0.530$$

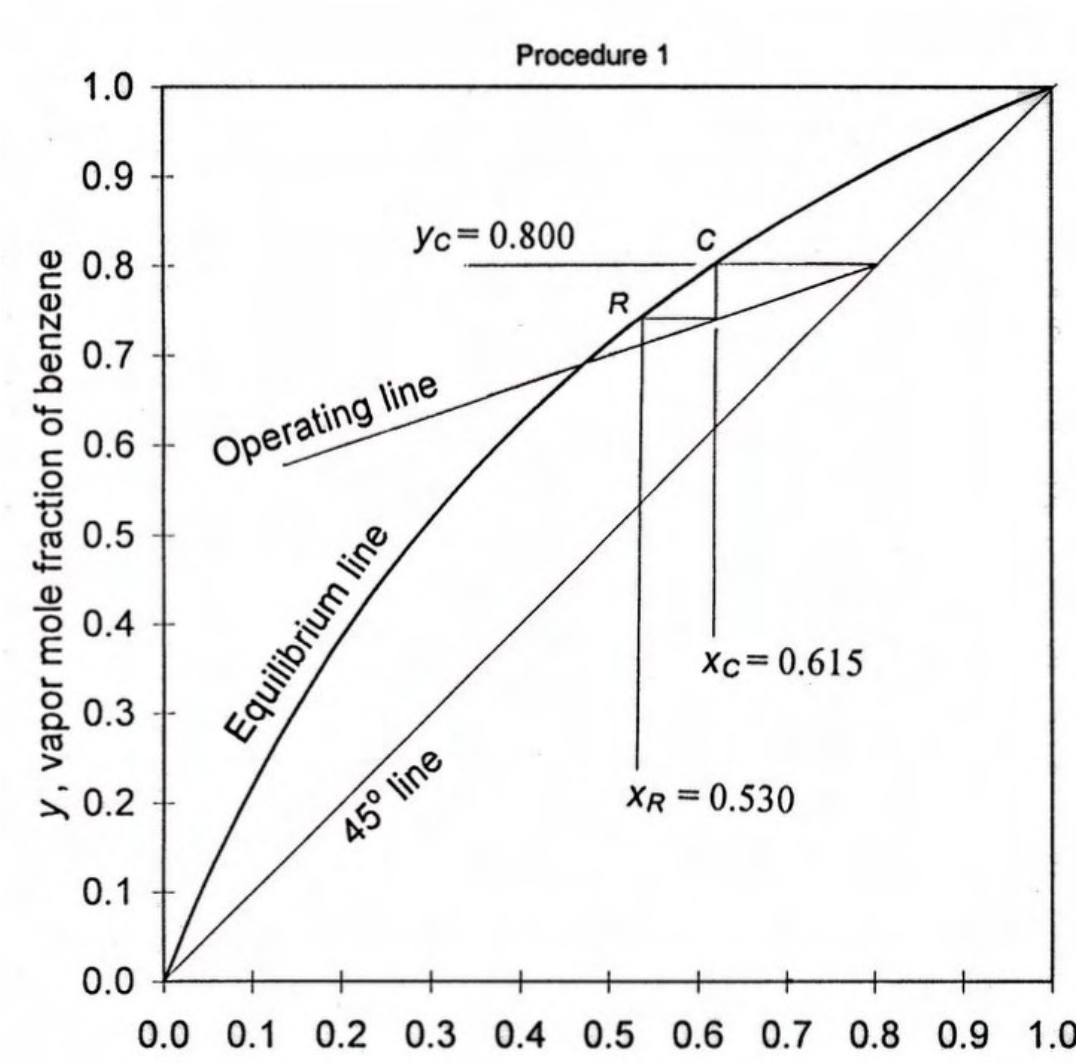
Overall total material balance, $F = 100 = D + B$ (3)

Overall benzene material balance, $x_F F = y_C D + x_R B$ or $70 = 0.8D + 0.530B$ (4)

Solving Eqs. (3) and (4), D = 62.9 mol/s or 62.9 mol/100 mol feed, and B = 37.1 mol/s.

Therefore, vapor generated = $V = 1.5D$ = 1.5(62.9) = 94.4 mol/s.

The operating line for the y-x diagram passes through the (y, x) point (0.8, 0.8) with a slope, L/V = 1/3, as shown in the diagram below.



Exercise 7.11 (continued)

Analysis: (continued)

Procedure 2:

The slope and top point of the operating line are the same as for Procedure 1. We just have to step off one more stage. Therefore from the results above, we have:

$y_C = 0.80$ $x_C = 0.615$ $y_1 = 0.738$ $x_1 = 0.530$

Benzene material balance around Stage 1,

$$y_R V + x_C L = y_1 V + x_1 L \qquad (5)$$

Solving for y_R, $y_R = y_1 + (x_1 - x_C)\left(\frac{L}{V}\right) = 0.738 + (0.530 - 0.615)\left(\frac{1}{3}\right) = 0.710$

The vapor from the reboiler is in equilibrium with the liquid bottoms (residue). From the left-hand part of Eq. (2),

$$x_R = \frac{y_R}{y_R + \alpha(1 - y_R)} = \frac{0.710}{0.710 + 2.5(1 - 0.710)} = 0.495$$

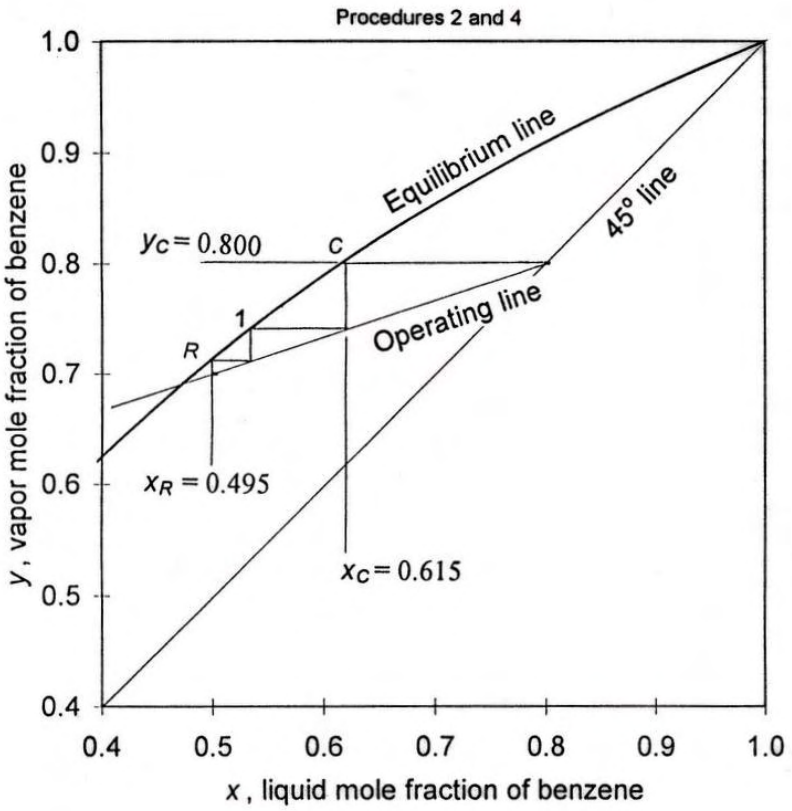
Overall total material balance, $F = 100 = D + B$ (6)

Overall benzene material balance, $x_F F = y_C D + x_R B$ or $70 = 0.8D + 0.495B$ (7)

Solving Eqs. (6) and (7), D = 67.2 mol/s or 67.2 mol / mol feed, and B = 32.8 mol/s.

Therefore, vapor generated = $V = 1.5D$ = 1.5(67.2) = 100.8 mol/s

The operating line for the y-x diagram passes through the (y, x) point (0.8, 0.8) with a slope, L/V = 1/3, as shown in the diagram below.



Exercise 7.11 (continued)

Analysis: (continued)

Procedure 3:

The slope and top point of the operating line are the same as for Procedures 1 and 2. We just have to extend Procedure 2 by stepping off a second equilibrium stage. From above, the results for the condenser and stage 1 are:

$y_C = 0.80$ $x_C = 0.615$ $y_1 = 0.738$ $x_1 = 0.530$ $y_2 = 0.710$ $x_2 = 0.495$

Benzene material balance around Stage 2,

$$y_R V + x_1 L = y_2 V + x_2 L \qquad (8)$$

Solving for y_R,

$$y_R = y_2 + (x_2 - x_1)\left(\frac{L}{V}\right) = 0.710 + (0.495 - 0.530)\left(\frac{1}{3}\right) = 0.698$$

The vapor from the reboiler is in equilibrium with the liquid bottoms (residue). From the left-hand part of Eq. (2),

$$x_R = \frac{y_R}{y_R + \alpha(1 - y_R)} = \frac{0.698}{0.698 + 2.5(1 - 0.698)} = 0.480$$

Overall total material balance, $F = 100 = D + B$ (10)

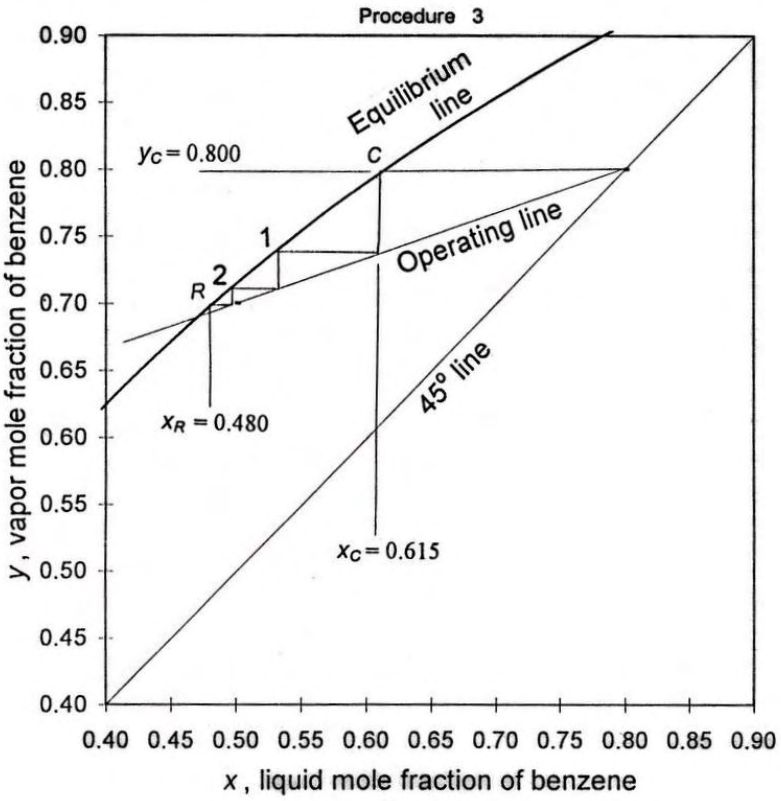
Overall benzene material balance, $x_F F = y_C D + x_R B$ or $70 = 0.8D + 0.480B$ (11)

Solving Eqs. (10) and (11), D = 68.8 mol/s or 68.8 mol / 100 mol feed, and B = 31.2 mol/s.

Therefore, vapor generated = $V = 1.5D$ = 1.5(68.8) = 103.2 mol/s

The operating line for the y-x diagram passes through the (y, x) point (0.8, 0.8) with a slope,

L/V = 1/3, as shown in the diagram below.



Exercise 7.11 (continued)

Analysis: (continued)

Procedure 4:

If the reflux bypasses the top stage, the vapor and liquid pass through that stage without change. Therefore, this procedure is the same as Procedure 2, i.e. just one stage in the column.

Procedure 5:

The slope and top point of the operating line are the same as for Procedure 1. We just have to add the feed to the stage in the column. Therefore from the results above, we have:

$y_C = 0.80$ $x_C = 0.615$ $y_1 = 0.738$ $x_1 = 0.530$

Benzene material balance around Stage 1, which now includes the feed,

$$x_F F + y_R \overline{V} + x_C L = y_1 V + x_1 \overline{L} \qquad (12)$$

Solving for y_R,

$$y_R = y_1\left(\frac{V}{\overline{V}}\right) + x_1\left(\frac{\overline{L}}{\overline{V}}\right) - x_C\left(\frac{L}{\overline{V}}\right) - x_F\left(\frac{F}{\overline{V}}\right) = 0.738\left(\frac{V}{\overline{V}}\right) + 0.530\left(\frac{\overline{L}}{\overline{V}}\right) - 0.615\left(\frac{L}{\overline{V}}\right) - 0.70\left(\frac{100}{\overline{V}}\right) \qquad (13)$$

Because the feed is a saturated liquid, , $V = \overline{V}$ and $\overline{L} = L + 100$

From above, $V = 1.5D$ and L/V = 1/3. Also, $\overline{L}/V = L/V + 100/V = 1/3 + 100/V$

Therefore, Eq. (13) becomes,

$$y_R = 0.738 + 0.530\left(\frac{1}{3} + \frac{100}{V}\right) - 0.615\left(\frac{1}{3}\right) - 0.70\left(\frac{100}{V}\right) = 0.710 - \frac{17}{V} = 0.710 - \frac{11.33}{D} \qquad (14)$$

The vapor from the reboiler is in equilibrium with the liquid bottoms (residue). From the left-hand part of Eq. (2),

$$x_R = \frac{y_R}{y_R + 2.5(1 - y_R)} \qquad (15)$$

Overall total material balance, $F = 100 = D + B$ (16)

Overall benzene material balance, $x_F F = y_C D + x_R B$ or $70 = 0.8D + x_R B$ (17)

Solving Eqs. (14), (15), (16), and (17),

$y_R = 0.565$, $x_R = 0.342$, $D = 78.3$ mol/s or 78.3 mol/100 mol feed, $B = 21.7$ mol/s

Therefore, vapor generated = $V = 1.5D = 1.5(78.3) = 117.5$ mol/s

The rectifying section operating line for the *y*-*x* diagram passes through the (*y*, *x*) point (0.8, 0.8) with a slope, $L/V = 1/3$, the *q*-line (feed line) is a vertical line, and the stripping section operating line passes throught the (*y, x*) point (0.565, 0.342) and the intersection of the other two lines, as shown in the diagram on the following page.

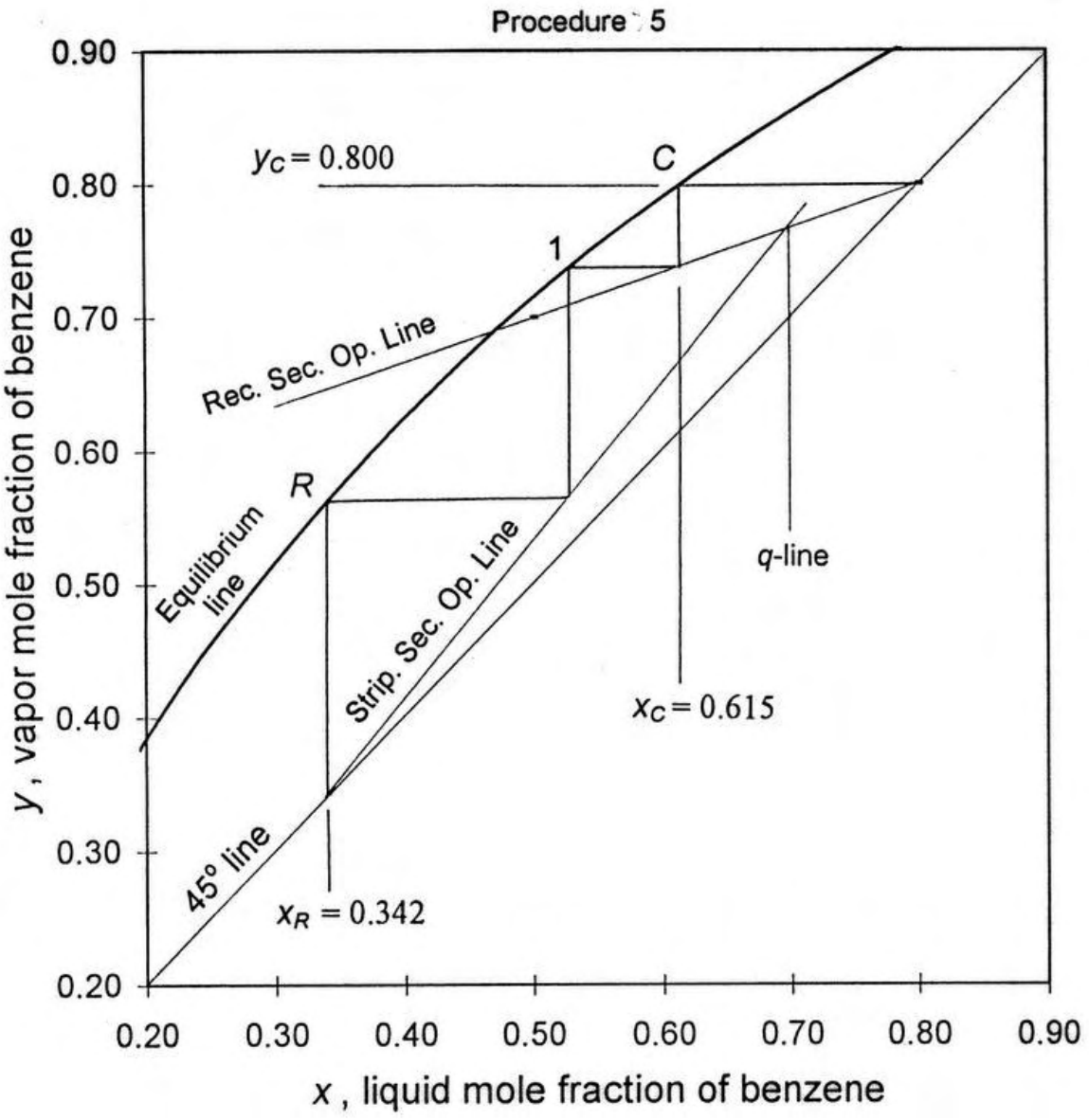
The results from the 5 procedures are summarized as follows:

Procedure	***D*/100 moles of feed**	***V*/mole of *D***	***x* of benzene in *B***
1	62.9	1.5	0.530
2	67.2	1.5	0.495
3	68.8	1.5	0.480
4	67.2	1.5	0.495
5	78.3	1.5	0.342

Exercise 7.11 (continued)

Analysis: Procedure 5: (continued)

(e) Procedure 5 is recommended because it produces by far the most distillate, which corresponds to the highest recovery of benzene.



Exercise 7.12

Subject: Distillation of a mixture of benzene (A) and toluene (B) at 101 kPa.

Given: Column consisting of a partial reboiler, one theoretical plate, and a total condenser. Produce a distillate of 75 mol% benzene from a saturated liquid feed of 50 mol% benzene.

Assumptions: Constant molar overflow. Constant relative volatility = $\alpha_{A,B} = 2.5$.

Find: Number of moles of distillate per 100 moles of feed for:

(a) Feed to the reboiler and no reflux.
(b) Feed to the reboiler and a reflux ratio, $L/D = 3$.
(c) Feed to the plate and a reflux ratio of 3.
(d) Same as (c) except a partial condenser.
(e) Feed to the reboiler with minimum reflux.
(f) Feed to the reboiler with total reflux.

Analysis: Either a graphical or analytical method can be used. Because the relative volatility is assumed constant, use an analytical method. For each part, the theoretical plate and the partial reboiler are equilibrium stages. Benzene is the more volatile component, so the *y*-*x* diagram is based on benzene. Because the relative volatility = constant = 2.5, the equilibrium relationship is given by Eq. (7-3),

$$y = \frac{\alpha x}{1 + x(\alpha - 1)} = \frac{2.5x}{1 + 1.5x} \qquad (1)$$

Take as a basis, 100 moles of feed. Therefore, the feed is 50 moles of A and 50 moles of B.

(a) With no reflux, separation occurs only in the reboiler. The vapor leaving the reboiler is totally condensed to become the distillate with $y_D = x_D = 0.75$. Solve Eq. (1) for equilibrium x,

$$x_B = \frac{y_D}{y_D + \alpha(1 - y_D)} = \frac{0.750}{0.750 + 2.5(1 - 0.750)} = 0.545 \qquad (2)$$

Because the distillate and bottoms have benzene mole fractions greater than the mole fraction of the feed (0.5), it is impossible to obtain a distillate with a benzene mole fraction of 0.75.

(b) From the reflux ratio, $L = 3D$, $V = L + D = 4D$. Therefore, $D/V = 1/4$ and $L/V = 3/4$. Use a subscript of D for distillate, R for reflux, B for streams leaving the reboiler, and 1 for the theoretical plate, when used. With 1 theoretical plate, from part (a),

$y_1 = 0.75 \qquad x_D = 0.75 \qquad x_1 = 0.545$

Benzene material balance around plate 1,

$$y_B V + x_D L = y_1 V + x_1 L \qquad (3)$$

Solving for y_B

$$y_B = y_1 + (x_1 - x_D)\left(\frac{L}{V}\right) = 0.750 + (0.545 - 0.750)\left(\frac{3}{4}\right) = 0.596$$

Exercise 7.12 (continued)

Analysis: (b) (continued)

The mole fraction of benzene in the bottoms product is in equilibrium with y_B =0.596. Therefore,
the form of Eq. (2) applies,

$$x_B = \frac{y_B}{y_B + \alpha(1-y_B)} = \frac{0.596}{0.596 + 2.5(1-0.596)} = 0.371$$

Overall total material balance, $F = 100 = D + B$ (4)
Overall benzene material balance, $x_F F = x_D D + x_B B$ or $50 = 0.75D + 0.371B$ (5)
Solving Eqs. (4) and (5), D = 34.2 moles or 34.2 mol/100 mol feed, and B = 65.8 moles.

(c) With the feed to the theoretical plate, the following results apply from part (b), $y_1 = 0.75$
$x_D = 0.75$ $x_1 = 0.545$
Benzene material balance around Stage 1, which now includes the feed,

$$x_F F + y_B \overline{V} + x_D L = y_1 V + x_1 \overline{L} \quad (6)$$

Solving for y_B,

$$y_B = y_1\left(\frac{V}{\overline{V}}\right) + x_1\left(\frac{\overline{L}}{\overline{V}}\right) - x_D\left(\frac{L}{\overline{V}}\right) - x_F\left(\frac{F}{\overline{V}}\right) = 0.750\left(\frac{V}{\overline{V}}\right) + 0.545\left(\frac{\overline{L}}{\overline{V}}\right) - 0.750\left(\frac{L}{\overline{V}}\right) - 0.50\left(\frac{100}{\overline{V}}\right) \quad (7)$$

Because the feed is a saturated liquid, , $V = \overline{V}$ and $\overline{L} = L + 100$
From above, $V = 4D$ and L/V = 3/4. Also, $\overline{L}/V = L/V + 100/V = 3/4 + 100/V$
Therefore, Eq. (7) becomes,

$$y_B = 0.750 + 0.545\left(\frac{3}{4} + \frac{100}{V}\right) - 0.750\left(\frac{3}{4}\right) - 0.50\left(\frac{100}{V}\right) = 0.596 - \frac{4.5}{V} = 0.596 - \frac{1.125}{D} \quad (8)$$

The vapor from the reboiler is in equilibrium with the liquid bottoms (residue). From the left-hand part of Eq. (2),

$$x_B = \frac{y_B}{y_B + 2.5(1-y_B)} \quad (9)$$

Overall total material balance, $F = 100 = D + B$ (10)
Overall benzene material balance, $x_F F = x_D D + x_B B$ or $50 = 0.75D + x_B B$ (11)
Solving Eqs. (8), (9), (10), and (11),
$y_B = 0.647$, $x_B = 0.423$, D = 23.5 moles or 23.5 mol/100 mol feed, B = 76.5 moles

(d) With a partial condenser, the mole fraction of the liquid reflux is that in equilibrium with the vapor distillate. Therefore, from the above results,
$y_D = 0.75$ $x_R = 0.545$ $y_1 = 0.596$ $x_1 = 0.371$
Benzene material balance around the theoretical plate, which includes the feed,

$$x_F F + y_B \overline{V} + x_R L = y_1 V + x_1 \overline{L} \quad (12)$$

Solving for y_B,

$$y_B = y_1\left(\frac{V}{\overline{V}}\right) + x_1\left(\frac{\overline{L}}{\overline{V}}\right) - x_R\left(\frac{L}{\overline{V}}\right) - x_F\left(\frac{F}{\overline{V}}\right) = 0.596\left(\frac{V}{\overline{V}}\right) + 0.371\left(\frac{\overline{L}}{\overline{V}}\right) - 0.545\left(\frac{L}{\overline{V}}\right) - 0.50\left(\frac{100}{\overline{V}}\right) \quad (13)$$

Exercise 7.12 (continued)

Analysis: (d) (continued)

Because the feed is a saturated liquid, , $V = \overline{V}$ and $\overline{L} = L + 100$

From above, $V = 4D$ and $L/V = 3/4$. Also, $\overline{L}/V = L/V + 100/V = 3/4 + 100/V$

Therefore, Eq. (13) becomes,

$$y_B = 0.596 + 0.371\left(\frac{3}{4} + \frac{100}{V}\right) - 0.545\left(\frac{3}{4}\right) - 0.50\left(\frac{100}{V}\right) = 0.466 - \frac{12.9}{V} = 0.466 - \frac{3.23}{D} \qquad (14)$$

The vapor from the reboiler is in equilibrium with the liquid bottoms (residue). From the left-hand part of Eq. (2),

$$x_B = \frac{y_B}{y_B + 2.5(1 - y_B)} \qquad (15)$$

Overall total material balance, $F = 100 = D + B$ (16)

Overall benzene material balance, $x_F F = y_D D + x_B B$ or $50 = 0.75D + x_B B$ (17)

Solving Eqs. (14), (15), (16), and (17),

$y_B = 0.405$, $x_B = 0.214$, $D = 53.4$ moles or 53.4/100 mol feed, $B = 46.6$ moles

(e) At minimum reflux, with the feed sent to the still pot (partial reboiler), an infinite number of theoretical plates is needed between the condenser and reboiler. This part is not completely specified. In order to compute the distillate, we must assume a bottoms benzene mole fraction less than that in the feed. Suppose we choose that mole fraction to be 0.45. Then the operating line will intersect the equilibrium line at $x = 0.45$, creating the pinch zone of infinite stages. The value of y at the intersection is given by Eq. (1):

$$y = \frac{2.5(0.45)}{1 + 1.5(0.45)} = 0.672$$

Therefore the operating line passes through the two points, as $\{y, x\}$, of {0.75, 0.75} and {0.672, 0.450}. Therefore, the slope = L/V = (0.75 - 0.672)/(0.75 - 0.45) = 0.260. Now compute the overall material balances:

Overall total material balance, $F = 100 = D + B$ (18)

Overall benzene material balance, $x_F F = y_D D + x_B B$ or $50 = 0.75D + 0.45B$ (19)

Solving Eqs. (18) and (19), $D = 16.67$ moles or 16.67 mol/100 mol feed, and $B = 83.33$ moles

Calculations for other values of the benzene mole fraction in the bottoms can be made in the same manner.

(f) At total reflux, there is no distillate, but there is a boilup. The moles of distillate per 100 moles of feed = 0.

Exercise 7.13

Subject: Distillation of a mixture of benzene and toluene at 101 kPa for specified reflux ratio and product compositions.

Given: Feed of 30 kg/h of saturated liquid feed containing 40 mass% benzene and 60 mass% toluene. Distillate to contain 97 mass% benzene and bottoms to contain 98 mass% toluene. Reflux ratio = 3.5 and feed is to optimal stage. Table of vapor-liquid equilibrium data in mole fractions. At 101 kPa.

Assumptions: Total condenser and partial reboiler. Saturated liquid reflux. Constant molar overflow.

Find: (a) Flow rates of distillate and bottoms.
(b) Number of equilibrium stages needed.

Analysis: First solve the material balance in mass units. Then convert to moles and mole fractions so that the McCabe-Thiele method can be used for part (b).

Overall total mass balance: $30 = D + B$ (1)

Overall benzene mass balance: $0.40(30) = 12 = 0.97D + 0.02B$ (2)

Solving Eqs. (1) and (2): $D = 12.1$ kg/h $B = 17.9$ kg/h

Converting to moles with molecular weights of 78.11 for benzene and 92.13 for toluene,

		Benzene		Toluene	
Product	**kmol/h**	**Mass fraction**	**Mole fraction**	**Mass fraction**	**Mole fraction**
Distillate	0.154	0.97	0.974	0.03	0.0235
Bottoms	0.196	0.02	0.026	0.98	0.9765
Total:	0.350	1.00	1.000	1.00	1.0000

(b) Because benzene is the more volatile component of the feed, the x and y coordinates will be those of benzene in the diagram on the next page.

. In moles, the feed consists of:

Component	**kmol/h**	**Mole fraction**
Benzene	0.154	0.44
Toluene	0.196	0.56
Total:	0.350	1.00

For a saturated liquid feed, the q-line is vertical and passes through $x = 0.44$. The slope of the rectifying operating line, L/V, is obtained from Eq. (7-7), using the specified reflux ratio = 3.5,

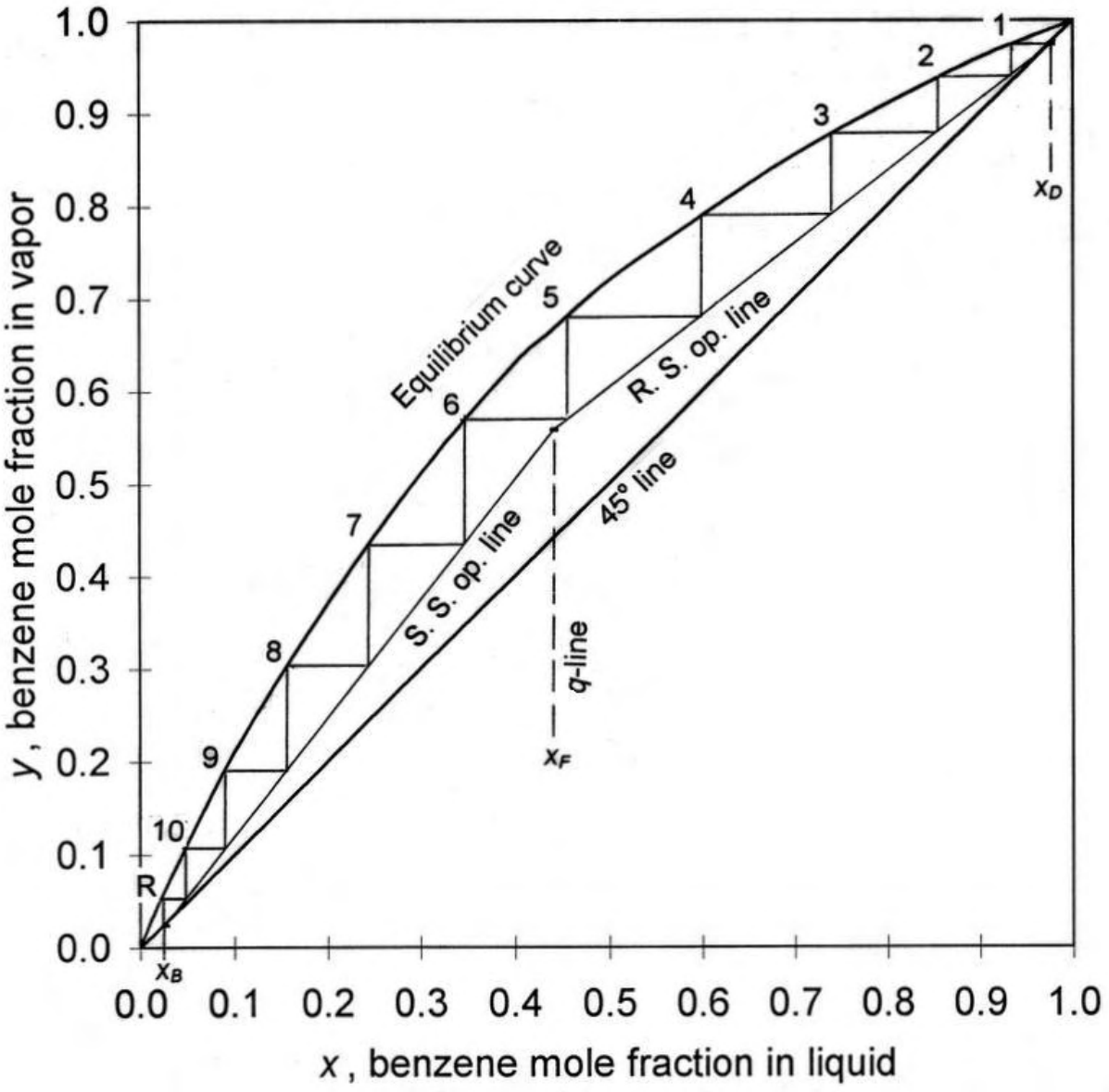
$$L/V = R/(1 + R) = 3.5/4.5 = 0.778$$

For saturated liquid reflux, the rectifying operating line passes through the point {0.974, 0.974}. See the McCabe-Thiele construction on the next page, where it is seen that slightly more than 10 stages + a partial reboiler acting as an equilibrium stage are required. The top 5 stages are in the rectifying section.

Exercise 7.13 (continued)

Analysis: (b) (continued)

McCabe-Thiele Diagram



Exercise 7.14

Subject: Distillation of a mixture of benzene and chlorobenzene with specified number of equilibrium stages, boilup ratio, and reflux ratio.

Given: Feed is a saturated liquid of 54.5 mol% benzene. Column contains two equilibrium plates with feed to the bottom plate. Column is equipped with total condenser and partial reboiler. Boilup is $V/F = 0.855$. Reflux ratio, $L/V = 0.5$. Vapor-liquid equilibrium data given.

Find: Compositions of distillate and bottoms, assuming constant molar overflow.

Analysis: Take as a basis, $F = 100$ mol/s. Therefore, vapor generated in reboiler = 0.855(100) = 85.5 mol/s. Since the feed is a saturated liquid, this vapor rate continues up the column to the condenser. $L/V = 0.5$, which is the slope of the operating line. Therefore, $L = 0.5(85.5) = 42.75$ mol/s. Therefore, the distillate rate = 85.5 - 42.75 = 42.75 mol/s. Passing to the reboiler is a liquid rate of 42.75 + 100 = 142.75 mol/s. The bottoms rate = 142.75 - 85.5 = 57.25 mol/s. The slope of the stripping section operating line is $\overline{L}/\overline{V} = 142.75/85.5 = 1.67$. The q-line is a vertical line because the feed is a saturated liquid. To solve for the compositions of the distillate and bottoms on a McCabe-Thiele diagram, we must locate the operating lines to obtain three equilibrium stages that satisfy an overall benzene material balance given by,

$$x_F F = 54.4 = x_D D + x_B B = 42.75 x_D + 57.25 x_B \qquad (1)$$

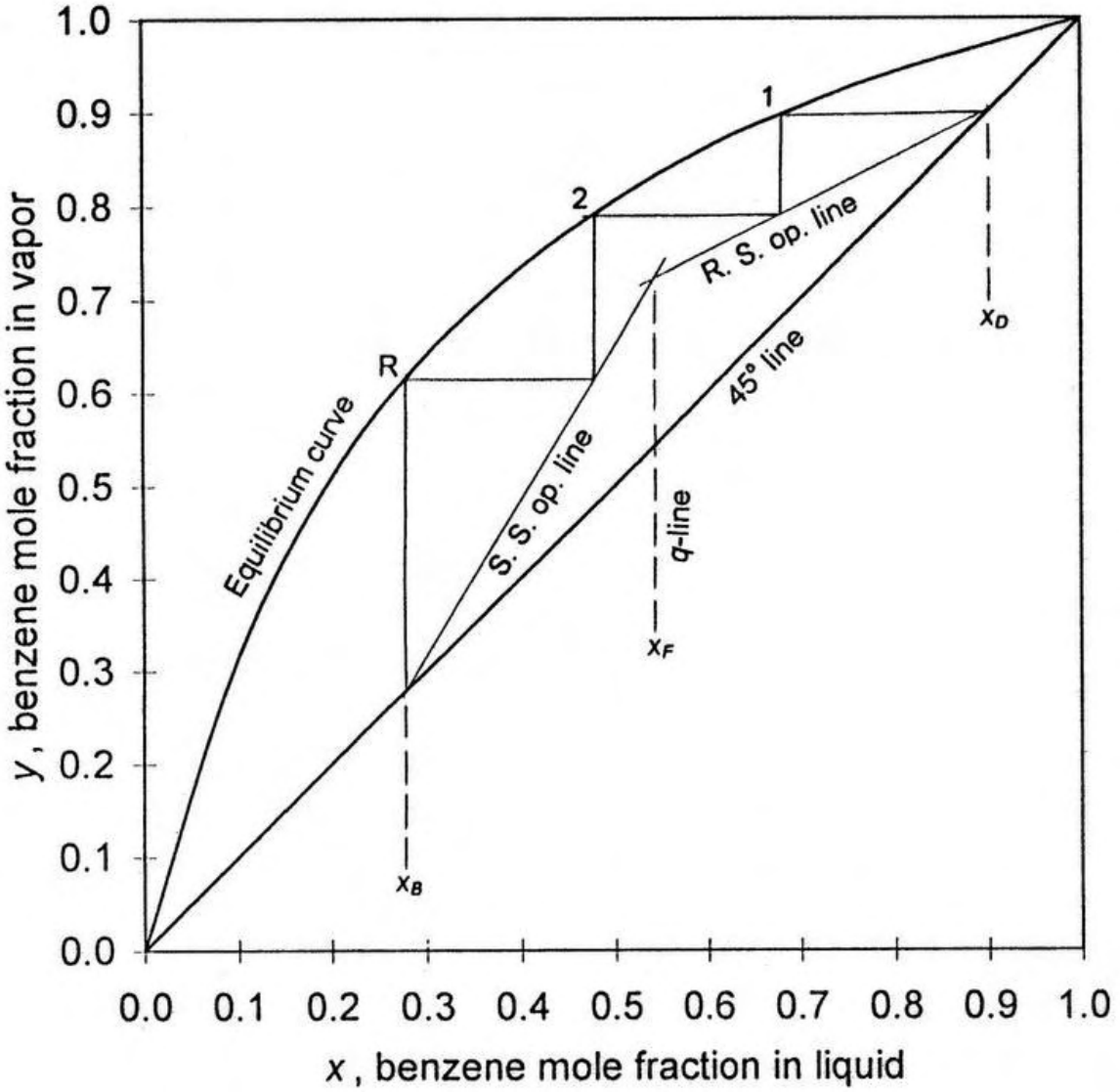
Solving Eq. (1),

$$x_B = 0.952 - 0.7467\, x_D \qquad (2)$$

Therefore, an approach to solving this exercise is to assume a value of x_D and then compute the value of x_B from Eq. (2). Then construct the McCabe-Thiele diagram with the above operating lines and q-line to see if three stages are required with the feed to the second plate.
See plot below, where benzene mole fractions are plotted because it is the more volatile component. It is seen that for benzene, $x_D = 0.90$ and $x_B = 0.28$.

Exercise 7.14 (continued)

McCabe-Thiele Diagram



Exercise 7.15

Subject: Effect of loss of plates in a distillation column separating a benzene-toluene mixture.

Given: Saturated vapor feed of 13,600 kg/h of 40 wt% benzene and 60 wt% toluene. Column with 14 plates above the feed location. Plate efficiency is 50%. Reflux ratio is 3.5. Previously, with 10 plates in the stripping section, column could achieve a distillate of 97 wt% benzene and a bottoms of 98 wt% toluene. Vapor-liquid equilibrium data in Exercise 7.13.

Assumptions: Constant molar overflow. Total condenser and partial reboiler.

Find: (a) If column with 10 inoperable plates can yield a distillate of 97 wt% benzene, assuming that we no longer can achieve the 98 wt% bottoms product.
(b) The distillate flow rate.
(c) The composition of the bottoms.

Analysis: (a) First convert the feed to kmol/h and mole fractions, using molecular weights of 78.11 for benzene and 92.13. The result is:

Component	kmol/h	Mole fraction
Benzene	69.65	0.44
Toluene	88.57	0.56
Total:	158.22	1.00

For a distillate of 97 wt% benzene, the mole fraction for benzene, the more volatile of the two components, is,

$$x_D = \frac{\frac{97}{78.11}}{\frac{97}{78.11}+\frac{3}{92.13}} = 0.974$$

With a reflux ratio of 3.5, from Eq. (7-7), the slope of the rectifying section operating line is,

$$L/V = R/(1 + R) = 3.5/4.5 = 0.778$$

The q-line is a horizontal line at $y = 0.44$. For 14 plates with 50% efficiency, the column has the equivalent of 7 equilibrium stages + 1 for the partial reboiler.
The McCabe-Thiele construction is shown on the next page, where it is seen that it is possible to obtain the desired distillate composition.
(b) and (c) From the McCabe-Thiele diagram, the mole fraction of benzene in the bottoms is $x_B = 0.24$. As a weight fraction, this corresponds to,

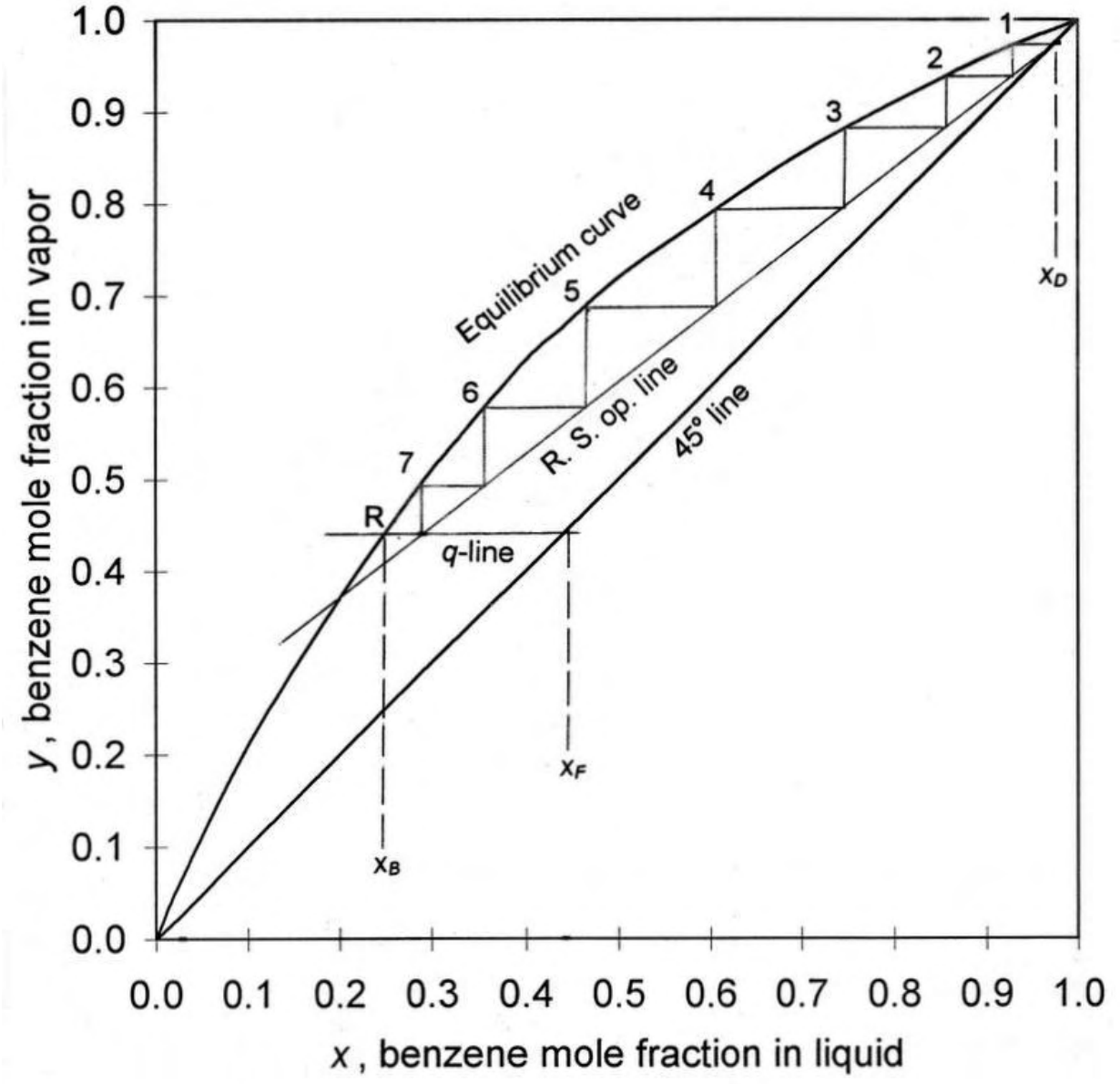
$$\frac{0.24(78.11)}{0.24(78.11)+0.76(92.13)} = 0.211 \text{ weight fraction or } 21.1 \text{ wt\% benzene}$$

Compute the distillate rate by overall molar material balances.
Overall total mass balance: $158.22 = D + B$ (1)
Overall benzene mass balance: $69.65 = 0.974D + 0.240B$ (2)
Solving Eqs. (1) and (2): $D = 43.16$ kmol/h $B = 115.06$ kmol/h
By weight, $D = 43.16[0.974(78.11) + 0.026(92.13)] = 3{,}387$ kg/h

Exercise 7.15 (continued)

Analysis: (a) (continued)

McCabe-Thiele Diagram



Exercise 7.16

Subject: Effect on the separation of A from B by distillation when 3 of 7 theoretical plates rust and drop to the bottom of the column.

Given: . Column has 7 theoretical plates + partial reboiler. Saturated liquid feed of 100 kmol/h of 50 mol% A is sent to plate 5 from the top. Distillate contains 90 mol% A. The $L/V = 0.75$ in the rectifying section. Vapor-liquid equilibrium data.

Assumptions: Constant molar overflow. Total condenser.

Find: Case 1: Column before the 3 plates rust and drop.
(a) Composition of the bottoms product.
(b) The L/V in the stripping section.
(c) The kmol/h of bottoms product.
Case 2: If plates 5, 6, and 7 counted down from the top are lost:
(a) Composition of bottoms product.
Case 3: Same as Case 2, except replace reflux with the same molar flow rate of product containing 80 mol% A:
(a) Composition of distillate.
(b) Composition of bottoms.

Analysis: Case 1: Apply the McCabe-Thiele method in terms of component A, which is more volatile than B. The rectifying section operating line passes through [0.90, 0.90] with a slope of 0.75. The q-line is vertical through $x = 0.50$. Step off 4 stages in the rectifying section. Then, by trial and error, find an x_B with a corresponding stripping section operating line that gives 4 equilibrium stages in the stripping section. The result is shown on the following page, where:

(a) Bottoms contains 7 mol% A and 93 mol% B.
(b) The slope of the stripping section operating line from the coordinates of the line is:

$$\bar{L}/\bar{V} = \{[0.90 - 0.75(0.90 - 0.50] - 0.07\}/(0.50 - 0.07) = 1.23$$

(c) By material balances, $F = D + B$ and $Fx_F = 50 = 0.9D + 0.07B$. Solving these two equations, distillate flow rate = 51.8 kmol/h and bottoms flow rate = 48.2 kmol/h

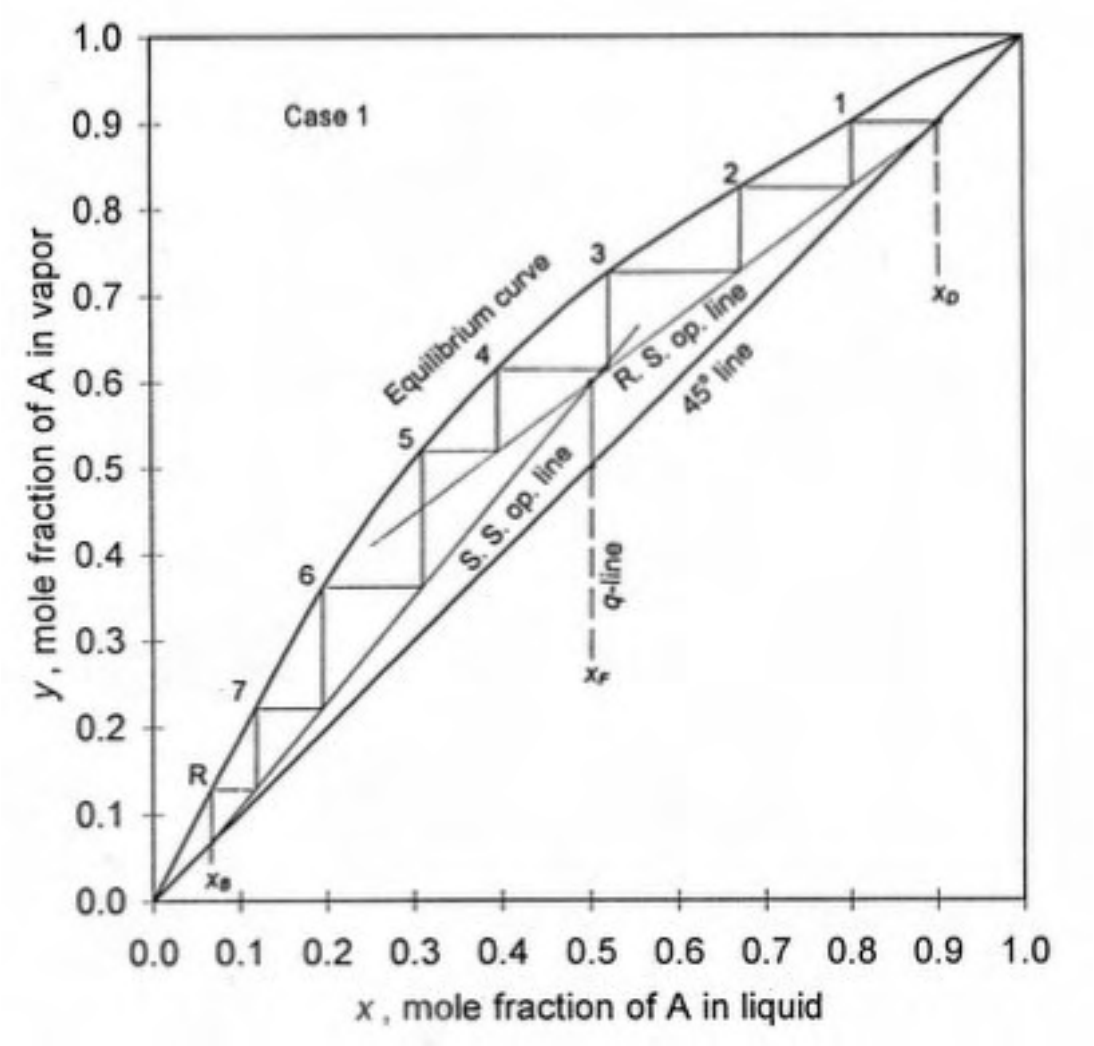
Case 2: We now have 4 equilibrium stages and a partial reboiler, with the feed being sent to the reboiler. Assume that utility rates are such that L/V and $\bar{L}/\bar{V}$ are the same as in Case 1. Then, on the McCabe-Thiele diagram, the values of x_D and x_B must shift so that 5 stages are stepped off, with the fifth, which is the reboiler, intersecting the stripping section operating line at the 45° line. This is shown on the McCabe-Thiele diagram on the following page.

(a) From this diagram, the mole fractions of benzene in the distillate and bottoms are 0.80 and 0.21, respectively.

Case 3: Since the distillate composition in Case 2 is 80 mol% benzene, the results would be the same as Case 2 if an 80 mol% benzene stream from another column were used as reflux.

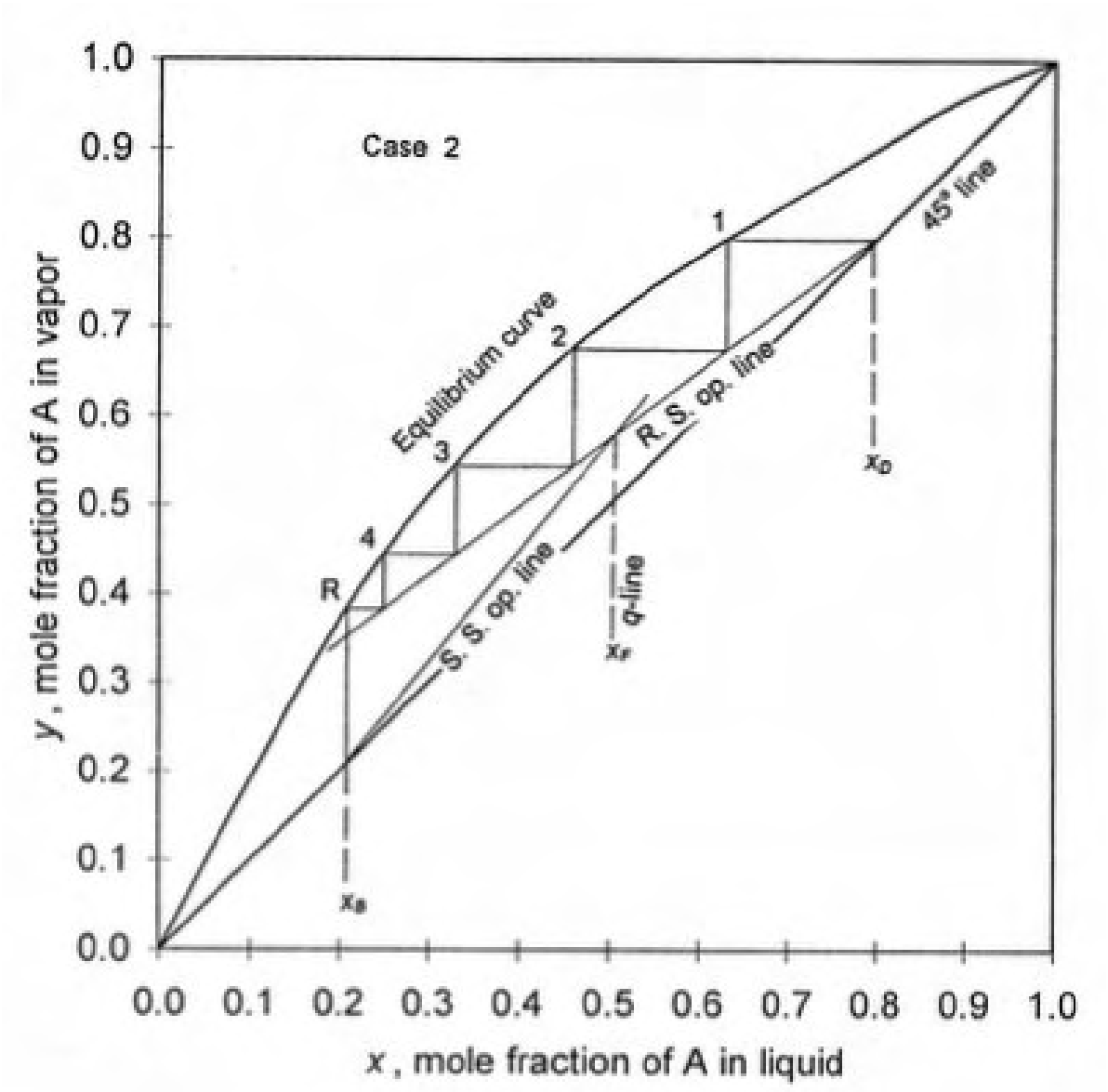
Exercise 7.16 (continued)

Analysis: Case 1 (continued)



Exercise 7.16 (continued)

Analysis: Case 2 (continued)



Exercise 7.17

Subject: Distillation of a mixture of benzene and toluene with different feed conditions.

Given: Column with 7 equilibrium plates, total condenser, and partial reboiler. Feed is 50 mol% benzene and 50 mol% toluene. Operation at 101 kPa to produce a distillate of 96 mol% benzene.
Equilibrium data from Exercise 7.13.

Assumptions: Constant molar overflow. Use a basis of 100 mol/s for the feed.

Find:

(a) For a saturated liquid feed sent to tray 5 from the top, (1) minimum reflux ratio, $R = L/D$, (2) bottoms composition for twice the minimum reflux ratio, and (3) moles of products per 100 moles of feed.

(b) Same as (a) except feed is saturated vapor to tray 5 from the top.

(c) For a saturated vapor feed to the reboiler and a reflux ratio, L/V, of 0.9, determine, (1) bottoms composition and (2) moles of products per 100 moles of feed.

Analysis:

(a)

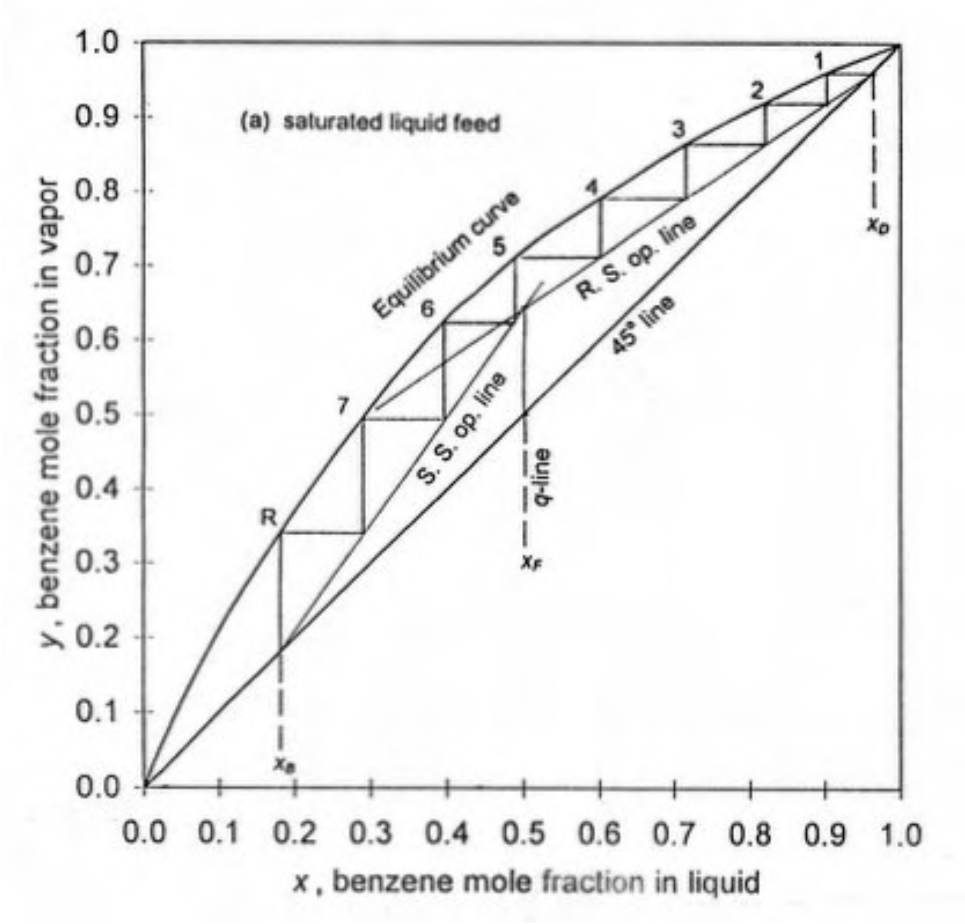
(1) For a saturated liquid feed, minimum reflux corresponds to a pinch point located at the intersection of a vertical q-line passing through $x_F = 0.5$ and the equilibrium curve. From the equilibrium data, this intersection is at $y = 0.72$ and $x = 0.5$. Then, the slope of the rectifying section operating line, $(L/V)_{min}$ is (0.96 - 0.72)/(0.96 - 0.50) = 0.522. From a rearrangement of Eq. (7-7), $R_{min} = (L/V)_{min} /[1 - (L/V)_{min}] = 0.522/(1 - 0.522) = 1.092$.

(2) Reflux ratio = 2(1.092) = 2.18. From Eq. (7-7), the slope of the rectifying section operating line = $L/V = R/(1 + R) = 2.18/3.18 = 0.686$. To determine the bottoms composition, use a McCabe-Thiele diagram in terms of benzene, the more volatile component. The q-line and the rectifying section operating line are fixed and 4 trays are stepped off from the top, starting at the distillate mole fraction for benzene, x_D , of 0.96. Then, the stripping section operating line is positioned by trial and error so that 3 more stages plus the reboiler stage are stepped off to arrive at the point where the assumed location of the stripping section operating line intersects the 45° line. The result is shown on the next page where it is seen that $x_B = 0.18$.

(3) The products are now computed by overall material balances: $F = 100 = D + B$ and $50 = x_D D + x_B B = 0.96D + 0.18B$. Solving these two equations, $D =$ 41.0 mol/100 mol feed and $B =$ 59.0 mol/100 mol feed.

Exercise 7.17 (continued)

Analysis: (a) (continued)



(b)

(1) For a saturated vapor feed, minimum reflux corresponds to a pinch point located at the intersection of a horizontal q-line passing through $x_F = y = 0.5$ and the equilibrium curve. From the equilibrium data, this intersection is at $y = 0.50$ and $x = 0.293$. Then, the slope of the rectifying section operating line, $(L/V)_{min}$ is (0.96 - 0.50)/(0.96 - 0.293) = 0.690. From a rearrangement of Eq. (7-7), $R_{min} = (L/V)_{min}/[1 - (L/V)_{min}] = 0.69/(1 - 0.69) = 2.23$.

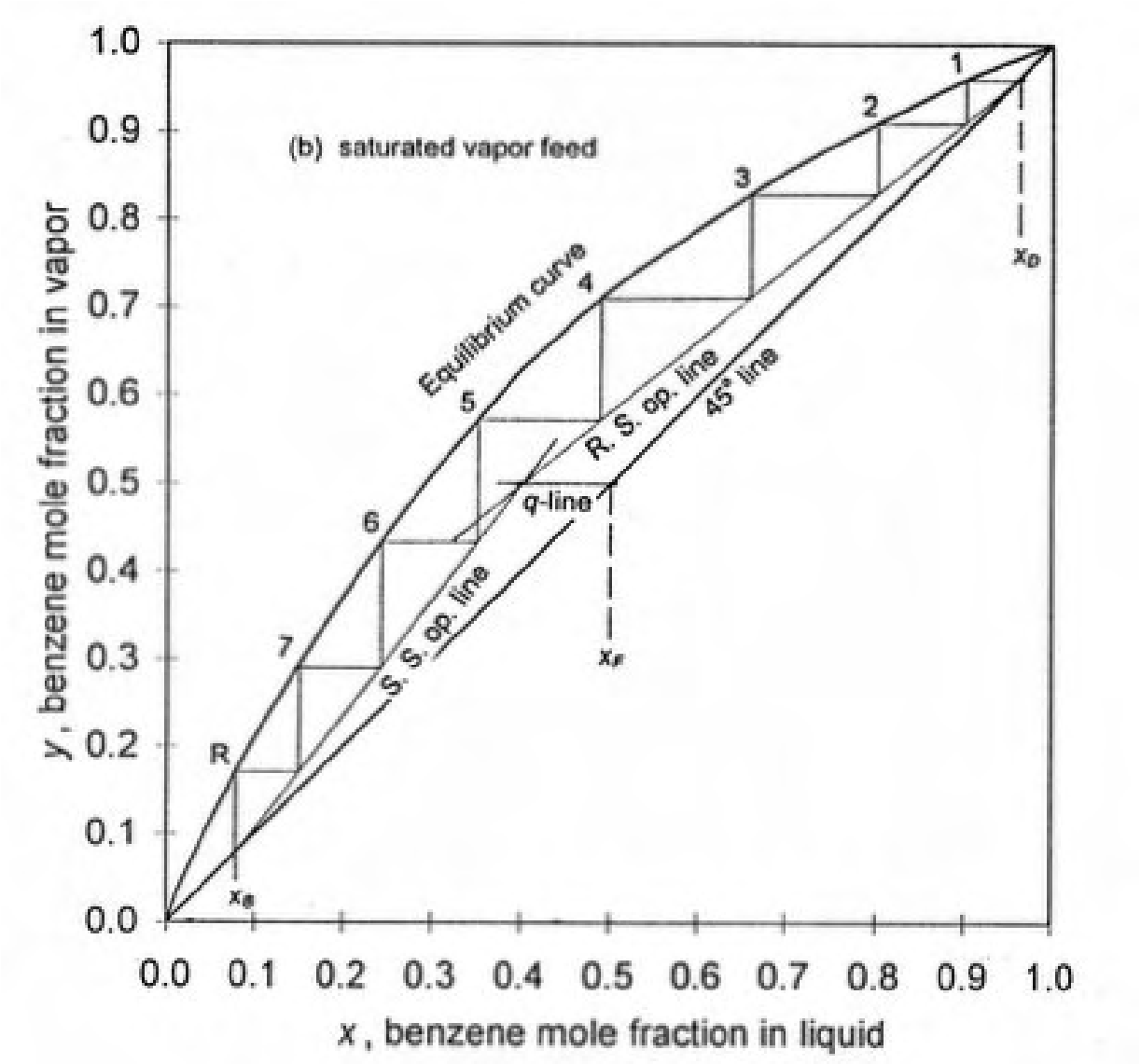
(2) Reflux ratio = 2(2.23) = 4.46. From Eq. (7-7), the slope of the rectifying section operating line = $L/V = R/(1 + R) = 4.46/5.46 = 0.817$. To determine the bottoms composition, use a McCabe-Thiele diagram in terms of benzene, the more volatile component. The q-line and the rectifying section operating line are fixed and 4 trays are stepped off from the top, starting at the distillate mole fraction for benzene, x_D , of 0.96. Then, the stripping section operating line is

positioned by trial and error so that 3 more stages plus the reboiler stage are stepped off to arrive at the point where the assumed location of the stripping section operating line intersects the 45° line. The result is shown below, where it is seen that $x_B = 0.08$.

Exercise 7.17 (continued)

Analysis: (b) (continued

(3) The products are now computed by overall material balances: $F = 100 = D + B$ and $50 = x_D D + x_B B = 0.96D + 0.08B$. Solving these two equations, $D =$ 47.7 mol/100 mol feed and $B = 52.3$ mol/100 mol feed.



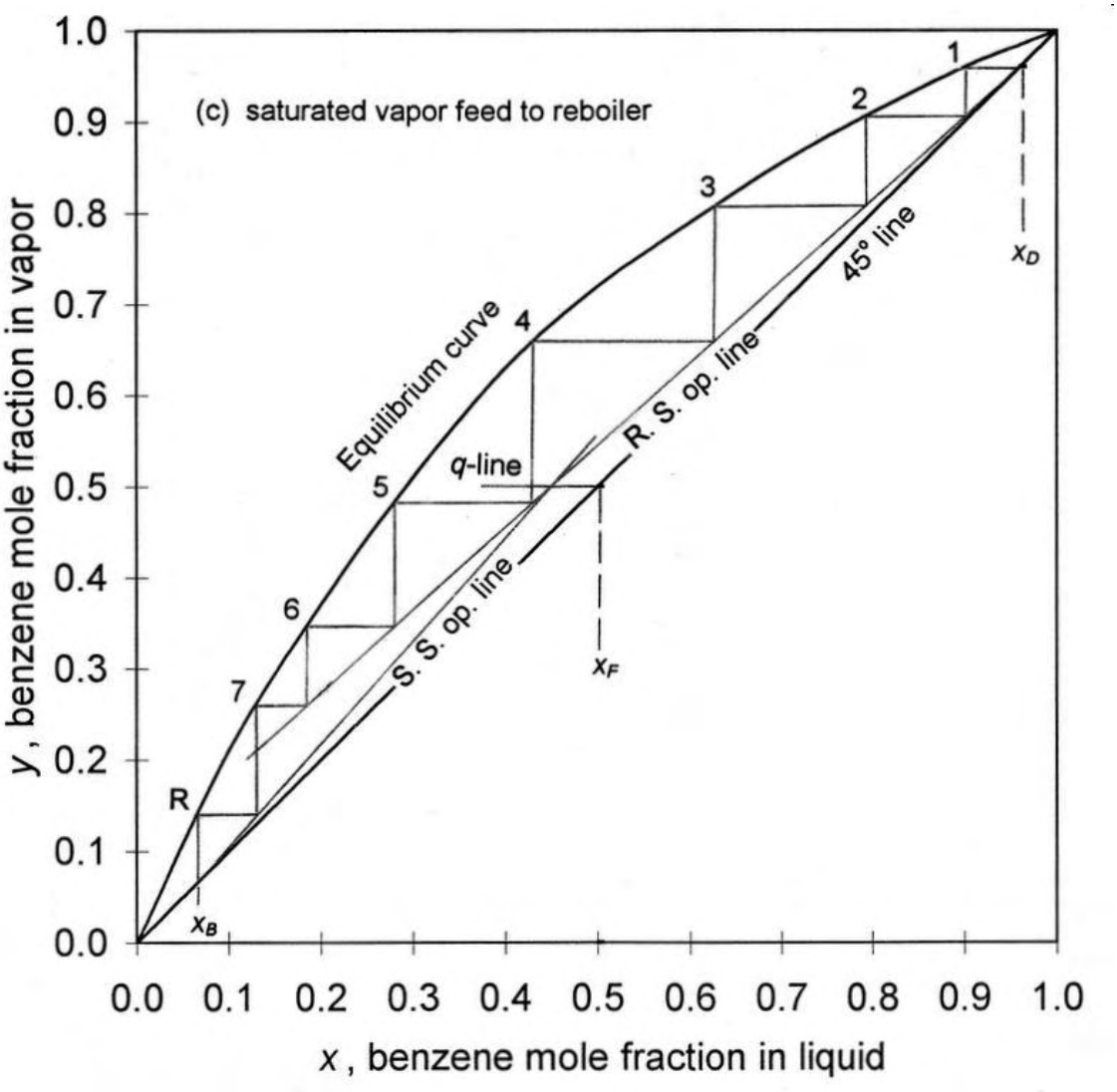
Exercise 7.17 (continued)

Analysis: (continued)

(c)

(1) A saturated vapor feed is fed to the reboiler. The slope of the rectifying section operating line, (L/V), is 0.9. To determine the bottoms composition, use a McCabe-Thiele diagram in terms of benzene, the more volatile component. The q-line and the rectifying section operating line are fixed and 7 trays are stepped off from the top, starting at the distillate mole fraction for benzene, x_D , of 0.96. Then, the stripping section operating line is positioned by trial and error so that the reboiler stage is stepped off to arrive at the point where the assumed location of the stripping section operating line intersects the 45° line. The result is shown below, where it is seen that $x_B = 0.07$.

(2) The products are now computed by overall material balances: $F = 100 = D + B$ and $50 = x_D D + x_B B = 0.96D + 0.07B$. Solving these two equations, $D =$ 48.3 mol/100 mol feed and $B = 51.7$ mol/100 mol feed.



Exercise 7.18

Subject: Conversion of a distillation column to a reboiled stripper to obtain very pure toluene from a mixture of benzene and toluene at 101 kPa.

Given: A column with 8 theoretical plates, a total condenser, and a partial reboiler. Feed contains 36 mol% benzene and 64 mol% toluene. Reboiler produces 100 kmol/h of vapor. To obtain nearly pure toluene bottoms, feed is introduced to the top plate as a saturated liquid, with no reflux. Vapor-liquid equilibrium data are in Exercise 7.13.

Assumptions: Constant molar overflow.

Find: (a) Minimum feed rate and corresponding bottoms composition.
(b) Bottoms rate and composition for a feed rate 25% above the minimum.

Analysis:

(a)

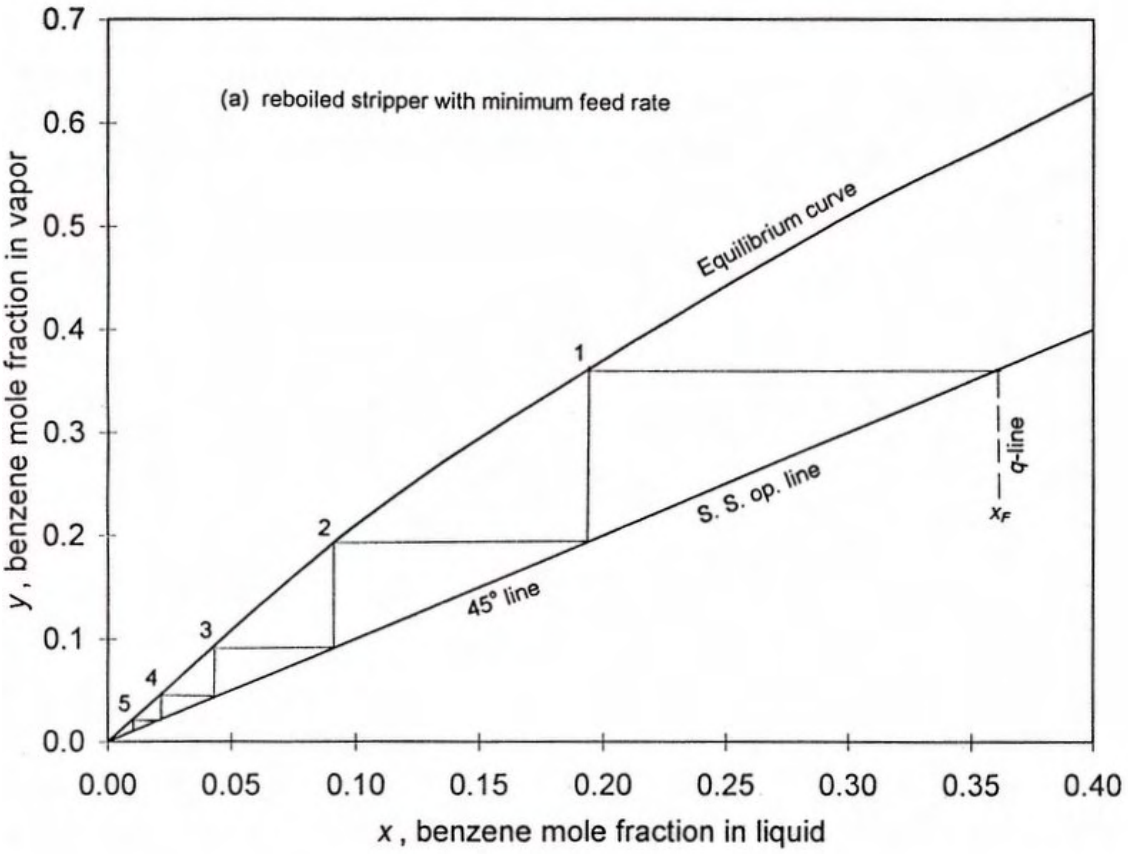
The minimum feed rate corresponds to a rate equal to the boilup rate so as to give an $\overline{L}/\overline{V} = 1.0$. Thus, the minimum feed rate = 100 kmol/h. Under these conditions, no bottoms product is withdrawn and the reboiler performs as a total reboiler. The vapor leaving the top of the column has the same composition as the feed. Therefore, we consider only a total of 8 equilibrium stages.

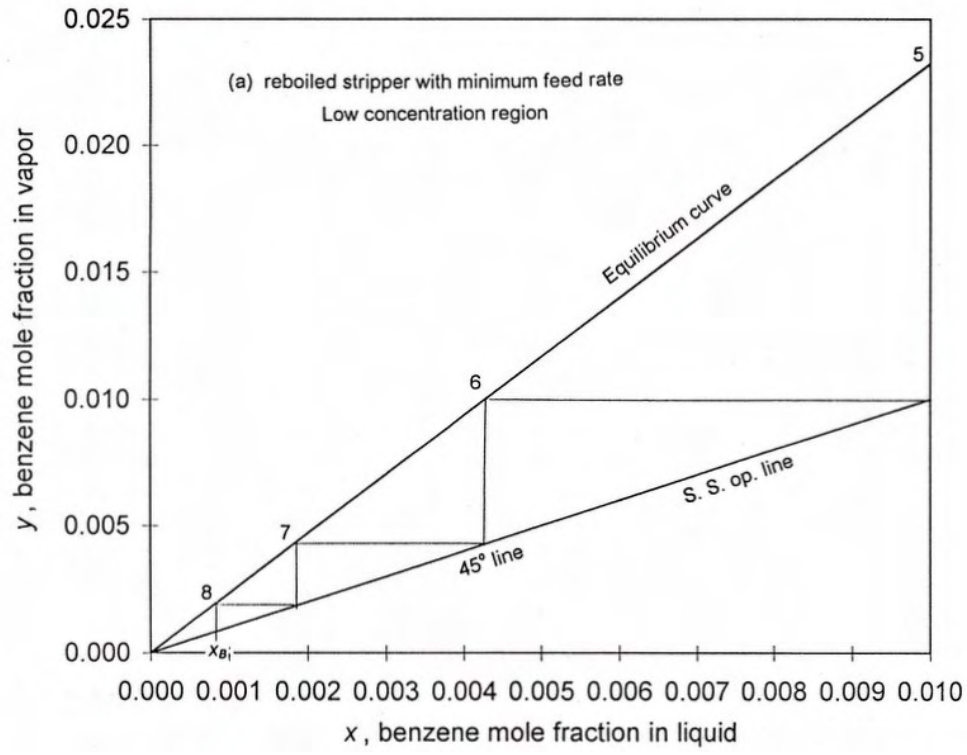
In the McCabe-Thiele diagram below, the stripping section operating line is coincident with the 45^{o} line. The 8 stages are stepped off from the top at $y = 0.36$ and $x = 0.36$. The mole fraction of benzene in the reboiler is found to be 0.008 from the low concentration region plot. Therefore, the corresponding toluene mole fraction = 0.992, which is quite pure.

Note that 2 diagrams below are used, with the second, covering the stages at the bottom of the column in the low concentration region. To obtain accuracy in this low-end region, the vapor-liquid equilibrium data for $x = 0.1$ and $x = 0.2$ were fitted to a quadratic equation passing through the origin, with the result, $y = 2.35x - 2.5x^2$.

Exercise 7.18 (continued)

Analysis: (a) (continued)

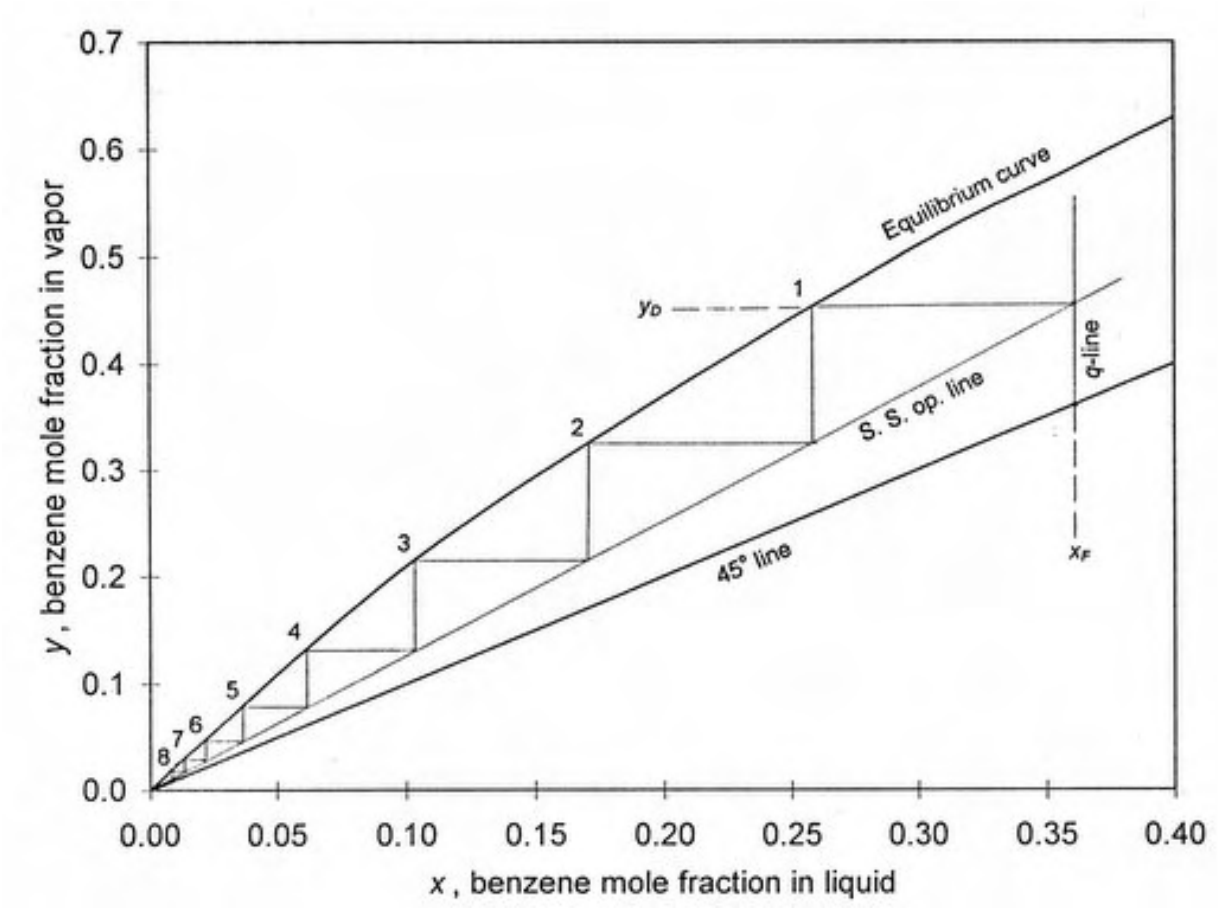




Exercise 7.18 (continued)

Analysis: (continued)

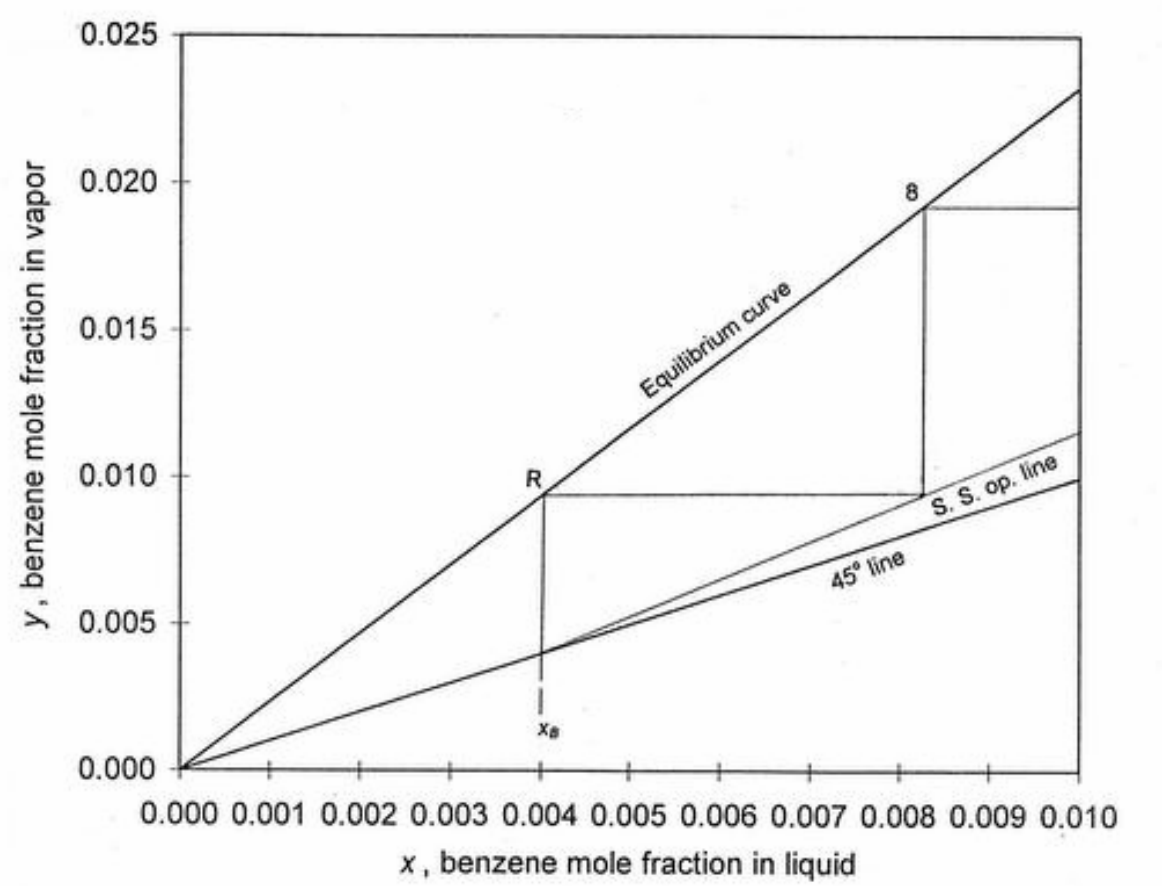
(b) F = Feed rate = $\overline{L}$ = 1.25(100) = 125 kmol/h. $\overline{V}$ = Vapor rate = 100 kmol/h. Therefore, with no condenser and constant molar overflow, $B = F - \overline{V}$ = 125 - 100 = 25 kmol/h. The slope of the stripping section operating line = $\overline{L}/\overline{V}$ = 125/100 = 1.25. The q-line is vertical for a saturated liquid feed, passing through x_F = 0.36. The stripping section operating line is positioned by trial and error so that 8 + 1 equilibrium stages will be stepped off. Because part (a) shows that a very low mole fraction of benzene is obtained in the bottoms, it is suspected that the operating line will intersect the 45° line almost at the origin. If this were true, then the operating line, with a slope of 1.25, would intersect the vertical q-line at 1.25(0.36) = 0.45. Use this as a first approximation and adjust it downward until only 9 stages can be stepped off. The final result is shown in the two plots on the next page, where the second plot is for the low concentration region. As seen, the mole percent of benzene in the bottoms = 0.004, giving 99.6 mol% toluene in the bottoms. The overhead vapor contains 0.449 mole fraction benzene. By material balances, $F = 125 = D + B$ and $0.36F = 0.449D + 0.004B$, D = 100.0 and B = 25.0 kmol/h.



Exercise 7.18 (continued)

Analysis: (b) (continued)

Low-concentration Region



Exercise 7.19

Subject: Normal and abnormal operation of a distillation column separating a methanol - water mixture at 101 kPa.

Given: Column with 7 theoretical plates, a total condenser, and a partial reboiler. A feed of 100 kmol/h of 50 mol% methanol in water is sent to plate 3 from the bottom. During normal operation, distillate is 90 mol% methanol and bottoms is 5 mol% methanol, with a reflux rate of 1 mole per mole distillate. During abnormal operation, the following data are obtained:

Stream	kmol/h	mol% methanol
Feed	100	51
Bottoms	62	12
Distillate	53	80
Reflux	94	-

Vapor-liquid equilibrium data are given at 101 kPa, where methanol is the more volatile species.

Assumptions: Constant molar overflow.

Find: Most probable cause for abnormal operation.
Recommended further tests.
If 90 mol% methanol distillate could be obtained by increasing the reflux ratio for a constant vapor rate.

Analysis:

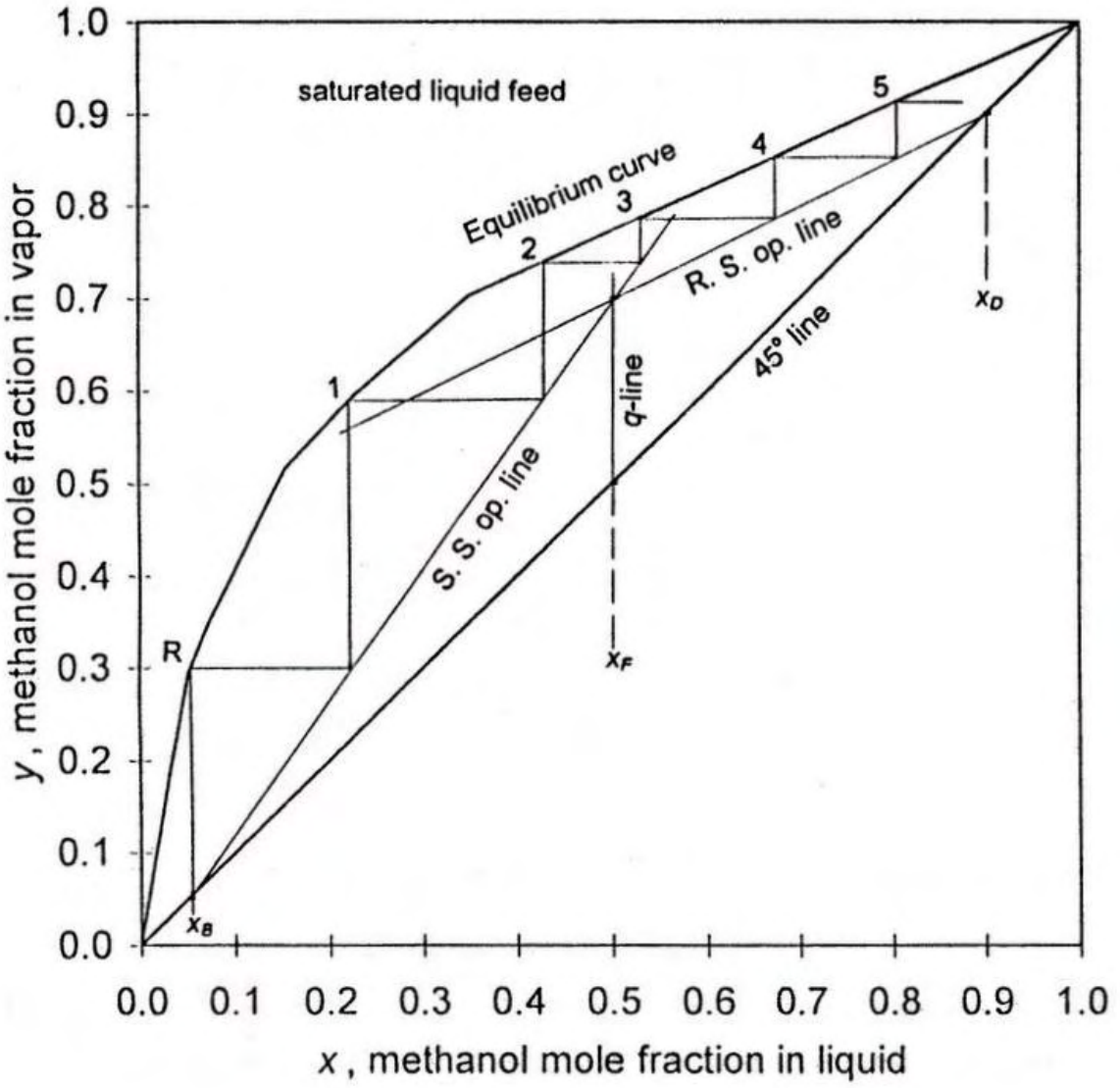
First determine whether the normal operation can be verified by the McCabe-Thiele method. With $L/D = R = 1$, from Eq. (7-7), the slope of the rectifying operating line = $L/V = R/(1 + R) = 1/2 = 0.5$. Also, $x_F = 0.5$, $x_D = 0.90$, and $x_B = 0.05$.

What is not known is the phase condition of the feed. If a saturated liquid feed is assumed, giving a vertical q-line as shown in the plot below, stepping stages up from the bottom, with the feed stage to plate 3 from the bottom, less than 2 theoretical plates are needed in the rectifying section, while 4 are present. The construction is shown on the next page.

Therefore, it appears that the feed is not a saturated liquid, but is partially vaporized.

Exercise 7.19 (continued)

Analysis: Normal Operation (continued)



By trial and error, using q-lines of various slopes, the following McCabe-Thiele diagram is consistent with the given data. It shows a q-line with a slope of -0.34.

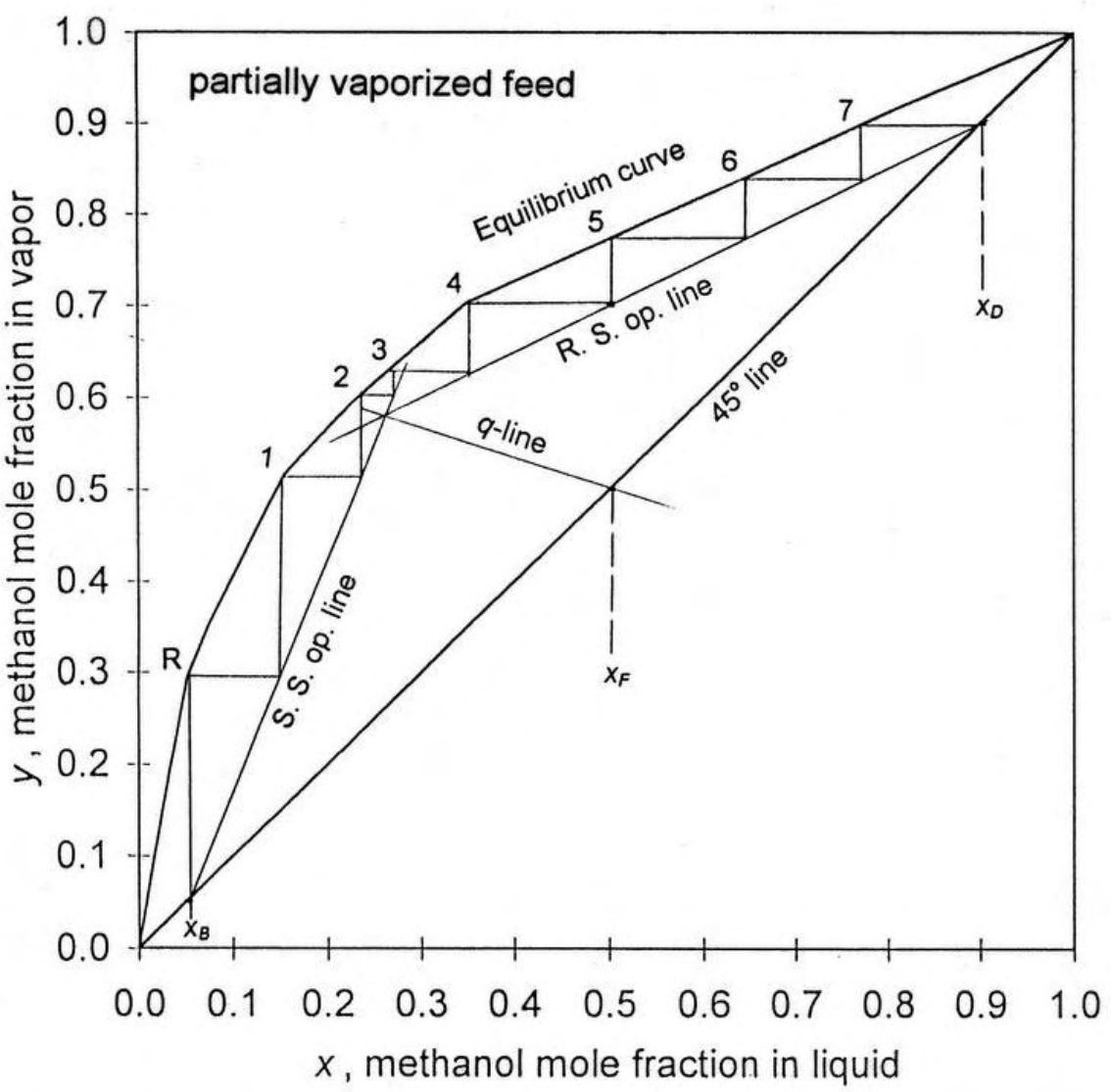
$$\text{slope} = q/(q-1)$$

Therefore, q = slope/(slope-1)=-0.34/(-0.34-1.0)=0.25

From Eq. (7-19), molar fraction vaporized $= 1-q = 1-0.25 = 0.75$

Exercise 7.19 (continued)

Analysis: Normal operation (continued)



The material balance for the normal operation is as follows, using the overall balances, $F = 100 = D + B$ and $0.5F = 0.5(100) = 50 = x_D D + x_B B = 0.90D + 0.05B$.

Stream	kmol/h	mol% methanol
Feed	100	50
Bottoms	47.06	5
Distillate	52.94	90
Reflux	52.94	90

Exercise 7.19 (continued)

Analysis: Abnormal operation

For the abnormal operation, first check the overall total material balance using the given data. F = 100 kmol/h. $D + B$ = 53 + 62 = 115 kmol/h. Therefore, it appears that we have 115 - 100 = 15 kmol/h more flow out of the distillation system. Now check the methanol overall material balance using the given data. Methanol flow rate in = 0.51(100) = 51 kmol/h. Methanol flow rate out = 0.80(53) + 0.12(62) = 49.84 kmol/h. Therefore, the methanol balance is close, with only about a 2% discrepancy. Now check the water overall material balance using the given data. Water flow in = 0.49(100) = 49 kmol/h. Water flow out = 0.20(53) + 0.88(62) = 65.16 kmol/h. Therefore, we have 65.16 - 49 = 16.16 kmol/h more water out than in. This is a significant discrepancy. It appears certain that water is leaking into the distillation system. Two possibilities are: (1) leakage of condenser cooling water into the condensate, or (2) leakage of reboiler steam into the boilup vapor. A reboiler steam leak may not be serious because the steam might not get to the top of the column to dilute the methanol product. A condenser cooling water leak could be very serious because part of it would end up in the distillate, thereby diluting the methanol product. Because of the impure methanol distillate for the abnormal operation, it appears that a condenser cooling water leak is the fault. Check this next.

We note that the distillate flow rate for the abnormal operation is almost exactly the same as that for the normal operation. A flow rate equal to that of he leakage passes out the bottom of the column. In normal operation, the water passing out in the distillate = 0.1(53) = 5.3 kmol/h, while for the abnormal operation, the water passing out in the distillate = 0.2(53) = 10.6 kmol/h. Thus, an additional 5.3 kmol/h of water leaves in the distillate. For the abnormal operation, the overhead vapor rate = 53 + 94 = 147 kmol/h and, therefore, 53/147 x 100% = 36% of the overhead vapor (total condensate) is distillate. Thus, if 15 kmol/h of water leaked into the overhead vapor, then, we would expect 0.36(15) = 5.4 kmol/h would be expected to leave with the distillate. This compares very well with the 5.3 kmol/h additional water calculated above by material balance. If the degree of fractionation within the column is about the same as for the normal operation, it could be concluded that a condenser cooling water leak is to blame.

To check the cooling water leak, could meter the cooling water in and out of the condenser and see if there is a difference.

If the vapor rate is kept constant and the reflux rate is increased, then the distillate rate must be decreased. Assume a vapor rate of 147 kmol/h, with 30 kmol/h to distillate and 117 kmol/h to reflux. Then, 30/117 x 100% = 25.6% of the overhead vapor is distillate. Therefore, the water leak to the distillate would be 0.256(15) = 3.84 kmol/h. If the fractionation were otherwise the same as for normal operation so that the overhead vapor was 90 mol% methanol, the dilution with leakage would result in 0.1(30 - 3.84) + 3.84 = 6.46 kmol/h of water in 30 kmol/h. Thus, methanol purity = (30 - 6.46)/30 x 100% = 78.5 mol%. However, the higher reflux ratio would increase the fractionation, so as to increase the purity above this value. A further increase in fractionation could be achieved, if the feed were condensed to a saturated liquid and additional heat was transferred in the reboiler. But, even if a pure methanol overhead vapor were achieved, the methanol purity after dilution with the water leakage would be : (30 - 3.84)/30 x 100% = 87.2 mol% methanol. Must eliminate the leak.

Exercise 7.20

Subject: Effect on reflux and boilup compositions of reducing the feed rate to a distillation column when the reflux and boilup rate are held constant

Given: Column with 3 theoretical plates, a total condenser, and a partial reboiler. Feed is a saturated liquid of 50 mol% A and 50 mol% B, fed to the bottom tray. At a feed rate of 100 kmol/h, desired products of distillate with 90 mol% A and bottoms of 20 mol% A can be achieved, when a reflux corresponding to $L/V = 0.75$ is used. Relative volatility of A to B is constant at 3.0.

Assumptions: Constant molar overflow. Saturated liquid reflux.

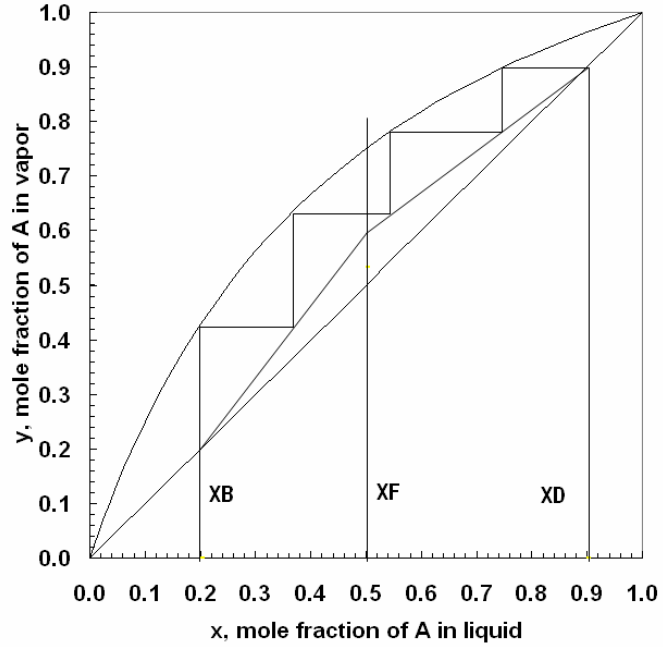
Find: Compositions of reflux and boilup when feed rate is inadvertently reduced to 25 kmol/h, while keeping the reflux and boilup flow rates constant.

Analysis: First, verify the separation for a feed rate of 100 kmol/h. This is shown in the McCabe-Thiele plot below in terms of mole fractions of A, the more volatile component. The equilibrium curve is computed from Eq. (7-3),

$$y = \frac{\alpha x}{1 + x(\alpha - 1)} = \frac{3x}{1 + 2x}$$

The given mole fractions are: $x_F = 0.50$ $x_D = 0.90$ $x_B = 0.20$

The rectification section operating line has a slope of 0.75 and passes through point {0.9, 0.9}. The q-line is vertical at $x = 0.5$. The plot shows almost perfect agreement with the desired separation for a feed rate of 100 kmol/h.



Exercise 7.20 (continued)

Analysis: (continued)

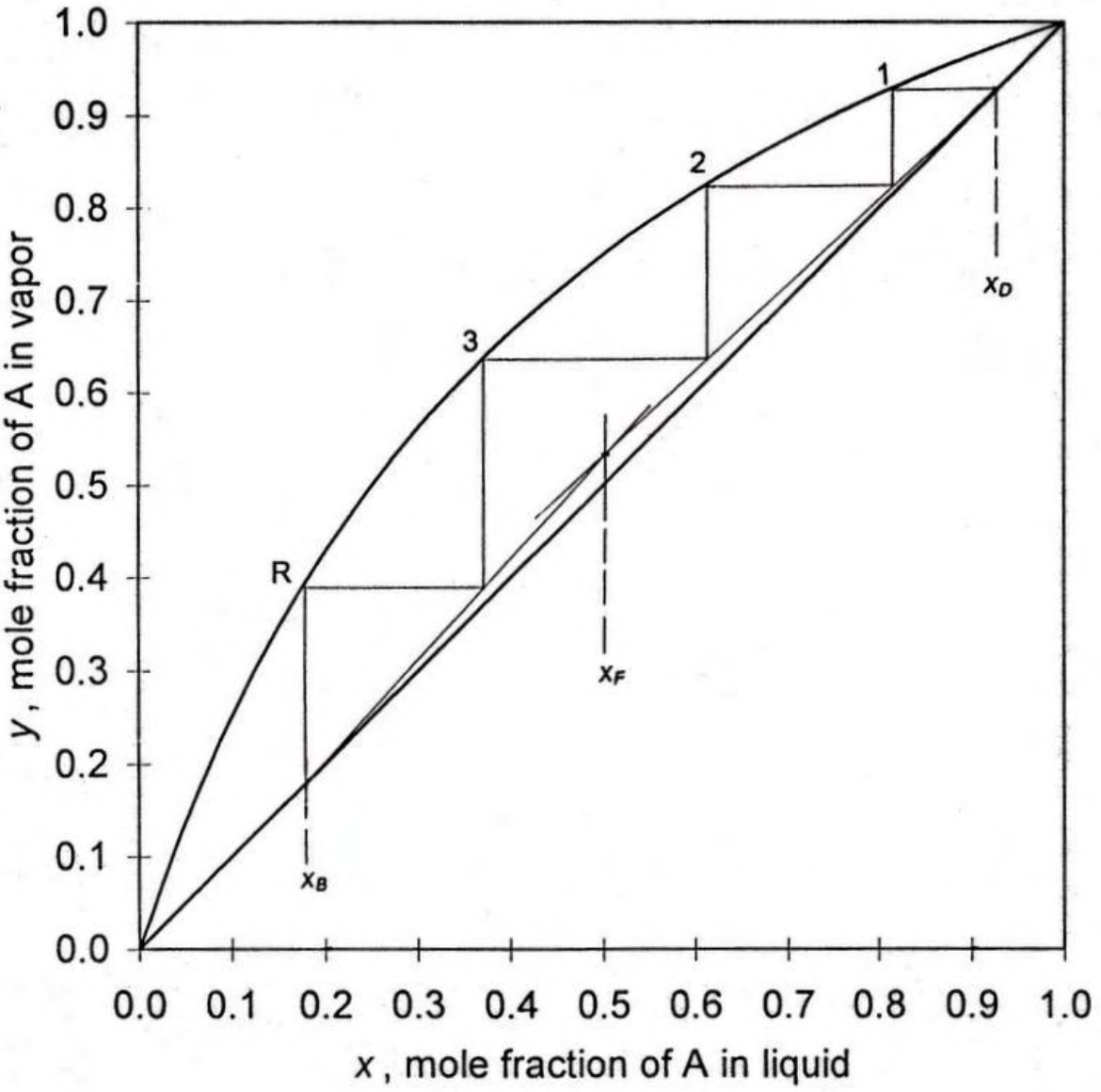
For the base case of F = 100 kmol/h, the material balance equations are $F = D + B$ and $x_F F = 50 = x_D D + x_B B = 0.90D + 0.20B$. Solving, these equations, along with $V = L + D$, $V/L = 0.75$, $\overline{V} = V$, and $\overline{L} = L + F$, gives the following results:

Stream	Flow rate, kmol/h	Mol% A	Mol% B
Feed	100.00	50	50
Distillate	42.86	90	10
Bottoms	57.14	20	80
Reflux, L	128.58		
Overhead vapor, V	171.44		
Liquid to reboiler, $\overline{L}$	228.58		
Vapor from reboiler, $\overline{V}$	171.44		

When the feed rate is reduced to 25 kmol/h, the reflux rate, L, is maintained at 128.58 kmol/h and the boilup, $\overline{V}$, is maintained at 171.44 kmol/h. Therefore by material balances, $\overline{L} = L + F$ = 128.58 + 25 = 153.58 and $B = \overline{L} - \overline{V}$ = 153.58 - 171.44 = -17.86 kmol/h. This is impossible. Therefore, the column can not be operated with the same boilup rate. That rate would have to be reduced to achieve a desired bottoms rate, e. g. the 57.14 % of the feed, as in the base case or 0.5714(25) = 14.29 kmol/h. If this were done, we would now have, $\overline{V} = \overline{L} - B$ = 153.58 - 14.29 = 139.29 kmol/h = V. Thus, in the rectifying section, L/V = 128.58/139.29 = 0.923 and in the stripping section, $\overline{L}/\overline{V}$ = 153.58/139.29 = 1.103. The resulting distillate and bottoms compositions are determined by positioning the operating lines so that 3 stages + a reboiler can be stepped off. The result is shown below, where the mole fractions of A are 0.93 in the distillate and reflux, 0.18 in the bottoms, and 0.38 in the reboiler vapor.

Exercise 7.20 (continued)

Analysis: (continued)



Exercise 7.21

Subject: Distillation of a saturated vapor of maleic anhydride (A) and benzoic acid (B) under vacuum at 13.3 kPa.

Given: Feed contains 90 mol% A and 10 mol% B. Distillate to contain 99.5 mol% anhydride and bottoms to contain 0.5 mol% acid. Vapor pressure data.

Assumptions: Raoult's law to compute *K*-values from vapor pressure data. Constant molar overflow.

Find: Number of theoretical plates needed if a reflux ratio, *L/D* = 1.6 times minimum.

Analysis: First compute an equilibrium *y, x* curve using Raoult's law with the vapor pressure data. Eq. (2-44) applies, as well as the sum of the mole fractions in the phases in equilibrium. Thus,

$$K_A = \frac{y_A}{x_A} = \frac{P_A^s\{T\}}{P} \quad , \quad K_B = \frac{y_B}{x_B} = \frac{P_B^s\{T\}}{P} \qquad (1,\ 2)$$

$$y_A + y_B = 1 \quad , \quad x_A + x_B = 1 \qquad (3,\ 4)$$

Equations (1) to (4) can be reduced to the following equations for the mole fractions of maleic anhydride (A) in terms of the *K*-values:

$$x_A = \frac{1 - K_B}{K_A - K_B} \quad , \quad y_A = K_A x_A \qquad (5, 6)$$

If the given vapor pressure data are fitted to Antoine equations, we obtain:

$$P_A^s = \exp\left(16.6541 - \frac{4088.12}{T + 203.924}\right) \qquad (7)$$

$$P_B^s = \exp\left(23.0155 - \frac{9336.97}{T + 321.434}\right) \qquad (8)$$

Where vapor pressure is in torr and temperature is in ^oC. Solving, Eqs. (1) to (8),
In solving the equations, P = 13.3 kPa or 99.8 torr. The results are tabulated on the next page. Below the table is a McCabe-Thiele plot of y_A versus x_A for determining the minimum reflux for x_D = 0.995 and a horizontal *q*-line at y = 0.90, which intersects the equilibrium curve at x = 0.572. Therefore, the slope of the rectifying section operating line at minimum reflux is $(L/V)_{min}$ = (0.995 - 0.90)/(0.995 - 0.572) = 0.225. From a rearrangement of Eq. (7-7), R_{min} = $(L/V)_{min}/[1 - (L/V)_{min}]$ = 0.225/(1-0.225) = 0.290. Therefore, the reflux ratio for operation = $1.6R_{min}$ = 1.6(0.290) = 0.464.

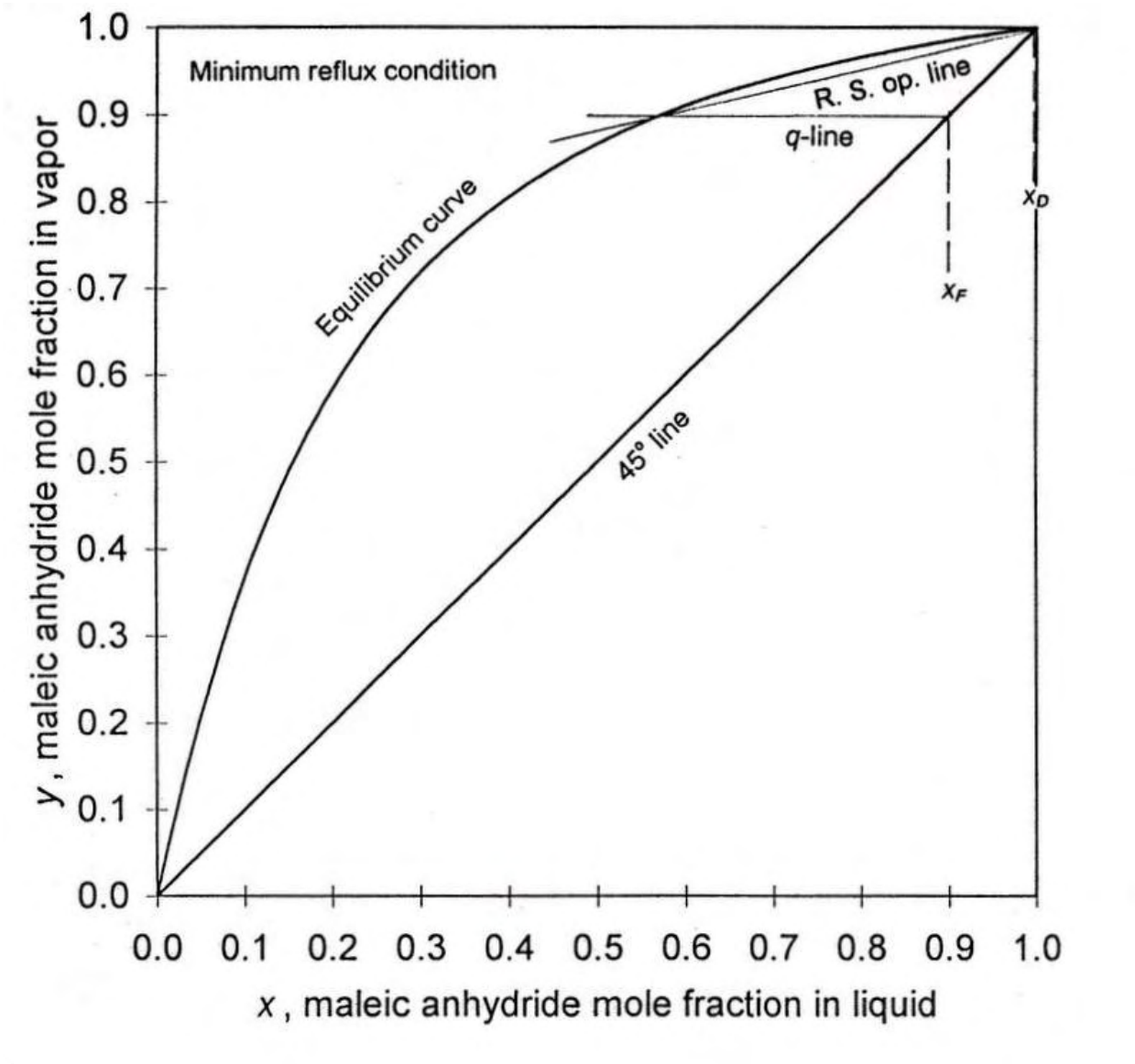
Exercise 7.21 (continued)

Analysis: (continued)

T, °C	P^s of A, torr	P^s of B, torr	K_A	K_B	x_A	y_A
135.3	99.8	13.1	1.000	0.131	1.000	1.000
136.5	104.1	13.8	1.043	0.138	0.953	0.993
137.8	108.9	14.6	1.092	0.147	0.903	0.986
140.3	118.8	16.3	1.191	0.164	0.814	0.970
142.8	129.5	18.2	1.297	0.183	0.733	0.951
145.3	140.9	20.3	1.411	0.203	0.659	0.931
147.8	153.1	22.6	1.534	0.226	0.592	0.908
150.3	166.2	25.1	1.665	0.251	0.530	0.882
152.8	180.2	27.9	1.805	0.279	0.472	0.853
157.8	211.1	34.2	2.115	0.343	0.371	0.784
160.3	228.1	37.8	2.286	0.379	0.326	0.744
162.8	246.3	41.8	2.468	0.419	0.284	0.700
165.3	265.6	46.2	2.661	0.463	0.244	0.650
167.8	286.1	50.9	2.867	0.510	0.208	0.596
170.3	307.9	56.1	3.085	0.562	0.173	0.535
172.8	331.1	61.8	3.317	0.619	0.141	0.468
175.3	355.6	68.0	3.563	0.681	0.111	0.395
177.8	381.6	74.7	3.824	0.748	0.082	0.313
180.3	409.2	81.9	4.100	0.821	0.055	0.224
182.8	438.3	89.9	4.392	0.901	0.028	0.125
185.3	469.1	98.5	4.701	0.987	0.004	0.017
185.7	474.2	99.9	4.751	1.001	0.000	0.000

Exercise 7.21 (continued)

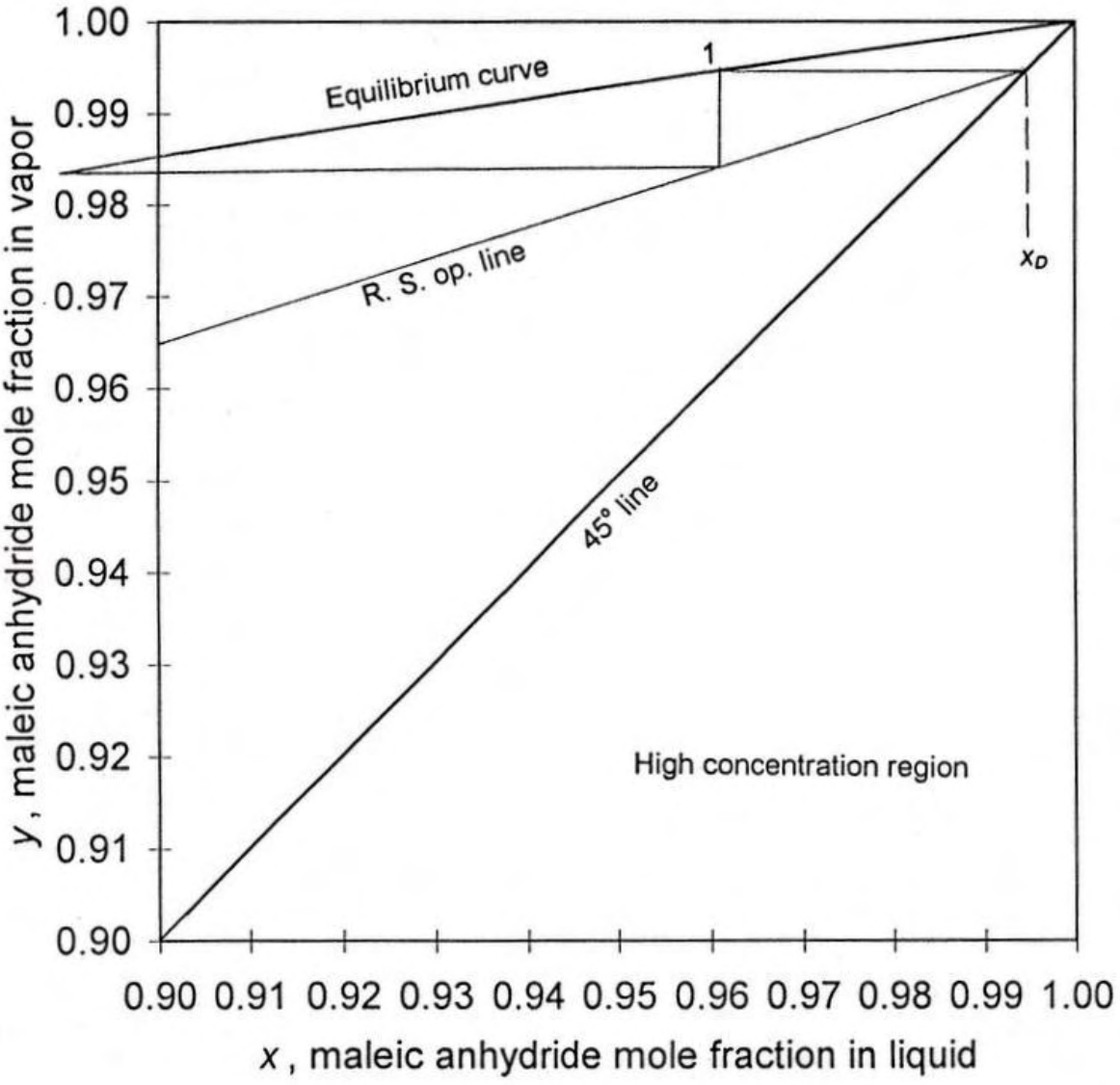
Analysis: (continued)



Exercise 7.21 (continued)

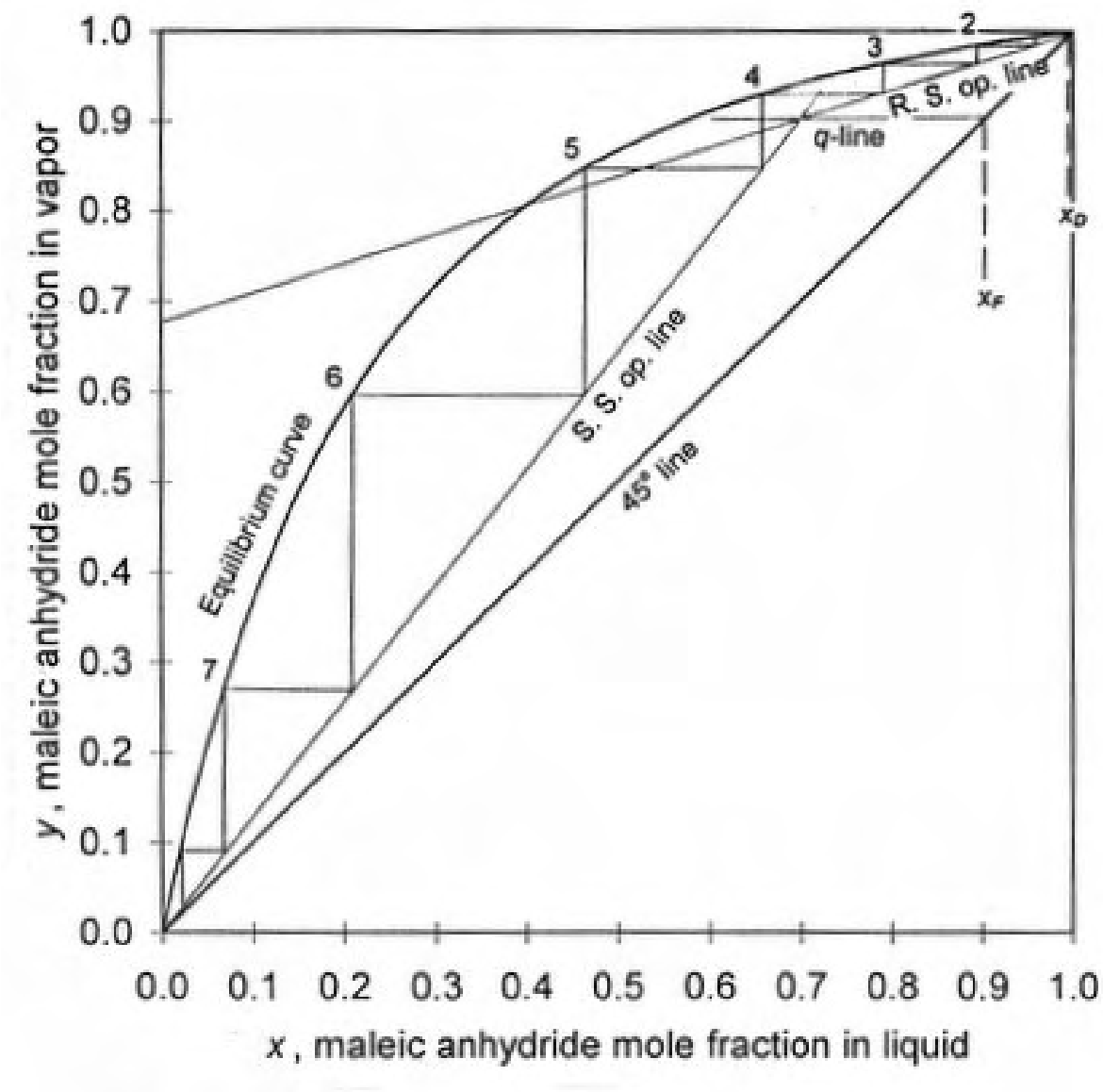
Analysis: (continued)

Now determine the tray requirements for actual operation. Using Eq. (7-7), with the operating reflux ratio of 0.464, $L/V = R/(1 + R) = 0.464/(1 + 0.464) = 0.317$. Because such high purity distillate and bottoms products are to obtained, use 3 McCabe-Thiele diagrams. The first diagram is for the high purity region of component A from y and $x = 0.9$ to 1.0. The operating line for the rectifying section begins at {0.995, 0.995} and, with a slope of 0.317, intersects the vertical axis for $x = 0.90$ at $y = 0.965$. The entire region is covered in the second diagram, the feed stage is located optimally. The low concentration region is covered in the third diagram. From these three diagrams, it is seen that 8 theoretical plates plus a partial reboiler are needed. The feed is sent to plate 4 from the top.



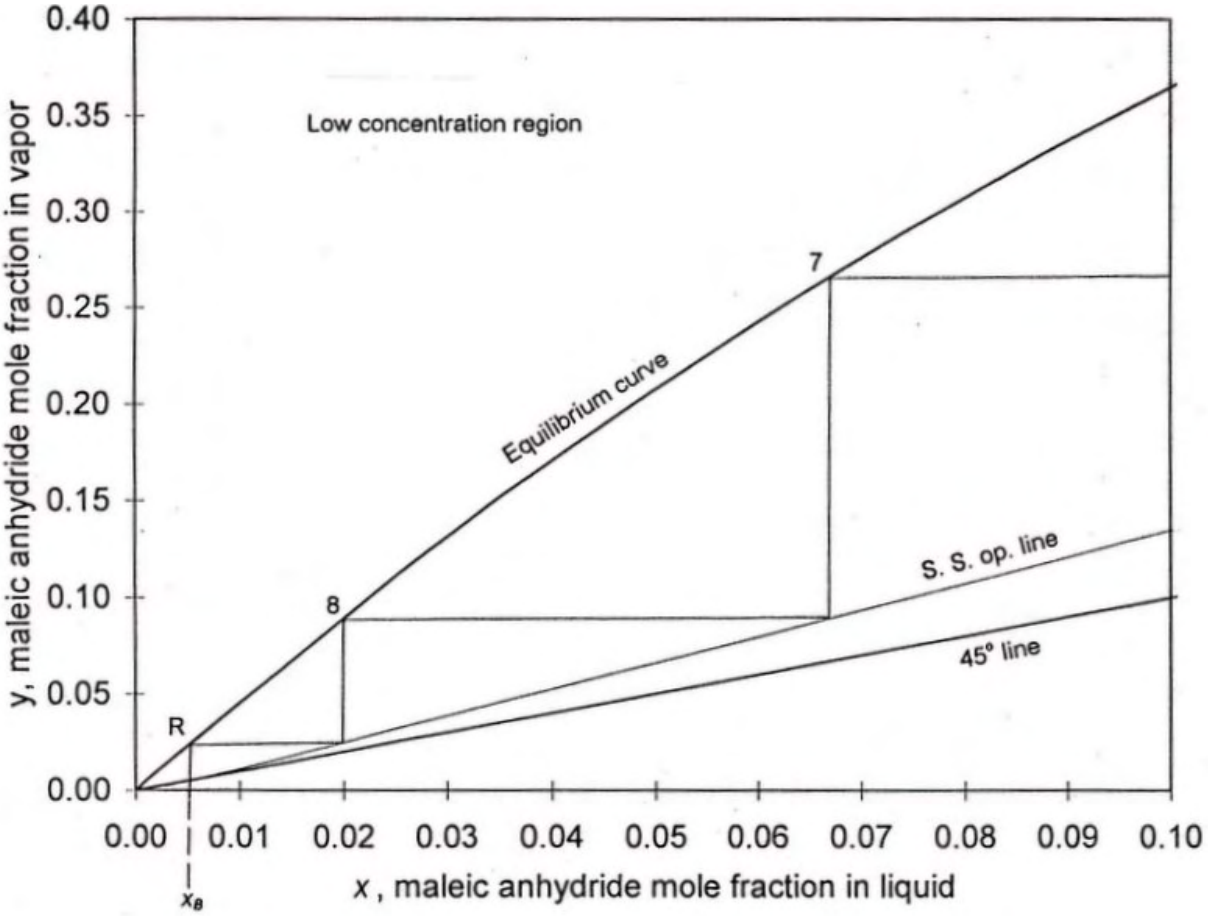
Exercise 7.21 (continued)

Analysis: (continued)



Exercise 7.21 (continued)

Analysis: (continued)



Exercise 7.22

Subject: Distillation of a mixture of A and B based on boilup, rather than reflux, requirements.

Given: A bubble-point feed mixture of 5 mol% A and 95 mol% B. Distillate to contain 35 mol% A and a bottoms to contain 0.2 mol% A. Relative volatility, $\alpha_{A,B} = 6$ = a constant. Column equipped with partial condenser and partial reboiler.

Assumptions: Constant molar overflow.

Find: Using algebraic methods,

(a) Minimum number of equilibrium stages.

(b) Minimum boilup ratio, $V_B = \overline{V} / B$.

(c) Number of equilibrium stages for a boilup ratio = 1.2 times minimum.

Analysis: From a rearrangement of the equilibrium equation, Eq. (7-3),

$$x = \frac{y}{y + \alpha(1 - y)} = \frac{y}{6 - 5y} \qquad (1)$$

(a) For minimum stages, have total reflux, so that $y = x$ for passing streams. Begin calculations from the top. $y_D = y_1 = 0.35$. From Eq. (1), $x_1 = 0.35/[6 - 5(0.35)] = 0.0824$. Therefore, $y_2 = x_1 = 0.0824$. From Eq. (1), $x_2 = 0.0824/[6\text{-}5(0.0824)] = 0.0147$. Therefore, $y_3 = x_2 = 0.0147$. From Eq. (1), $x_3 = 0.0147/[6\text{-}5(0.0147)] = 0.0025$. This is close to but not quite equal to the desired value of 0.002. Thus, we need just slightly more than 3 minimum equilibrium stages.

(b) For minimum boilup ratio, the stripping section operating line connects the two points for $\{y, x\}$ of {0.002, 0.002} and {y in equilibrium with $x = 0.05$}. From a rearrangement of Eq. (1), the y in equilibrium with $x = 0.05$ is: $y = \alpha x/[1 + x(\alpha - 1)] = 6(0.05)/[1 + 0.05(6 - 1)] = 0.24$. The slope of the operating line = $(\overline{L} / \overline{V})$ = (0.24 - 0.002)/(0.05 - 0.002) = 4.96. From a rearrangement of Eq. (7-12), $(V_B)_{min}$ = 1/ [$(\overline{L} / \overline{V})$ - 1] = 1/(4.96 - 1) = 0.253.

(c) The boilup ratio = V_B = 1.2(0.253) = 0.3036. From Eq. (7-12), the slope of the stripping section operating line = $\overline{L} / \overline{V} = (V_B + 1)/V_B = (0.3036 + 1)/0.3036 = 4.294$. This line intersects the vertical q-line ($x_F = 0.05$) at 0.002 + 4.294(0.05 - 0.002) = 0.2081. Therefore, the slope of the rectifying line = L/V = (0.35 - 0.2081)/(0.35 - 0.05) = 0.4730. From a rearrangement of Eq. (7-8), $R = (L/V)/[1 - (L/V)] = 0.473/(1 - 0.473) = 0.8975$. The equation for the rectifying section operating line, using Eq. ((7-9), with a modification for a partial condenser as determined from Fig. 7.18, is,

$$y_{n+1} = \left(\frac{R}{R+1}\right)x_n + \left(\frac{1}{R+1}\right)y_D = 0.473x_n + 0.184\,5 \qquad (2)$$

Exercise 7.22 (continued)

Analysis: (c) (continued)

The equation for the stripping section operating line, using Eq. (7-12) is,

$$y_{m+1} = \left(\frac{V_B + 1}{V_B}\right) x_m - \left(\frac{1}{V_B}\right) x_B = 4.294 x_m - 0.00659 \qquad (3)$$

We can now calculate stage by stage down from the top, starting from $y_D = 0.35$, alternating between the equilibrium curve, Eq. (1) and the appropriate operating line, Eq. (2) or (3). We begin using Eq. (2), but switch to Eq. (3), when $x < x_F = 0.05$. The calculations are terminated when $x < x_B = 0.002$. The calculations can be done with a spreadsheet, with the following results, given as mole fractions of A leaving an equilibrium stage. The optimal feed stage is the top plate.

Equilibrium stage	y_A	x_A
Partial condenser	0.350	0.0824
1	0.223	0.0458
2	0.190	0.0376
3	0.155	0.0296
4	0.121	0.0224
5	0.0894	0.0161
6	0.0626	0.0110
7	0.0407	0.00701
8	0.0235	0.00400
Partial reboiler	0.0106	0.00178

The calculations show that besides the partial condenser and partial reboiler, 8 equilibrium stages are needed in the column.

Exercise 7.23

Subject: Distillation of a mixture of methanol and water with a subcooled liquid feed.

Given: Liquid feed of 14,460 kg/h methanol and 10,440 kg/h water at $q = 1.12$. Distillate of 99 mol% methanol and a bottoms of 99 mol% water are desired. Column has a total condenser and a partial reboiler. Operation at 1 atm with a reflux ratio of $L/D = R = 1.0$. Vapor-liquid equilibrium data in Exercise of 7.19.

Assumptions: Constant molar overflow.

Find: Feed stage location and number of equilibrium stages.

Analysis: First, determine feed composition in mol%. Using molecular weights of 32.04 for methanol and 18.02 for water,

Component	kg/h	kmol/h	Mol%
Methanol	14,460	451.3	43.79
Water	10,440	579.4	56.21
Total:	24,900	1,030.7	100.00

Using the vapor-liquid equilibrium data, a *y-x* plot for the McCabe-Thiele method is made and smoothed with a spreadsheet, noting that methanol is the more volatile. Therefore, $x_F = 0.4379$, $x_D = 0.99$, $x_B = 0.01$.

From Eq. (7-26), slope of *q*-line = $q/(q - 1) = 1.12/(1.12 - 1) = 9.333$. Therefore, on the McCabe-Thiele diagram, a line is drawn with a slope of 9.333 that intersects the point {0.438,0.438}.

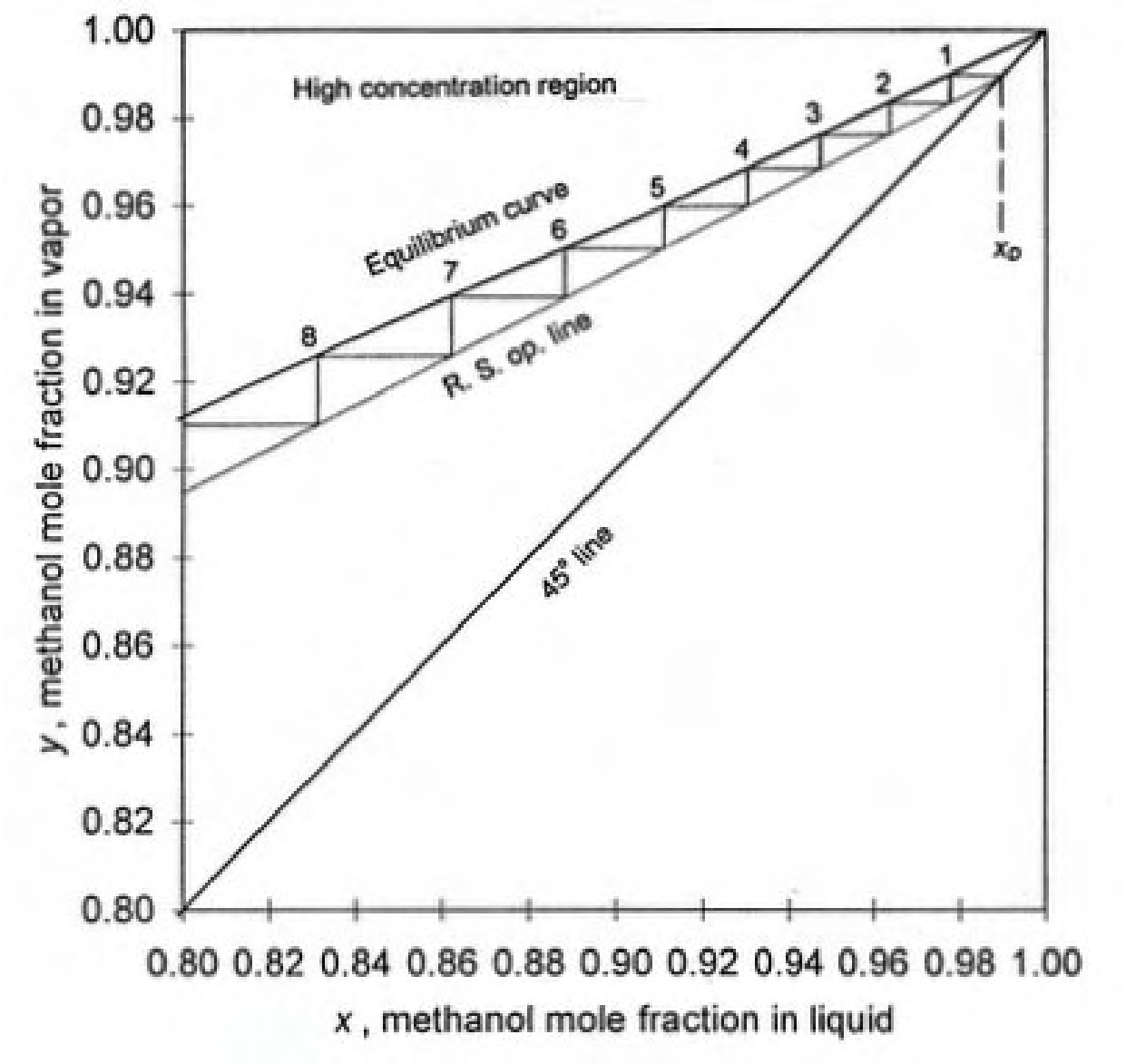
From Eq. (7-7), the slope of the rectifying section operating line = $L/V = R/(R + 1) = 1/(1 + 1) = 0.5$. This line is drawn on the McCabe-Thiele diagram with a slope of 0.5 that intersects the point {0.99,0.99}. The stripping section operating line is drawn to intersect the point {0.01,0.01} and the point where the *q*-line intersects the rectifying section operating line.

In the McCabe-Thiele graphs below, the first for the high mole-fraction region, it is seen that the specified reflux ratio is, fortunately, above the minimum value for the specified distillate mole fraction.

From the plots, it is seen that 20 theoretical stages plus a partial reboiler are needed. The optimal feed stage is number 17 down from the top.

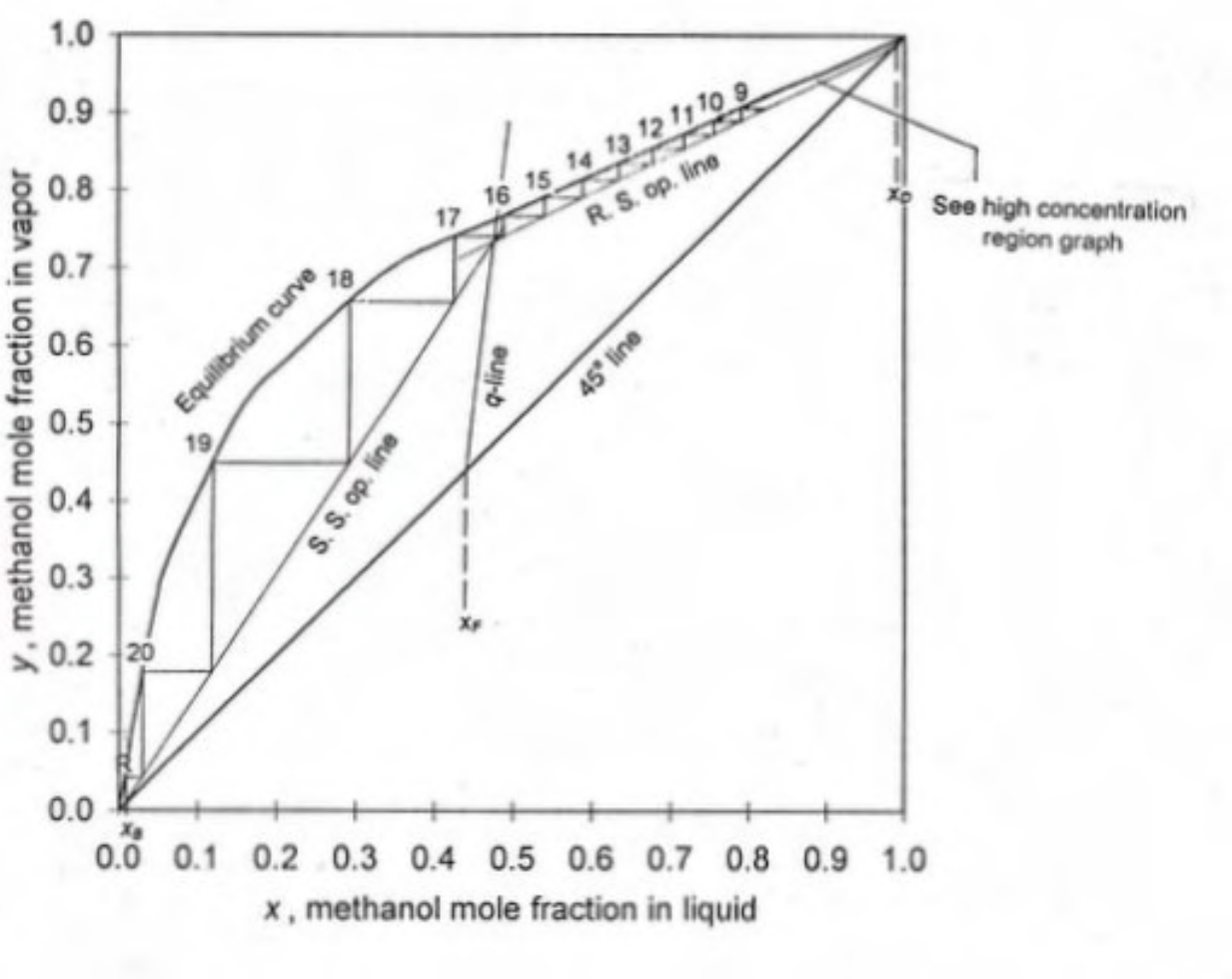
Exercise 7.23 (continued)

Analysis: (continued)



Exercise 7.23 (continued)

Analysis: (continued)



Exercise 7.24

Subject: Partial separation of a benzene-toluene mixture with a partial reboiler and a partial condenser.

Given: Saturated liquid feed of 69.4 mol% benzene (B) in toluene (T) fed to a partial reboiler. Vapor from the reboiler passes to a partial condenser. Vapor from the partial condenser passes to a total condenser. Reflux from the partial condenser is sent to the partial reboiler. Distillate is to contain 90 mol% benzene ($y_D = 0.9$) at a rate of 25 moles per 100 moles of feed. The relative volatility of benzene with respect to toluene = $\alpha = 2.5$.

Find: Moles of vapor generated in the reboiler per 100 moles of feed by analytical and graphical methods.

Analysis: First compute overall material balance. The total condenser need not be considered.
Basis: 100 moles of feed.

Overall total material balance: $F = 100 = D + B = 25 + B$ (1)

Solving Eq. (1), $B = 75$ moles

Overall benzene material balance: $Fx_F = 69.4 = Dy_D + Bx_B = 25(0.9) + 75x_B$ (2)

Solving Eq. (2), $x_B = 0.625$

Analytical Method:

Write material balances around the partial reboiler and partial condenser, using subscripts B for streams leaving the reboiler and D for streams leaving the partial condenser.

Partial reboiler:

Total material balance: $F + L_D = B + V_B$ or $100 + L_D = 75 + V_B$ (3)

Benzene material balance: $Fx_F + L_Dx_D = Bx_B + V_By_B$

or $69.4 + L_Dx_D = 75(0.625) + V_By_B = 46.9 + V_By_B$ (4)

Partial condenser:

Total material balance: $V_B = D + L_D = 75 + L_D$ (5)

Benzene material balance: $V_By_B = Dy_D + L_Dx_D = 75(0.9) + L_Dx_D = 67.5 + L_Dx_D$ (6)

Assume equilibrium in the partial condenser and partial reboiler. Using the given α with its definition in Eq. (7-2). For the partial condenser,

$\alpha = 2.5 = y_D\,(1 - x_D)/x_D(1 - y_D) = 0.9(1 - x_D)/x_D(1 - 0.9) = 9(1 - x_D)/x_D$ (7)

Solving Eq. (7), $x_D = 0.783$

For the partial reboiler,

$\alpha = 2.5 = y_B\,(1 - x_B)/x_B(1 - y_B) = y_B\,(1 - 0.625)/0.625(1 - y_B) = 0.6\,y_B/(1 - y_B)$ (8)

Solving Eq. (8), $y_B = 0.806$

Eqs. (3) through (6), are 4 equations in 2 unknowns, V_B and L_D. We only need 2 of the 4 equations. Using Eqs. (3) and (4),

$100 + L_D = 75 + V_B$ (3)

$69.4 + L_D(0.783) = 46.9 + V_B(0.806)$ (9)

Solving Eqs. (3) and (9),

$L_D = 98$ moles /100 moles of feed and $V_B = 123$ moles/100 moles of feed

Exercise 7.24 (continued)

Analysis: (continued)

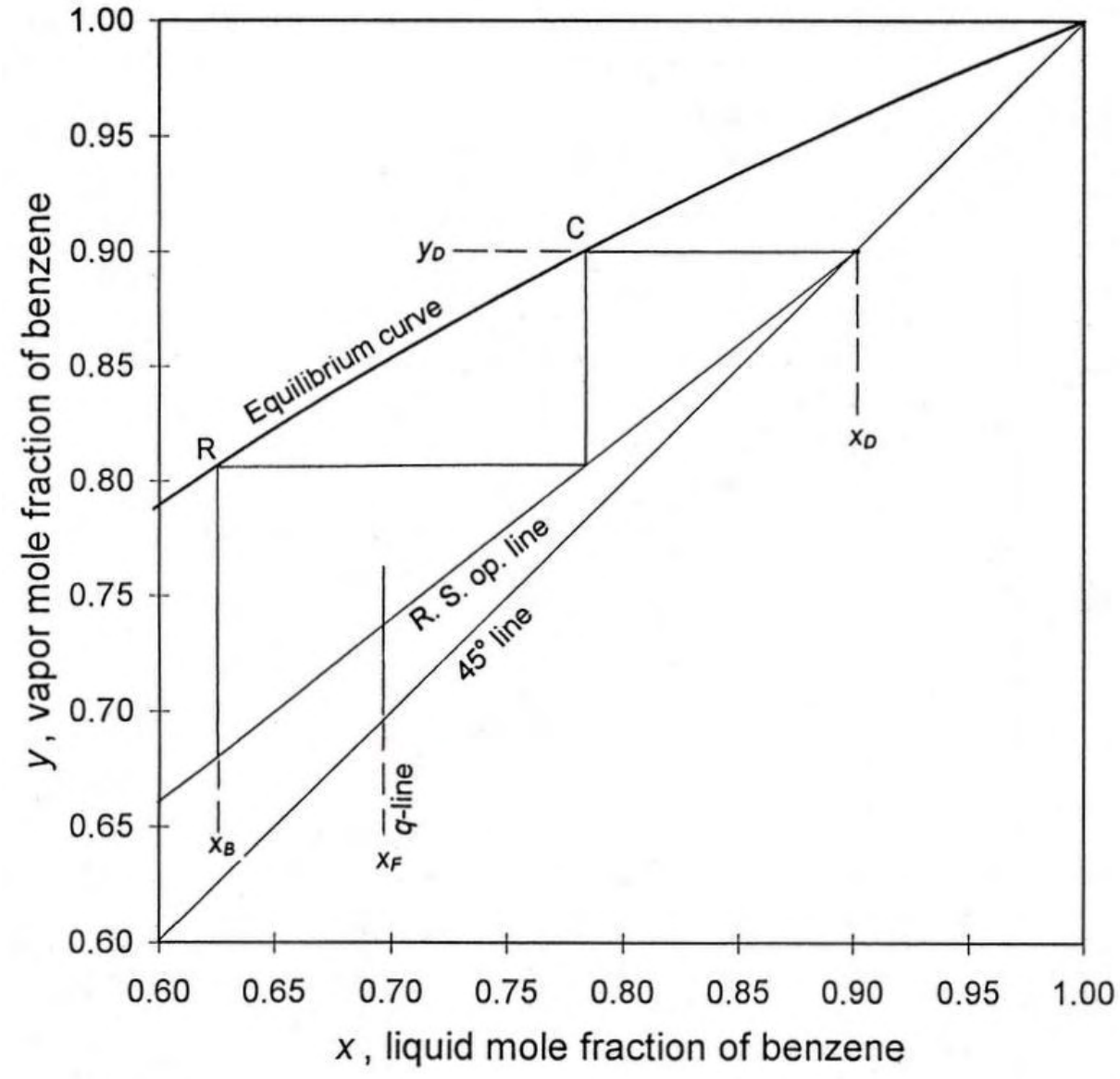
Graphical Method:

On the McCabe-Thiele diagram below, the equilibrium curve is obtained from Eq. (7-3),

$$y = \frac{\alpha x}{1 + x(\alpha - 1)} = \frac{2.5x}{1 + 1.5x}$$

The rectification section operating line is located, as shown, so that two equilibrium steps, one for the partial condenser and one for the partial reboiler, are stepped off between $x_C = 0.9$ (from the total condenser) and $x_B = 0.625$. The measured slope of the operating line = $L_D/V_B = 0.8$. Combining this with Eq. (3),

V_B = 125 moles/100 moles of feed, which is close to the analytical value.



Exercise 7.25

Subject: Rectification of a mixture of benzene and chlorobenzene at total reflux.

Given: Feed of 100 kmol of 20 mol% benzene and 80 mol% chlorobenzene. Column has 4 theoretical plates, a total condenser, a reflux drum, and a still to vaporize the feed. At an operating pressure of 1 atm, relative volatility of benzene with respect to chlorobenzene = α = 4.13. Operate at total reflux with holdups only in the reflux drum and the still. Want liquid in the still with 0.1 mol% benzene.

Assumptions: Perfect mixing to give uniform compositions in the reflux drum and the still.

Find: Moles of liquid in the still at steady state.

Analysis: This exercise can be solved analytically or graphically. Since benzene is the more volatile component, Eq. (7-3) gives the equilibrium relation at the still or any of the 4 plates, n, as,

$$y_n = \frac{\alpha x_n}{1 + x_n(\alpha - 1)} = \frac{4.13 x_n}{1 + 3.13 x_n} \qquad (1)$$

At total reflux, numbering stages up from the bottom,

$$x_{n+1} = y_n \qquad (2)$$

Analytical Method:

Start at the bottom, stage 1, with $x_1 = 0.001$. Solve for y_1 (vapor leaving the still) with Eq. (1). Then, from Eq. (2), $x_2 = y_1$. Continue in this manner, solving alternately Eq. (1) and then Eq. (2), until y_5 (vapor leaving the top plate) is reached. Then, x in the reflux drum = y_5. The results from a spreadsheet are,

Equilbrium stage	***x***	***y***
1 (still)	0.00100	0.00412
2 (bottom plate	0.00412	0.01679
3	0.01679	0.06587
4	0.06587	0.22554
5 (top plate)	0.22554	0.54603
reflux drum	0.54603	

By overall total material balance, $F = 100 = D + B$ (3)

By overall benzene material balance,

$$Fx_F = (100)(0.20) = 20 = Dx_D + Bx_B = D(0.54603) + B(0.001) \qquad (4)$$

Solving Eqs. (3) and (4), D = distillate in reflux drum = 36.51 kmoles

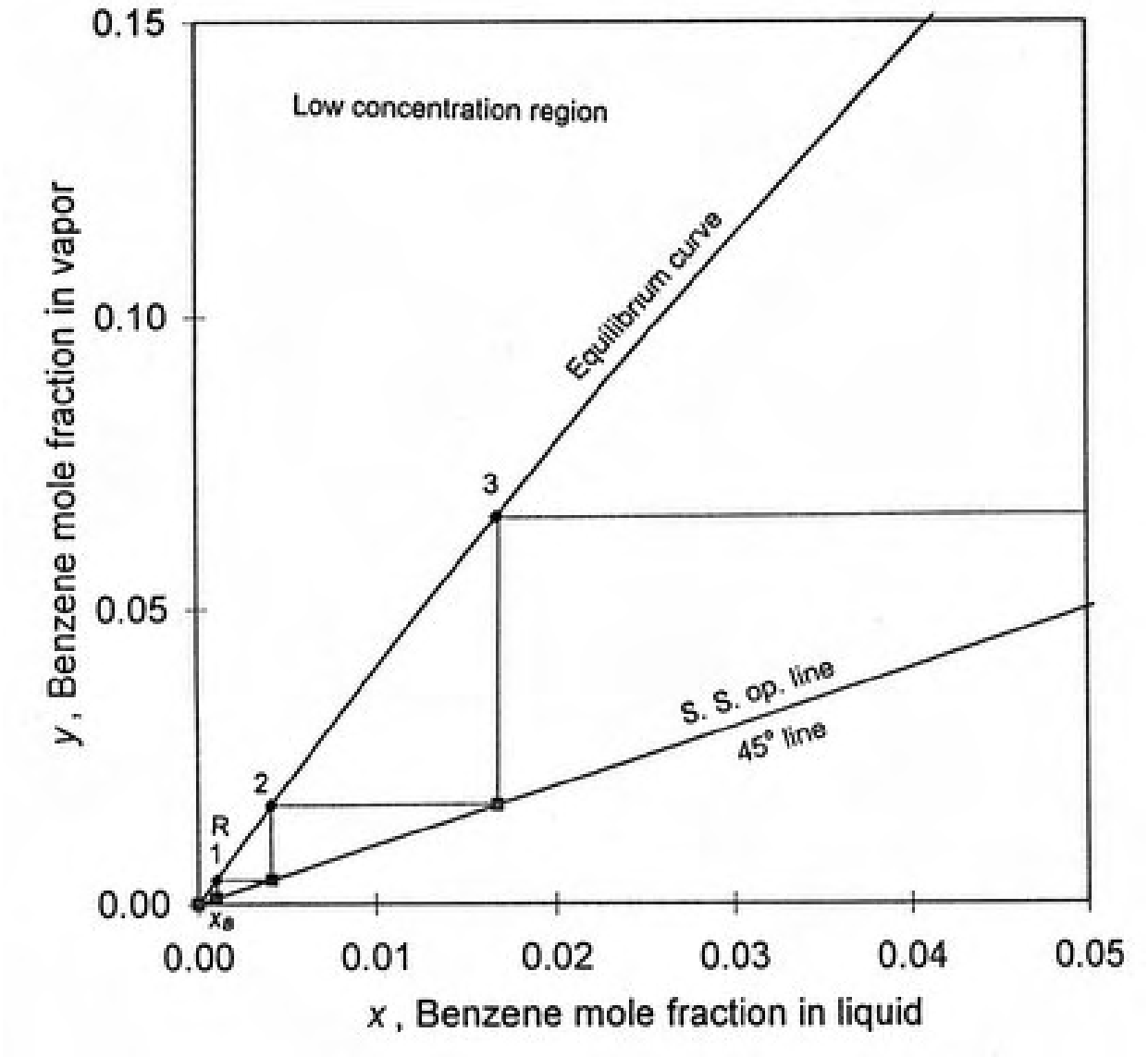
B = bottoms in still = 63.49 kmoles

Exercise 7.25 (continued)

Graphical Method:

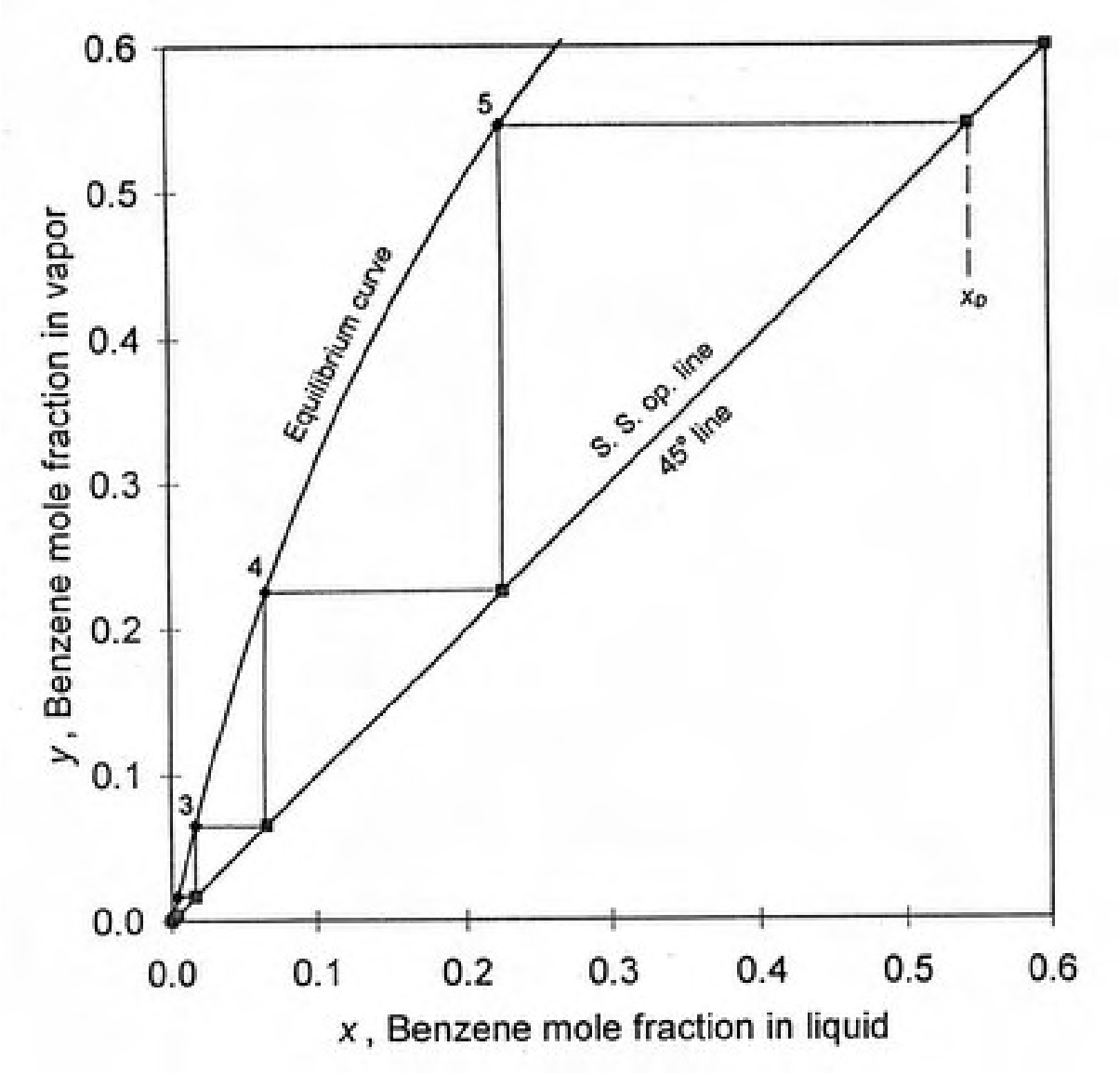
On the McCabe-Thiele plot on the next page, the equilibrium curve is computed from Eq. (1). The rectification section operating line is the 45° line. Five stages are stepped off from the bottoms of $x_B = 0.001$. The resulting y_5 is essentially the same as that for the analytical method.

Thus, again, B = bottoms in still = 63.49 kmoles.



Exercise 7.25 (continued)

Analysis: Graphical method (continued)



Exercise 7.26

Subject: Distillation of acetone and isopropanol, taking into account tray efficiency.

Given: Saturated liquid feed of 50 mol% acetone and 50 mol% isopropanol. Column is equipped with a total condenser, and a partial reboiler. Reflux ratio, *L/D,* is 0.5. Murphree vapor efficiency = 50%. Vapor-liquid equilibrium data at 1 atm are given, with acetone being the more volatile component.

Assumptions: Constant molar overflow.

Find: Number of actual trays required to achieve a distillate of 80 mol% acetone and a bottoms of 25 mol% acetone, inserting the feed at the optimal location.

Analysis: In the McCabe-Thiele diagram below, the equilibrium curve is plotted from the given data. The *q*-line is vertical, passing through $x = 0.5$. The rectification operating line has a slope, *L/V*, from Eq. (7-9), of $R/(R + 1) = 0.5/1.5 = 0.333$. This operating line passes through the point, $y = 0.8$, $x = 0.8$. From Eq. 7-9), the equation for the rectifying section operating line is,

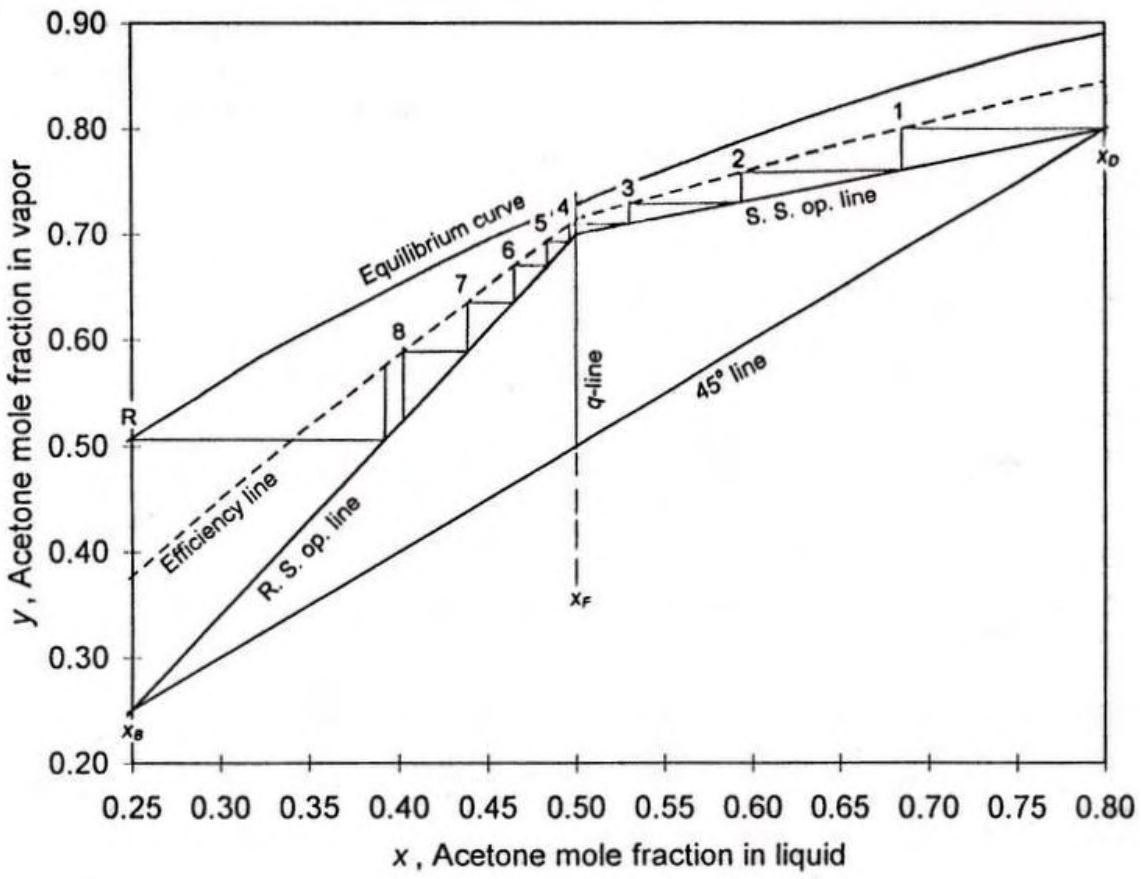
$$y = \left(\frac{R}{R+1}\right)x + \left(\frac{1}{R+1}\right)x_D = 0.333x + 0.667(0.8) = 0.333x + 0.533$$

From this equation, the intersection of the rectifying section operating line and the vertical *q*-line is at $y = 0.333(0.5) + 0.533 = 0.70$. The stripping section operating line passes through the $\{y, x\}$ points $\{0.70, 0.50\}$ and $\{0.25, 0.25\}$, giving it the equation, $y = 1.80x\text{-}0.20$.

Except for the reboiler stage, the stages are stepped off from an efficiency line, which for a Murphree vapor efficiency of 0.5 is positioned vertically half way between the equilibrium curve and the operating line, as governed by Eq. (7-41), $E_{MV} = 0.5 = (y_n - y_{n+1})/(y_n^* - y_{n+1})$, where y_{n+1} is the location on the operating line, y_n is the location on the efficiency line, and y_n^* is the location on the equilibrium line. However, the reboiler is assumed to have a 100% efficiency. As seen in the plot, just over 8 trays are required plus the partial reboiler. The feed plate is 4 from the top.

Exercise 7.26 (continued)

Analysis (continued)



Exercise 7.27

Subject: Distillation of carbon disulfide and carbon tetrachloride.

Given: Partially vaporized feed ($q = 0.5$) of 40 mol% CS_2. Operation with a reflux ratio, L/D, of 4 and a Murphree vapor efficiency of 80%. Partial reboiler and total condenser. Vapor-liquid equilibrium data.

Assumptions: Constant molar overflow.

Find: For a distillate of 95 mol% CS_2 and a bottoms of 5 mol% CS_2, determine:
(a) Minimum reflux ratio, minimum boilup ratio, and minimum number of stages.
(b) Number of trays.

Analysis: (a) In the McCabe-Thiele plot on the next page, rectifying section and stripping section operating lines are shown for determining minimum reflux and boilup ratios. Note that the q-line has a slope given in Eq. (7-26) as $q/(q - 1) = 0.5/(0.5 - 1) = -1$ and intersects the point {0.4, 0.4}. The rectifying section operating line intersects the point {0.95, 0.95} and the point where the equilibrium curve and the q-line intersect. The slope of that line is measured to be $L/V = 0.642$. From Eq. (7-9), $L/V = R/(R + 1)$. Rearranging,

$$R_{min} = (L/V)/[1 - (L/V)] = 0.642/(1 - 0.642) = 1.79$$

The stripping section operating line intersects the point {0.05, 0.05} and the point where the equilibrium curve and the q-line intersect. The slope of that line is measured to be $\bar{L}/\bar{V} = 2.043$. From Eq. (7-14), $\bar{L}/\bar{V} = (V_B + 1)/V_B$. Rearranging,

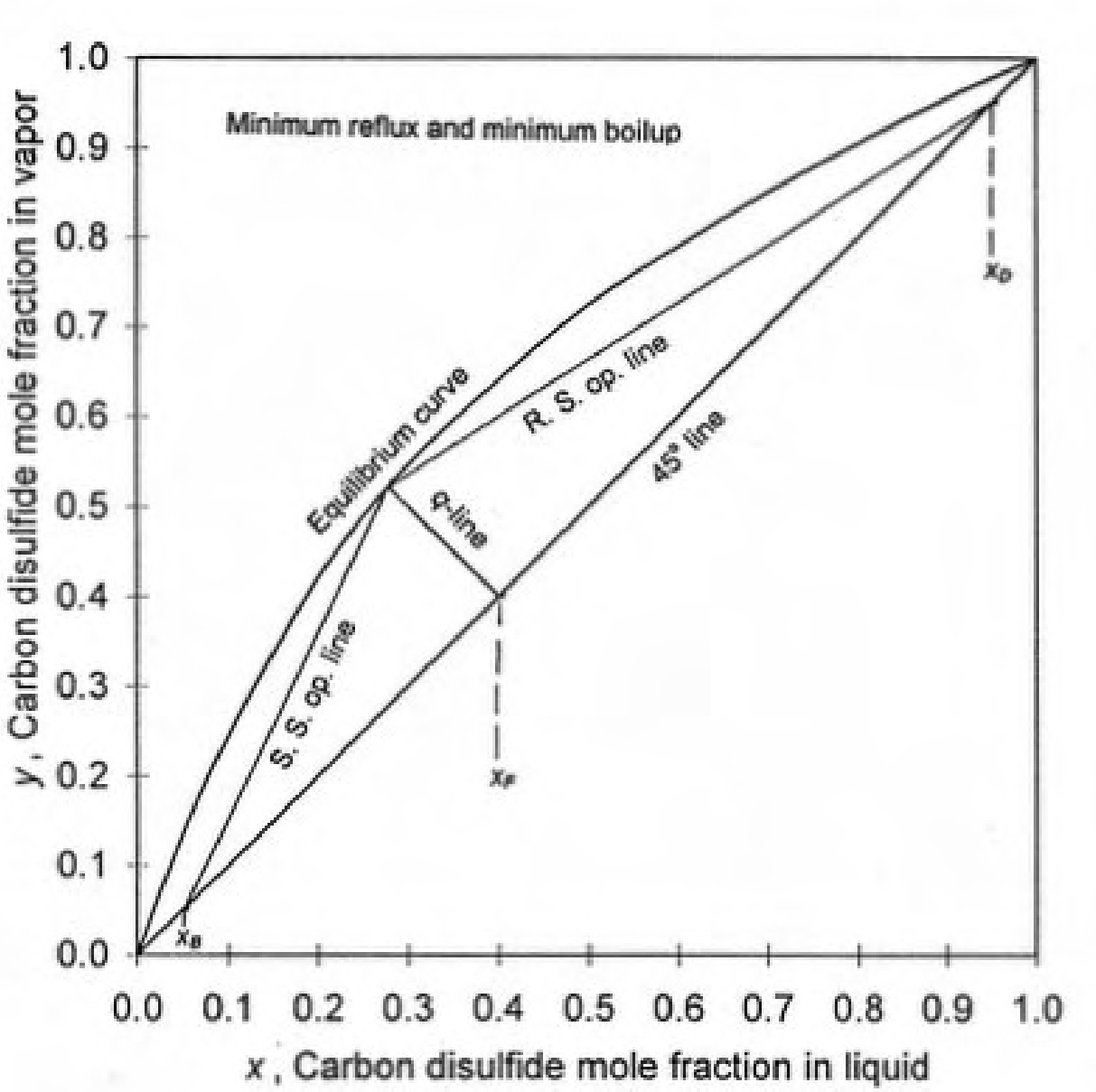
$$(V_B)_{min} = \left(\frac{\bar{V}}{B}\right)_{min} = \frac{1}{(\bar{L}/\bar{V}) - 1} = \frac{1}{2.043 - 1} = 0.959$$

The McCabe-Thiele plot for minimum stages at total reflux is also shown on the next page. The operating lines are coincident with the 45° line. It is seen that 6 equilibrium stages are needed.

(b) For a reflux ratio, $R = L/D$, of 4, the slope of the rectifying section operating line from Eq. (7-9) is $L/V = R/(R + 1) = 4/5 = 0.8$. This line and the stripping section operating line are shown on the third McCabe-Thiele diagram below. Except for the reboiler stage, the stages are stepped off from an efficiency line, which for a Murphree vapor efficiency of 0.8 is positioned 80% of the vertical distance from the operating line to the equilibrium curve, as governed by Eq. (7-41), $E_{MV} = 0.8 = (y_n - y_{n+1})/(y_n^* - y_{n+1})$, where y_{n+1} is the location on the operating line, y_n is the location on the efficiency line, and y_n^* is the location on the equilibrium line. However, the reboiler is assumed to have a 100% efficiency. As seen in the plot, just over 9 trays are required plus the partial reboiler. Call it 10 trays plus the reboiler. The feed plate is 7 from the top.

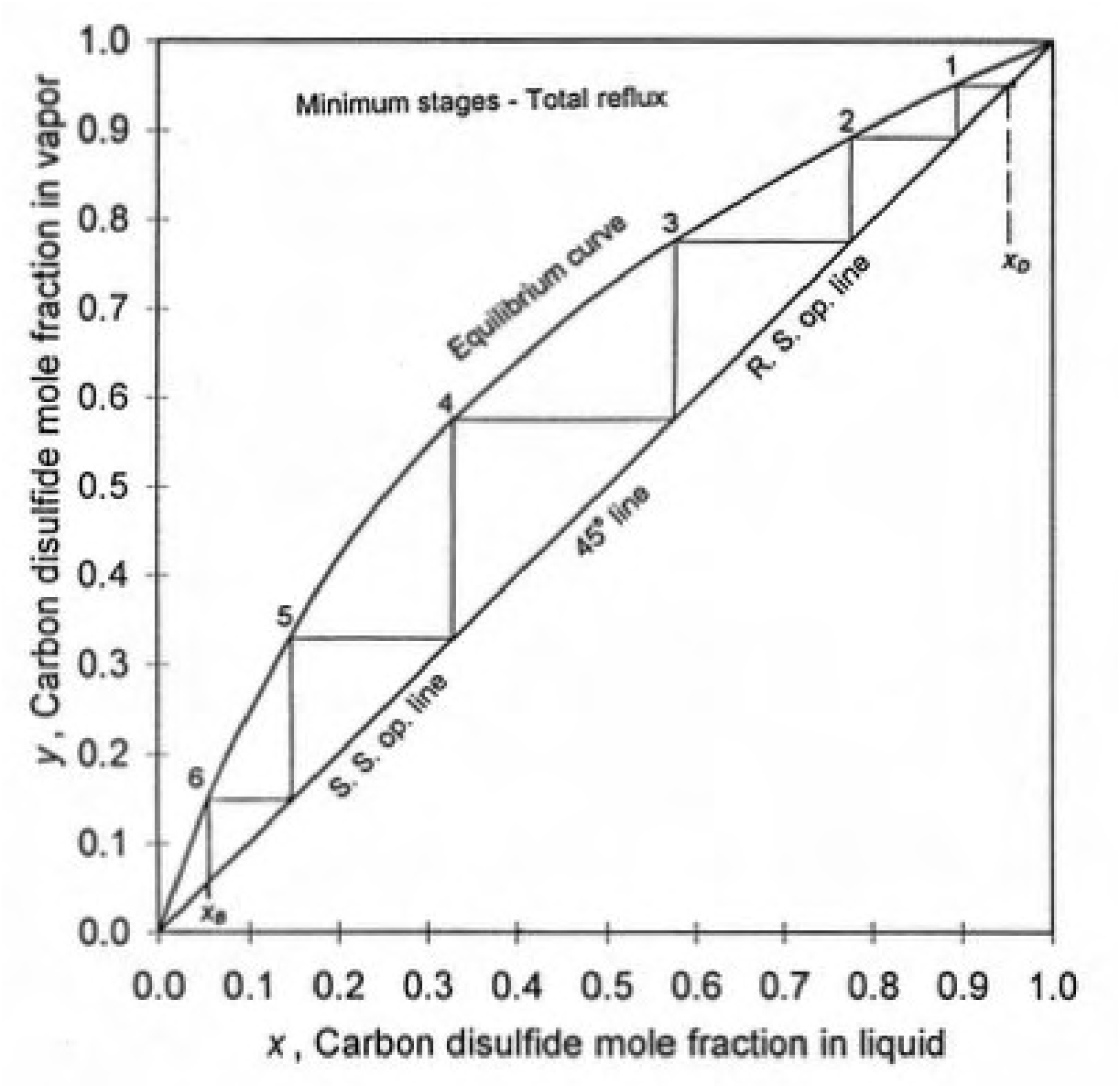
Exercise 7.27 (continued)

Analysis: (a) (continued)



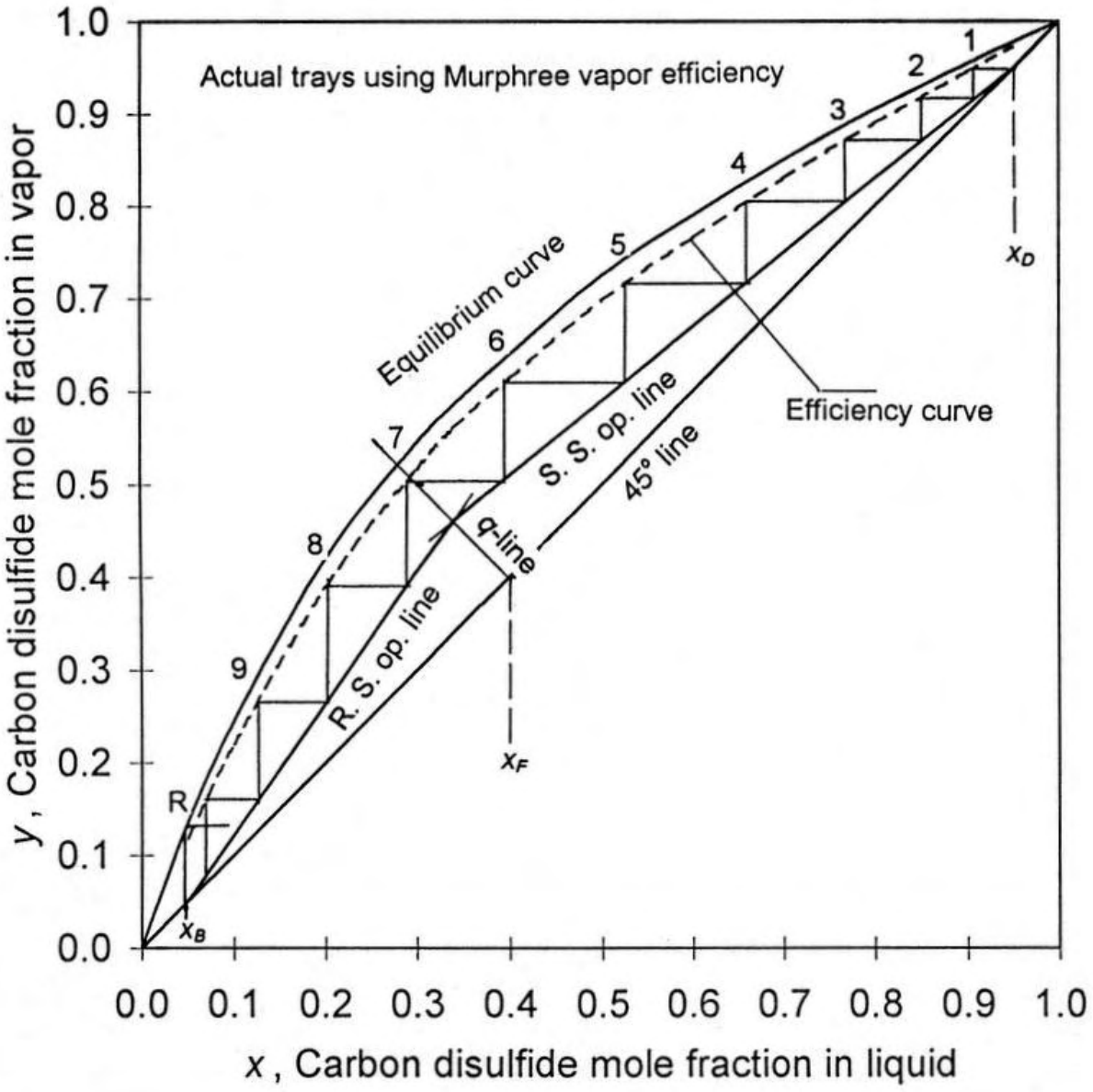
Exercise 7.27 (continued)

Analysis: (a) (continued)



Exercise 7.27 (continued)

Analysis: (b) (continued)



Exercise 7.28

Subject: Preliminary design calculations for the distillation of a benzene-toluene mixture.

Given: Bubble-point feed of 50 mol% benzene and 50 mol% toluene. Equipment to include a partial reboiler, total condenser, and a bubble-cap tray column with an overall plate efficiency of 65%. Column to operate at 1 atm to produce a distillate of 95 mol% benzene and a bottoms of 95 mol% toluene. Vapor-liquid equilibrium data from Exercise 7.13. Enthalpy data for reboiler.

Assumptions: Constant molar overflow and saturated liquid reflux.

Find: (a) Minimum reflux ratio (infinite stages).
(b) Minimum number of actual plates (total reflux).
(c) Number of actual plates for $R = 1.5\ R_{min}$.
(d) Kilograms per hour of products for a feed of 907.3 kg/h.
(e) Kg/h of saturated steam at 273.7 kPa for reboiler heat duty using given enthalpy data.
(f) Rigorous enthalpy balance around the reboiler.

Analysis: McCabe-Thiele plots are made in terms of benzene mole fractions, since benzene is the more volatile component. The equilibrium curve is plotted from the data in Exercise 7.13.

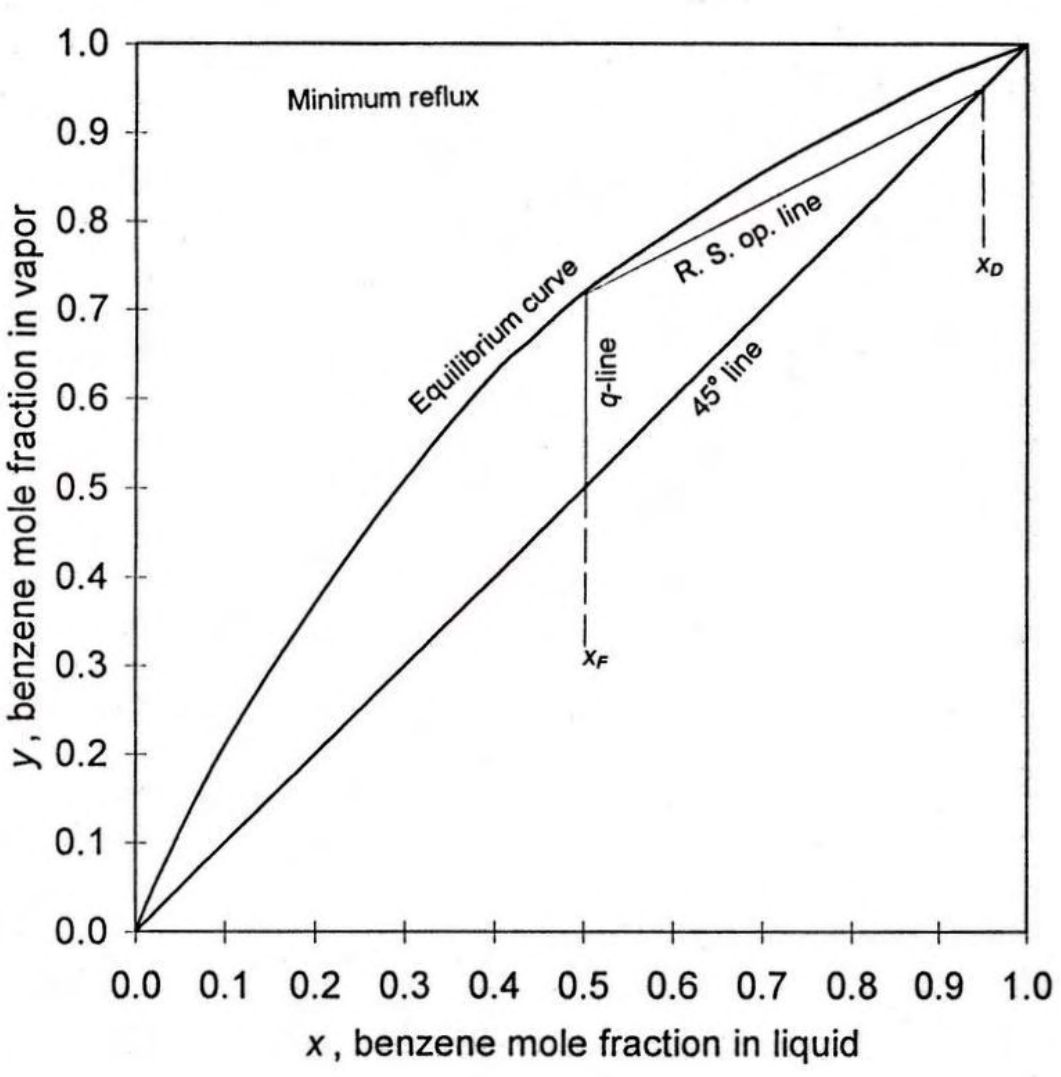
(a) For a saturated liquid feed, minimum reflux corresponds to a pinch point located at the intersection of a vertical q-line passing through $x_F = 0.5$ and the equilibrium curve as shown in the McCabe-Thiele diagram below. From the equilibrium data, this intersection is at $y = 0.72$ and $x = 0.5$. Then, the slope of the rectifying section operating line, $(L/V)_{min}$ is (0.95 - 0.72)/(0.95 - 0.50) = 0.511. From a rearrangement of Eq. (7-7), $R_{min} = (L/V)_{min} / [1 - (L/V)_{min}] = 0.511/(1 - 0.511) = 1.045$.

(b) The McCabe-Thiele plot for minimum stages at total reflux is shown below. The operating lines are coincident with the 45° line. Equilibrium stages are stepped off starting from $x_B = 0.05$ to $x_D = 0.95$. It is seen that just less than 7 equilibrium stages are needed. Call it $N_t = 7$. From Eq. (6-21), for an overall plate efficiency of 65%, i.e. $E_o = 0.65$, the actual minimum number of plates = $N_a = N_t / E_o = 7/0.65 = 10.8$.

(c) Operating reflux ratio = $R = 1.5\ R_{min} = 1.5(1.045) = 1.57$. From Eq. (7-7), the slope of the operating line for the rectifying section = $L/V = R/(1 + R) = 1.57(1 + 1.57) = 0.611$. On the McCabe-Thiele diagram on the next page, the rectifying section operating line has this slope and passes through the point, y=0.95, x=0.95. the stripping section operating line passes through the point, y=0.05, x=0.05 and intersects the vertical q-line at the point where the rectifying section operating line intersects the q-line. As seen, the equilibrium stages are stepped off starting at the top, with a switch from the rectifying section to the stripping section to minimize the number of stages and, thus, locating the optimal feed stage. The result is just over 10 equilibrium stages plus a partial reboiler. Call it 11 equilibrium stages plus a partial reboiler. Applying Eq. (6-21), $N_a = 11/0.65 = 16.9$ or 17 actual plates plus the partial reboiler.

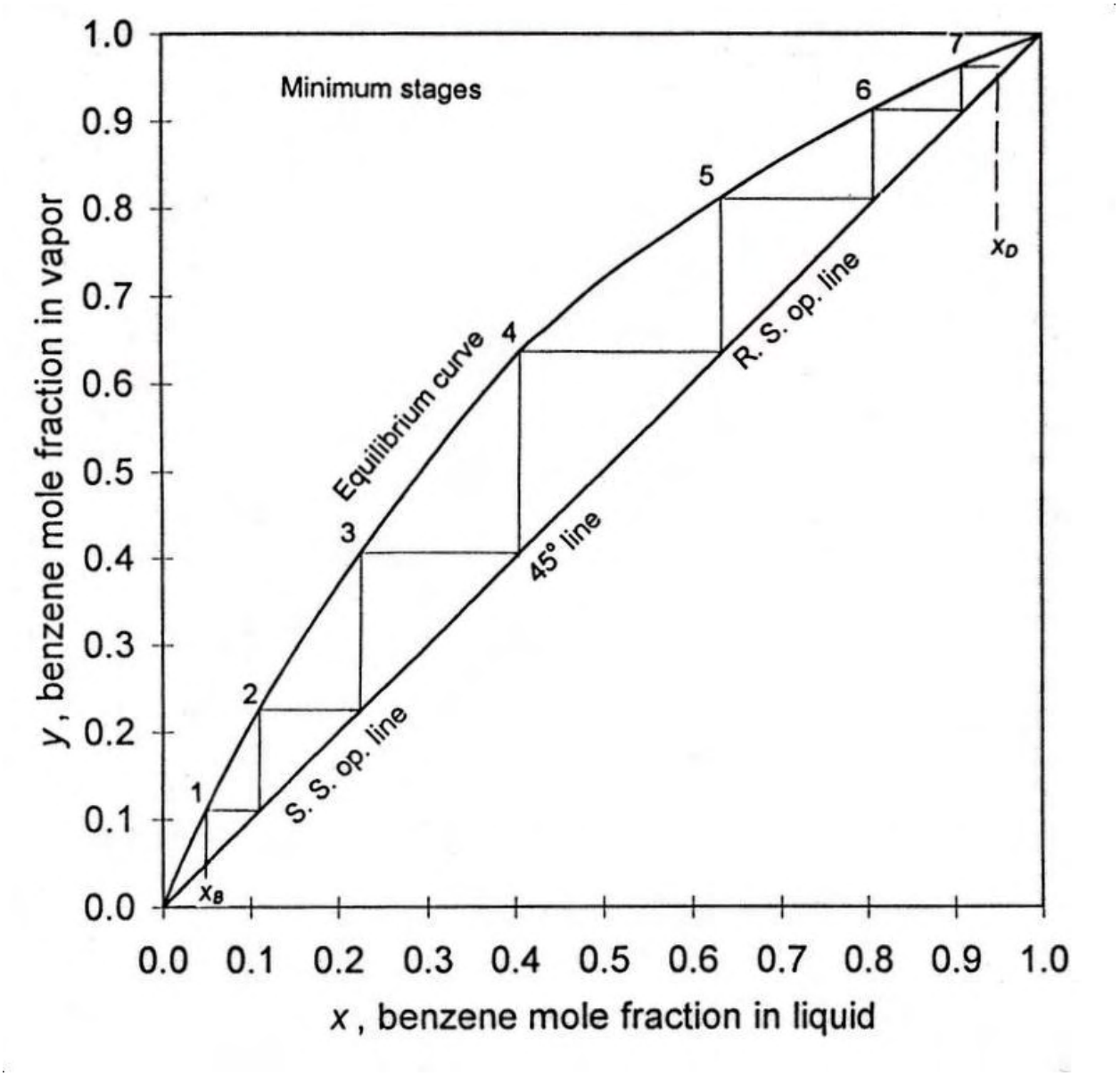
Exercise 7.28 (continued)

Analysis: (continued)



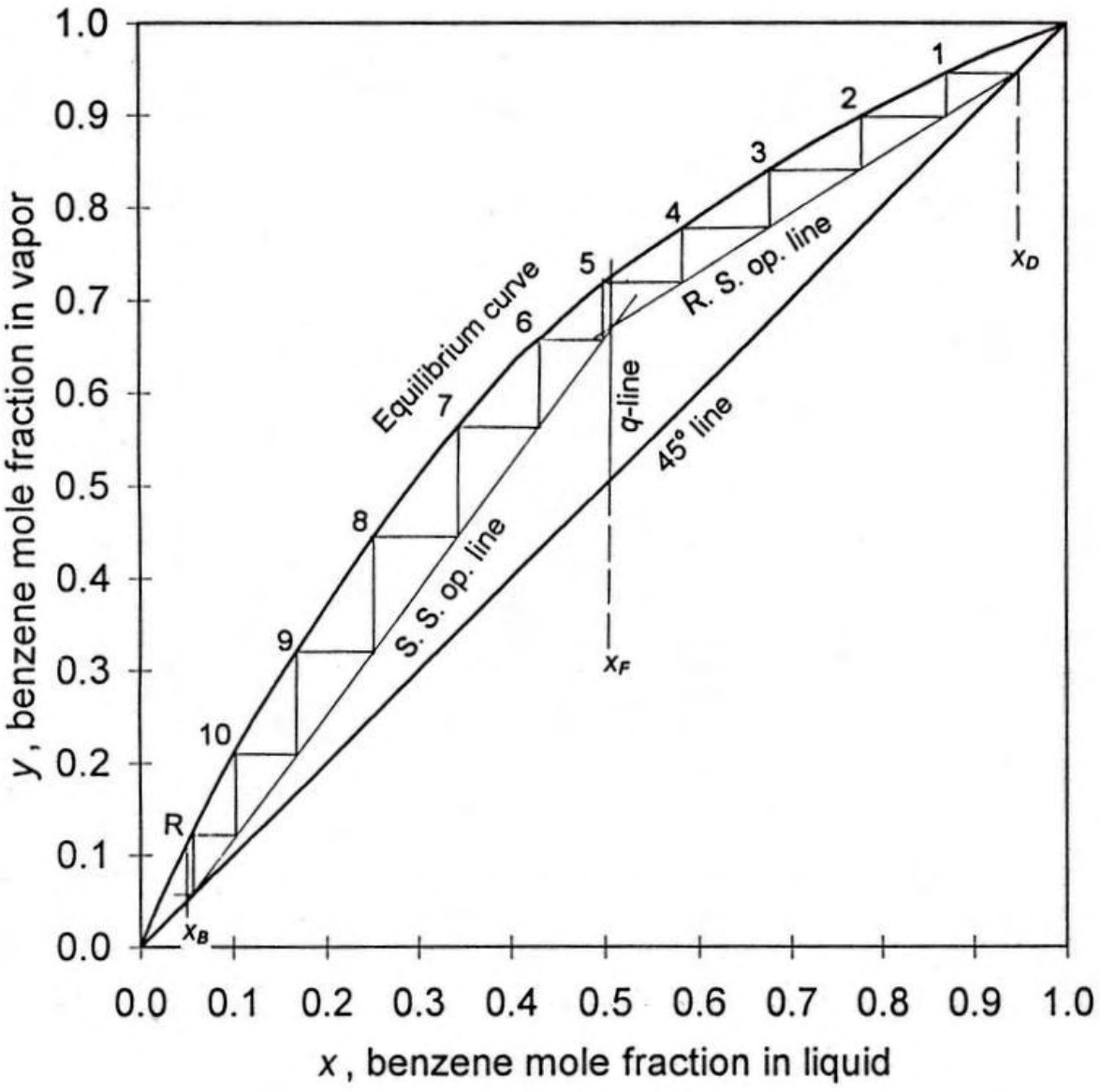
Exercise 7.28 (continued)

Analysis: (continued)



Exercise 7.28 (continued)

Analysis: (continued)



Exercise 7.28 (continued)

Analysis: (continued)

(d) MW of benzene = 78.11. MW of toluene = 92.14.

Let F = kmol/h of feed. Then by mass material balance with an equimolar feed,

$$0.5F\,(78.11) + 0.5F(92.14) = 907.3$$

Solving, F = 10.66 kmol/h. For the equimolar feed, the component flow rates in the feed are:

5.33 kmol/h each for benzene and toluene

Next calculate the distillate and bottoms flow rates from,

overall total mole balance: $F = n_F = 10.66 = D + B$ (1)

overall benzene mole balance: $Fx_F = 5.33 = 0.95D + 0.05B$ (2)

Solving Eqs. (1) and (2), D = 5.33 kmol/h and B = 5.33 kmol/h

Therefore in terms of mass flow rates, total total distillate rate is,

$m_D = 0.95(5.33)(78.11) + 0.05(5.33)(92.14)$ = 420.1 kg/h

Therefore the bottoms rate = m_B = 907.3 - 420.1 = 487.2 kg/h

(e) First compute the kmol/h of vapor leaving the reboiler, using the assumption of constant molar overflow. From part (c), the reflux ratio = 1.57. Therefore, the reflux rate = 1.57(5.33) = 8.37 kmol/h. Below the feed stage, the liquid rate = 8.37 + 10.66 = 19.03 kmol/h. The vapor rate leaving the reboiler = 19.03 - 5.33 = 13.70 kmol/h. From the plot above, the composition of the reboiler vapor = 12 mol% benzene. Neglecting the sensible heat and using the enthalpy data given, after converting from Btu/lbmol to kJ/kmol, the reboiler heat duty is,

$Q_R = 2.324[0.12(13.7)(18{,}130 - 4{,}900) + 0.88(13.7)(21{,}830 - 8{,}080)] = 436{,}000$ kJ/kmol.

From Perry's Handbook, latent heat of vaporization of steam at 273.7 kPa (404 K) = 2,172 kJ/kg

Therefore, we need 436,000/2,172 = 200.7 kmol/h or 3,616 kg/h.

(f) A rigorous enthalpy balance around the reboiler takes into account the sensible heat effect since the temperature of the liquid entering the reboiler is not the same as the temperatures of the equilibrium liquid and vapor leaving the reboiler. Let N = conditions leaving the reboiler and N-1 be the conditions leaving the stage above the reboiler. Then,

$$Q_R = V_N H_{V_N} + L_N H_{L_N} - L_{N-1} H_{L_{N-1}}$$

Note that in the simplified enthalpy balance of part (e), the following equation was applied,

$$Q_R = V_N \left(H_{V_N} - H_{L_N} \right)$$

Since, $V_N = L_N - L_{N-1}$, this is equivalent to assuming $H_{L_N} = H_{L_{N-1}}$

Exercise 7.29

Subject: Preliminary design for the distillation of a mixture of ethanol and water at 1 atm.

Given: Bubble-point feed containing 20 mol% ethanol in water. Unit consisting of a perforated-tray column, partial reboiler, and total condenser. Distillate to contain 85 mol% alcohol and a 97% recovery of alcohol. Vapor-liquid equilibrium data.

Assumptions: Constant molar overflow.

Find: (a) Molar concentrations in the bottoms product.
(b) Minimum values of L/V, L/D, and V_B/B.
(c) Minimum number of equilibrium stages and actual plates for $E_o = 0.55$.
(d) Number of actual plates for $L/V = 0.80$.

Analysis: From the vapor-liquid equilibrium data for 1 atm., it is seen that ethanol is more volatile than water for ethanol mole fractions in the liquid from 0 to 0.8943, which is the azeotrope concentration. The distillate composition is within this region.

(a) Take a basis of $F = 100$ kmol/h.

Overall total material balance: $F = 100 = D + B$ (1)

Ethanol recovery: $0.97Fx_F = 0.97(100)(0.20) = 19.4 = Dx_D = 0.85D$ (2)

Solving Eq. (2), $D = 22.82$ kmol/h. From Eq. (1), $B = 100 - 22.82 = 77.18$ kmol/h

Ethanol in bottoms = 20 - 19.4 = 0.6 kmol/h

Therefore, ethanol mole fraction in bottoms = 0.6/77.18 = 0.00777

Water mole fraction in bottoms = 1.0 - 0.00777 = 0.99223

(b) In the McCabe-Thiele diagram on the next page, the given equilibrium data are plotted. For a bubble-point liquid feed, the q-line is vertical at $x_F = 0.2$. The minimum reflux in terms of L/V is obtained from the slope of the rectifying section operating line, which passes through the point, $y = x_D = 0.85$ and is tangent to the equilibrium curve, rather than being drawn through the intersection of the q-line and the equilibrium curve because that would cause the operating line to mistakenly cross over the equilibrium curve.

The slope of the operating line = $(L/V)_{min} = 0.65$.

From Eq. (7-27), $R_{min} = (L/D)_{min} = 0.65/(1-0.65) = 1.86$.

The liquid rate in the rectifying section = $L = 1.86D = 1.86(22.82) = 42.44$ kmol/h.

Below the feed plate, $\overline{L} = L + F = 42.44 + 100 = 142.44$ kmol/h.

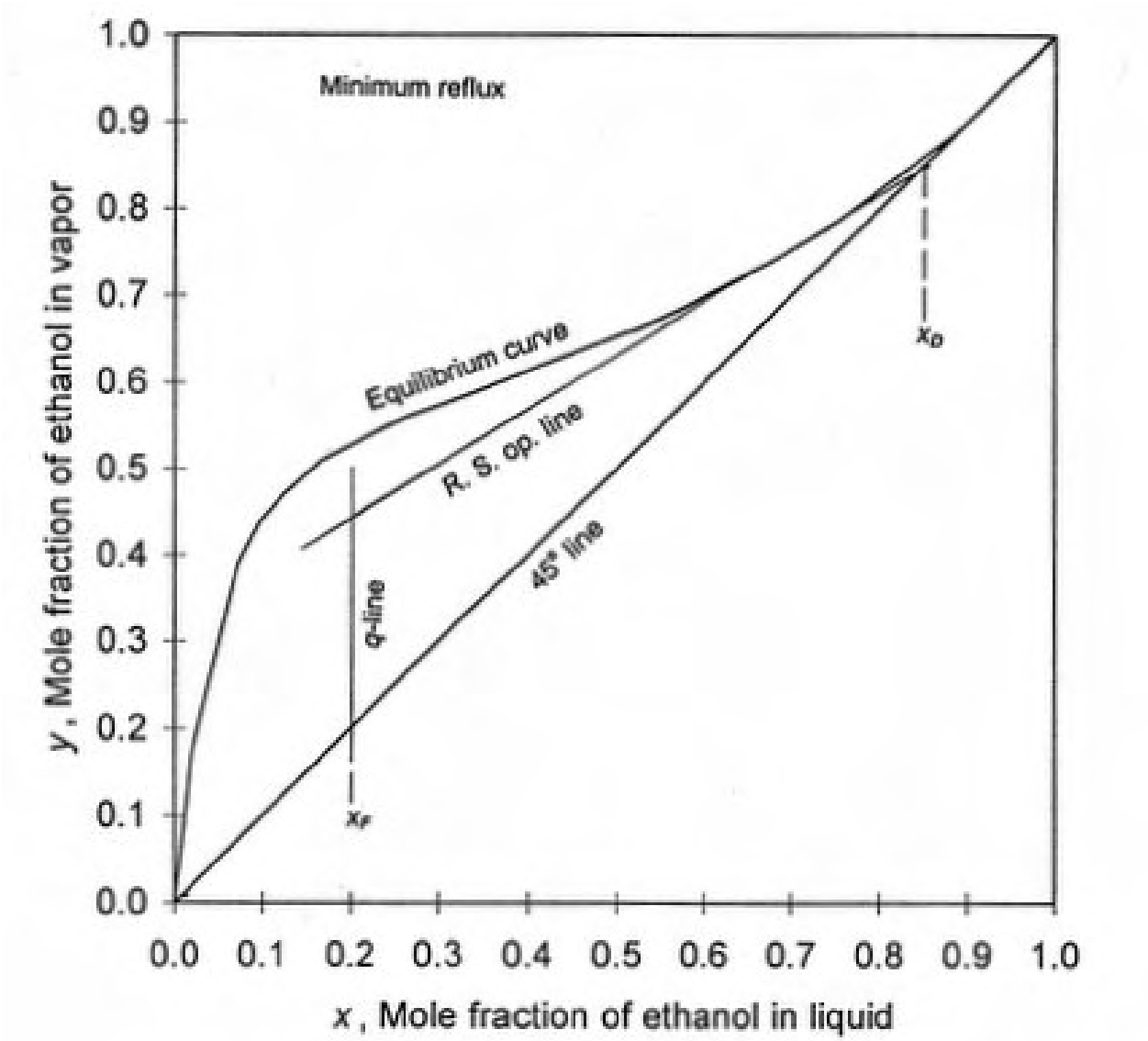
Vapor rate from the reboiler = $V_B = \overline{L} - B = 142.44 - 77.18 = 65.26$ kmol/h.

Therefore, boilup ratio = $V_B/B = 65.26/77.18 = 0.846$.

(c) In the second McCabe-Thiele diagram on the next page, the minimum number of stages is determined by stepping off stages between the equilibrium curve and the 45° line (total reflux) from the points 0.85 and 0.00777 on the 45° line. The result is approximately 10 minimum equilibrium stages. For a stage efficiency of 0.55, using Eq. (6-21), $N_a = N_t/E_o =$ 10/0.55 = 18.2 minimum plates.

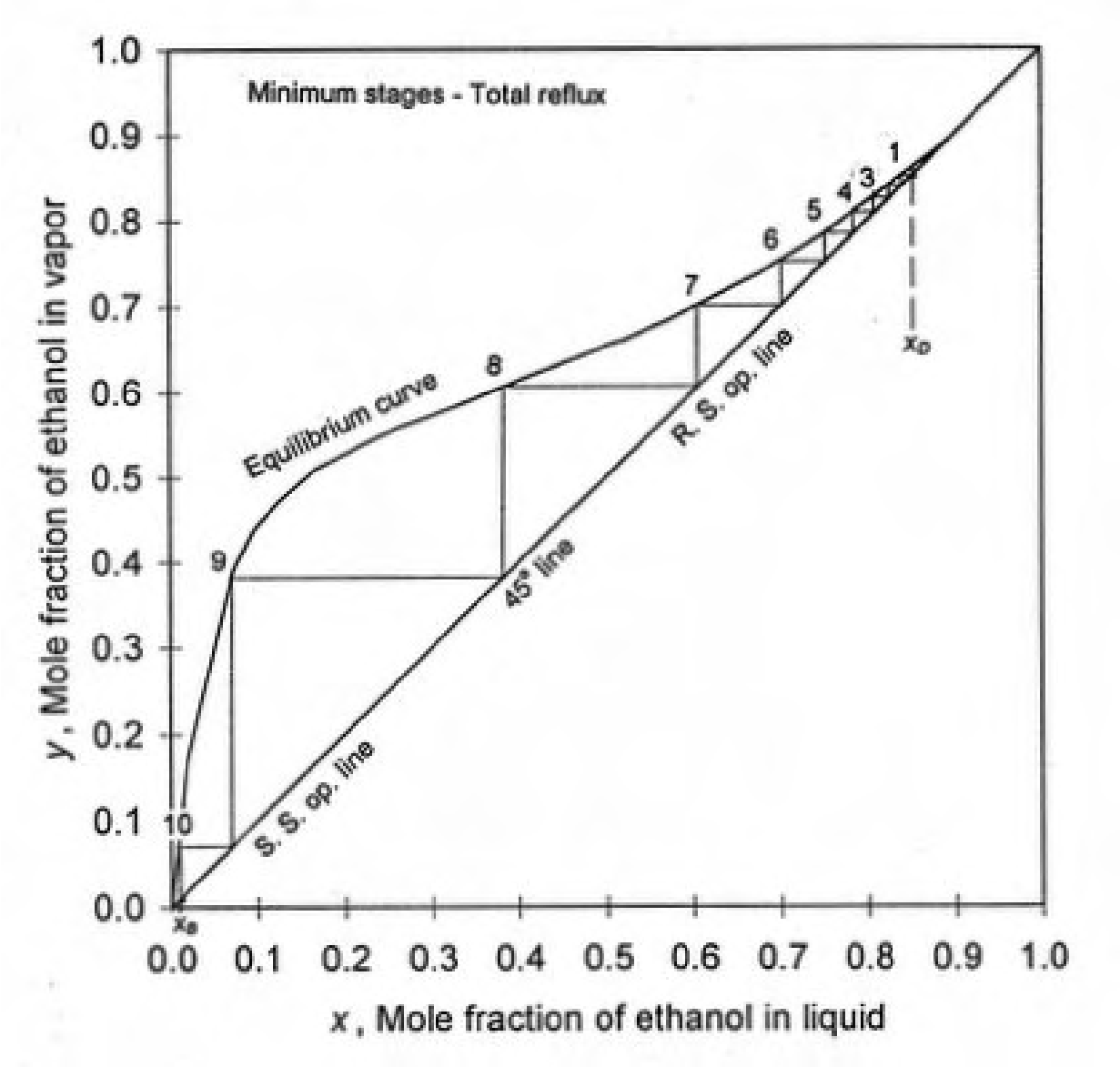
Exercise 7.29 (continued)

Analysis: (b and c) (continued)



Exercise 7.29 (continued)

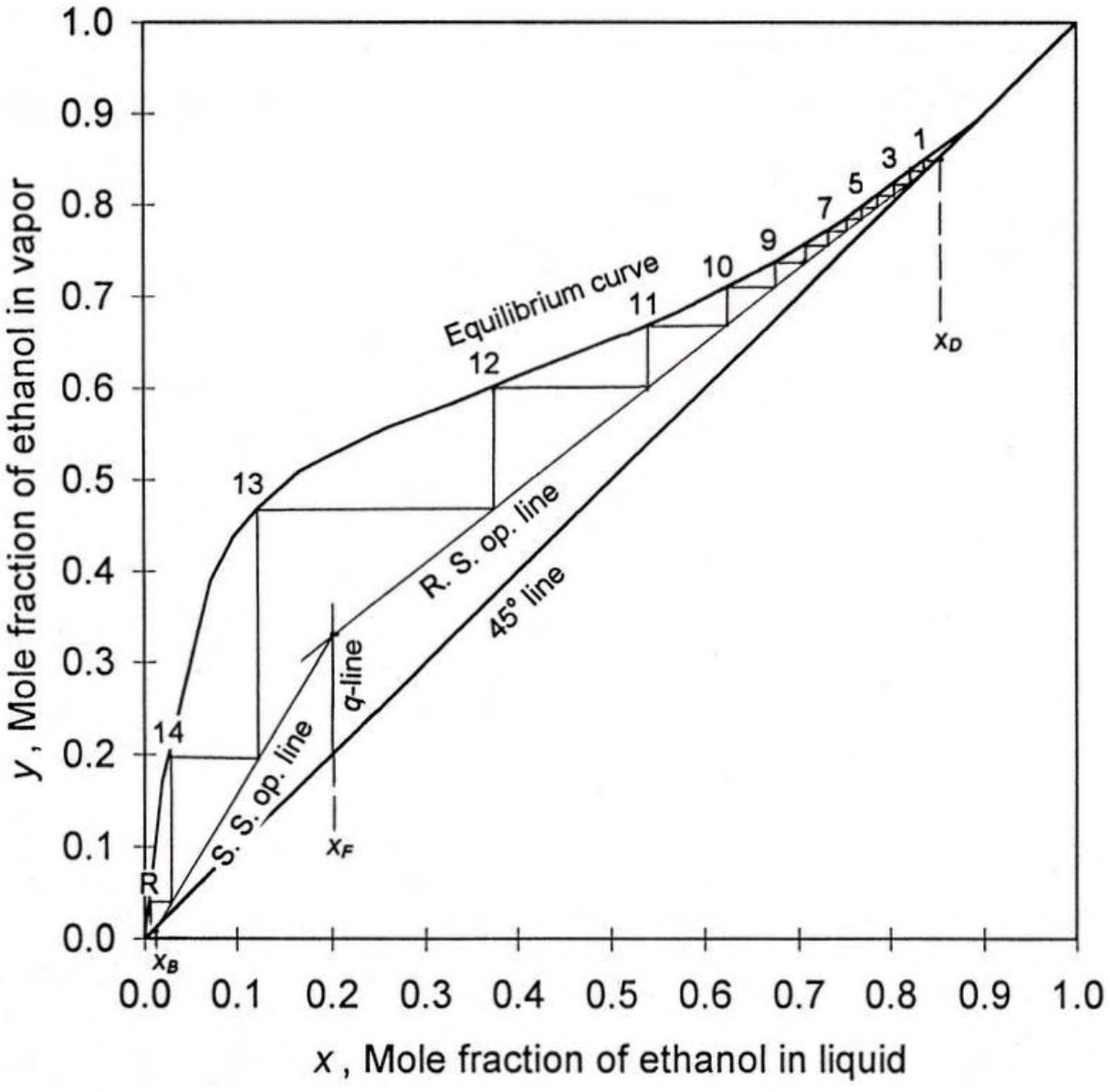
Analysis: (b and c) (continued)



Exercise 7.29 (continued)

Analysis: (continued)

(d) For an operating reflux ratio = L/V = 0.8, the reflux ratio, R = L/D = 0.8/(1-0.8) = 4. On the McCabe-Thiele diagram below, the rectifying section operating line has a slope of 0.8 and passes through the point, y=0.85, x=0.85. the stripping section operating line passes through the point, y=0.00777, x=0.0777 and intersects the vertical q-line at the point where the rectifying section operating line intersects the q-line. As seen, the equilibrium stages are stepped off starting at the top, with a switch from the rectifying section to the stripping section to minimize the number of stages and, thus, locating the optimal feed stage. The result is just less than 15 equilibrium stages. Call it 14 equilibrium stages plus a partial reboiler. Applying Eq. (6-21), N_a = 14/0.55 = 25.5 or 26 actual plates plus the partial reboiler as an equilibrium stage.



Exercise 7.30

Subject: Recovery by distillation with open steam of solvent A from water in two feeds.

Given: Two saturated liquid feeds, each containing 50 kmol/h of A. Feed 1 contains 40 mol% A and Feed 2 contains 60 mol% A. Unit consists of a column and a total condenser. Open steam is used in lieu of a partial reboiler. Relative volatility = 3.0 for A with respect to water. Distillate is to contain 95 mol% A with a 95% recovery.

Assumptions: Constant molar overflow. Open steam enters bottom stage as saturated vapor. Both feeds enter at optimal locations.

Find: For an overall plate efficiency of 70% and an $R = L/D$ = 1.33 times minimum, determine the number of actual plates. Compute the bottoms composition. Determine analytically the location of all three operatiing lines.

Analysis: The total flow rate of Feed 1 = 50/0.4 = 125 kmol/h. The total feed rate of Feed 2 = 50/0.6 = 83.3 kmol/h. The total feed rate of A = 50 + 50 = 100 kmol/h. For a recovery of 95% of A in the distillate, the flow rate of A in the distillate = 0.95(100) = 95 kmol/h. With a mole fraction of 0.95 for A in the distillate, the total flow rate of the distillate = 95/0.95 = 100 kmol/h.

From Eq. (7-3) for $\alpha = 3$, the equilibrium mole fractions of A are related by,

$$y = \frac{\alpha x}{1+(\alpha-1)x} = \frac{3x}{1+2x} \qquad (1)$$

Equation (1) is plotted in the McCabe-Thiele diagram on the next page. Because Feed 2 is richer in A than Feed 1, Feed 2 enters the column above Feed 1. At minimum reflux, the pinch condition will occur at either Feed 1 or Feed 2. Assume that the pinch occurs at Feed 2. For a saturated liquid feed, using Eq. (1), the upper section operating line will intersect the equilibrium curve for $x_F = 0.6$ at $y = 3(0.6)/[1 + 2(0.6)] = 0.818$. Therefore, the slope of this operating line is,

$$(L/V)_{min} = (0.95 - 0.818)/(0.950 - 0.6) = 0.377$$

Correspondingly, using Eq. (7-17), $R = L/D = (L/V)_{min}/[1 - (L/V)_{min}] = 0.377/(1 - 0.377) = 0.605$ and $L_{min} = 0.605(100) = 60.5$ kmol/h.

Now check the middle section to see if the operating line there is below the equilibrium curve.

The liquid rate in the middle section = $L' = L + F_2 = 60.5 + 83.3 = 143.8$ kmol/h.

The vapor rate in the middle section = $V' = V = L + D = 60.5 + 100 = 160.5$ kmol/h.

Therefore the slope of the operating line in the middle section = $L'/V' = 143.8/160.5 = 0.896$.

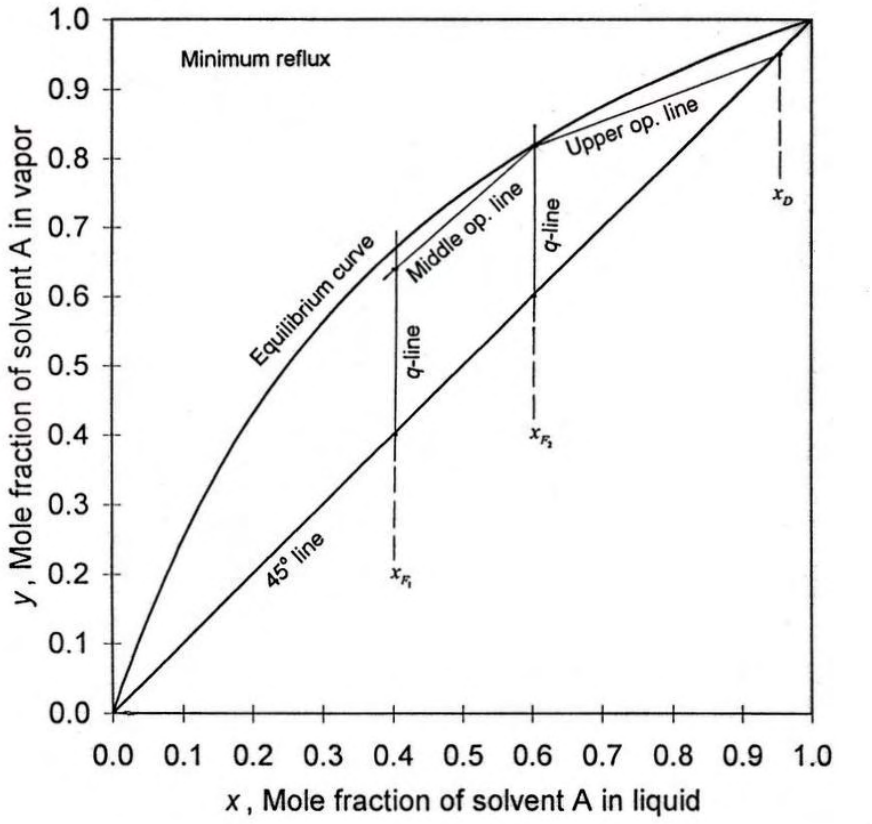
As seen in the McCabe-Thiele diagram on the next page, this operating line does not cross over the equilibrium curve. Therefore, the pinch does occur at Feed 2 (the upper feed).

For an operating reflux ratio of 1.33 times minimum, $L = 1.33(60.5) = 80.5$ kmol/h.

The vapor rate in the upper section = $L + D = 80.5 + 100 = 180.5$ kmol/h.

Exercise 7.30 (continued)

Analysis: (continued)



Therefore the upper section operating line has a slope, L/V = 80.5/180.5 = 0.446 and passes through the point $y = x = 0.95$. It intersects the vertical q-line at $x = 0.6$ and for the slope of

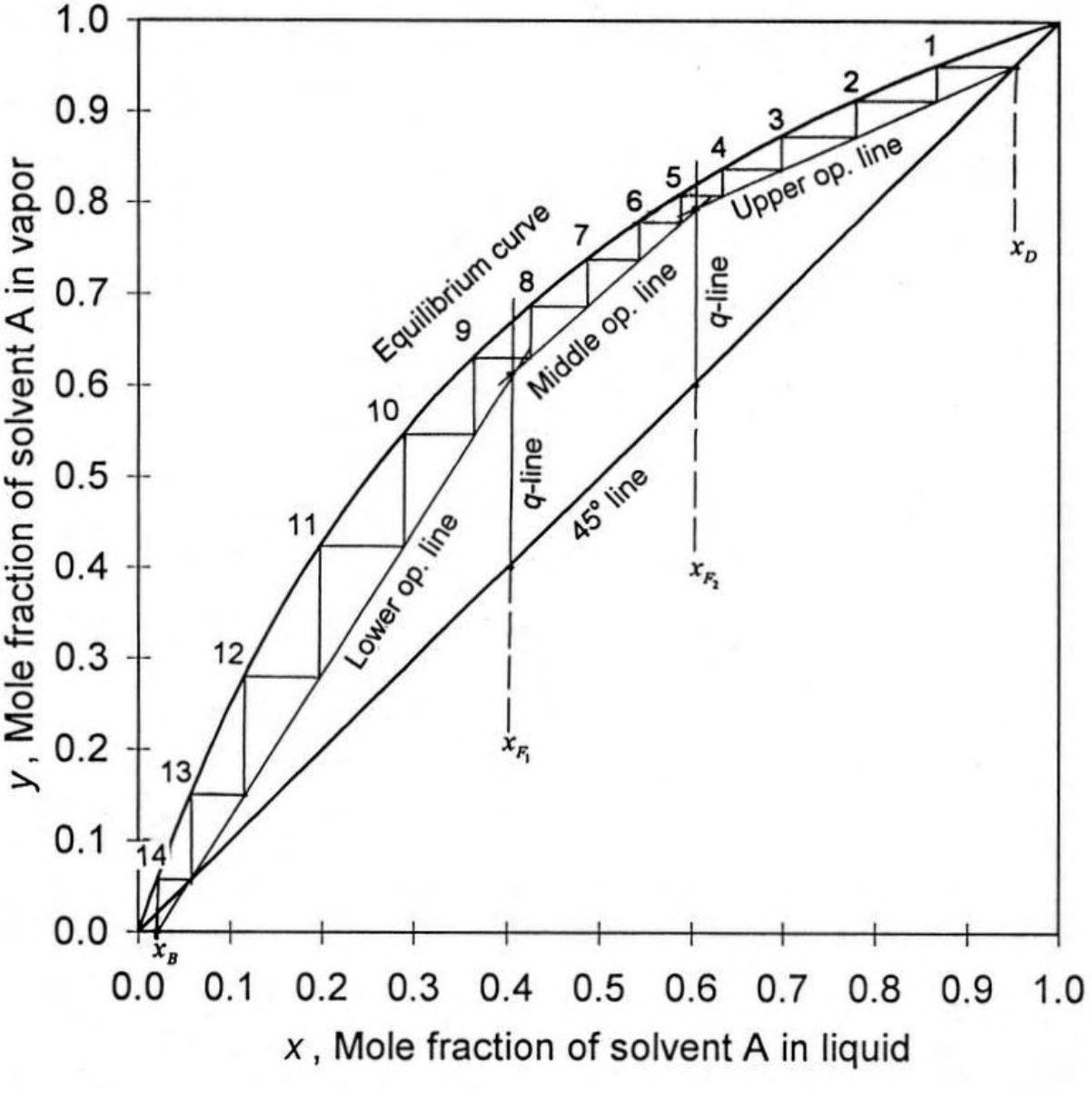
$$0.446 = (0.95 - y)/(0.95 - 0.6),\ y = 0.794.$$

For the middle section, $L' = L + F_2$ = 80.5 + 83.3 = 163.8 kmol/h and $V' = V$ = 180.5 kmol/h
Therefore, the middle section operating line has a slope of L'/V' = 163.8/180.5 = 0.908 and intersects the q-line for $x = 0.6$ at $y = 0.794$. It intersects the vertical q-line at $x = 0.4$ and for the slope of $0.908 = (0.794 - y)/(0.6 - 0.4)$, $y = 0.613$.
For the lower section, $L'' = L' + F_1$ = 163.8 + 125 = 288.8 kmol/h and $V''=V'$ = 180.5 kmol/h
Therefore, the lower section operating line has a slope of L''/V'' = 288.8/180.5 = 1.60 and intersects the q-line for $x = 0.4$ and $y = 0.613$. As seen in Fig. 7.27(c), the mole fraction of A in the bottoms, x_B , is determined from the intersection of the operating line for the lower section with the y-axis. Thus, $1.60 = (0.613 - 0)/(0.4 - x_B)$. Solving, x_B = 0.0169 for component A.
Since the bottoms contains 5 kmol/h of A, the bottoms rate = B = 5/0.0169 = 295.9 kmol/h.
Thus, the bottoms contains 290.9 kmol/h of water. But, the flow rate of water entering in the two feeds = 125 + 83.3 - 100 = 108.3 kmol/h.
Therefore, the open steam flow rate = 290.9 + 5 - 108.3 = 187.6 kmol/h

In the McCabe-Thiele diagram on the next page, the three operating lines are drawn and the equilibrium stages are stepped off so as to place the two feeds at their optimal locations. As seen, the number of equilibrium stages required = N_t = 14. From Eq. (6-21), for a plate efficiency of 70%, the actual number of trays = $N_a = N_t/E_o$ = 14/0.7 = 20 plates.

Exercise 7.30 (continued)

Analysis: (continued)



Exercise 7.31

Subject: Distillation of a mixture of n-hexane and n-octane in a column with an intercooler.

Given: Saturated liquid feed of 40 mol% hexane in octane. Intercooler at second stage from the top removes heat so as to condense 50 mol% of the vapor rising from the third. Distillate is to contain 95 mol% of hexane and bottoms is to contain 5 mol% of hexane. Reflux ratio, L/D, at the top, is equal to 0.5. Vapor-liquid equilibrium data for 1 atm is plotted in Fig. 4.4.

Assumptions: Constant molar overflow. Total condenser and partial reboiler. Operating pressure of 1 atm.

Find: (a) Equations to locate operating lines.
(b) Number of equilibrium stages if optimal feed stage location is used.

Analysis: First compute overall material balance. Take a basis of $F = 100$ kmol/h.

Overall total mole balance: $F = 100 = D + B$ (1)

Overall hexane mole balance: $Fx_F = 40 = Dx_D + Bx_B = 0.95D + 0.05B$ (2)

Solving Eqs. (1) and (2), $D = 38.9$ kmol/h and $B = 61.1$ kmol/h

(a) For a reflux ratio of 0.5, in the section above the intercooler, $L = 0.5D = 19.45$ kmol/h. The overhead vapor rate is $V = L + D = 19.45 + 38.9 = 58.35$ kmol/h. The slope of the operating line = $L/V = 19.45/58.35 = 0.333$. Using Eq. (7-6), the equation for the operating line is, $y = 0.333x + Dx_D/V = 0.333x + (38.9)(0.95)/(58.35) = 0.333x + 0.633$ (3)

Now consider the section of stages between the intercooler at stage 2 from the top and the feed stage. Because 50 mol% of the vapor from this section is condensed at stage 2 by the intercooler, the vapor rate in this section = $V' = 2V = 2(58.35) = 116.7$ kmol/h. The liquid rate in this section is $L' = V' - D = 116.7 - 38.9 = 77.8$ kmol/h. The slope of the operating line = $L'/V' = 77.8/116.7 = 0.667$. In this section, by hexane material balance, $yV' = xL' + x_D D$ or,

$y = (L'/V')x + Dx_D/V' = 0.667x + (38.9)(0.95)/116.7 = 0.667x + 0.317$ (4)

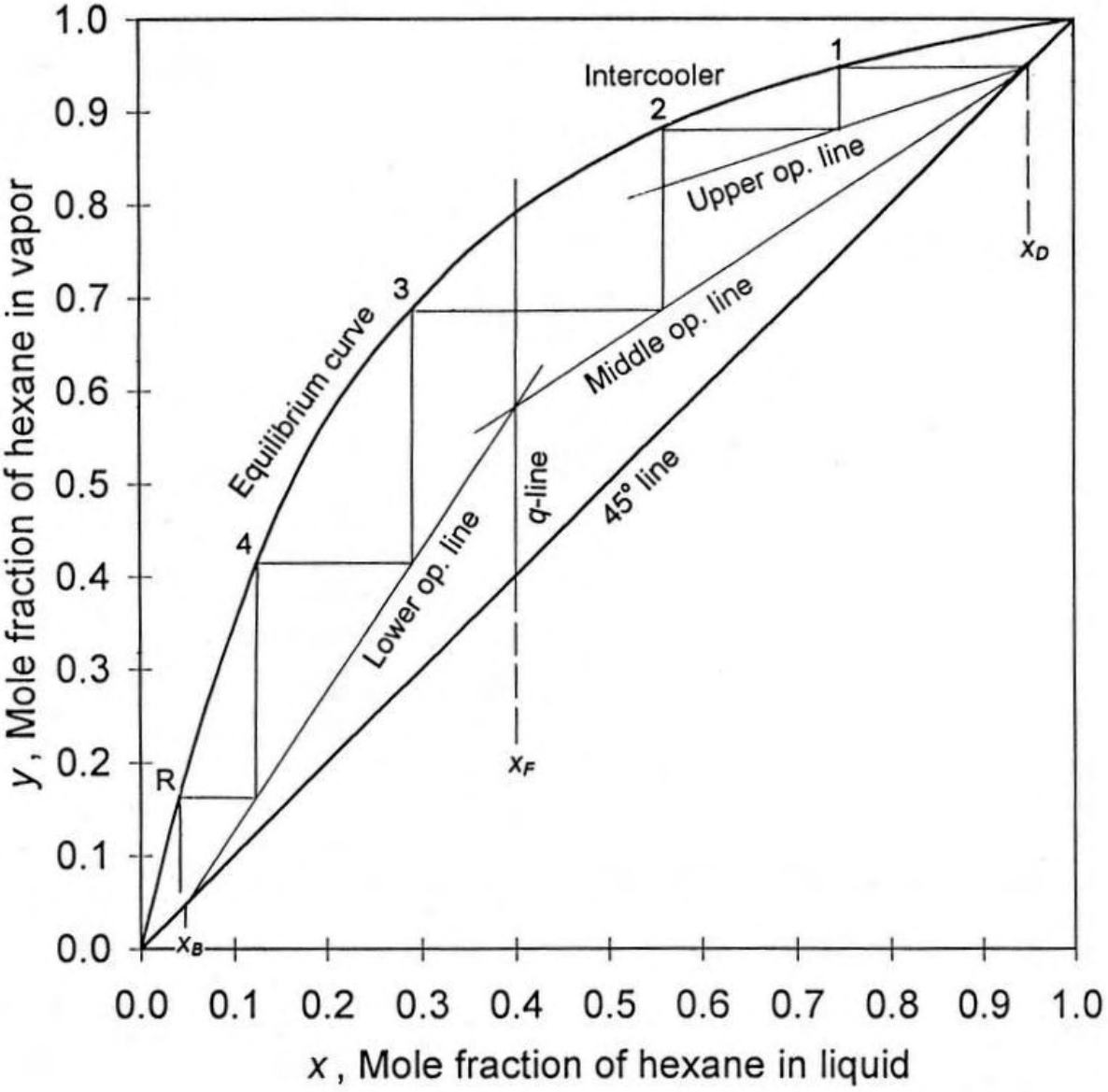
In the section below the feed stage, for a saturated liquid feed, $L'' = L' + F = 77.8 + 100 = 177.8$ kmol/h. The vapor rate = $V'' = V' = 116.7$ kmol/h. The slope of the operating line = $L''/V'' = 177.8/116.7 = 1.524$. From Eq. (7-11),

$y = (L''/V'')x - Bx_B/V'' = 1.524x - (61.1)(0.05)/116.7 = 1.524x - 0.026$ (5)

(b) A McCabe-Thiele diagram in terms of hexane, the more volatile component, is shown on the next page, where the equilibrium curve is obtained from Fig. 4.4 and the operating lines for the three sections are drawn from Eqs. (3), (4), and (5). The q-line is vertical, passing through $x = 0.4$. Note that the upper and middle section operating lines both pass through the point {0.95, 0.95}. The theoretical stages are stepped off starting from the top, switching to the middle section operating line after stage 2, and switching to the stripping section so as to locate the feed stage optimally. The result is just slightly less than 5 equilibrium stages or, say, 4 stages plus a partial reboiler.

Exercise 7.31 (continued)

Analysis: (continued)



Exercise 7.32

Subject: Distillation of a mixture of ethyl alcohol and water at 1 atm using open steam instead of a reboiler.

Given: 100 kmol/h of a saturated liquid feed containing 12 mol% ethyl alcohol in water. Distillate to contain 85 mol% alcohol with a recovery of 90%. Reflux ratio, $L/D = 3$ with saturated liquid reflux. Feed stage located optimally. Vapor-liquid equilibrium data in Exercise 7.29.

Assumptions: Constant molar overflow. Total condenser.

Find: (a) Open steam requirement, kmol/h
(b) Number of equilibrium stages
(c) Optimal feed stage location.
(d) Minimum reflux ratio.

Analysis: First compute material balance. Because the ethanol mole fraction in the distillate is less than that of the azeotrope (89.43 mol% in Exercise 7.29), the ethanol is always the more volatile component. The feed contains 12 kmol/h of ethanol and 88 kmol/h of water. For a 90% recovery, the distillate contains 0.9(12) = 10.8 kmol/h of ethanol. Since the distillate is 85 mol% ethanol, the total distillate rate = D = 10.8/0.85 = 12.7 kmol/h. The bottoms contains 12 - 10.8 = 1.2 kmol/h of ethanol. The distillate contains 12.7 - 10.8 = 1.9 kmol/h of water. The bottoms contains 88 - 1.9 + open steam = 89.9 + open steam in kmol/h.

(a) For a reflux ratio of 3, $L = 3D = 3(12.7) = 38.1$ kmol/h. Overhead vapor rate = $V = L + D = 38.1 + 12.7 = 50.8$ kmol/h. Below the feed stage, $L' = L + F = 38.1 + 100 = 138.1$ kmol/h. Boilup rate = $V' = V =$ 50.8 kmol/h = flow rate of open steam.

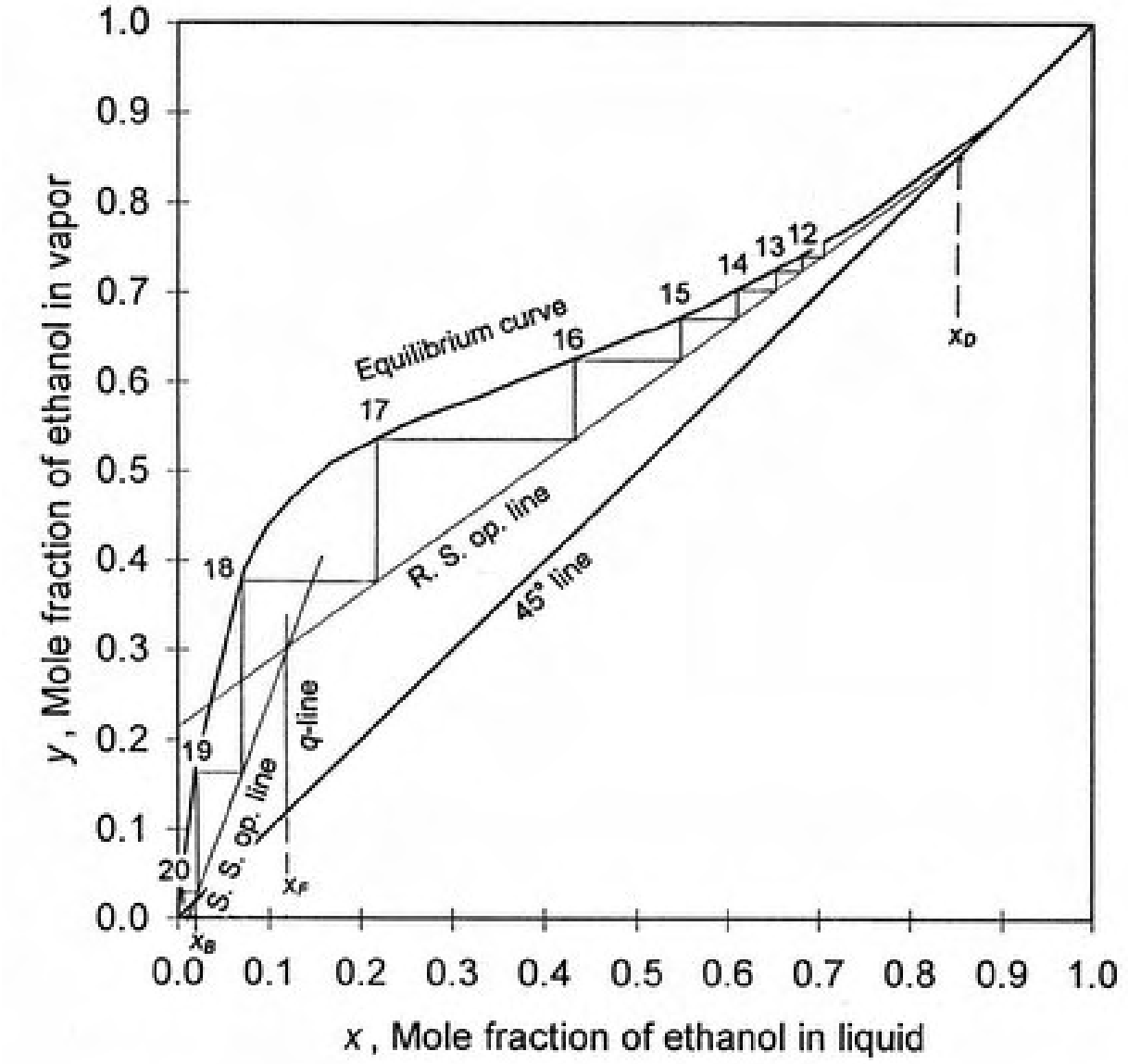
(b) The bottoms rate = 138.1 kmol/h. The bottoms consists of 1.2 kmol/h of ethanol and 138.1 - 1.2 = 136.9 kmol/h of water. The mole fraction of ethanol in the bottoms = 1.2/138.1 = 0.0087. The McCabe-Thiele diagram is given on the next page, where the equilibrium curve is obtained from Exercise 7.29 and the q-line is vertical at $x = 0.12$. The rectifying section operating line passes through the point {0.85, 0.85}and has a slope, $L/V = 38.1/50.8 = 0.75$. The stripping section operating line has a slope, $L'/V' = 138.1/50.8 = 2.72$ and, as shown in Fig. 7.27(c), passes through the point $x = x_B = 0.0087$ at $y = 0$. Because the stages are so crowded at the high mole fraction end, a second McCabe-Thiele diagram is shown for the region above $y = x = 0.7$. As shown, with the use of the two diagrams, just less than 20 equilibrium stages are needed.

(c) From the first McCabe-Thiele plot, the optimal feed stage is Stage 18 from the top.

(d) From the third McCabe-Thiele diagram on the next page, the minimum reflux in terms of L/V is obtained from the slope of the rectifying section operating line, which passes through the point, $y = x_D = 0.85$ and is tangent to the equilibrium curve, rather than being drawn through the intersection of the q-line and the equilibrium curve because that would cause the operating line to mistakenly cross over the equilibrium curve. The slope of the operating line = $(L/V)_{min} = 0.667$. From Eq. (7-27), $R_{min} = (L/D)_{min} = 0.667/(1-0.667) = 2.0$.

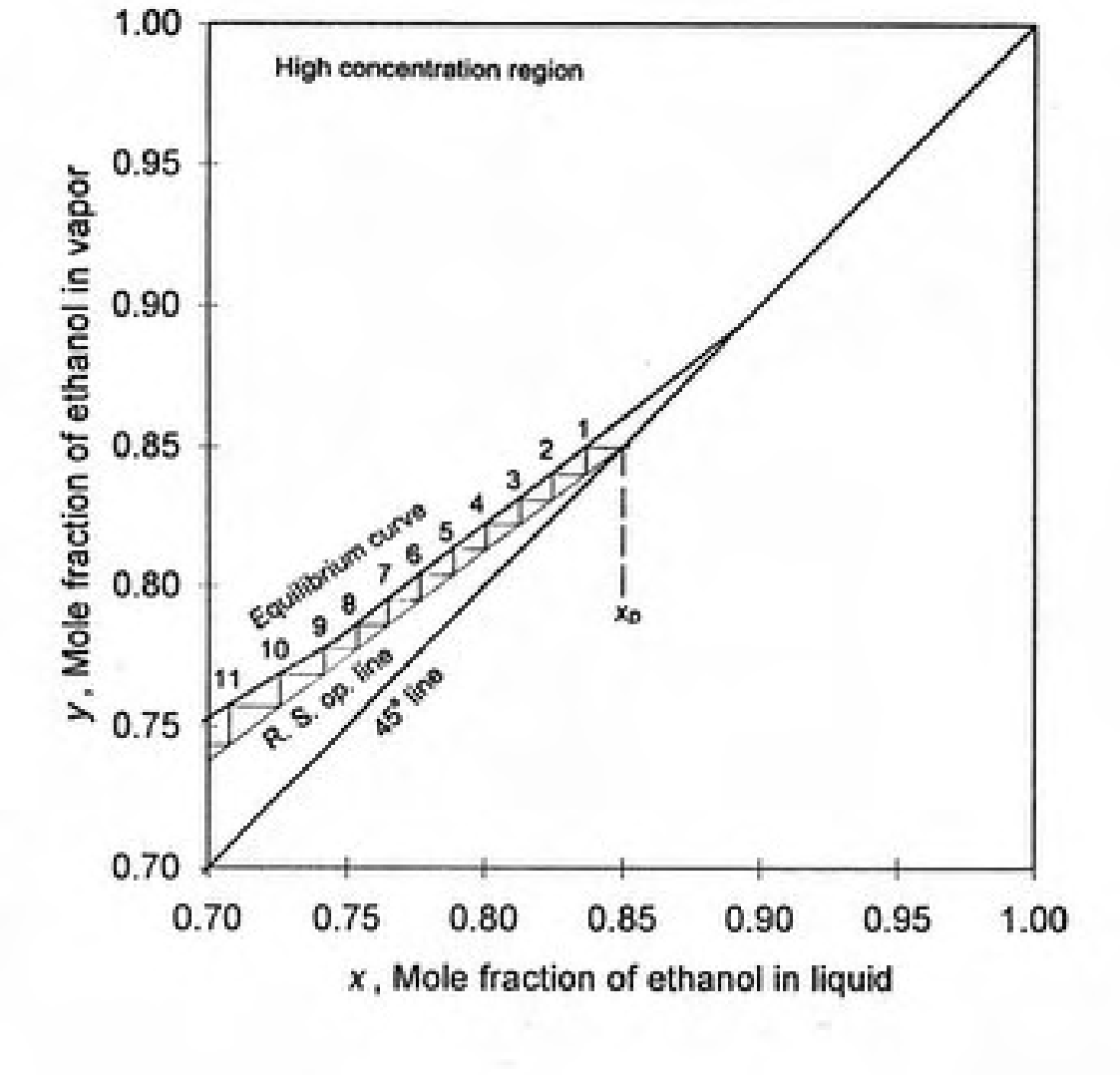
Exercise 7.32 (continued)

Analysis: (b, c, and d) (continued)



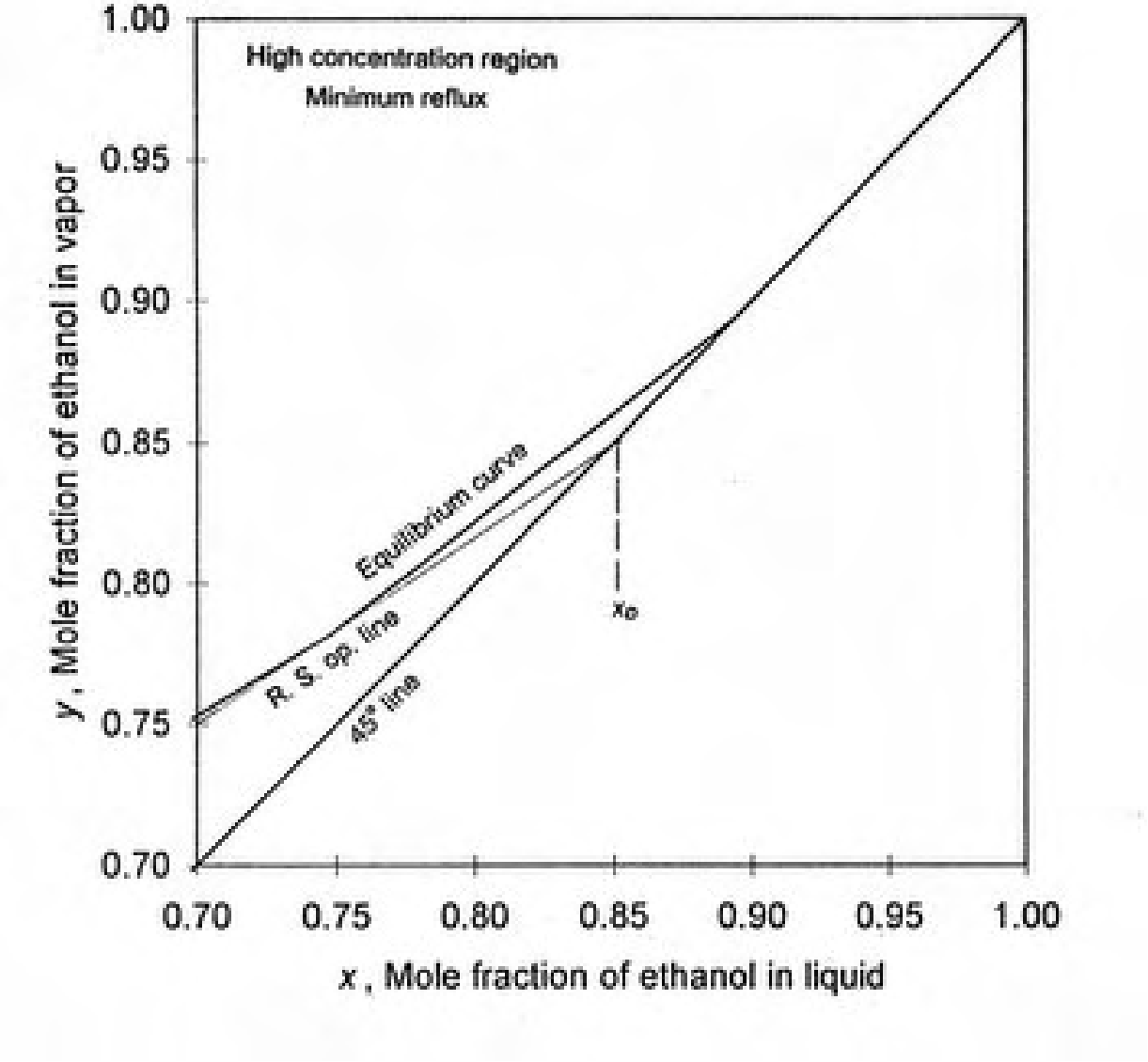
Exercise 7.32 (continued)

Analysis: (b, c, and d) (continued)



Exercise 7.32 (continued)

Analysis: (b, c, and d) (continued)



Exercise 7.33

Subject: Distillation of a mixture of isopropyl alcohol and water at 1 atm using either a partial reboiler or open steam.

Given: Bubble-point feed containing 10 mol% isopropyl alcohol in water. Distillate to contain 67.5 mol% isopropyl alcohol with a 98% recovery. Vapor-liquid equilibrium data , with an azeotrope at 68.54 mol% alcohol.

Assumptions: Constant molar overflow. Total condenser.

Find: For a reflux ratio, $R = L/D = 1.5$ times minimum, determine number of stages, if:

(a) Partial reboiler is used.

(b) Open saturated steam is used.

and

(c) Minimum number of equilibrium stages.

Analysis: In the composition region of operation, the alcohol is the most volatile component. First, compute the distribution of the alcohol. Take a basis of 100 kmol/h of feed.
Then, the feed contains 10 kmol/h alcohol and 90 kmol/h of water. For a recovery of 98 mol%, alcohol, distillate contains 9.8 kmol/h of alcohol. For an alcohol purity of 67.5 mol%, the distillate rate = $D = 9.8/0.675 = 14.52$ kmol/h. Water in the distillate = 14.52 - 9.8 = 4.72 kmol/h.
Alcohol in the bottoms = 10 - 9.8 = 0.2 kmol/h.

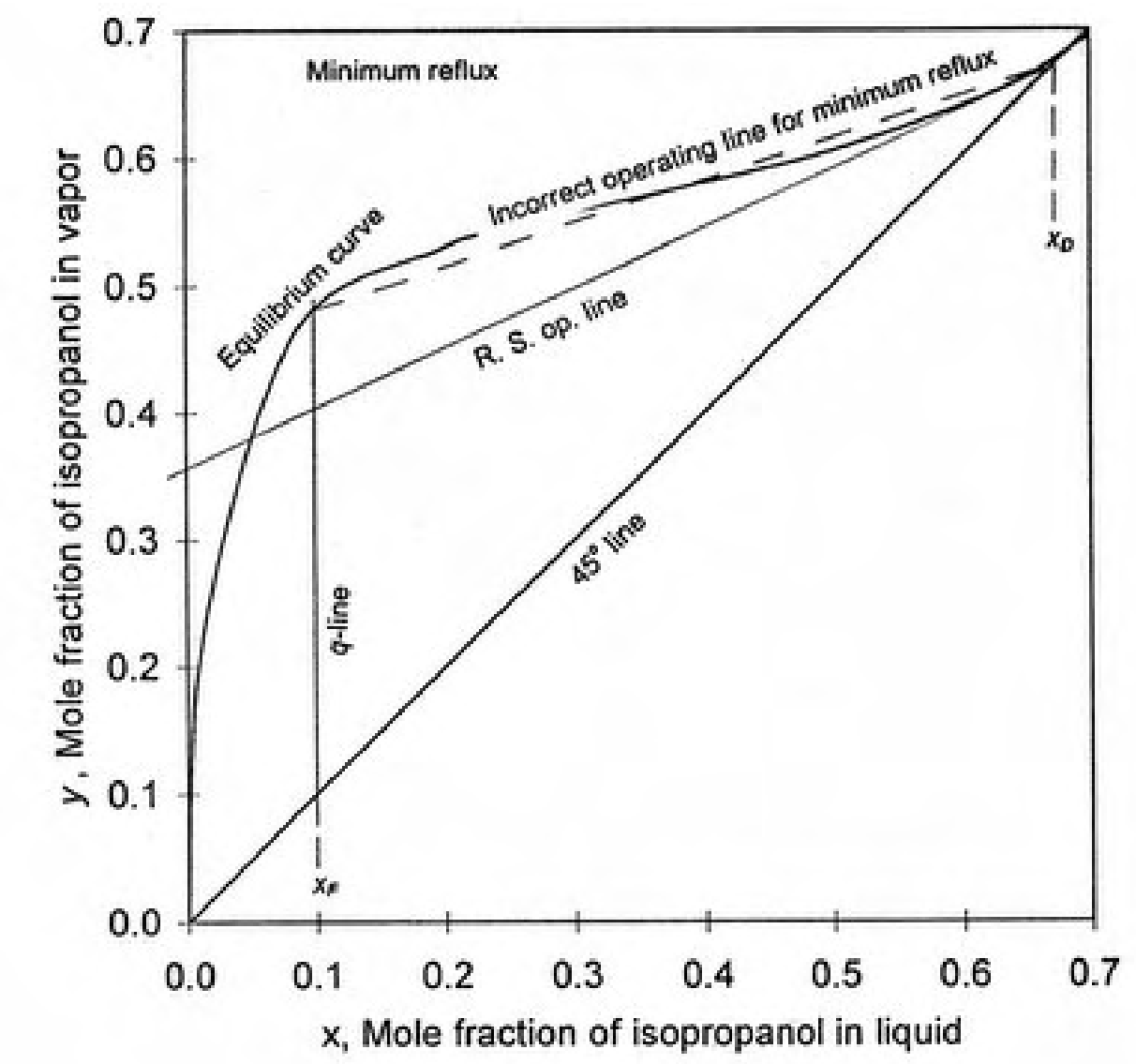
(a) With a partial reboiler, no other water enters the system. Therefore, water in the bottoms = 90 - 4.72 = 85.28 kmol/h. Total bottoms rate = $B = 85.28 + 0.2 = 85.48$ kmol/h.

Mole fraction of alcohol in bottoms = 0.2/85.48 = 0.0023. The minimum reflux is determined from the McCabe-Thiele diagram on the next page, where the equilibrium curve is drawn from the given data and the q-line is vertical, passing through $x = 0.10$. The rectifying section operating line for minimum reflux usually is a straight line that connects the distillate mole fraction on the 45^o line to the intersection of the equilibrium curve and the q-line as shown by the dashed line on the diagram. However, in this case the line mistakenly crosses over the equilibrium curve. Therefore, instead, the operating line is drawn tangent to the equilibrium curve from the point $x = x_D = 0.675$ as shown on the diagram by a solid line. The slope of the operating line = $L/V = 0.467$. From Eq. (7-27), $R_{min} = (L/D)_{min} = 0.467/(1-0.467) = 0.876$.
The operating reflux ratio = $R = 1.5R_{min} = 1.5(0.876) = 1.314$. From Eq. (7-7), $L/V = R/(1+R) = 1.314/(1+1.314) = 0.568$. On a set of three McCabe-Thiele diagrams on the next page, the rectifying section operating line has this slope and passes through the point, y=0.675, x=0.675. the stripping section operating line passes through the point, y=0.0023, x=0.0023 and intersects the vertical q-line at the point where the rectifying section operating line intersects the q-line. As seen, the equilibrium stages are stepped off starting at the top, with a switch from the rectifying section to the stripping section to minimize the number of stages and, thus, locating the optimal feed stage. To achieve accuracy, one diagram covers the high-concentration region, one the

middle region, and one the low-concentration region. The result is between 14 and 15 equilibrium stages. Call it 14 stages plus a partial reboiler.

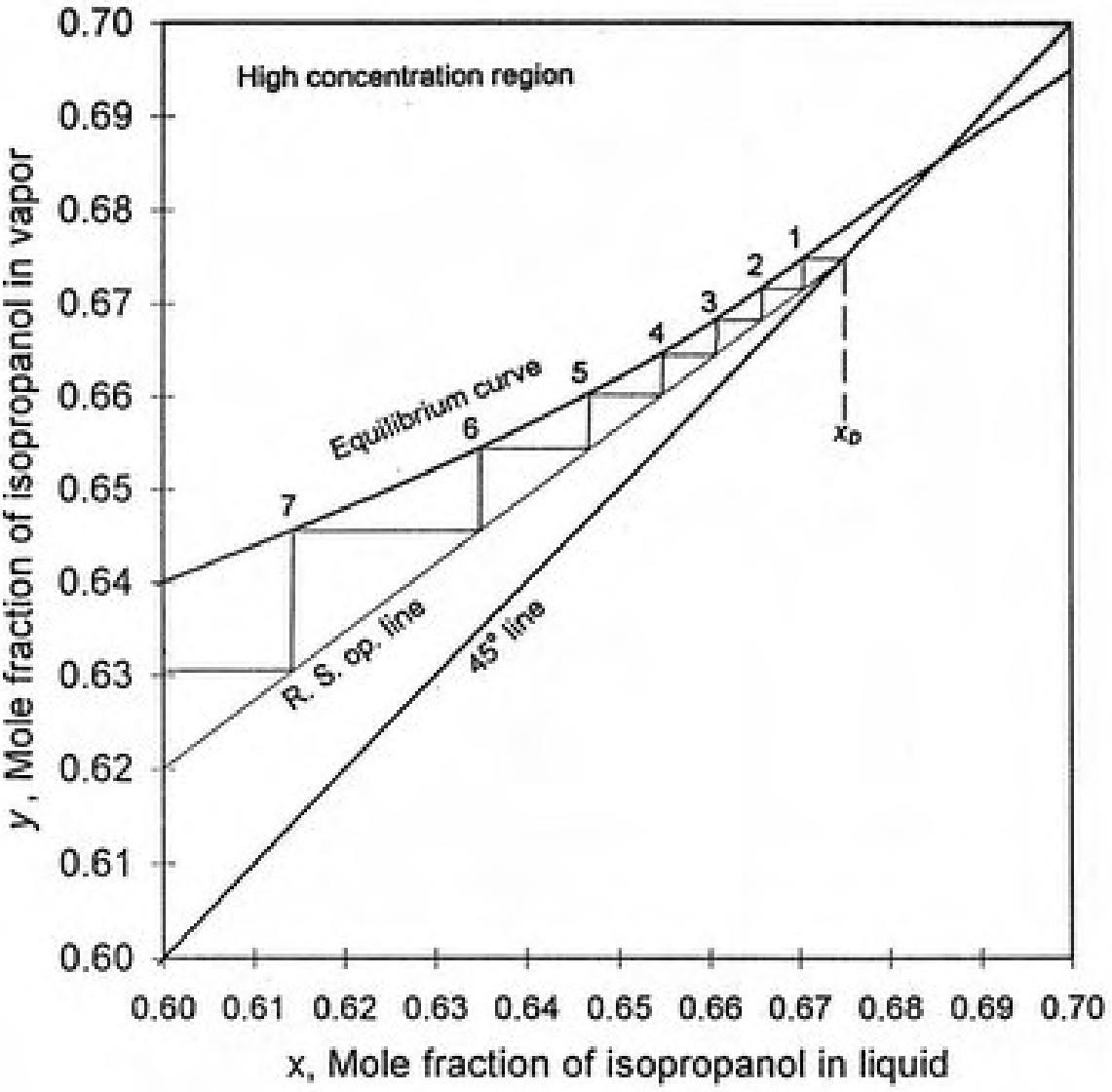
Exercise 7.33 (continued)

Analysis: (a) (continued)



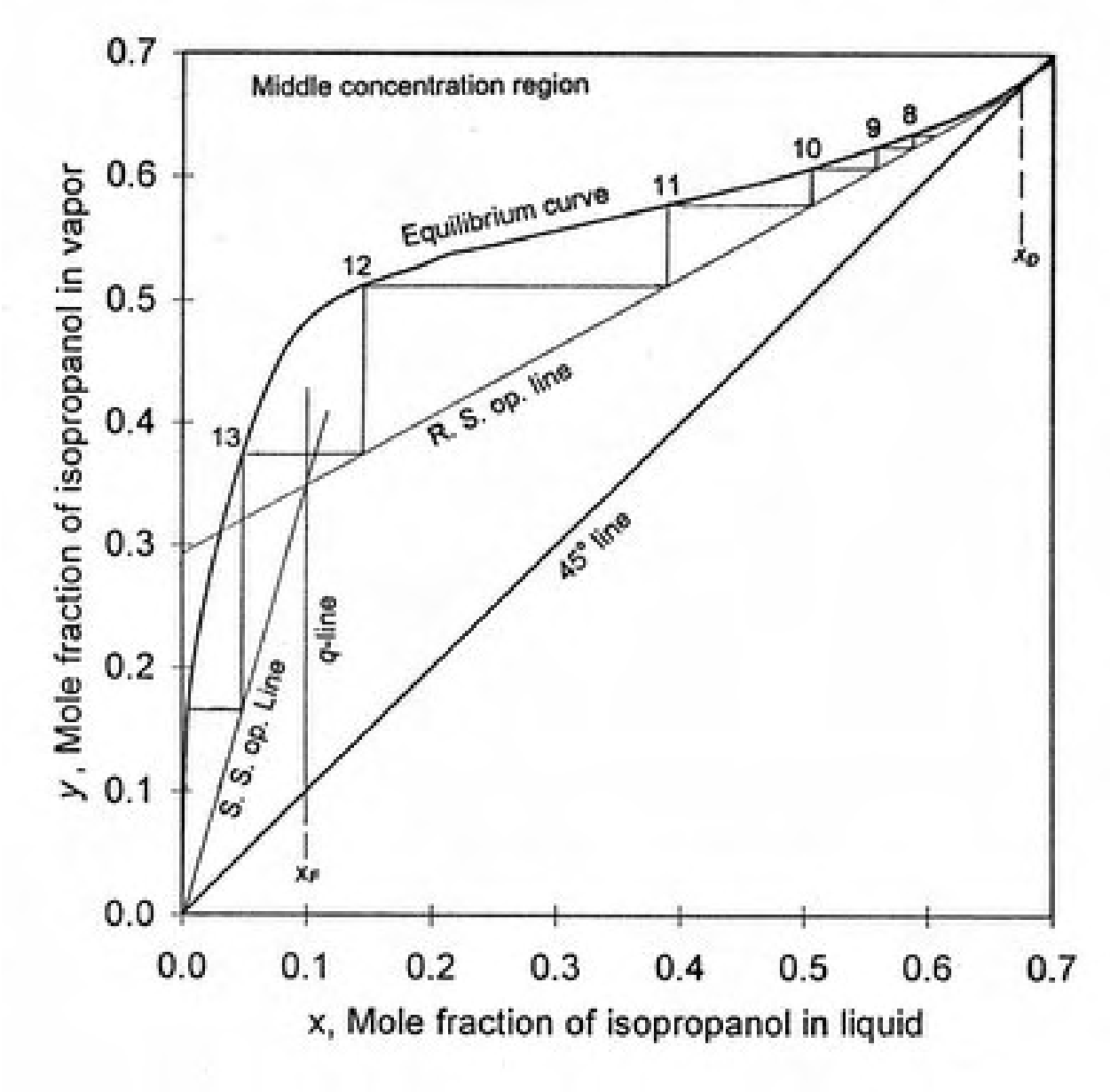
Exercise 7.33 (continued)

Analysis: (a) (continued)



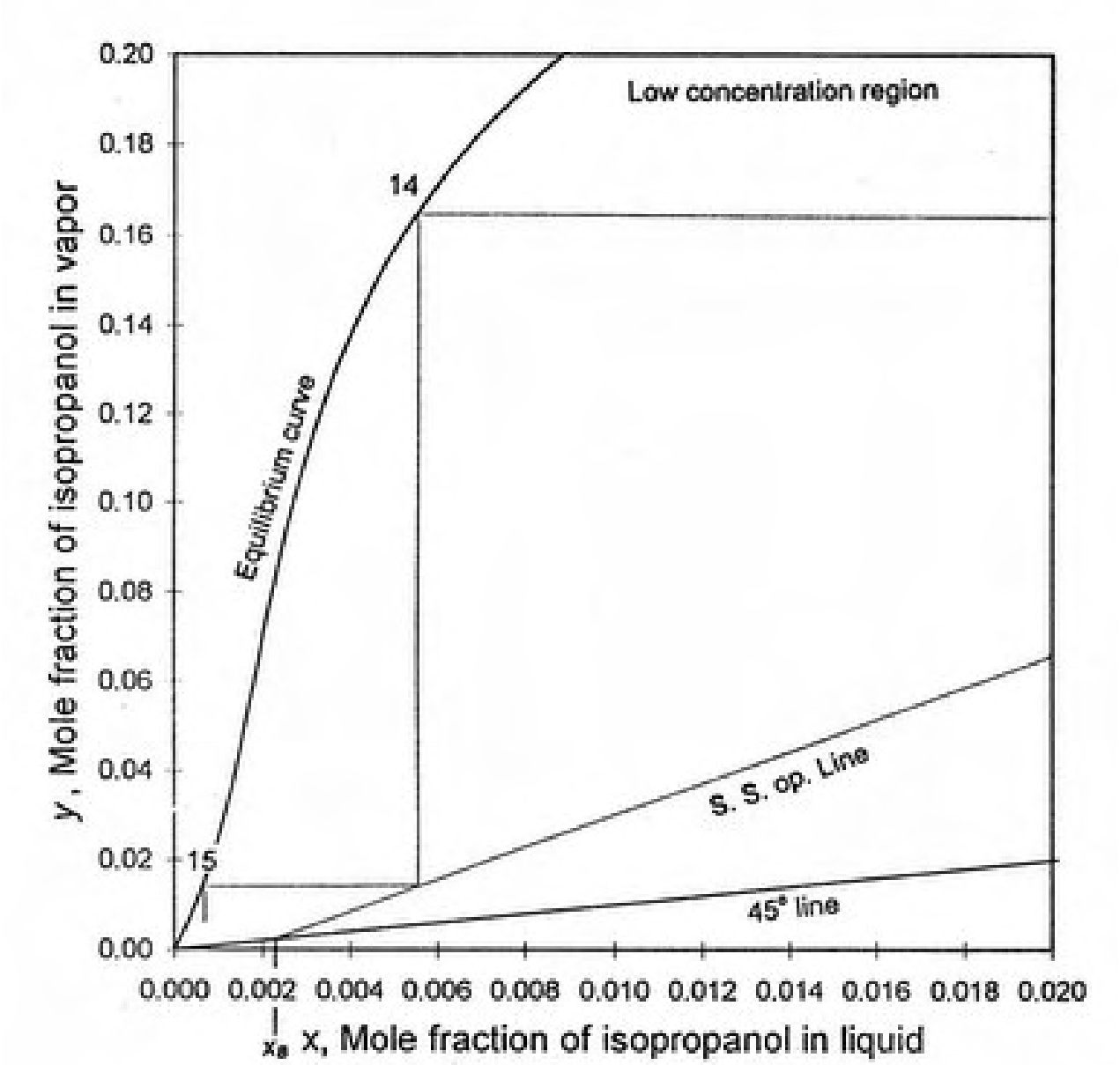
Exercise 7.33 (continued)

Analysis: (a) (continued)



Exercise 7.33 (continued)

Analysis: (a) (continued)



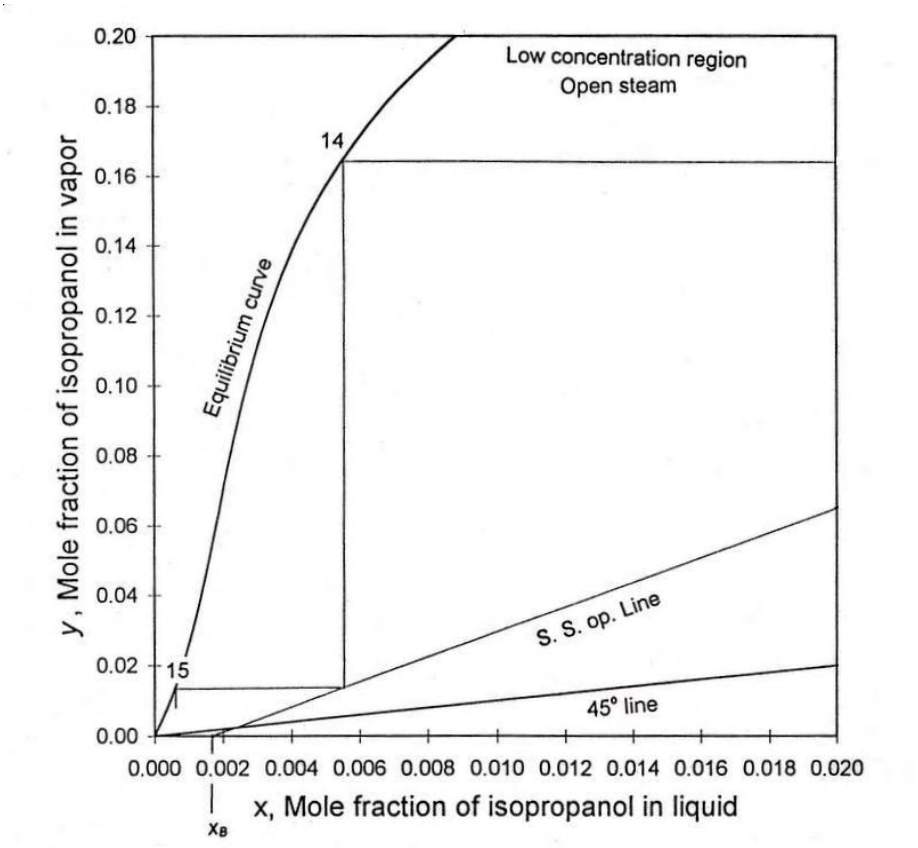
Exercise 7.33 (continued)

Analysis: (continued)

(b) When open (live) steam is used with the same reflux ratio, the rectification section operating line and the *q*-line are identical to part (a) for a partial reboiler. Thus, the part (a) McCabe-Thiele diagram for the high concentration region applies for open steam.

However, the stripping section operating line and the bottoms mole fraction change as follows. The liquid rate in the rectification section = $L = 1.314D = 1.314(14.52) = 19.08$ kmol/h. The vapor rate in the rectifying section = $V = L + D = 19.08 + 14.52 = 33.6$ kmol/h. The liquid rate below the feed stage = $L' = L + F = 19.08 + 100 = 119.08$ kmol/h. The vapor rate in the stripping section = $V' = V = 33.6$ kmol/h = open steam flow rate. The bottoms rate = $B = L' = 119.08$ kmol/h. The mole fraction of isopropanol in the bottoms = 0.2/119.08 = 0.00168. The change to the part (a) McCabe-Thiele diagrams on the preceding page for the middle concentration region is extremely small because the location of the stripping section operating line changes only slightly.

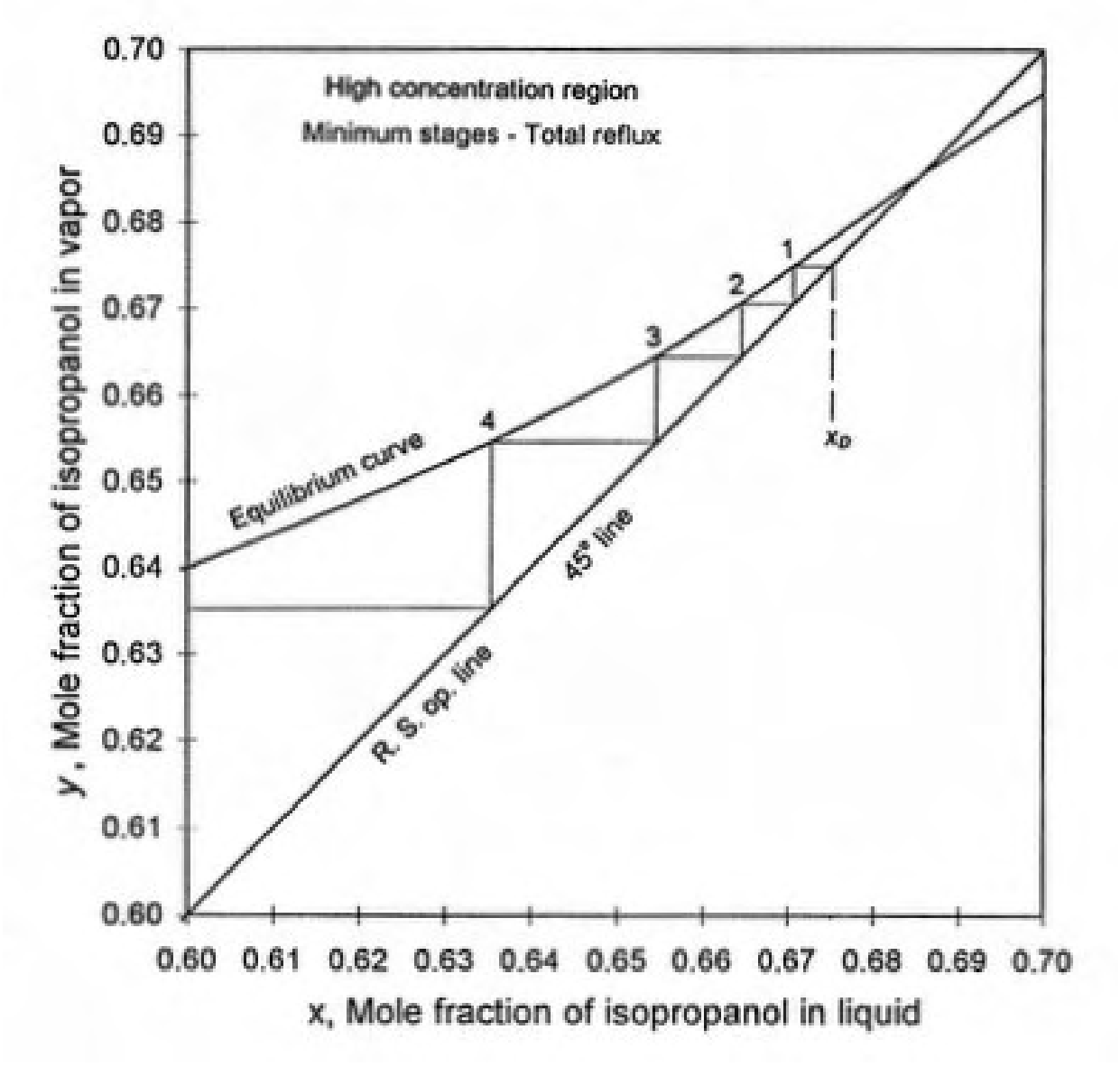
However, the change is important in the low-concentration region. The new McCabe-Thiele diagram for the low concentration region is shown below. The operating line for the stripping section has a slope of $L'/V' = 119.08/33.6 = 3.54$ and passes through the point $\{y = 0, x = 0.00168\}$. The number of stages remains about the same as for part (a). Thus, without a reboiler, use 15 equilibrium stages in the column.



Exercise 7.33 (continued)

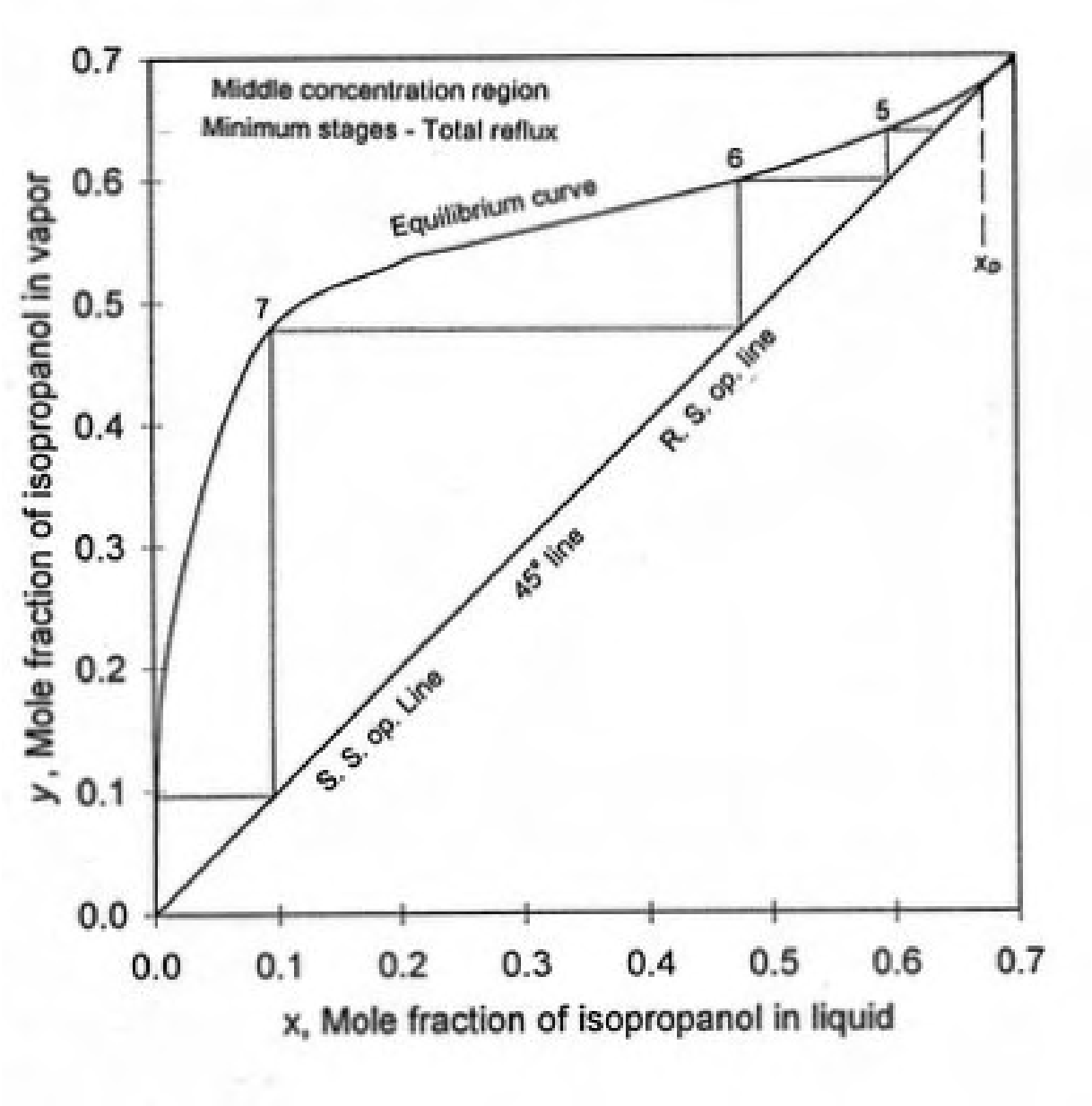
Analysis: (c) (continued)

(c) The minimum number of stages is determined as shown in the McCabe-Thiele diagrams on the next page by stepping off stages between the equilibrium curve and the 45° line from x_B = 0.0023 and x_D = 0.675. The number of minimum equilibrium stages = just more than 8 equilibrium stages.



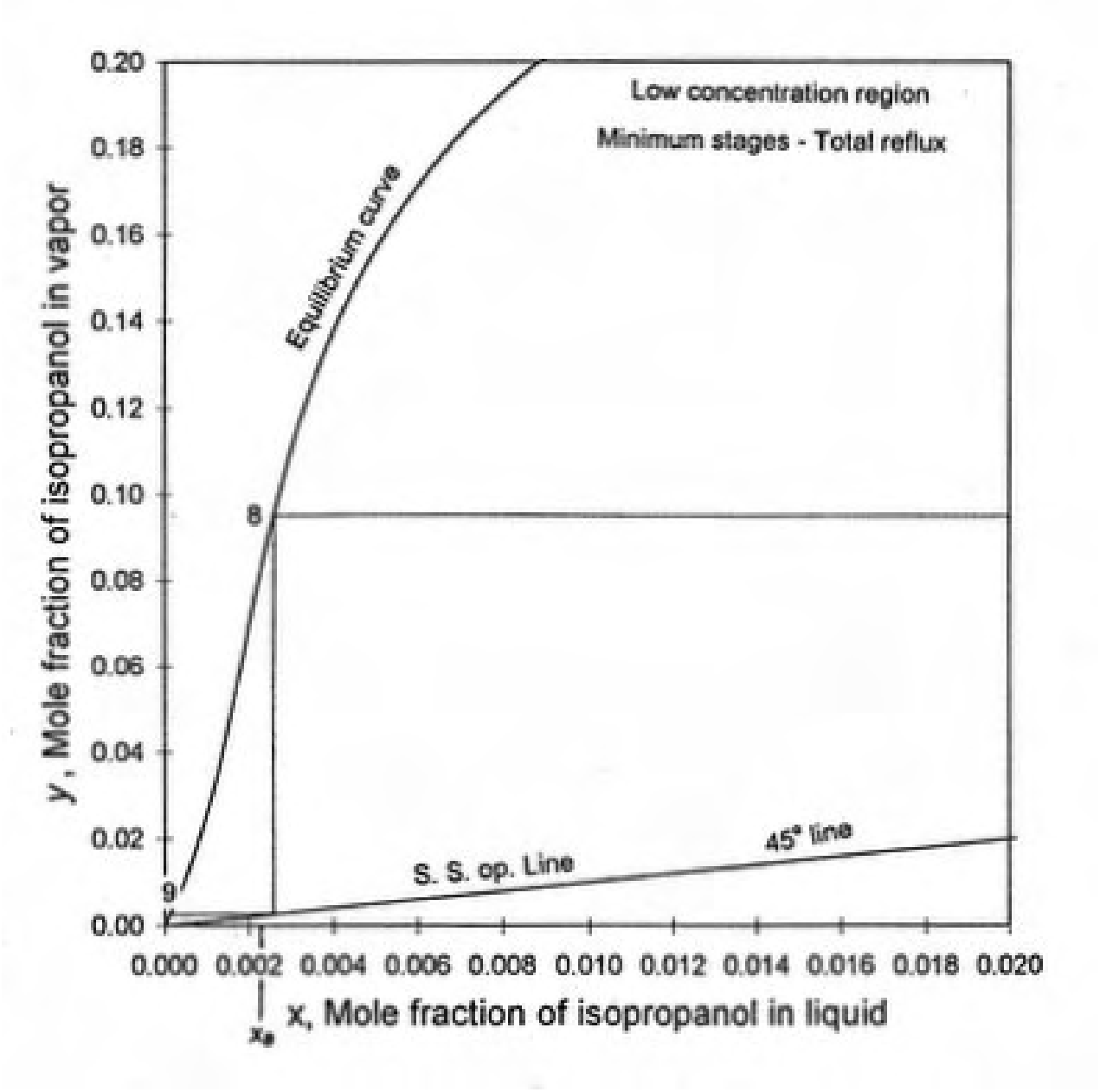
Exercise 7.33 (continued)

Analysis: (c) (continued)



Exercise 7.33 (continued)

Analysis: (c) (continued)



Exercise 7.34

Subject: Stripping of isopropyl alcohol from water at 1 atm using either a partial reboiler or open (live) steam.

Given: Bubble-point liquid feed containing 10 mol% alcohol. Vapor overhead to contain 40 mol% alcohol. Boilup, $V/F = 0.246$. Vapor-liquid equilibrium data from Exercise 7.33.

Assumptions: Constant molar overflow.

Find: Determine the number of equilibrium stages for: (1) Partial reboiler, (2) Open steam.

Analysis:

Take a basis of $F = 100$ kmol/h. Vapor rate leaving top of column = $V = 0.246F = D = 0.246(100) = 24.6$ kmol/h. Alcohol in overhead vapor = $0.4(24.6) = 9.84$ kmol/h. Water in the overhead vapor = $24.6 - 9.84 = 14.76$ kmol/h.

(1)

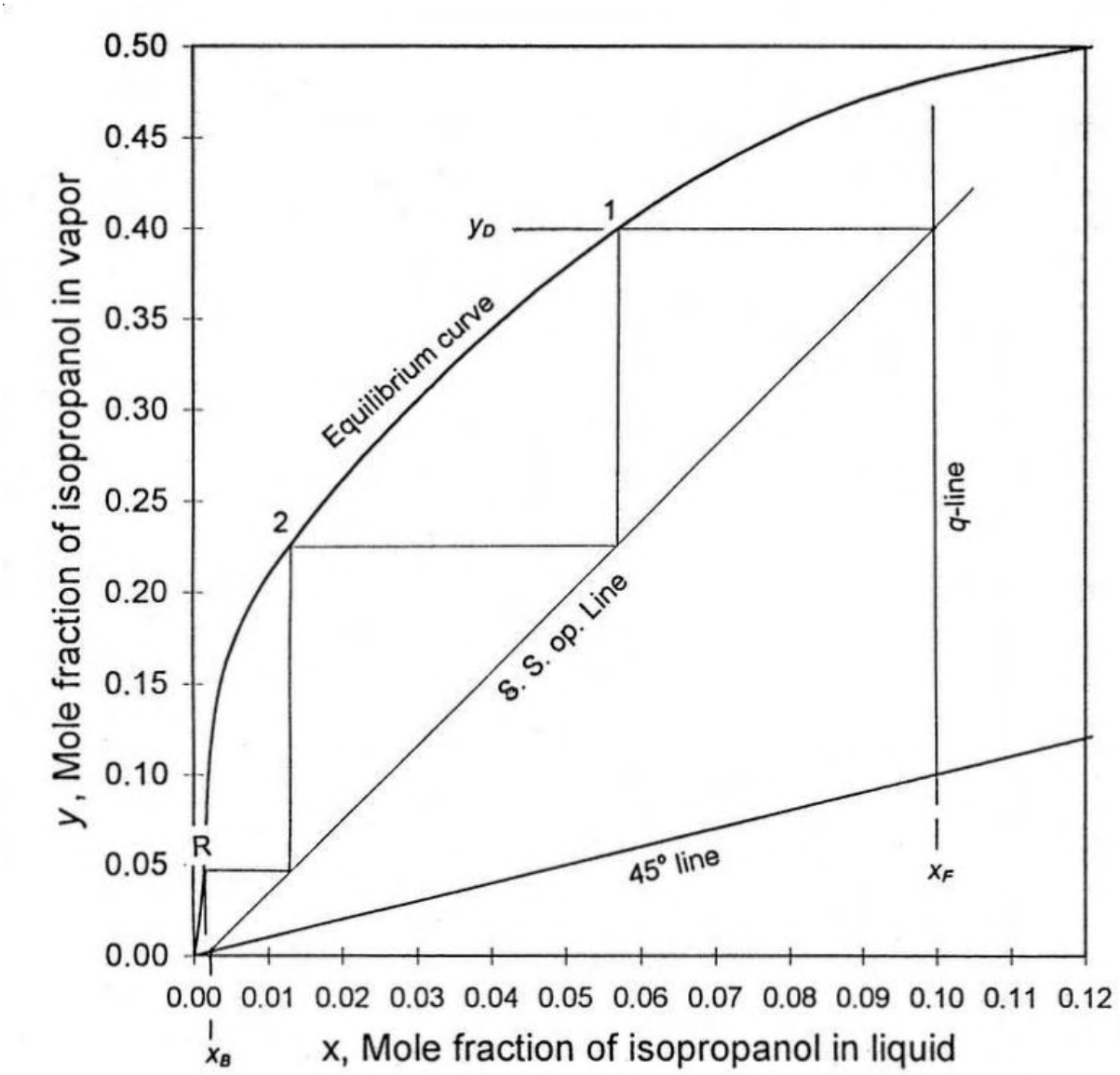
With a partial reboiler, bottoms rate = $B = F - D = 100 - 24.6 = 75.4$ kmol/h. Alcohol in bottoms = $10 - 9.84 = 0.16$ kmol/h. Mole fraction of alcohol in bottoms = $x_B = 0.16/75.4 = 0.0021$. With isopropanol as the most volatile component, the McCabe-Thiele diagram is given below, where the equilibrium curve is obtained from the data in Exercise 7.33 and the q-line is vertical through $x = 0.10$. The stripping section operating line passes through the point $\{x=0.0021, y=0.0021\}$with a slope = $L/V = F/V = 100/24.6 = 4.065$. It also passes through the point $\{x=0.1, y=0.4\}$. From the plot, the number of equilibrium stages = just less than 3. Call it 2 equilibrium stages in the column + partial reboiler.

(2)

The open steam rate = $V = 24.6$ kmol/h. The liquid rate = $L = 100$ kmol/h. Therefore, the slope of the stripping section operating line is the same as for part (1), i.e. $L./V = 100/24.6 = 4.065$. Now the mole fraction of alcohol in the bottoms = $x_B = 0.16/100 = 0.0016$. Thus, as shown in the McCabe-Thiele diagram below, the operating line passes through the points $\{x=0.0016, y=0\}$and $\{x=0.10, y=0.40\}$, with the slope of 4.065. Now, The number of equilibrium stages is equal to 3, all of them in the column.

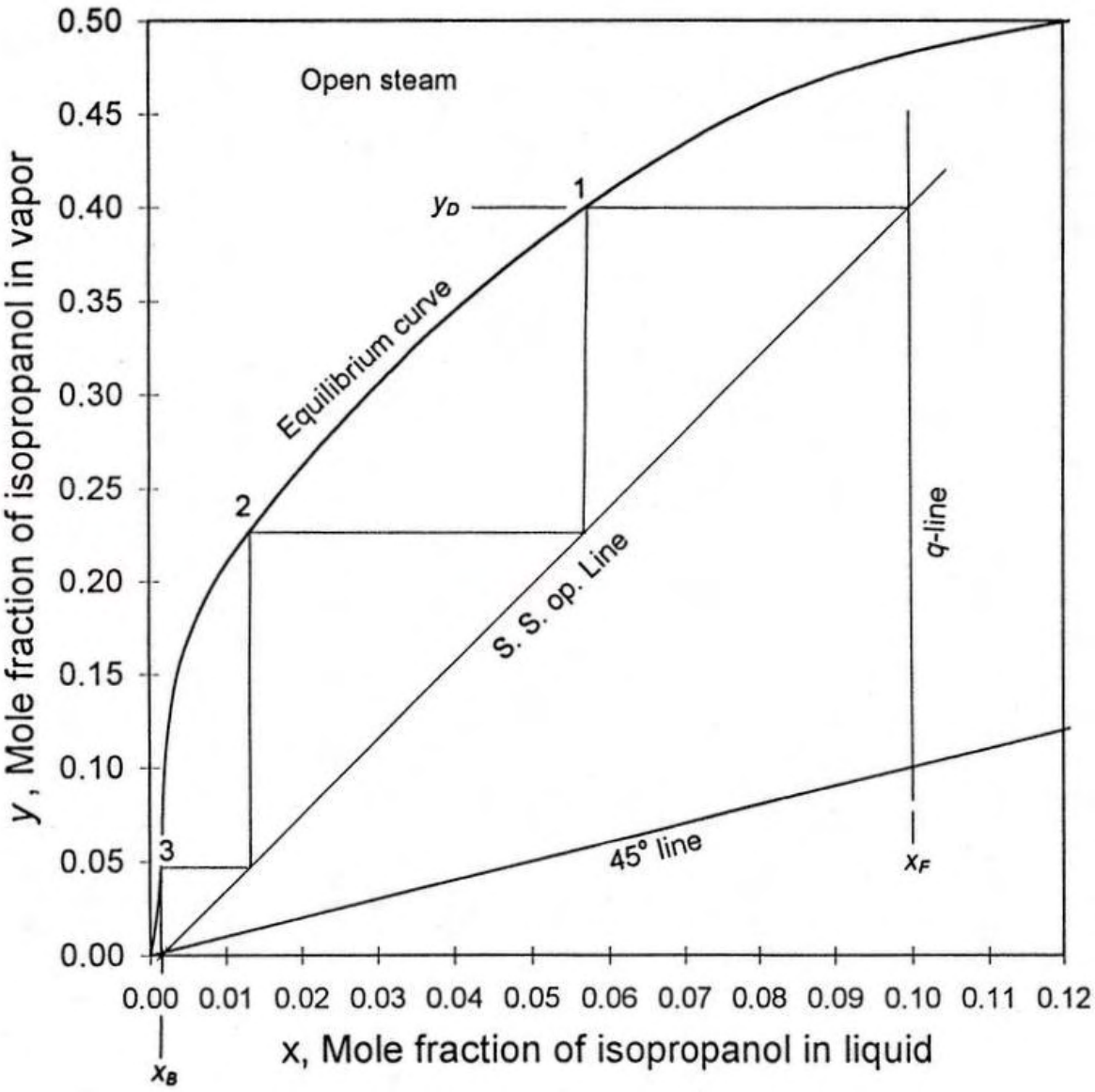
Exercise 7.34 (continued)

Analysis: Partial Reboiler Case:



Exercise 7.34 (continued)

Analysis: Open Steam Case:



Exercise 7.35

Subject: Distillation of two feeds of mixtures of water and acetic acid at 1 atm.

Given: Feed 1 is a bubble-point liquid of 100 kmol/h containing 75 mol% water. Feed 2 is 50 mol% vaporized of 100 kmol/h containing 50 mol% water. Unit consists of a plate column, total condenser, and partial reboiler. Distillate is to contain 98 mol% water. Bottoms is to contain 5 mol% water. Reflux ratio, $L/D = R = 1.2$ times minimum. Vapor-liquid equilibrium data.

Assumptions: Constant molar overflow.

Find: Optimal feed stage locations and number of equilibrium stages.

Analysis: Water is the more volatile component. Compute flow rates of distillate and bottoms.
Overall total material balance: $F_1 + F_2 = 100 + 100 = 200 = D + B$ (1)
Overall water balance: $(0.75)(100) + 0.5(100) = 125 = x_D D + x_B B = 0.98D + 0.05B$ (2)
Solving Eqs. (1) and (2), $D = 123.66$ kmol/h and $B = 76.34$ kmol/h.

Assume the minimum reflux is controlled by the upper feed. This is verified in the McCabe-Thiele diagram below, where the equilibrium curve is plotted from the data, the q-line for Feed 1 is vertical through the point, $x = 0.75$, the q-line for Feed 2 has a slope of -1 starting from $x = 0.50$, and the operating line for the upper section between Feed 1 and the condenser is drawn through the two points, {x=0.98, y=0.98} and the intersection of the equilibrium curve and the q-line for Feed 1. From the plot, for the upper section, $L/V = (0.98\text{-}0.828)/(0.98\text{-}0.75) = 0.661$. From Eq. (7-27), $R = L/D = (L/V)/[1 - (L/V)] = 0.661/(1 - 0.661) = 1.95$. Therefore, $L = 1.95D = 1.95(123.66) = 241.1$ kmol/h and $V = L + D = 241.1 + 123.66 = 364.8$ kmol/h. In the middle section, between the two feeds, $L' = L + F_1 = 241.1 + 100 = 341.1$ kmol/h and $V' = V = 364.8$ kmol/h. Therefore, the slope of the middle section operating line = $L'/V' = 341.1/364.8 = 0.935$. As seen in the diagram below, this line does not cause a pinched region at Feed 2. Therefore, the assumption is correct and $R_{min} = 1.95$.

For an operating reflux ratio of 1.2 times minimum, $L = 1.2(241.1) = 289.3$ kmol/h. The vapor rate in the upper section = $V = L + D = 289.3 + 123.66 = 413$ kmol/h. Therefore the upper section operating line has a slope, $L/V = 289.3/413 = 0.700$ and passes through the point $y = x = 0.98$. It intersects the vertical q-line at $x = 0.75$ and, for the slope of $0.700 = (0.98 - y)/(0.98 - 0.75)$, at $y = 0.819$.

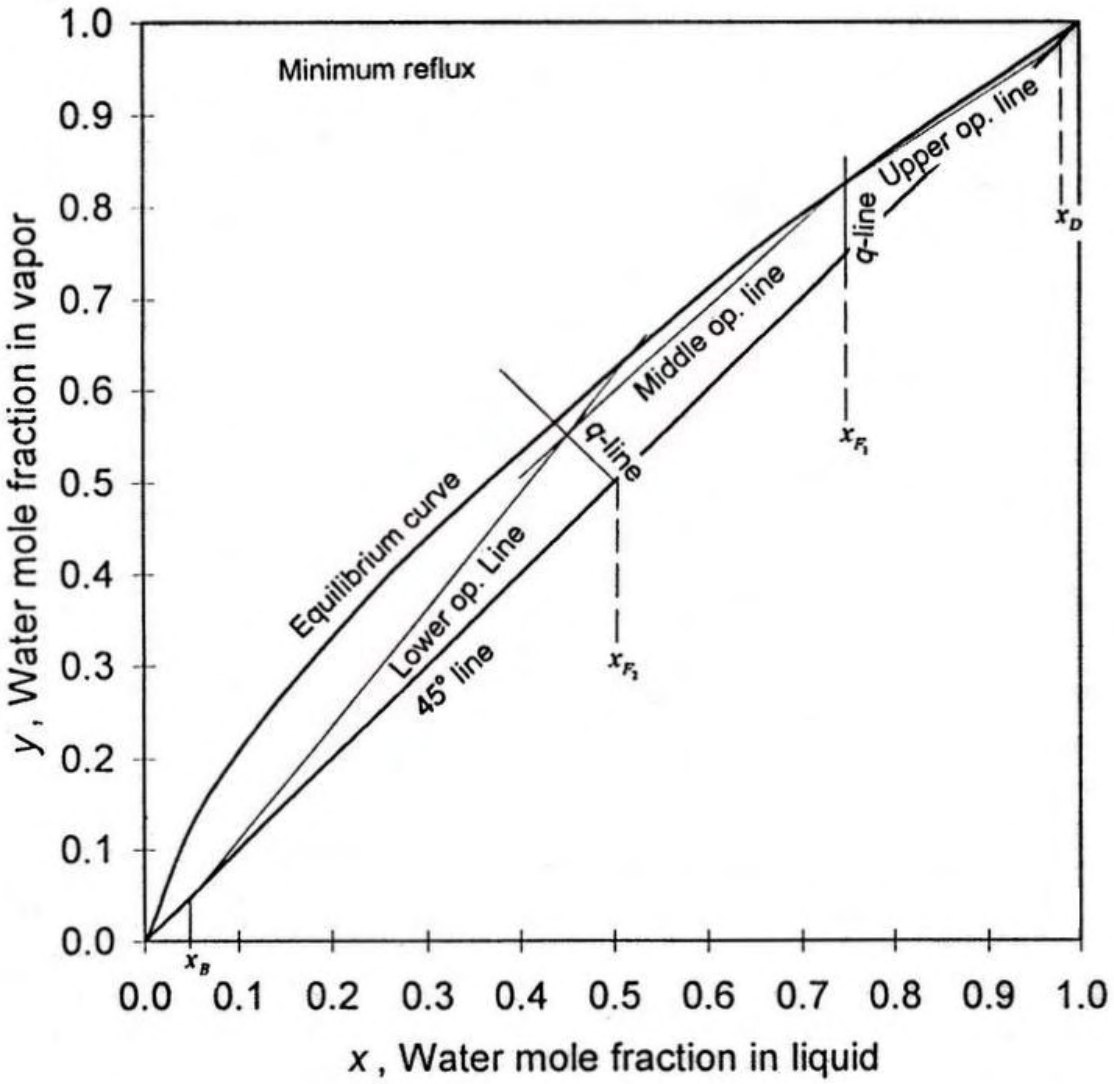
For the middle section, $L' = L + F_1 = 289.3 + 100 = 389.3$ kmol/h and $V' = V = 413$ kmol/h. Therefore, the middle section operating line has a slope of $L'/V' = 389.3/413 = 0.943$ and intersects the q-line for $x = 0.75$ at $y = 0.819$. It intersects the q-line for Feed 2 at $y = 0.543$.

For the lower section, $L'' = L' + 0.5F_2 = 389.3 + 50 = 439.3$ kmol/h and $V'' = V' - 0.5F_2 = 413 - 50 = 363$ kmol/h. Therefore, the lower section operating line has a slope of $L''/V'' = 439.3/363 = 1.210$ and intersects the q-line for Feed 2 at $y = 0.543$ and the 45° line at $x_B = 0.05$.

In the McCabe-Thiele diagrams below and on the next page for the high, middle, and low mole fraction regions, the three operating lines are drawn and the equilibrium stages are stepped off so as to place the two feeds at their optimal locations. As seen, the number of equilibrium stages required = just less than 33 equilibrium stages. Call it 32 equilibrium stages in the column and a partial reboiler. Optimal feed stages are located at Stages 17 and 27 from the top.

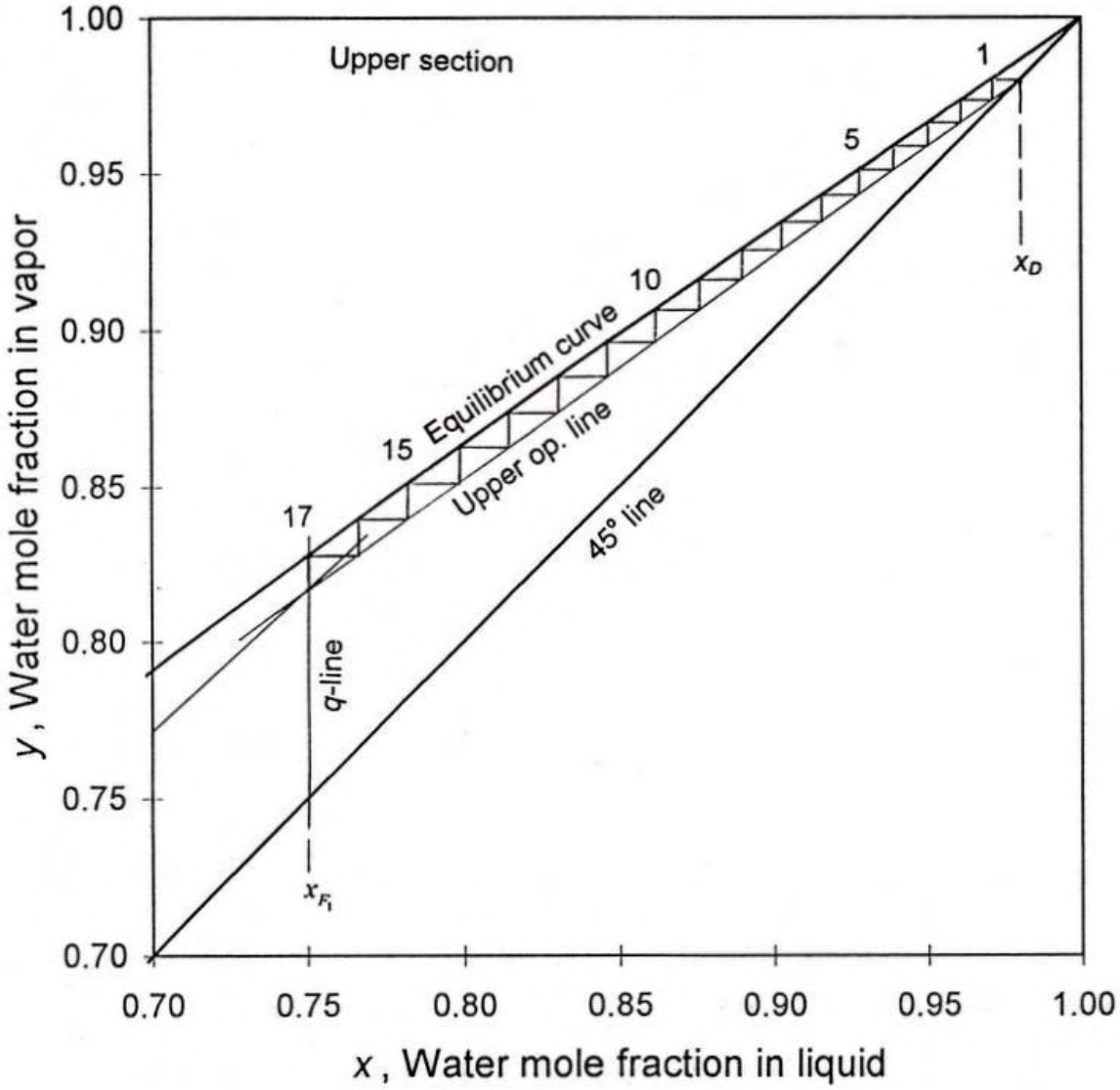
Exercise 7.35 (continued)

Analysis: (continued)



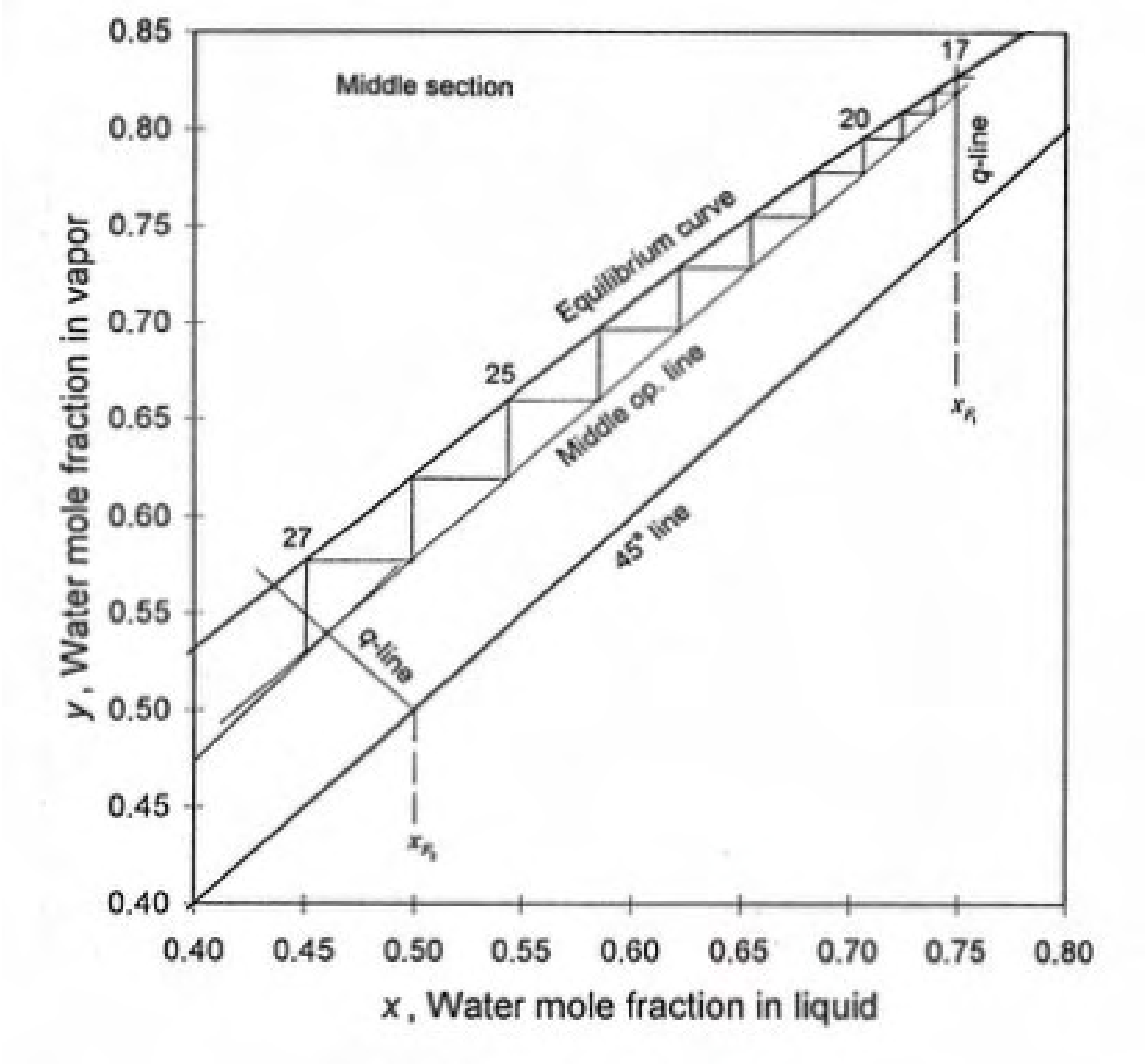
Exercise 7.35 (continued)

Analysis: (continued)



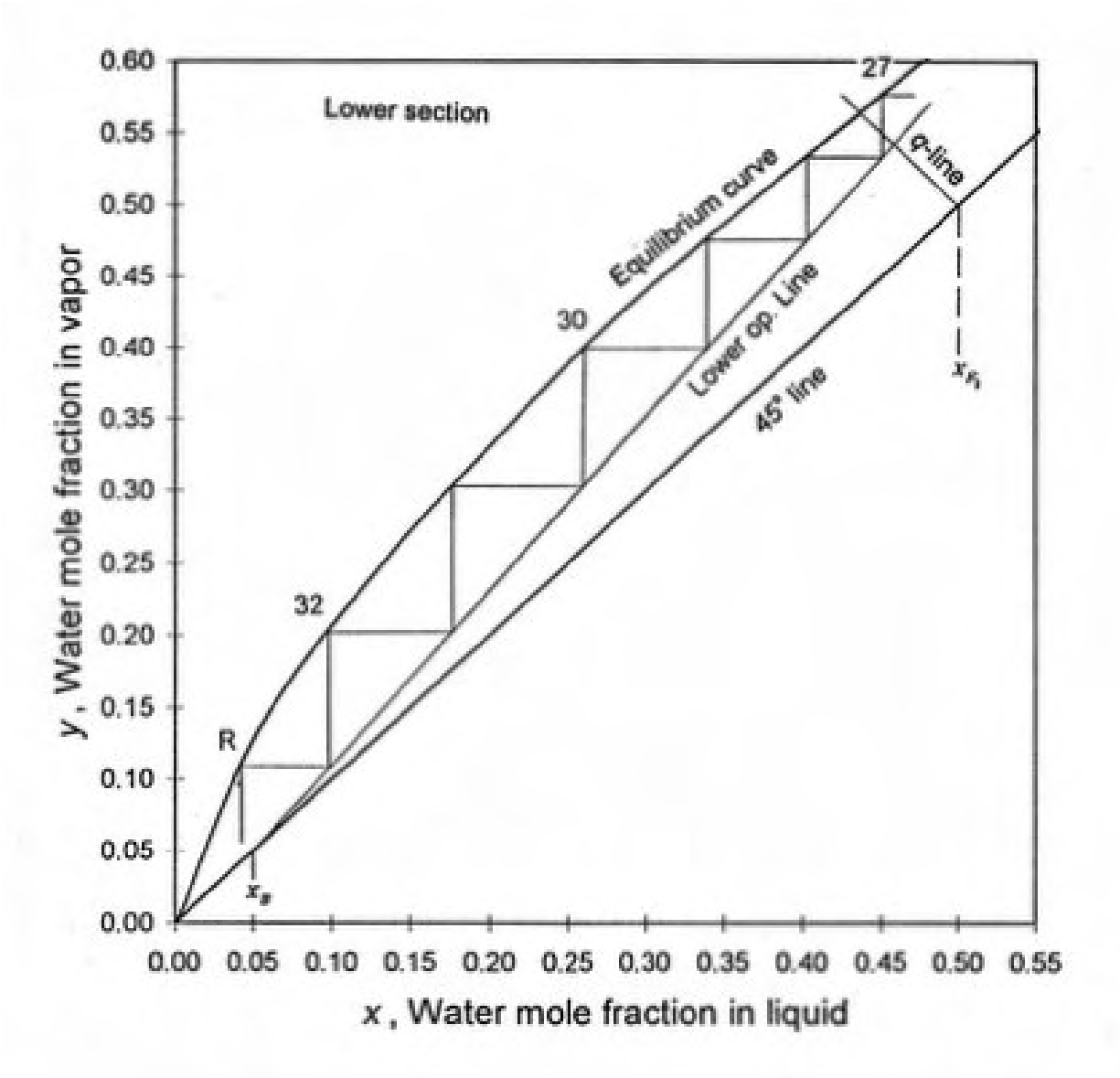
Exercise 7.35 (continued)

Analysis: (continued)



Exercise 7.35 (continued)

Analysis: (continued)



Exercise 7.36

Subject: Distillation at 1 atm of a mixture of methanol (M) and ethanol (E) to obtain a distillate, bottoms, and a liquid sidestream.

Given: 100 kmol/h of a 25 mol% vaporized mixture of 75 mol% methanol in ethanol. Distillate is 96 mol% methanol and bottoms is 5 mol% methanol. Unit consists of a total condenser, plate column, and partial reboiler. Sidestream is 15 kmol/h of 20 mol% methanol. Reflux ratio, R = 1.2 times minimum.

Assumptions: Constant molar overflow. Raoult's law K-values.

Find: Number of theoretical stages and optimal locations of feed and sidestream.

Analysis: First compute the material balance.

Overall total material balance: $F = 100 = D + B + S = D + B + 15$ (1)

Overall methanol material balance: $75 = 0.96D + 0.05B + 0.20(15)$ (2)

Solving Eqs. (1) and (2), D = 74.45 kmol/h and B = 10.55 kmol/h

Now determine the equilibrium curve. At 1 atm (14.696 psia), methanol boils at 64.7°C and ethanol boils at 78.4°C. From Fig. 2.4, the vapor pressure of ethanol at 64.7°C = 8.2 psia. The vapor pressure of methanol at 78.4°C = 25 psia. For the Raoult's law K-value, Eq. (2-44) applies. Combining this equation with the definition of the relative volatility of Eq. (2-21), gives, for methanol with respect to the less volatile ethanol, $\alpha_{M,E} = (P^s)_M / (P^s)_E$. At 64.7°C, $\alpha_{M,E}$ = 14.696/8.2 = 1.79. At 78.4°C, $\alpha_{M,E}$ = 25/14.696 = 1.70. Since these values are close (within about 5%), use an equilibrium curve based on a constant $\alpha = (1.70 + 1.79)/2 = 1.745$. From Eq. (7-3), the curve is computed from,

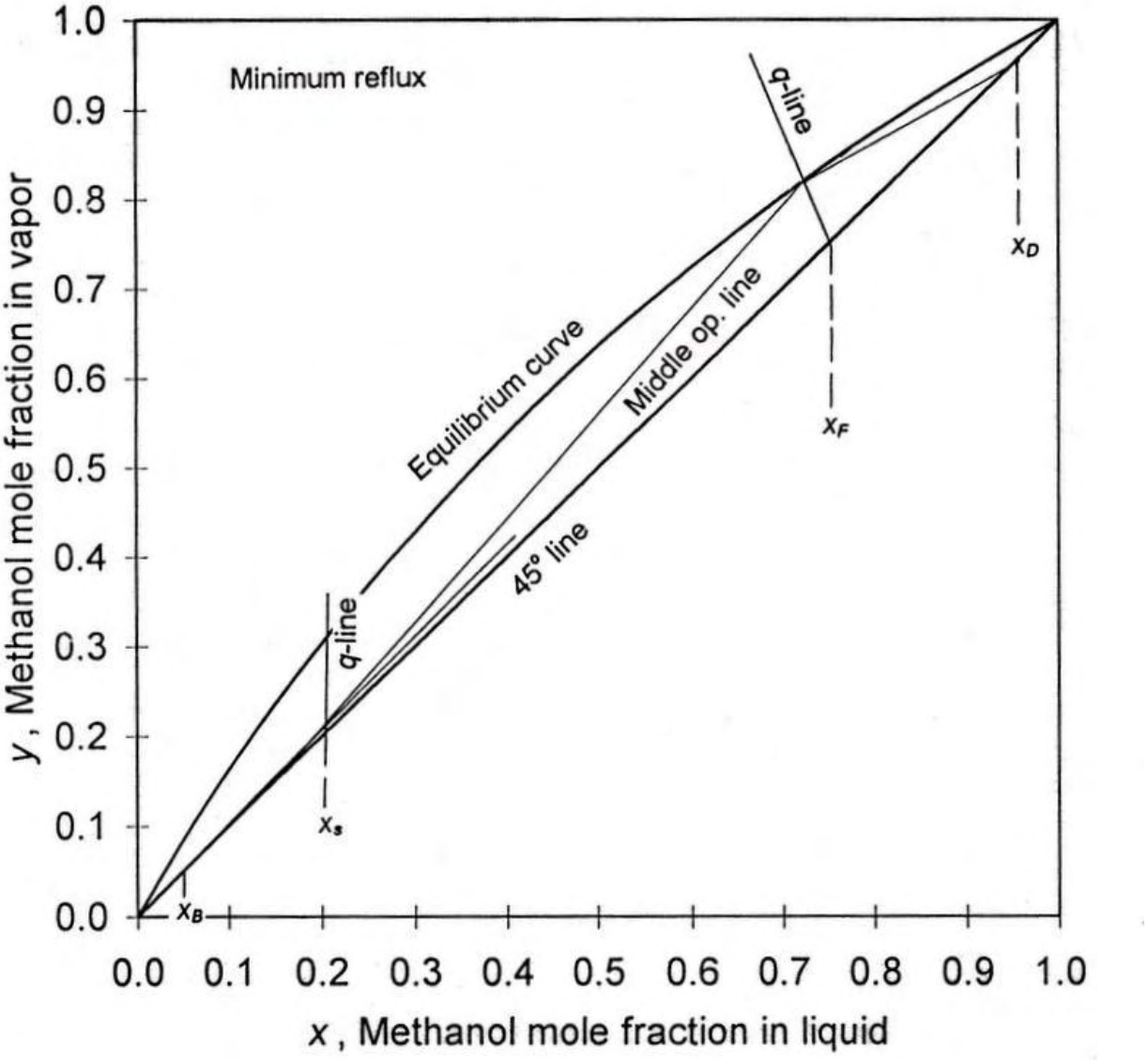
$$y = \alpha x/[1 + x(\alpha-1)] = 1.745x/(1+0.745x) \qquad (3)$$

The McCabe-Thiele diagram on the next page shows the operating lines for determining the minimum reflux ratio. It assumes that the pinch region occurs at the feed stage and not at the sidestream stage. From Eq. (7-18), q for 25 mol% vaporized = 0.75. From Eq. (7-26), the slope of the q-line = $q/(q-1)$ = 0.75/(0.75-1) = -3. The upper section operating line intersects the q-line and equilibrium curve at y=0.823 and x=0.727. Thus, slope of the upper section operating line = L/V = (0.96-0.823)/(0.96-0.727) = 0.588. From Eq. (7-27), $R_{min} = (L/V)/[1 - (L/V)]$ = 0.588/(1-0.588) = 1.427. Therefore, L = 1.427(74.45) = 106.3 kmol/h and $V = L + D$ = 106.3 + 74.45 = 180.75 kmol/h. In the middle section between the feed stage and sidestream stage, for 25 mol% vaporization, $L' = L + 0.75(100)$ = 106.3 + 75 = 181.3 kmol/h and $V' = V - 0.25(100)$ = 180.75 - 25 = 155.75 kmol/h. Thus, L'/V' = 181.3/155.75 = 1.164. The middle section operating line has this slope and passes through y=0.823 and x=0.727. In the lower section operating line below the sidestream, for a liquid sidestream flow rate of 15 kmol/h, $L'' = L' - S$ = 181.3 - 15 = 166.3 kmol/h and $V'' = V'$ = 155.75 kmol/h. Thus, L''/V'' = 166.3/155.75 = 1.068. This line passes through the point y=0.05 and x = 0.05 with the slope of 1.068. It also intersects the middle section operating line at the sidestream composition, x_s = 0.20. These three operating lines are drawn in the McCabe-Thiele diagram, showing that the middle section operating line lies below

Exercise 7.36 (continued)

Analysis: (continued)

the equilibrium curve. Therefore, the assumption that the minimum reflux is controlled by the feed stage is verified and the minimum reflux ratio is 1.427.



For actual operation, reflux ratio = $1.2R_{min}$ = 1.2(1.427) = 1.712. Reflux rate in upper section = L = $1.2L_{min}$ = 1.2(106.3) = 127.6 kmol/h. Vapor rate = $V = L + D$ = 127.6 + 74.45 = 202.05 kmol/h. Slope of upper section operating line = L/V = 127.6/202.05 = 0.632. For constant molar overflow, the flow rates in the other sections are:

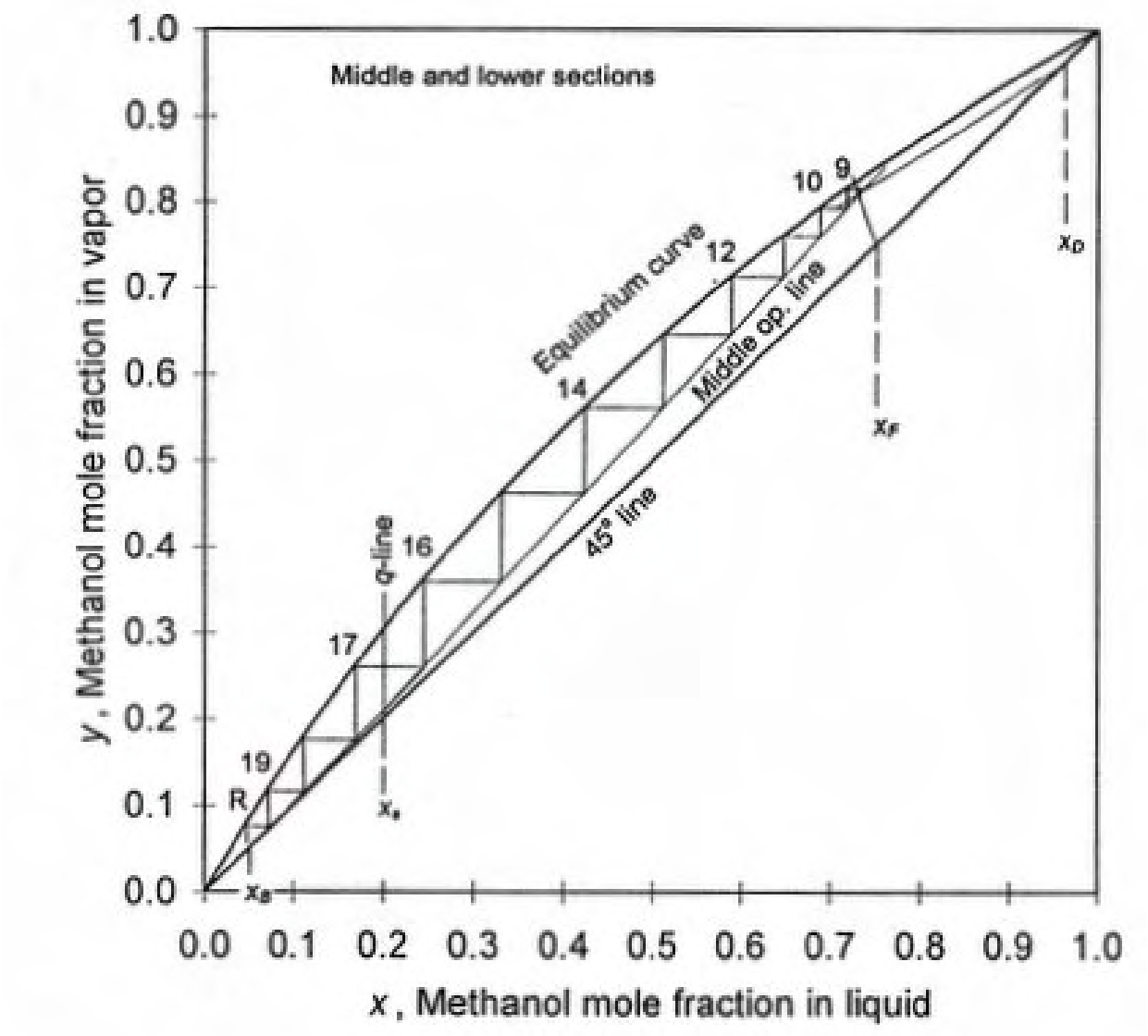
Middle section: L' = 202.6 kmol/h V' = 177.05 kmol/h L'/V' = 1.144

Lower section: L'' = 187.6 kmol/h V'' = 177.05 kmol/h L''/V'' = 1.060

Exercise 7.36 (continued)

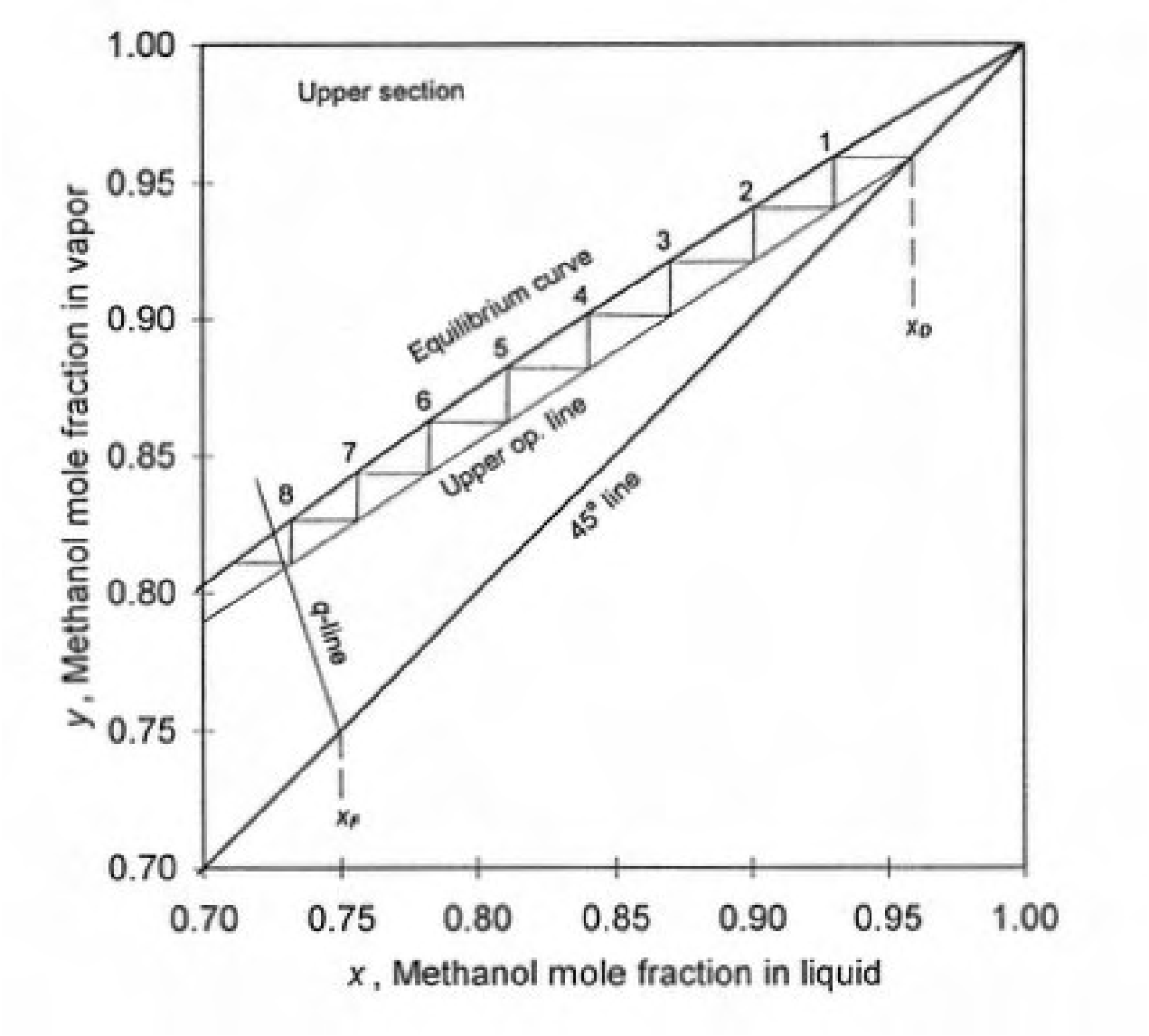
Analysis: (continued)

In the McCabe-Thiele diagrams below, upper, middle, and lower operating lines are based on these values starting from the upper line, which passes through the point $x = 0.96$ on the 45^{o} line. Equilibrium stages are stepped off starting from the distillate composition and switching operating lines at the appropriate times to determine the optimal feed stage and sidestream stage locations. A separate McCabe-Thiele diagram is used for the upper section to achieve better accuracy. As seen 19 equilibrium stages plus a partial reboiler are required. The optimal feed stage is 9 from the top and the optimal sidestream stage is 17 from the top.



Exercise 7.36 (continued)

Analysis: (continued)



Exercise 7.37

Subject: Distillation at 1 atm of a mixture of toluene and phenol for a given boilup ratio, with an alternative using an interreboiler.

Given: 1,000 kmol/h of a saturated liquid feed of 25 mol% toluene. Distillate is 98 mol% toluene and bottoms is 2 mol% toluene. The base unit consists of a total condenser, a plate column, and a partial reboiler, with a boilup ratio, $V_B = \bar{V} / B = 1.15$ times minimum. The alternative unit adds an interreboiler midway in the stripping section to provide 50% of the boilup. A table of *T-y-x* phase equilibrium data

Assumptions: Constant molar overflow.

Find: For each unit, determine the number of theoretical stages. For the alternative unit, determine the temperature of the interreboiler stage.

Analysis: Toluene is the more volatile unit.

Base unit:

From the McCabe-Thiele diagram below, the minimum boilup ratio is determined from the slope of the stripping section operating line that intersects the equilibrium curve at the feed composition of $x_F = 0.25$.

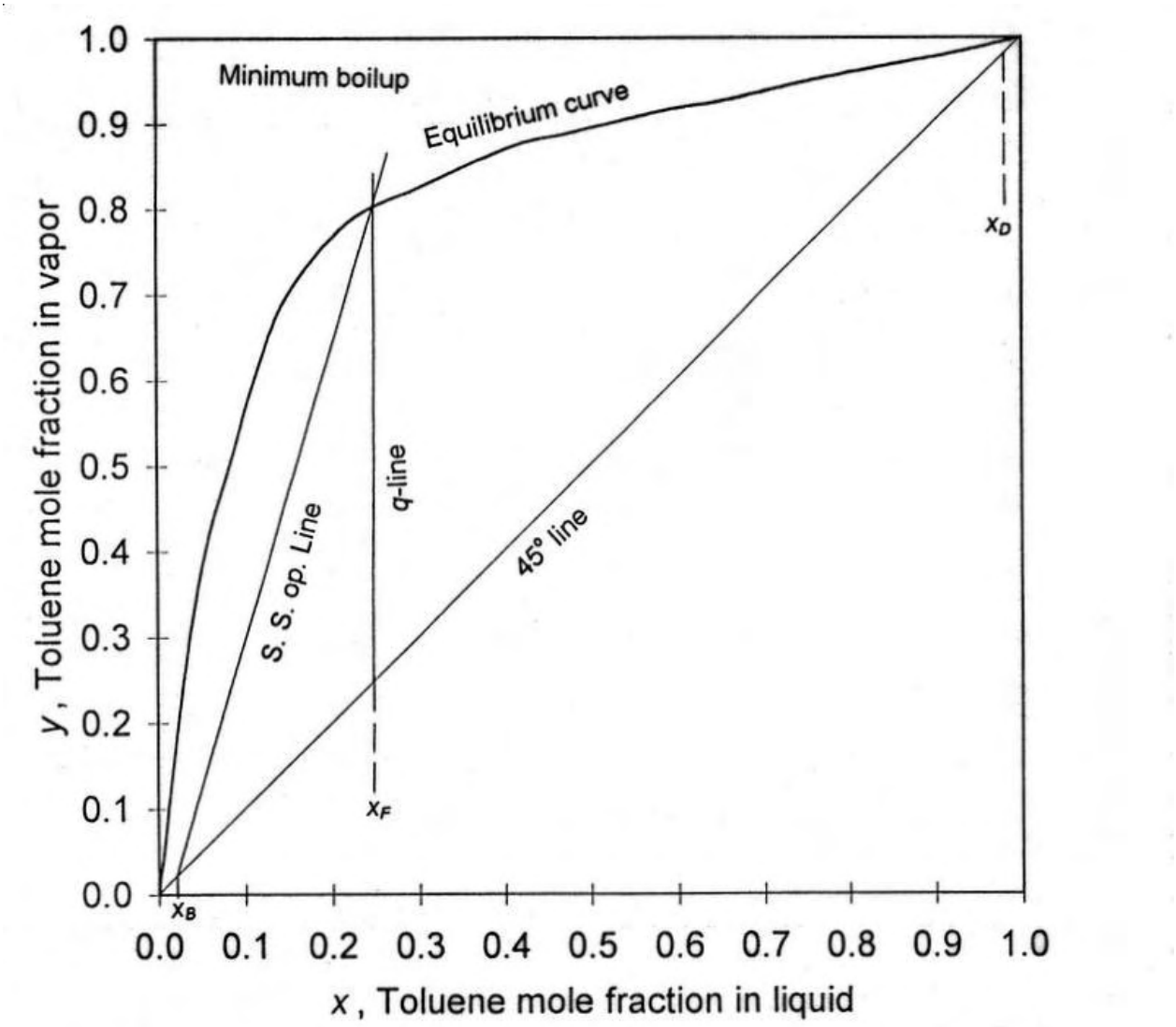
$$\left(\bar{L}/\bar{V}\right)_{\min} = \frac{0.815 - 0.02}{0.25 - 0.02} = 3.46$$

From Eq. (7-28),

$$\left(V_B\right)_{\min} = \frac{1}{\left(\bar{L}/\bar{V}\right)_{\min} - 1} = \frac{1}{3.46 - 1} = 0.407$$

Exercise 7.37 (continued)

Analysis: Base Case (continued)



For column operation, $V_B = 1.15(V_B)_{min} = 1.15(0.407) = 0.468$

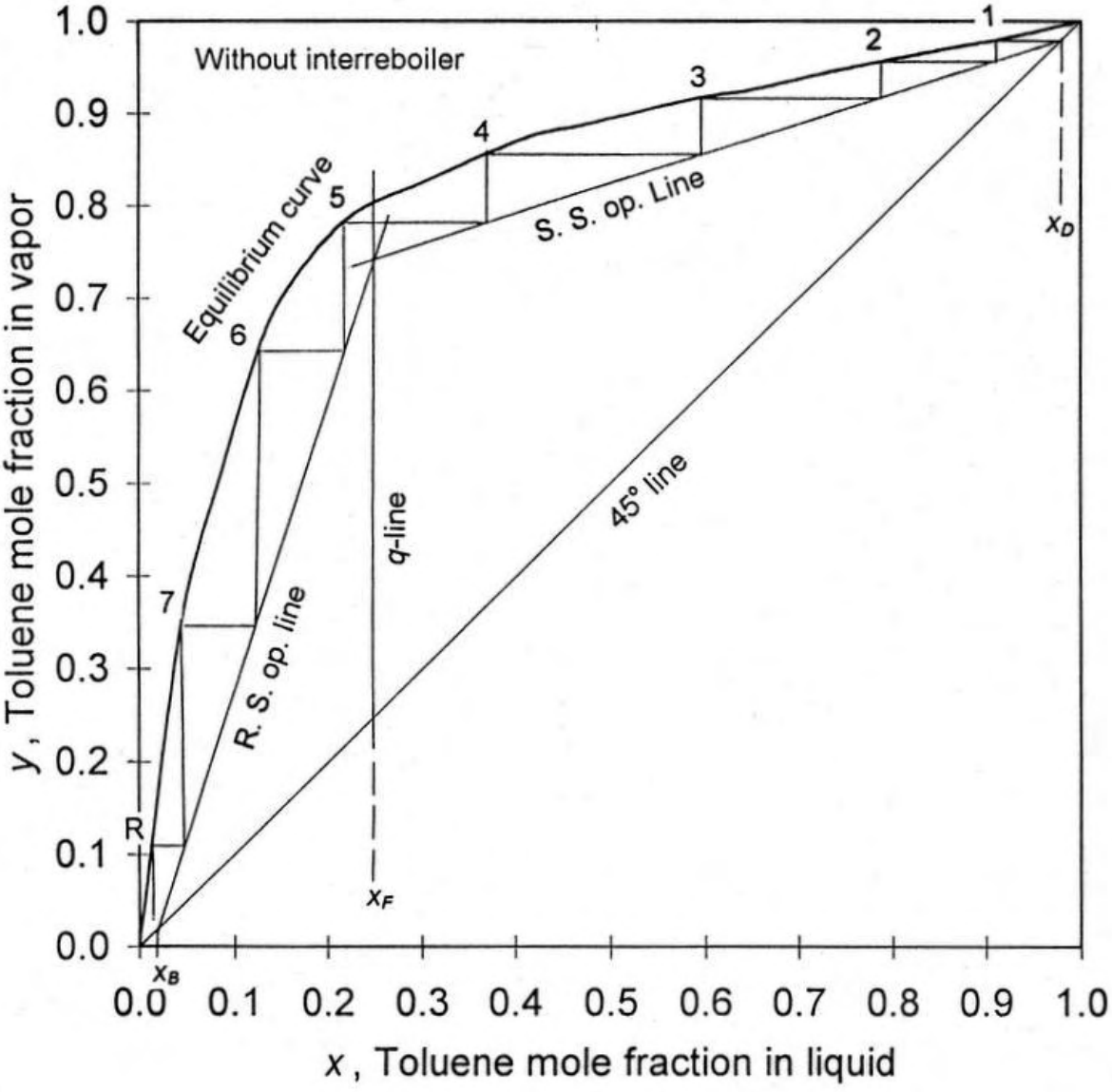
From Eq. (7-12), the slope of the stripping section operating line is,

$$\overline{L}/\overline{V} = \frac{V_B + 1}{V_B} = \frac{0.468 + 1}{0.468} = 3.14$$

As shown in the McCabe-Thiele diagram, below, a line of this slope is drawn through the point $x = y = 0.02$ until it intersects the q-line. Equilibrium stages are stepped off, starting from the distillate point at $y = x = 0.98$. The optimal feed stage location is located as shown at stage 5 from the top. The total number of stages required is just less than 8, with one of those stages being the partial reboiler.

Exercise 7.37 (continued)

Analysis: Base Case (continued)



Exercise 7.37 (continued)

Analysis: (continued)

Alternative unit with Interreboiler:

For column operation with an interreboiler that provides 50% of the reboiler duty, the operating boilup ratio between the reboiler and the interreboiler is 50% of 0.468 or 0.234. From Eq. (7-12), the slope of the operating line in this region is:

$$\bar{L}/\bar{V} = \frac{V_B + 1}{V_B} = \frac{0.234 + 1}{0.234} = 5.27$$

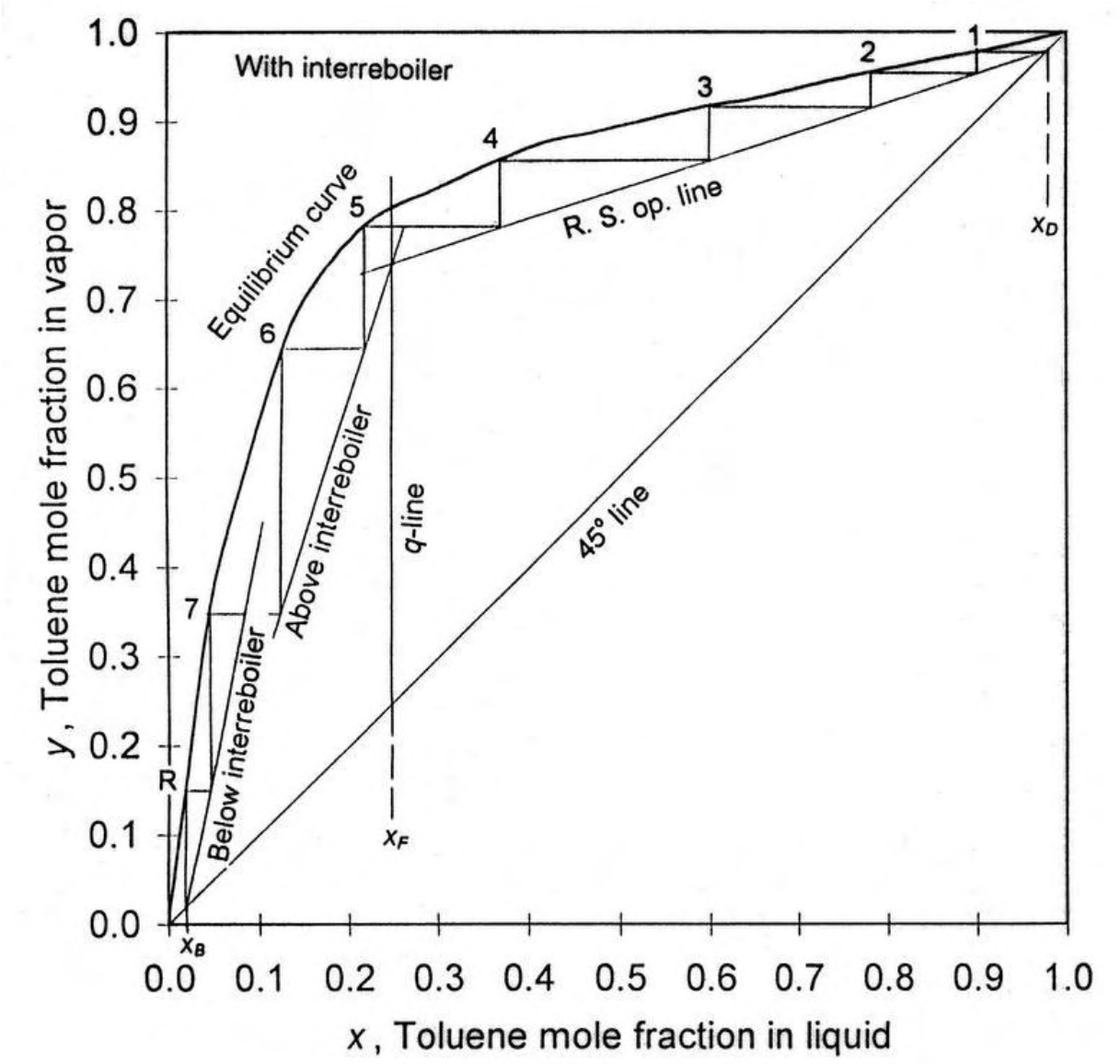
Between the interreboiler and the feed stage, the slope of the operating line remains at 3.14, based on a material balance around the column section from the bottoms to the region between the interreboiler and the feed stage. These two operating lines are shown in the McCabe-Thiele diagram below, where both pass through the point $y = x = 0.02$. Stepping off stages from the bottom, it is seen that 3 stages are needed below the feed stage. The first stage is the partial reboiler. The interreboiler is located at the second equilibrium stage. A total of 8 equilibrium stages is required, just slightly more than that when all of the heat input is to the partial reboiler at the bottom of the column.

The vapor composition of the interreboiler stage is 0.345, which from the given *T*-*y*-*x* phase equilibrium data corresponds to a temperature of approximately 173°C. The interreboiler could also be located at the third stage from the bottom. The would increase the number of stages by about half of a stage and lower the temperature of the interreboiler stage to 162°C.

Exercise 7.37 (continued)

Analysis: (continued)

Alternative unit with Interreboiler:



Exercise 7.38

Subject: Effect of the addition of an intercondenser and interreboiler to a distillation column separating n-butane and n-pentane.

Given: Distillate and bottoms compositions of actual operation (before addition of intercondenser and interreboiler) compared to design specification.

Assumptions: Constant molar overflow. Constant relative volatility. Column is large enough in diameter to handle increased reflux and boilup. Raoult's law (ideal solutions and ideal gas law).

Find: Whether the addition can improve the operation because of the increased reflux and boilup produced by the intercondenser and interreboiler.

Analysis:

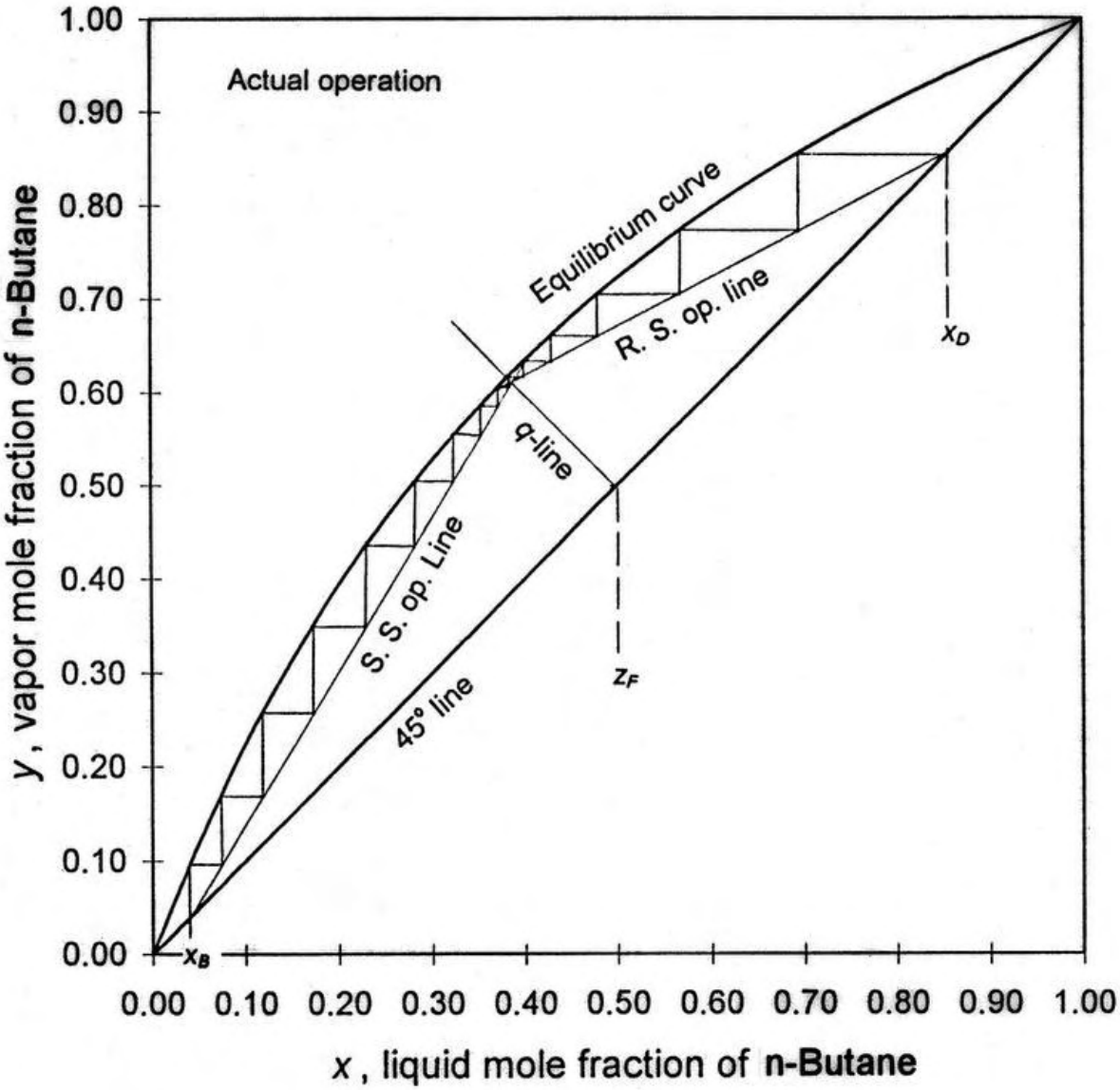
First, estimate the average relative volatility for nC_4/nC_5. Assume a distillate temperature of 120°F so that cooling water can be used in the condenser. This corresponds to a saturation pressure of about 70 psia. Using Fig. 2.8 with Eqs. (2-21) and (2-44), the relative volatility of butane with respect to pentane is $\alpha = 1.1/0.38 = 2.9$. Assuming a 5 psi pressure drop, gives a bottoms pressure of 75 psia and a corresponding temperature of 200°F. Using Fig. 2.8 with Eqs. (2-21) and (2-44), $\alpha = 2.1/0.9 = 2.3$. Take the average relative volatility as 2.6 and draw a *y*-*x* equilibrium curve using Eq. (7-3),

$$y = \frac{\alpha x}{1 + x(\alpha - 1)} = \frac{2.6x}{1 + 1.6x} \qquad (1)$$

The equilibrium curve, based on Eq. (1) is shown below in a McCabe-Thiele diagram. Included on the diagram are arbitrary operating lines and a *q*-line for an equimolar feed that is 50 mol% vaporized. Using these lines, 15 equilibrium stages are stepped off between the compositions of the actual operation, $x_D = 1 - 0.1349 = 0.8651$ and $x_B = 0.0428$. The slope, *L/V*, of the rectifying section operating line is 0.52.

Exercise 7.38 (continued)

Analysis: Actual operation before addition (continued)



Exercise 7.38 (continued)

Analysis: Addition (continued)

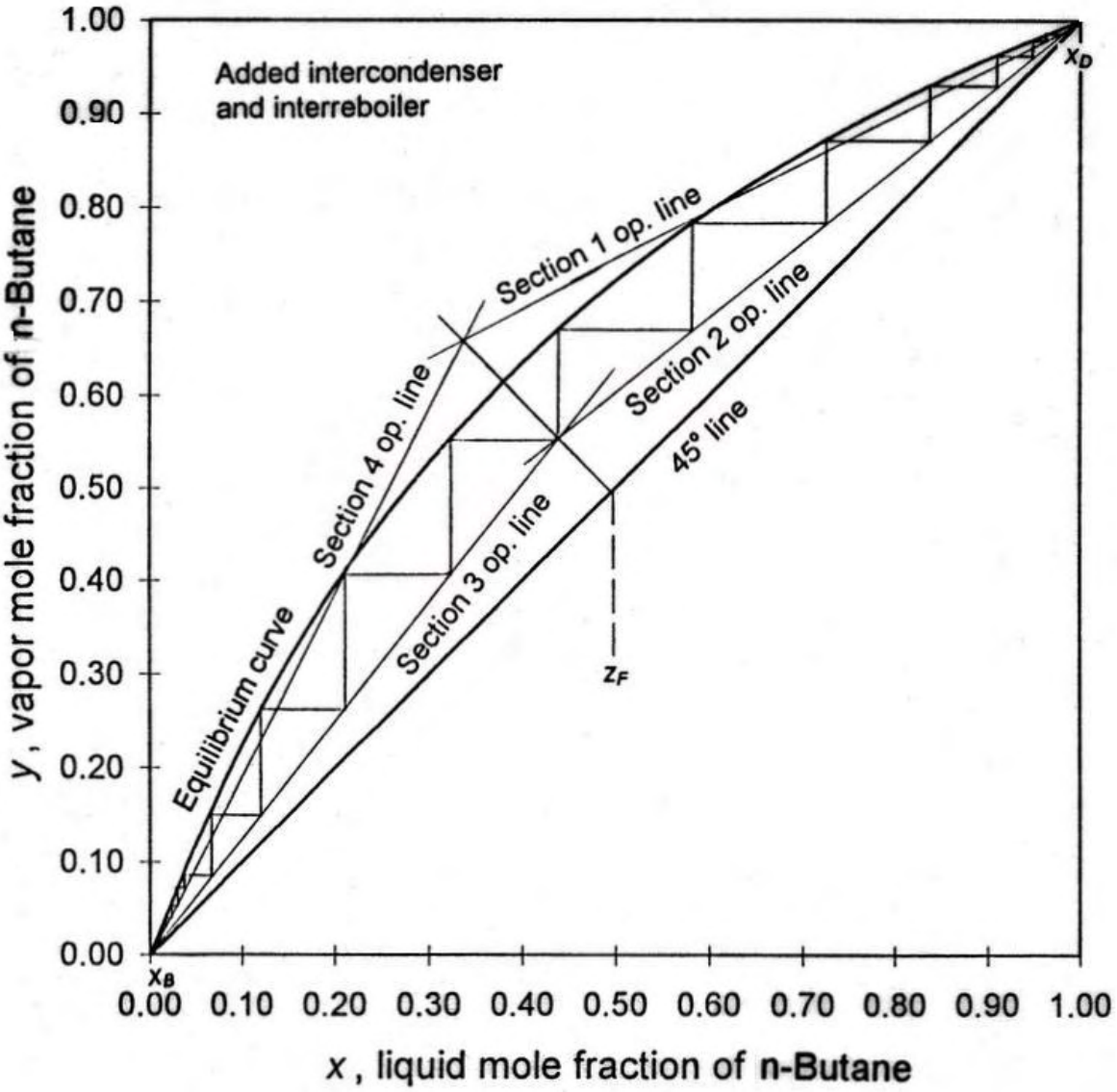
When an interreboiler is added between the reboiler and the feed stage and an intercondenser is added between the feed stage and the overhead condenser, the column is made up of 4 sections instead of 2. Each section has its own operating line as shown in the McCabe-Thiele diagram below. In order to maintain the same reflux ratio and boilup ratio, the intercondenser is designed to condense a molar flow rate equal to that produced by the interreboiler. Thus, in Section 2 between the intercondenser and the feed stage, the *L/V* ratio is higher than the value in Section 1 between the overhead condenser and the intercondenser. Thus, the two operating lines above the feed stage have different slopes, but by material balance both lines pass through the distillate composition on the 45^o line.

Correspondingly, in Section 3 between the interreboiler and the feed stage, the *L/V* ratio is lower than the value in Section 4 between the reboiler and the interreboiler. Thus, the two operating lines below the feed stage have different slopes, but by material balance both lines pass through the bottoms composition on the 45^o line. Also note that by material balance, the operating lines for Sections 1 and 4 intersect on the 45^o line, and the operating lines for Sections 2 and 3 intersect on the 45^o line. Starting from $x_D = 0.9974$, stages are stepped off from the top between the operating line for Section 1 and the equilibrium curve for a few stages before switch to the operating line for Section 2. Then 5 stages are stepped off until the feed stage is reached. Then, 4 stages are stepped off between the operating line for Section 3 and the equilibrium curve before switching to the operating line for Section 4.

The switches are made to maintain the same number of total stages, 15, and the same location for the feed stage. Other combinations of arbitrary operating lines and a *q*-line can be used to illustrate the potential of an intercondenser and interreboiler. The important thing to note is that the addition of an intercondenser and interreboiler increases the distance between the equilibrium curve and the operating lines for Sections 2 and 3 so that the steps in Sections 2 and 3 accomplish larger composition changes.

Exercise 7.38 (continued)

Analysis: Addition (continued)



Exercise 7.39

Subject: Distillation of a mixture of para-dichlorobenzene (P) and ortho-dichlorobenzene (O), two close-boiling isomers, using the McCabe-Thiele diagram, with the Kremser equation to accurately calculate the separations at the two ends of the column.

Given: Feed of 62 mol% P and 38 mol% O that is slightly vaporized with $q = 0.9$. Distillate is liquid of 98 mol% P. Bottoms is 96 mol% O. Pressures at top and bottom are 20 psia and 15 psia, respectively. Reflux ratio, $R = 1.15$ times minimum.

Assumptions: Constant molar overflow. Total condenser and partial reboiler. Average relative volatility based on Raoult's law.

Find: Number of theoretical stages from McCabe-Thiele diagram, using Kremser supplement for the two ends of the column.

Analysis: From a simulation program or handbook, the temperatures at the top and bottom of the column, based on the given pressures and product compositions, are determined to be approximately 350 and 380°F. From vapor pressure data, e.g. from CHEMCAD, using Eq. (7-1),

$$\alpha_{P,O} \text{ at } 350^\circ\text{F} = \frac{P_P^s}{P_O^s} = \frac{15.65}{13.41} = 1.167 \quad \text{and} \quad \alpha_{P,O} \text{ at } 380^\circ\text{F} = \frac{P_P^s}{P_O^s} = \frac{23.16}{19.98} = 1.159$$

Take the average relative volatility as (1.167 + 1.159)/2 = 1.163.
From Eq. (7-26), the slope of the q-line = $q/(q - 1)$ = 0.9/(0.9 - 1) = -9. Feed is 10 mol% vaporized.

Apply the Fenske-Underwood-Gilliland method to obtain an initial estimate of reflux and stage requirements. Can use the SHOR model in CHEMCAD. The results are:

$N_{min} = 48$, $R_{min} = 9.37$ $R = 1.15R_{min} = 10.77$ $N = 103$ (102 + reboiler)
N of feed = stage 50 from the top

To construct the equilibrium curve for the McCabe-Thiele method, use Eq. (7-3),

$$y_P = \frac{\alpha_{P\text{-}O} x_P}{1 + x_P(\alpha_{P\text{-}O} - 1)} = \frac{1.163 x_P}{1 + 0.163 x_P} \qquad (1)$$

From Eq. (7-9), the slope of the rectifying section operating line is,

$$L/V = R/(R+1) = 10.77/(10.77 + 1) = 0.9150$$

Exercise 7.39 (continued)

Analysis: (continued)

This line passes through $x = 0.98$ on the 45° line. The equation for this line is given by Eq. (7-9),

$$y = \left(\frac{L}{V}\right)x + \left(\frac{1}{R+1}\right)x_D = 0.915x + \left(\frac{1}{11.77+1}\right)(0.98) = 0.915x + 0.08326 \qquad (2)$$

Below the feed stage, with 10 mol% vaporization of the feed, $\overline{L}/\overline{V} = 1.0535$. From a rearrangement of Eq. (7-12), the boilup ratio, V_B, is 18.6916. The equation of the stripping section operating line is given by Eq. 7-14),

$$y = \left(\frac{\overline{L}}{\overline{V}}\right)x - \left(\frac{1}{V_B}\right)x_D = 1.0535x - \left(\frac{1}{18.6916}\right)(0.04) = 1.0535x - 0.00214 \qquad (3)$$

The equation for the q-line is given by Eq. (7-26),

$$y = \left(\frac{q}{q-1}\right)x - \left(\frac{1}{q-1}\right)z_F = \left(\frac{0.9}{0.9-1}\right)x - \left(\frac{1}{0.9-1}\right)(0.62) = -9x + 6.2 \qquad (4)$$

Based on Eqs. (1) to (4), the McCabe-Thiele diagram in terms of P, the more volatile component, is drawn below for three regions: (2) $x = 0.2$ to 0.4, (3) $x = 0.4$ to 0.6, and (4) $x = 0.6$ to 0.8, in order to gain accuracy. In these three regions, 28 stages are stepped off in the rectifying section up to $x = 0.8$, and 34.3 stages are stepped off in the stripping section down to $x = 0.2$.

Let region (1) extend from $x = 0.8$ to 0.98 (i.e. x_D). Apply the Kremser equation, Eq. (7-39) to this region. Apply this equation to the heavy component, O. Obtain the K-value for O from the top α of 1.167, taking the K-value for P = 1.00. Therefore, $K_O = 1/1.167 = 0.857$. Therefore, the absorption factor, $A = L/KV = 0.915/0.857 = 1.067$. Other quantities needed in Eq. (7-39) are: $x_o = 1 - (x_D)_P = 1 - 0.98 = 0.02$ $\qquad y_1 = x_o = 0.02$

From Eq. (2), for $x_N = 0.8$, y_{N+1} for P = 0.8153. Therefore, for O, $y_{N+1} = 1 - 0.8153 = 0.1847$.

$$N_R = \frac{\log\left[\frac{1}{A} + \left(1 - \frac{1}{A}\right)\left(\frac{y_{N+1} - x_o K}{y_1 - x_o K}\right)\right]}{\log A} = \frac{\log\left[\frac{1}{1.067} + \left(1 - \frac{1}{1.067}\right)\left(\frac{0.1847 - 0.02(0.857)}{0.02 - 0.02(0.857)}\right)\right]}{\log 1.067} = 23.6$$

Let region (5) extend from $x = 0.04$ (i.e. x_B) to 0.20. Apply the Kremser equation, Eq. (7-40) to this region. Apply this equation to the light component, P. Obtain the K-value for P from the bottom α of 1.159, taking the K-value for O = 1.00. Therefore, $K_P = 1.159$. Therefore, the absorption factor in the stripping section is $\overline{A} = \overline{L}/K\overline{V} = 1.0535/1.159 = 0.9085$. Other values needed in Eq. (7-40) are $x_1 = x_B = 0.04$ and $x_{N+1} = 0.20$. Therefore,

$$N_S = \frac{\log\left[\overline{A} + (1 - \overline{A})\left(\frac{x_{N+1} - x_1/K}{x_1 - x_1/K}\right)\right]}{\log\left(\frac{1}{\overline{A}}\right)} = \frac{\log\left[0.9085 + (1 - 0.9085)\left(\frac{0.20 - 0.04/1.159}{0.04 - 0.04/1.159}\right)\right]}{\log\left(\frac{1}{0.0985}\right)} = 13.5$$

Exercise 7.39 (continued)

Analysis: (continued)

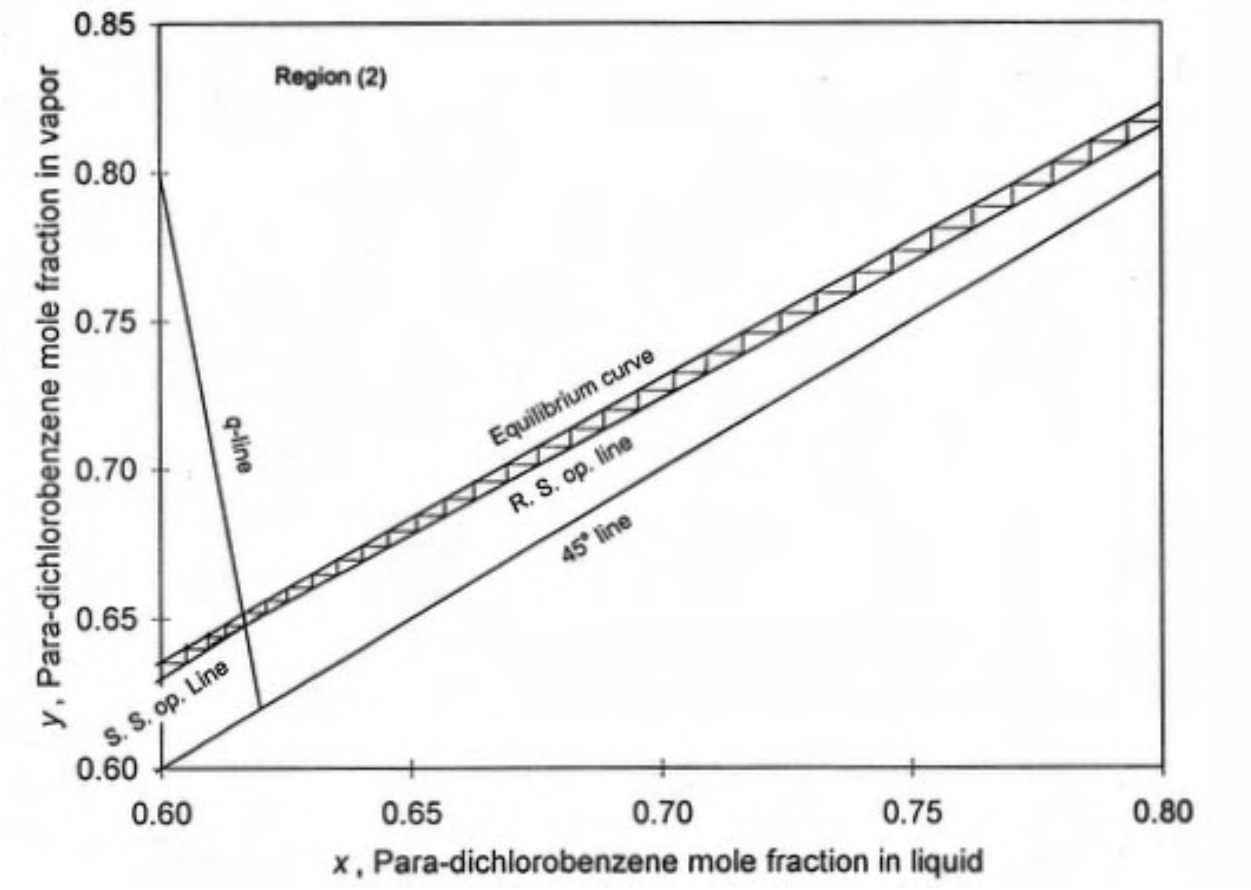
Summing the above results,

Number of equilibrium stages in the rectifying section = 28 + 23.6 = 51.6 stages

Number of equilibrium stages in the stripping section = 34.3 + 13.5 = 47.8 stages

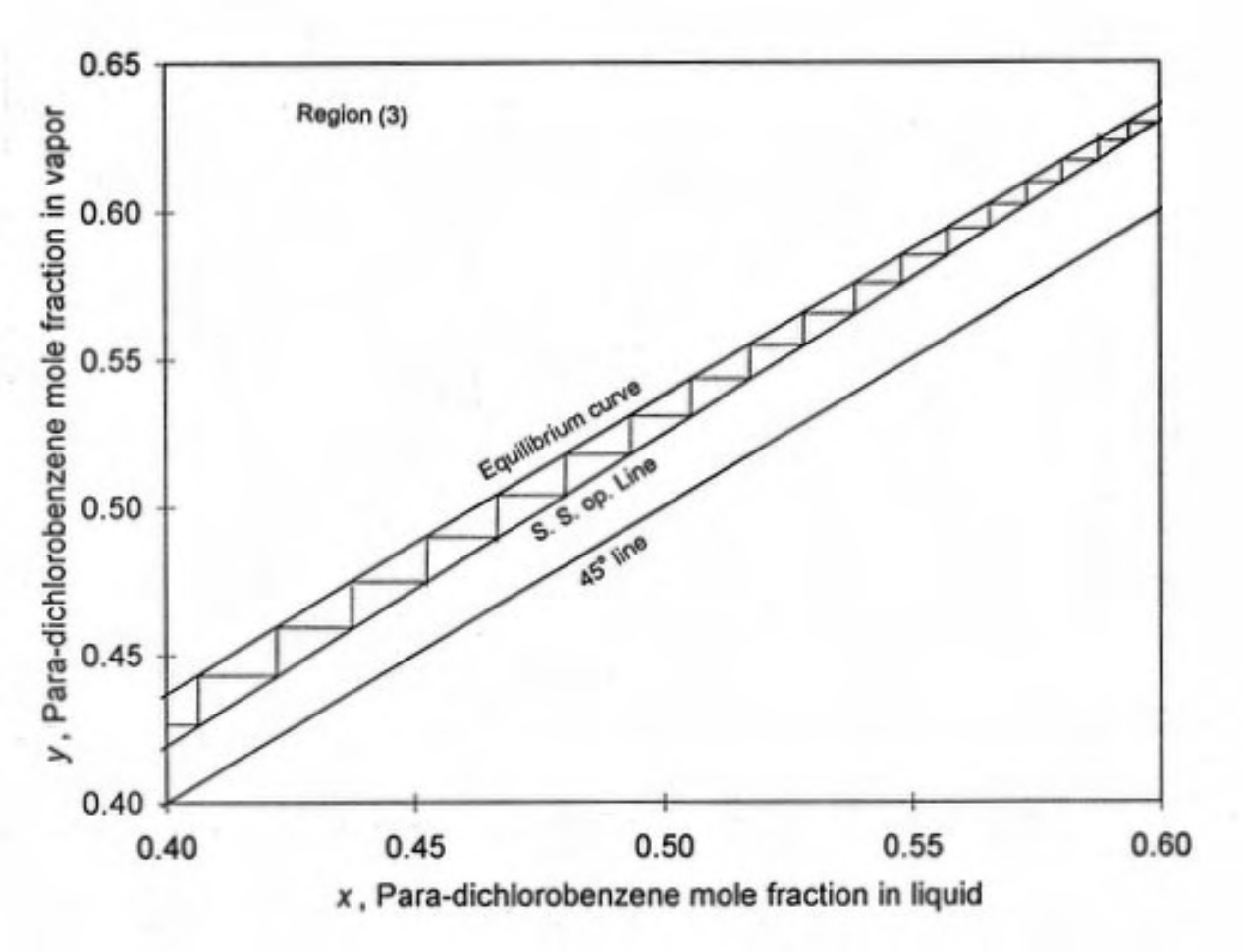
Call it 99 stages in the column plus a partial reboiler with the feed to stage 52 from the top.

This compares to 102 stages in the column plus a partial reboiler with the feed to stages 50 from top as determined by the Fenske-Underwood-Gilliland method.



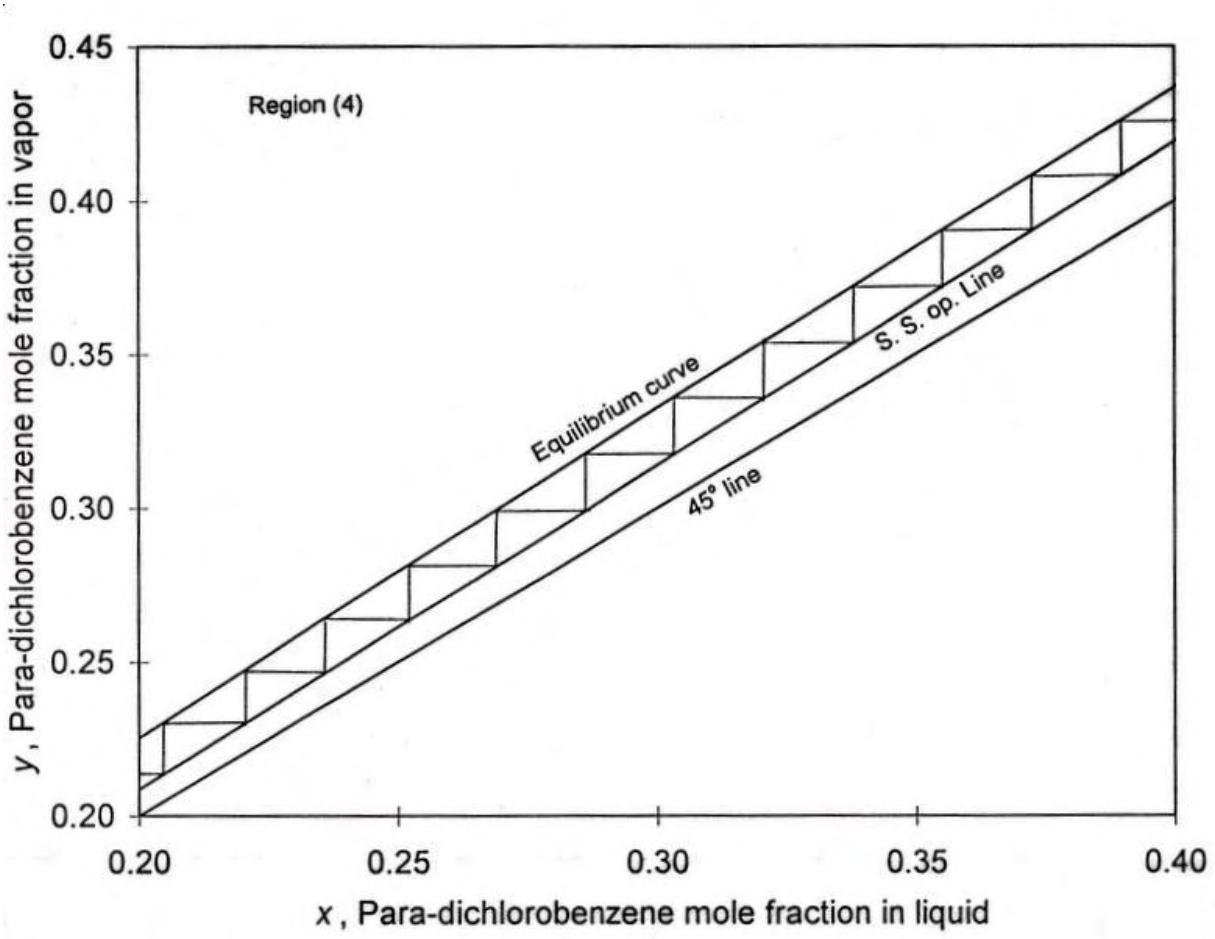
Exercise 7.39 (continued)

Analysis: (continued)



Exercise 7.39 (continued)

Analysis: (continued)



Exercise 7.40

Subject: Use of a McCabe-Thiele diagram to determine stage requirements for the distillation of air into nitrogen and oxygen using a Linde double column.

Given: As shown in Fig. 7.45, the distillation consists of an upper column (UC) operating at 1 atm, on top of a lower column (LC) operating at 4 to 5 atm. Compressed air, containing 79 mol% N_2 is condensed to supply heat in the reboiler of LC, and then is fed as liquid air to an intermediate tray of LC. Bottoms liquid from LC, containing about 55 mol% N_2, is the feed to an intermediate tray in UC. The reboiler of UC is the condenser for LC. Condensate from the top of LC is nearly pure N_2, which is sent as reflux to the top of UC. The reboiler at the bottom of UC provides almost pure O_2 boilup for UC. Nearly pure liquid O_2 is withdrawn from the UC reboiler sump at the bottom of UC. The UC has no condenser. Nearly pure gaseous N_2 leaves the top of UC. This is consistent with the fact that N_2 with a normal boiling point of -195.8°C (77.4 K) is more volatile than O_2 with a normal boiling point of -183°C (90.2 K).

Assumptions: Constant molar overflow. Constant relative volatility at each pressure.

Find: Construction lines on a McCabe-Thiele diagram that enable the determination of stage requirements.

Analysis: In LC, the N_2 composition ranges from 55 mol% at the bottom to about 99 mol% at the top, with a feed of 79 mol%. Based on calculations using *K*-values from the SRK equation of state at 4.5 atm, the average relative volatility in LC is 2.5. In UC, the N_2 composition ranges from about 1 mol% at the bottom to 99 mol% at the top, with a feed of 55 mol%. Based on calculations using *K*-values from the SRK equation of state at 1 atm, the average relative volatility in UC is 4.0. Using Eq. (7-3), equilibrium curves for these constant α cases are shown in the McCabe-Thiele diagram on the next page. However, so as not to clutter the diagram, the curve for UC at 1 atm is based on N_2, using,

$$y_{N_2} = \frac{\alpha_{N_2-O_2} x_{N_2}}{1 + x_{N_2}\left(\alpha_{N_2-O_2} - 1\right)} = \frac{4x_{N_2}}{1 + 3x_{N_2}} \qquad (1)$$

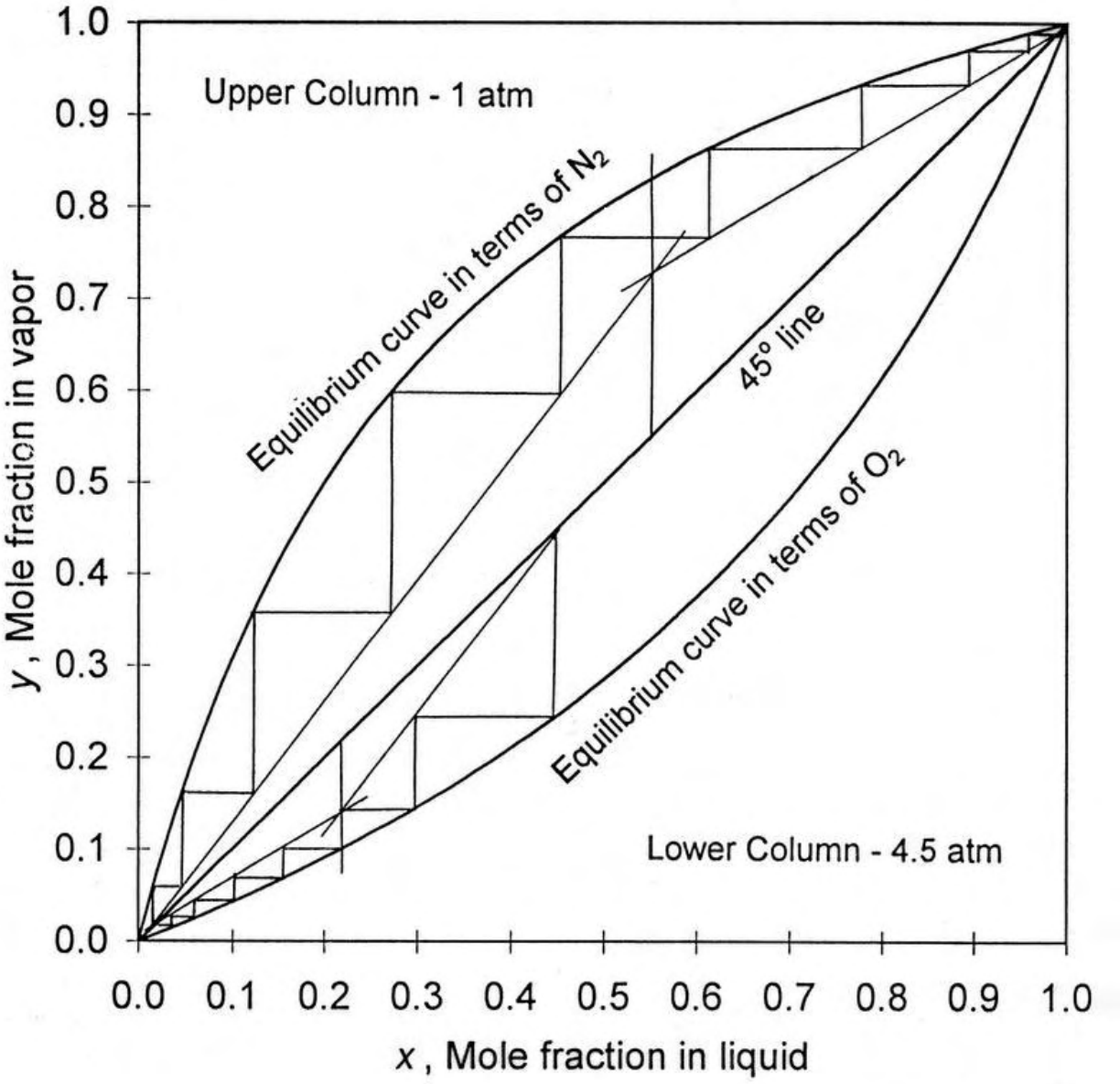
while the curve for LC at 4.5 atm is based on O_2, using,

$$y_{O_2} = \frac{\alpha_{O_2-N_2} x_{O_2}}{1 + x_{O_2}\left(\alpha_{O_2-N_2} - 1\right)} = \frac{(1/2.5)x_{O_2}}{1 + x_{O_2}\left(1/2.5 - 1\right)} = \frac{0.4x_{O_2}}{1 - 0.6x_{O_2}} \qquad (2)$$

Note that the equilibrium curve for 1 atm is above the 45° line, while that for 4.5 atm is below the 45° line. Typical operating lines and *q*-lines are shown for determining the stage requirements.

Exercise 7.40 (continued)

Analysis: (continued)



Exercise 7.41

Subject: Comparison of measured with predicted plate efficiency for distillation of a methanol-water mixture.

Given: Performance data for a distillation column. Vapor-liquid equilibrium data.

Assumptions: Partial reboiler is an equilibrium stage. Constant molar overflow.

Find: (a) Overall plate efficiency from performance data.
(b) Predicted plate efficiency from Drickamer-Bradford correlation.
(c) Predicted plate efficiency from O'Connell correlation.
(d) Predicted efficiency from Chan-Fair correlation.

Analysis: (a) Convert the performance data for feed and product flow rates and compositions from mass units into mole units, molecular weights of 32.04 for methanol and 18.02 for water. The results are as follows:

	Flow rate, lbmol/h:			**Mole fraction:**		
Component	**Feed**	**Distillate**	**Bottoms**	**Feed**	**Distillate**	**Bottoms**
Methanol	709.1	702.7	6.4	0.360	0.915	0.0053
Water	1260.8	65.3	1195.5	0.640	0.085	0.9947
Total:	1969.9	768.0	1201.9	1.000	1.000	1.0000

Use the McCabe-Thiele method, based on methanol mole fractions, to find the number of equilibrium stages needed. The slope of the rectifying section operating line is given by Eq. (7-7). $L/V = R/(R+1)$=0.947/(1.947)=0.486. This line intersects the 45° line at $x = 0.915$.
The slope of the stripping section operating line is given by Eq. (7-12).
$\bar{L}/\bar{V} = (V_B + 1)/V_B$ = (1.138 + 1)/1.138 = 1.88. This line intersects the 45°i line at $x = 0.0056$.
The McCabe-Thiele diagram is given below in two parts to achieve accuracy. From the two parts of the diagram, it is observed that the two operating lines do not intersect on the *q*-line. This is probably because the assumption of constant molar overflow is not valid and the operating lines have some curvature. Assuming the feed stage in the actual column is near the optimal location, the questionable McCabe-Thiele diagram gives 5 equilibrium stages in the stripping section, one of which is the partial reboiler, and 4.2 equilibrium stages in the rectifying section. Thus, the total equilibrium stages in the column = N_t = 8.2 + the partial reboiler. The column contains 12 plates + the partial reboiler. From Eq. (6-21), the overall plate efficiency is,

$$E_o = N_t/N_a = 8.2/12 = 0.68 \text{ or } 68\%.$$

The column contains 5 plates in the rectifying section. This is equivalent to a plate efficiency in that section of 4.2/5 = 0.84 or 84%. The stripping section contains 6 plates plus the feed plate.

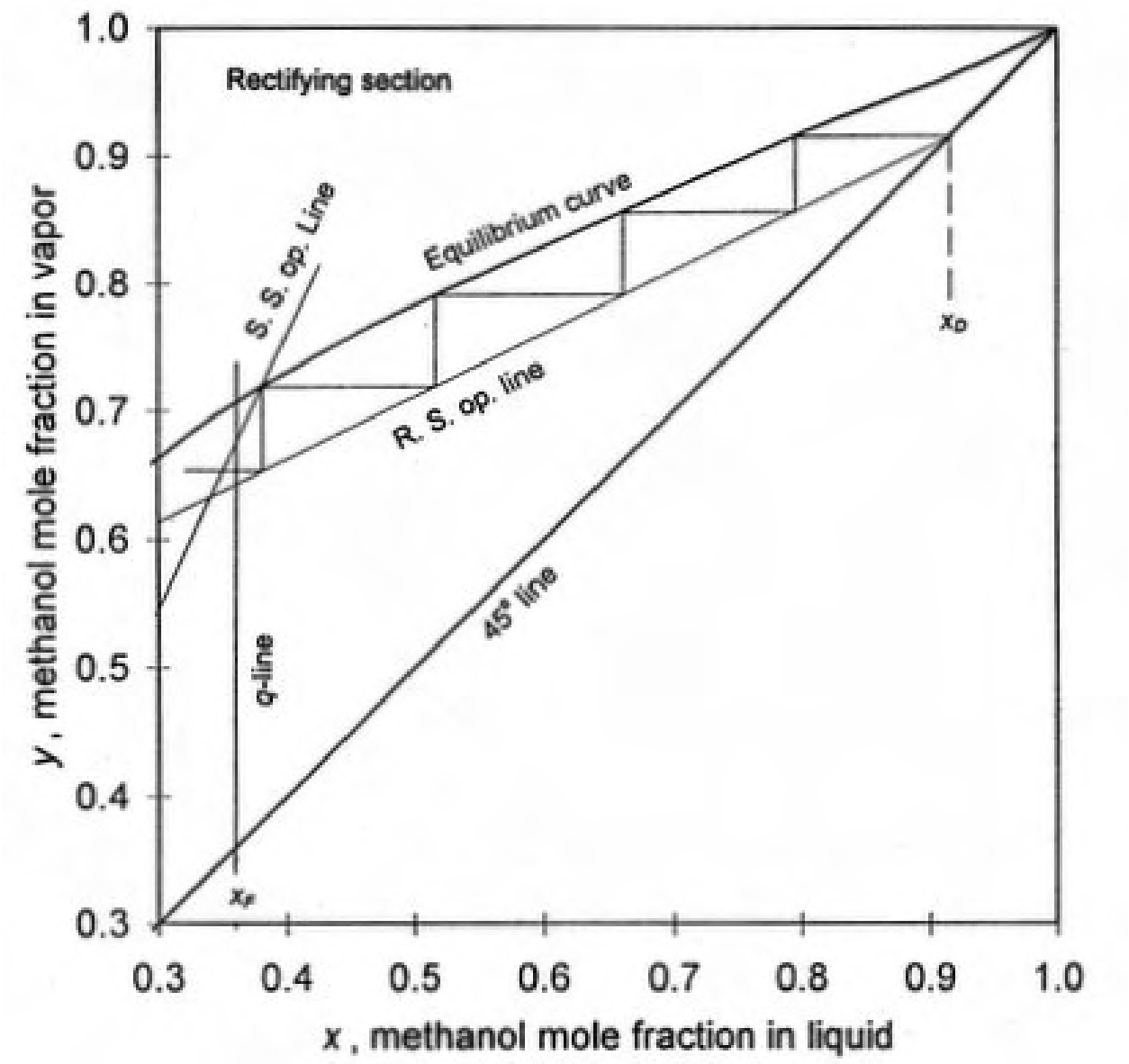
Exercise 7.41 (continued)

Analysis: (a) (continued)

Therefore, the efficiency in this section is 4/7 = 0.57 or 57%.

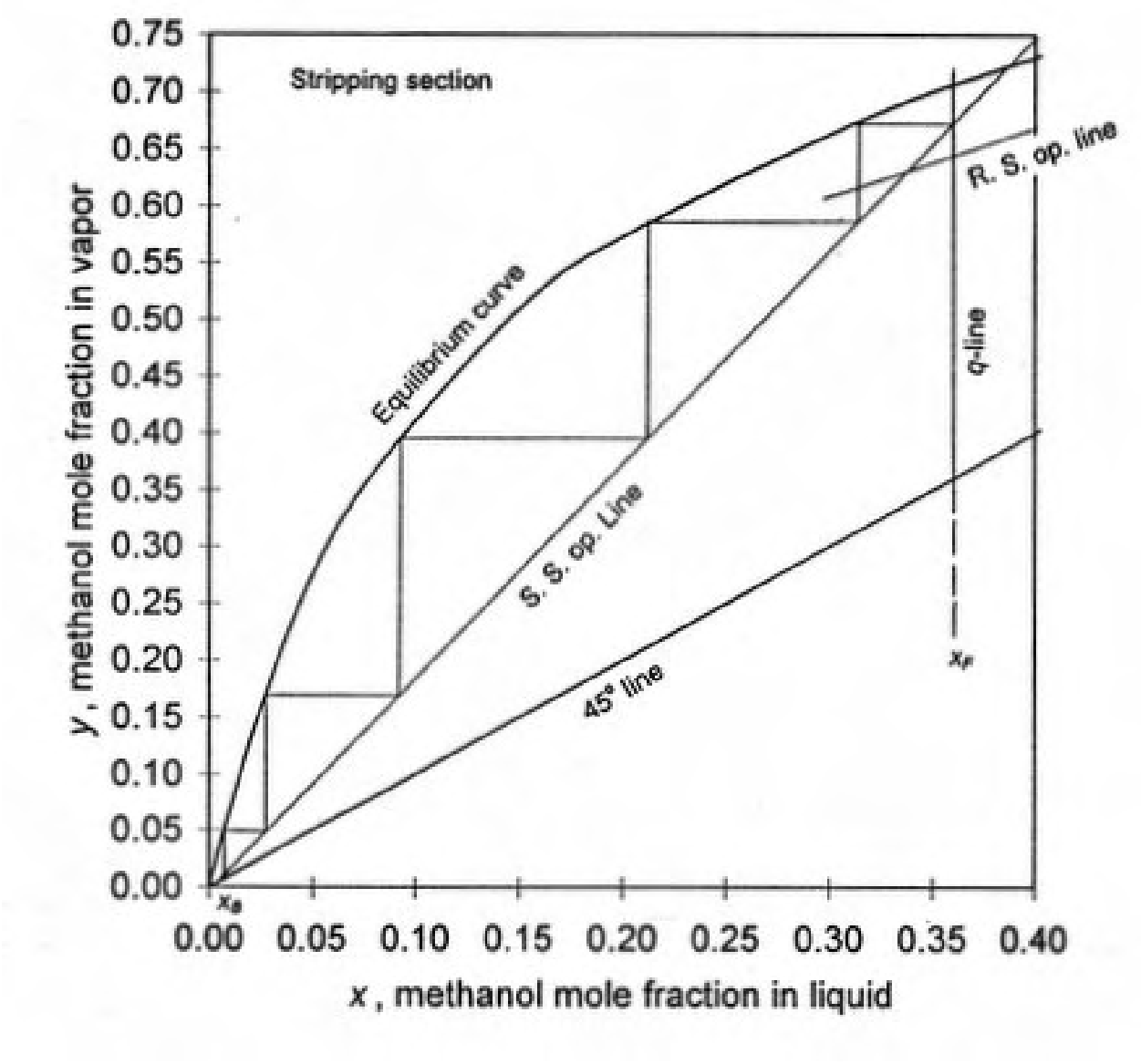
Note these results are subject to degree of curvature of the operating lines and the placement of the feed in the McCabe-Thiele method. In the McCabe-Thiele method, if one more equilibrium stage is added to the stripping section, so as to give 5 stages plus the partial reboiler, then the rectifying section only needs 3.8 equilibrium stages. Then the overall plate efficiency is 73%, with

71% in the stripping section and 76% in the rectifying section. This still does not account for the effect of curvature of the operating lines.



Exercise 7.41 (continued)

Analysis: (a) (continued)



(b) From Eq. (7-42), $E_o = 13.3 - 66.7 \log \mu$

Take the viscosity as that of the feed = 0.34 cP

$$E_o = 13.3 - 66.7 \log (0.34) = 44.6\%$$

This is poor agreement with the performance data.

(c) From Eq. (7-43), $E_o = 50.3(\alpha\mu)^{-0.226}$

At the feed composition, $x = 0.36$ and $y = 0.71$. Therefore, from Eqs (2-19) and (2-21 combined, the relative volatility is, $\alpha = (y/x)/[(1 - y)/(1 - x)] = (0.71/0.36)/(0.29/0.64) = 4.4$

Exercise 7.41 (continued)

Analysis:

$$E_o = 50.3[(4.4)(0.34)]^{-0.226} = 45.9\%$$

Now correct for length of liquid path from Fig. 7.5. Column diameter = 6 ft. Assume length of liquid path = 70% of column diameter = 0.7(6) = 4.2 ft. From Fig. 7.5, correction to be added = 10%. Therefore corrected E_o = 45.9 + 10 = 55.9%
This also appears to be low.

(d) From Eq. (6-56), $N_{OG} = -\ln(1 - E_{OV})$. Therefore, $E_{OV} = 1 - \exp(-N_{OG})$
Use Eqs. (6-62, (6-64), (6-66), and (6-67) as in Example 6.7. Carry out the calculations at the bottom tray based on methanol diffusion. Conditions are:

	Gas	Liquid
Molar flow rate, kmol/h	630	1,192
Molecular weight	18.5	18.0
Density, kg/m^3	0.657	940

Estimate liquid diffusivity of methanol in water at 212°F = 373 K. From Perry's Handbook, D_L = 1.6 x 10^{-5} cm^2/s at 25°C. The viscosity of water at 212°F = 0.25 cP. Using Eq. (3-39) to correct for temperature and viscosity, D_L = 1.6 x 10^{-5} (373/298)(1/0.25) = 8 x 10^{-5} cm^2/s

Estimate gas diffusivity of methanol in water vapor from Eq. (3-36). T = 373 K

$M_{AB} = 2/[(1/32) + (1/18)] = 23$. Using Table 3.1,

$$\sum_{V_{\text{methanol}}} = 15.9 + 2.31(4) + 6.11 = 31.3, \qquad \sum_{V_{\text{water}}} = 13.1$$

$$D_V = \frac{0.00143(373)^{1.75}}{(15.1/14.7)23^{1/2}[31.3^{1/3} + 13.1^{1/3}]^2} = 0.30\ \text{cm}^2/\text{s}$$

Required tray dimensions: D_T = 6 ft, $A = 3.14(6)^2/4 = 28.3$ ft^2 = 2.63 m^2
$A_a = 0.91\ A = 0.91(2.63) = 2.39$ m^2 = 23,900 cm^2, L_w = 42.5 in. = 1.08 m

Tray conditions: $\phi_\varepsilon = 1 - 0.617 = 0.383$, $q_L = 47{,}300/(60)(8.33) = 94.6$ gpm = 5,970 cm^3/s
From Eq. (6-54), $C_l = 0.362 + 0.317\exp[-3.5(2)] = 0.362$

From Eq. (6-51),
$$h_l = 0.383\left[2.0 + 0.362\left(\frac{94.6}{(42.5)(0.383)}\right)^{2/3}\right] = 1.21 \text{ in.} = 3.08 \text{ cm}^2$$

f = 0.40, From Eq. (6-64), $\bar{t}_L = (3.08)(23{,}900)/5{,}970 = 12.3$ s

Exercise 7.41 (continued)

Analysis: (d) (continued)

The continuity equation is,

$$m_V = U_a A_a \rho_V, \text{ so } U_a, \text{ft/s} = \frac{m_V}{A_a \rho_V} = \frac{630(18.5)(2.205)/3600}{28.3(0.91)(0.657/16.02)} = 6.8 \text{ ft/s} = 2.07 \text{ m/s}$$

From Eq. (6-65), $$\bar{t}_G = \frac{(0.617)(3.08)}{(0.383)(6.8)(2.54)(12)} = 0.024 \text{ s}$$

From below Eq. (6-67), $F = U_a \rho_V^{0.5} = 2.07(0.657)^{0.5} = 1.68 \text{ (kg/m)}^{0.5}/\text{s}$

From Eq. (6-67), $k_L \bar{a} = 78.8(8 \times 10^{-5})^{0.5}(1.68 + 0.425) = 1.48 \text{ s}^{-1}$

From Eq. (6-66), $$k_G \bar{a} = \frac{1{,}030(0.30)^{1/2}\left[0.40 - 0.842(0.40)^2\right]}{3.08^{1/2}} = 85.3 \text{ s}^{-1}$$

From Eq. (6-63), $N_L = k_L \bar{a} \bar{t}_L = 1.48(12.3) = 18.2$

From Eq. (6-62), $N_G = k_G \bar{a} \bar{t}_G = 85.3(0.024) = 2.05$

From the vapor-liquid equilibrium data at the bottom of the column,

$K_{\text{methanol}} = 0.156/0.0246 = 6.34$

Absorption factor = $KV/L = (6.34)(630)/1{,}192 = 3.35$

From Eq. (6-61), $$\frac{1}{N_{OG}} = \frac{1}{N_G} + \frac{(KV/L)}{N_L} = \frac{1}{2.05} + \frac{3.35}{18.2} = 0.488 + 0.184 = 0.672$$

$N_{OG} = 1/0.672 = 1.488$

Thus, the gas-phase resistance is more important than the liquid-phase resistance.

From Eq. (6-56), $E_{OV} = 1 - \exp(-N_{OG}) = 1 - \exp(-1.488) = 0.774$ or 77.4%

This is in very good agreement with the performance data.

Exercise 7.42

Subject: Estimation of efficiencies, E_{MV} and E_o from E_{OV} for methanol-water mixture, as measured with a small Oldershaw column.

Given: Column conditions from Exercise 7.41.

Find: E_{MV} and E_o

Analysis: Case 1: Assume complete mixing on the trays.

$E_{MV} = E_{OV} = 0.65$ or 65%

Case 2: Assume plug flow of liquid with no longitudinal diffusion. Take conditions at the top of the column.

From Eq. (7-7), $L/V = R/(R + 1) = 0.947/(1 + 0.947) = 0.486$

From Eq. (6-33), $\lambda = m/(L/V)$

From the vapor-liquid equilibrium data given in Exercise 7.41,

$m = dy/dx = (1 - 0.915)/(1 - 0.793) = 0.41$

$\lambda = 0.41/0.486 = 0.844$

From Eq. (6-32),

$$E_{MV} = \frac{1}{\lambda}\left[\exp(\lambda E_{OV}) - 1\right] = \frac{1}{0.844}\left\{\exp\left[0.844(0.65)\right] - 1\right\} = 0.754 \text{ or } 75.4\%$$

The actual value of E_{MV} probably lies inbetween 65% and 75.4%, or say 70%.

From Eq. (6-37), assuming that the equilibrium and operating lines are straight,

$$E_o = \frac{\log\left[1 + E_{MV}(\lambda - 1)\right]}{\log \lambda} = \frac{\log\left[1 + 0.70(0.844 - 1)\right]}{\log(0.844)} = 0.68 \text{ or } 68\%$$

Exercise 7.43

Subject: Estimation of column diameter at top tray of a distillation column separating benzene from monochlorobenzene.

Given: Conditions at the top tray in Fig. 7.46.

Find: Column diameter for a valve tray at 85% of flooding.

Analysis: Use Fig. 6.24, where the value of F_{LV} is needed.

V = 336.5 lbmol/h, L = 274.7 lbmol/h

Because both the vapor and liquid are almost pure benzene, take M_V and M_L = 78.1

From Perry's Handbook, the liquid density of benzene at 204°F and 23 psia = ρ_L = 52 lb/ft^3

From the ideal gas law, $\rho_V = PM_V/RT$ = (23)(78.1)/[(10.73)(664)] = 0.252 lb/ft^3

$$F_{LV} = \frac{LM_L}{VM_V}\left(\frac{\rho_V}{\rho_L}\right)^{1/2} = \frac{(274.7)(78.1)}{(336.5)(78.1)}\left(\frac{0.252}{52}\right)^{0.5} = 0.057$$

Assume 24-inch tray spacing. From Fig. 6.24, C_F = 0.37

From below Eq. (6-44), A_d/A = 0.1

From the Handbook of Chemistry and Physics, for benzene under its own vapor, σ = 30 dyne/cm.

From below Eq. (6-42), $F_{ST} = (30/20)^{0.2}$ = 1.084

Assume that the foaming factor, F_F = 1.0 and take F_{HA} = 1.0

.

From Eq. (6-42),

$$C = 1.084(1.0)(1.0)(0.37) = 0.40 \text{ ft/s}$$

From Eq. (6-40),

$$U_f = C\left(\frac{\rho_L - \rho_V}{\rho_V}\right)^{1/2} = 0.40\left(\frac{52 - 0.252}{0.252}\right)^{0.5} = 5.73 \text{ ft/s}$$

From Eq. (6-44),

$$D_T = \left[\frac{4VM_V}{fU_f\pi(1 - A_d/A)\rho_V}\right]^{1/2} = \left[\frac{4(336.5/3600)(78.1)}{0.85(5.73)(3.14)(1-0.1)(0.252)}\right]^{0.5} = 2.9 \text{ ft}$$

Exercise 7.44

Subject: Diameters and heights for separation of propylene from propane in two columns.

Given: Feed and product conditions and numbers of trays for sieve-tray columns in Fig. 7.47.

Assumptions: Constant molar overflow. 85% of flooding.

Find: Column diameters, tray efficiencies, numbers of actual trays, and column heights.

Analysis:

Column diameters: Assume that the diameter of the second column is controlled at the top tray, and than the diameter of the first column is controlled by the bottom tray.

Top tray of second column: Use the properties of pure propylene.

Distillate rate = 3.5 + 360 - 12.51 = 350.99 lbmol/h

With an R = 15.9, L = 15.9(350.99) = 5,580 lbmol/h. $V = L + D$ = 351 + 5,580 = 5,931 lbmol/h.

From Perry's Handbook, at 116°F = 576°R = 320 K, vapor density = ρ_V = 2.64 lb/ft^3 and liquid density = ρ_L = 29.0 lb/ft^3.

$$F_{LV} = \frac{LM_L}{VM_V}\left(\frac{\rho_V}{\rho_L}\right)^{1/2} = \frac{(5{,}580)(42.1)}{(5{,}931)(42.1)}\left(\frac{2.64}{29.0}\right)^{0.5} = 0.284$$

Assume 24-inch tray spacing. From Fig. 6.24, C_F = 0.25

From below Eq. (6-44), A_d/A = 0.1+ (0.284 - 0.1)/9 = 0.120

Assume surface tension, σ, = 10 dyne/cm. From below Eq. (6-42), $F_{ST} = (10/20)^{0.2}$ = 0.87

Assume that the foaming factor, F_F = 1.0 and take F_{HA} = 1.0.

From Eq. (6-42), C = 0.87(1.0)(1.0)(0.25) = 0.22 ft/s

From Eq. (6-40), $U_f = C\left(\frac{\rho_L - \rho_V}{\rho_V}\right)^{1/2} = 0.22\left(\frac{29.0 - 2.64}{2.64}\right)^{0.5} = 0.70$ ft / s

From Eq. (6-44),

$$D_T = \left[\frac{4VM_V}{fU_f\pi(1 - A_d/A)\rho_V}\right]^{1/2} = \left[\frac{4(5931/3600)(42.1)}{0.85(0.70)(3.14)(1-0.12)(2.64)}\right]^{0.5} = 8.0 \text{ ft}$$

Bottom tray of first column: Use the properties of pure propane.

L in first column = L in second column + feed = 5,580 + 360 + 240 = 6,180 lbmol/h.

V in first column = L in first column - B = 6,180 - (600 - 351) = 5,931 lbmol/h

From Perry's Handbook, at 136°F = 596°R = 331 K, vapor density = ρ_V = 2.93 lb/ft^3 and liquid density = ρ_L = 27.0 lb/ft^3.

Exercise 7.44 (continued)

Analysis: (continued)

$$F_{LV} = \frac{LM_L}{VM_V}\left(\frac{\rho_V}{\rho_L}\right)^{1/2} = \frac{(6{,}180)(44.1)}{(5{,}931)(44.1)}\left(\frac{2.93}{27.0}\right)^{0.5} = 0.343$$

Assume 24-inch tray spacing. From Fig. 6.24, $C_F = 0.22$
From below Eq. (6-44), $A_d/A = 0.1 + (0.343 - 0.1)/9 = 0.127$
Assume surface tension, σ, = 10 dyne/cm. From below Eq. (6-42), $F_{ST} = (10/20)^{0.2} = 0.87$
Assume that the foaming factor, $F_F = 1.0$ and take $F_{HA} = 1.0$.
From Eq. (6-42), $C = 0.87(1.0)(1.0)(0.22) = 0.19$ ft/s

From Eq. (6-40), $U_f = C\left(\frac{\rho_L - \rho_V}{\rho_V}\right)^{1/2} = 0.19\left(\frac{27.0 - 2.93}{2.93}\right)^{0.5} = 0.55 \text{ ft/s}$

From Eq. (6-44),

$$D_T = \left[\frac{4VM_V}{fU_f\pi(1 - A_d/A)\rho_V}\right]^{1/2} = \left[\frac{4(5{,}931/3600)(44.1)}{0.85(0.55)(3.14)(1-0.127)(2.93)}\right]^{0.5} = 8.8 \text{ ft}$$

Tray Efficiencies: Use Fig. 7.32. Need relative volatility and average liquid viscosity.
From Fig. 2.8, *K*-values and relative volatilities are:

Component	Propylene	Propane
K-value at 116°F, 280 psia	1.00	0.87
K-value at 136°F, 300 psia	1.14	1.00

At the top, $\alpha = 1.00/0.87 = 1.15$. At the bottom, $\alpha = 1.14/1.00 = 1.14$
At the top, propylene viscosity = 0.45 cP. At the bottom, propane viscosity = 0.44 cP.
At the top, $\alpha\mu = 1.15(0.45) = 0.52$. From Fig. 7.32, $E_o = 60\%$.
At the bottom, $\alpha\mu = 1.14(0.44) = 0.50$. From Fig. 7.32, $E_o = 62\%$.

Actual trays and column heights:
Actual tray requirements are 90/0.62 = 145 trays for the bottom column and
90/0.60 = 150 trays for top column.
Column heights are:

Bottom column = 144(2) + 4 + 10 = 302 ft
Top column = 149(2) + 4 + 10 = 312 ft

Exercise 7.45

Subject: Sizing of a vertical flash drum.

Given: Flash temperature and pressure, with product flow rates in Fig. 7.48.

Find: Drum height and diameter.

Analysis: To determine minimum drum diameter, use Eq. (6-44) with $f = 0.85$ and $A_d = 0$. The flooding velocity is obtained from Eqs. (6-40) and (6-42), using $F_{ST} = 1.0$, $F_{HA} = 1.0$ and $F_F = 1.0$, with C_F from the 24-inch plate spacing curve in Fig. 6.24. The value of F_{LV} is obtained first, using the conditions in Fig. 7.48.

$$M_V = [187.6(58.1) + 176.4(72.2) + 82.5(86.2)]/446.5 = 68.9$$
$$M_L = [112.4(58.1) + 223.6(72.2) + 217.5(86.2)]/553.5 = 74.8$$

From a simulation program, $\rho_V = 1.13$ lb/ft^3, compared to 0.965 from the ideal gas law and $\rho_L = 33.2$ lb/ft^3. Also given, $V = 446.5$ lbmol/h and $L = 553.5$ lbmol/h

In Fig. 6.24, $F_{LV} = \dfrac{LM_L}{VM_V}\left(\dfrac{\rho_V}{\rho_L}\right)^{1/2} = \dfrac{553.6(74.8)}{446.5(68.9)}\left(\dfrac{1.13}{33.2}\right)^{1/2} = 0.248$

From Fig. 6.24, $C_F = 0.27$ ft/s. From Eq. (6.42), $C = (1)(1)(1)0.27 = 0.27$ ft/s.
From Eq. (6-40),

$$U_f = C\left(\frac{\rho_L - \rho_V}{\rho_V}\right)^{1/2} = 0.27\left(\frac{33.2 - 1.13}{1.13}\right)^{1/2} = 1.44 \text{ ft/s}$$

From Eq. (6-44),

$$D_T = \left[\frac{4VM_V}{fU_f \pi \rho_V}\right]^{1/2} = \left[\frac{4(446.5/3600)(68.9)}{0.85(1.44)(3.14)(1.13)}\right]^{1/2} = 2.81 \text{ ft}$$

Assume a liquid residence time, t, of 5 minutes (0.0833 h), half full

.

From Eq. (7-44), vessel volume = $V_V = \dfrac{2LM_L t}{\rho_L} = \dfrac{2(553.5)(74.8)(0.0833)}{33.2} = 208 \text{ ft}^3$

Now compute the height, H, from Eq. (7-45). $H = \dfrac{4V_V}{\pi D_T^2} = \dfrac{4(208)}{3.14(2.81)^2} = 33.6$ ft

Thus, $H/D = 33.6/2.81 = 12.0$. This is too large, so re-dimension the volume to give $H/D = 4$.
From Eq. (7-46),

$$D_T = \left(\frac{V_V}{\pi}\right)^{1/3} = \left(\frac{208}{3.14}\right)^{1/3} = 4.05 \text{ ft}$$

From Eq. (7-46), $H = 4D_T = 4(4.05) = 16.2$ ft

Exercise 7.46

Subject: Sizing of a horizontal reflux drum.

Given: Flow conditions leaving reflux drum in Fig. 7.49.

Find: Drum length and diameter.

Analysis:

Liquid rate leaving drum = (3 + 1)120 = 480 lbmol/h
Assume properties of pure n-hexane. From Fig. 2.4, boiling point of nC_6 at 1 atm = 150°F.
From Fig. 2.3, $\rho_L = 0.63$ g/cm^3 = 39 lb/ft^3
Assume a liquid residence time in the reflux drum of 5 minutes (0.0833 h), half full.
From Eq. (7-44),

$$V_V = \frac{2LM_L t}{\rho_L} = \frac{2(480)(86.2)(0.0833)}{39} = 177 \text{ ft}^3$$

From Eq. (7-46),

$$D_T = \left(\frac{V_V}{\pi}\right)^{1/3} = \left(\frac{177}{3.14}\right)^{1/3} = 3.83 \text{ ft}$$

From Eq. (7-46), $H = 4D_T = 4(3.83) = 15.3$ ft

Might use a drum of 4 ft diameter and 16 ft long.

Exercise 7.47

Subject: Sizing of a sieve-tray distillation column separating methanol and water.

Given: Column top and bottom conditions in Fig. 7.50.
Assumptions: Column feed is a bubble-point liquid. Constant molar overflow.
Find: (a) Column diameters at top and bottom. Should column be swaged?
(b) Length and diameter of horizontal reflux drum.

Analysis: First, compute the liquid and vapor flow rates at the top and bottom of the column.
Molecular weight of distillate = 0.9905(32.04) + 0.0095(18.02) = 31.91
Distillate flow rate = D = 462,385/31.91 = 14,490 lbmol/h
Molecular weight of bottoms = 0.0101(32.04) + 0.9899(18.02) = 18.16
Bottoms flow rate = B = 188,975/18.16 = 10,410 lbmol/h
From these values and the given compositions, the overall material balance is:

Lbmol/h:

Component	Feed	Distillate	Bottoms
Methanol	14,457	14,352	105
Water	10,443	138	10,305
Total:	24,900	14,490	10,410

From the reboiler duty, assuming the bottoms is pure water, can compute the boilup rate.
Heat of vaporization of water at 262.5°F = 937 Btu/lb = 16,885 Btu/lbmol
Boilup rate = V = 442,900,000/16,885 = 26,230 lbmol/h
Assume constant molar overflow with saturated liquid feed. Therefore, overhead vapor rate also is equal to 26,230 lbmol/h. The reflux rate = V - D = 26,230 - 14,490 = 11,740 lbmol/h
A more accurate calculation by CHEMCAD with an overall energy balance gives a reflux rate of 15,800 lbmol/h and an overhead vapor rate of 30,300 lbmol/h. But use the constant molar overflow values.

(a) **Column diameter at the bottom:**

From a simulation program, at 262.5°F and 40 psia, ρ_V = 0.0994 lb/ft^3 and ρ_L =57.9 lb/ft^3.
V = 26,230 lbmol/h and L = 10,410 + 26,230 = 36,640 lbmol/h
In Fig. 6.24,

$$F_{LV} = \frac{LM_L}{VM_V}\left(\frac{\rho_V}{\rho_L}\right)^{1/2} = \frac{36{,}640(18.2)}{26{,}230(18.29)}\left(\frac{0.0994}{57.9}\right)^{1/2} = 0.058$$

From Fig. 6.24, for 24-inch plate spacing, C_F = 0.27 ft/s.
For Eqs. (6-40) and (6-42), use F_{HA} = 1.0 and F_F = 1.0. For water, σ = 51 dyne/cm
Therefore, F_{ST} = (51/20)$^{0.2}$ = 1.21. From Eq. (6.42), C = 1.21(1)(1)0.37 = 0.45 ft/s.

Exercise 7.47 (continued)

Analysis: (a) (continued)

From Eq. (6-40), $U_f = C\left(\frac{\rho_L - \rho_V}{\rho_V}\right)^{1/2} = 0.45\left(\frac{57.9 - 0.0994}{0.0994}\right)^{1/2} = 10.9$ ft/s

Since $F_{LV} < 0.1$, from below Eq. (6-44), $A_d/A = 0.1$. Assume $f = 0.80$.

From Eq. (6-44), $D_T = \left[\frac{4VM_V}{fU_f\pi(1 - A_d/A)\rho_V}\right]^{1/2} = \left[\frac{4(26,230/3600)(18.2)}{0.80(10.9)(3.14)(1-0.1)(0.0994)}\right]^{1/2} = 14.7$ ft

Column diameter at the top:

From a simulation program, at 189°F and 33 psia, $\rho_V = 0.1566$ lb/ft^3 and ρ_L =45.3 lb/ft^3.
V = 26,230 lbmol/h and L = 11,740 lbmol/h
In Fig. 6.24,

$$F_{LV} = \frac{LM_L}{VM_V}\left(\frac{\rho_V}{\rho_L}\right)^{1/2} = \frac{11,740(34)}{26,230(34)}\left(\frac{0.1566}{45.3}\right)^{1/2} = 0.026$$

From Fig. 6.24, for 24-inch plate spacing, $C_F = 0.38$ ft/s
For Eqs. (6-40) and (6-42), use $F_{HA} = 1.0$ and $F_F = 1.0$. For methanol, $\sigma = 17$ dyne/cm
Therefore, $F_{ST} = (17/20)^{0.2} = 0.97$
From Eq. (6.42), $C = 0.97(1)(1)0.38 = 0.37$ ft/s.
From Eq. (6-40),

$$U_f = C\left(\frac{\rho_L - \rho_V}{\rho_V}\right)^{1/2} = 0.37\left(\frac{45.3 - 0.1566}{0.1566}\right)^{1/2} = 6.28 \text{ ft/s}$$

Since $F_{LV} < 0.1$, from below Eq. (6-44), $A_d/A = 0.1$. Assume $f = 0.80$.
From Eq. (6-44),

$$D_T = \left[\frac{4VM_V}{fU_f\pi(1 - A_d/A)\rho_V}\right]^{1/2} = \left[\frac{4(26,230/3600)(34)}{0.80(6.28)(3.14)(1-0.1)(0.1556)}\right]^{1/2} = 21.2 \text{ ft}$$

Therefore, column would be swaged.

(b) Sizing of reflux drum.
Assume a liquid residence time in the reflux drum of 5 minutes (0.0833 h), half full.

From Eq. (7-44),

$$V_V = \frac{2LM_L t}{\rho_L} = \frac{2(26,230)(34)(0.0833)}{45.3} = 3,280 \text{ ft}^3$$

From Eq. (7-46),

$$D_T = \left(\frac{V_V}{\pi}\right)^{1/3} = \left(\frac{3,280}{3.14}\right)^{1/3} = 10.1 \text{ ft}$$

From Eq. (7-46), $H = 4D_T = 4(10.1) = 40.4$ ft

Exercise 7.48

Subject: Tray hydraulics for methanol-water separation'

Given: Data from Exercise 7.41.

Find: (a) Percent of flooding.
(b) Tray pressure drop in psi.
(c) Weeping potential.
(d) Entrainment rate.
(e) Downcomer froth height.

Analysis: Use the material balance from Exercise 7.41. Make calculations at the top and bottom trays.

(a) **At the top of the column**, the reflux rate is 0.947(768) = 727 lbmol/h. The overhead vapor rate = 727 + 768 = 1,495 lbmol/h. Use the entrainment flooding correlation of Fig. 6.24, with densities from a simulation program, where the abscissa is,

$$F_{LV} = \frac{LM_L}{VM_G}\left(\frac{\rho_V}{\rho_L}\right)^{1/2} = \frac{727(30.9)}{1{,}495(30.9)}\left(\frac{0.0703}{47.2}\right)^{1/2} = 0.0188 \qquad (1)$$

From Fig. 6.24, for 24-inch tray spacing, $C_F = 0.38$ ft/s. Because $F_{LV} < 1$, $A_d/A = 0.1$.
$F_{HA} = 1.0$, $F_F = 1.0$, and since $\sigma = 20$ dynes/cm, $F_{ST} = 1.0$.
From Eq. (6-24), $C = F_{ST}F_FF_{HA}C_F = (1)(1)(1)(0.38) = 0.38$ ft/s

From Eq. (6-40), $U_f = C\left[(\rho_L - \rho_V)/\rho_V\right]^{1/2} = 0.38\left[(47.2 - 0.0703)/0.0703\right]^{1/2} = 9.84$ ft / s

From a rearrangement of Eq. (6-44), solving for the fraction of flooding,

$$f = \frac{4VM_V}{D^2U_f\pi(1 - A_d/A)\rho_V} = \frac{4(1{,}495/3{,}600)(30.9)}{6^2(9.84)(3.14)(1-0.1)(0.0703)} = 0.73 \text{ or } 73\%$$

At the bottom of the column, the boilup rate from Exercise 7.41 is 1.138(1,209) = 1,376 lbmol/h. The liquid rate leaving the bottom tray = 1,376 + 1,201.9 = 2,578 lbmol/h. Use the entrainment flooding correlation of Fig. 6.24, with densities and molecular weights from a simulation program, where the abscissa is,

$$F_{LV} = \frac{LM_L}{VM_G}\left(\frac{\rho_V}{\rho_L}\right)^{1/2} = \frac{2{,}578(18.1)}{1{,}376(18.8)}\left(\frac{0.0408}{59.5}\right)^{1/2} = 0.0473$$

From Fig. 6.24, for 24-inch tray spacing, $C_F = 0.37$ ft/s. Because $F_{LV} < 1$, $A_d/A = 0.1$.
$F_{HA} = 1.0$, $F_F = 1.0$, and since $\sigma = 20$ dynes/cm, $F_{ST} = (58/20)^{0.2} = 1.24$
From Eq. (6-24), $C = F_{ST}F_FF_{HA}C_F = (1.24)(1)(1)(0.37) = 0.46$ ft/s

From Eq. (6-40), $U_f = C\left[(\rho_L - \rho_V)/\rho_V\right]^{1/2} = 0.46\left[(59.5 - 0.04)/0.0408\right]^{1/2} = 17.6$ ft / s

From a rearrangement of Eq. (6-44), solving for the fraction of flooding,

$$f = \frac{4VM_V}{D^2U_f\pi(1 - A_d/A)\rho_V} = \frac{4(1{,}376/3{,}600)(18.8)}{6^2(17.6)(3.14)(1-0.1)(0.0408)} = 0.39 \text{ or } 39\%$$

Exercise 7.48 (continued)

Analysis: (continued)

(b) Vapor pressure drop per tray is given by Eq. (6-49), $h_t = h_d + h_l + h_\sigma$ (2)

From Eq. (6-50), $h_d = 0.186\left(\frac{u_o^2}{C_o^2}\right)\left(\frac{\rho_V}{\rho_L}\right)$ (3)

Column area = $A = \pi D^2/4 = 3.14(6)^2/4 = 28.3$ ft^2
Take downcomer area = $A_d = 0.1(28.3) = 2.83$ ft^2
Bubbling area = $A_a = A - 2A_d = 28.3 - 2(2.83) = 22.6$ ft^2
Hole area = $A_h = 0.1(22.6) = 2.26$ ft^2

Consider first, the conditions at the top of the column.

From the continuity equation, $u_o = m/A_h\rho_V$ (4)
$u_o = (1{,}495/3{,}600)(30.9)/[(2.26)(0.0703)] = 80.7$ ft/s and $C_o = 0.73$

From Eq. (3), $h_d = 0.186\left(\frac{80.7^2}{0.73^2}\right)\left(\frac{0.0703}{47.2}\right) = 3.39$ inches of liquid

Superficial velocity based on bubbling area = $U_a = 80.7(2.26/22.6) = 7.97$ ft/s

From Eq. (6-53), $K_s = U_a\left(\frac{\rho_V}{\rho_L - \rho_V}\right)^{1/2} = 7.97\left(\frac{0.0703}{47.2 - 0.0703}\right)^{1/2} = 0.31$ ft/s

From Eq. (6-52), $\phi_e = \exp(-4.257K_s^{0.91}) = \exp[-4.257(0.31)^{0.91}] = 0.23$
From Eq. (6-54), $C_l = 0.362 + 0.317\exp(-3.5h_w) = 0.362 + 0.317\exp[-3.5(2.0)] = 0.362$
Weir length = $L_w = 42.5$ in.
Volumetric liquid rate = $q_L = 727(30.9)/[60(8.33)(47.2/62.4)] = 59.4$ gpm

From Eq. (6-51), $h_l = \phi_e\left[h_w + C_l\left(\frac{q_L}{L_w\phi_e}\right)^{2/3}\right] = 0.23\left[2 + 0.362\left(\frac{59.4}{(42.5)0.23}\right)^{2/3}\right] = 0.74$ in. liquid

From Eq. (6-55), with maximum bubble size = D_H = 3/16 inch = 0.00476 m and liquid density = 47.2 lb/ft^3 or 756 kg/m^3,
$h_\sigma = 6\sigma / g\rho_L D_{B_{\max}} = 6(20/1000)/(9.8)(756)(0.00476) = 0.0034$ m = 0.13 in. liquid

From Eq. (2), $h_t = h_d + h_l + h_\sigma = 3.39 + 0.74 + 0.13 = 4.26$ inches liquid = 0.115 psi/tray.

Consider next, the conditions at the bottom tray of the column.

From the continuity equation, $u_o = m/A_h\rho_V$ (4)
$u_o = (1{,}376/3{,}600)(18.1)/[(2.26)(0.0408)] = 75.0$ ft/s and $C_o = 0.73$

From Eq. (3), $h_d = 0.186\left(\frac{75.0^2}{0.73^2}\right)\left(\frac{0.0408}{59.5}\right) = 1.35$ inches of liquid

Superficial velocity based on bubbling area = $U_a = 75.0(2.26/22.6) = 7.5$ ft/s

From Eq. (6-53), $K_s = U_a\left(\frac{\rho_V}{\rho_L - \rho_V}\right)^{1/2} = 7.5\left(\frac{0.0408}{59.5 - 0.0408}\right)^{1/2} = 0.196$ ft/s

From Eq. (6-52), $\phi_e = \exp(-4.257K_s^{0.91}) = \exp[-4.257(0.196)^{0.91}] = 0.381$

Exercise 7.48 (continued)

Analysis: (b) (continued)
From Eq. (6-54), $C_l = 0.362 + 0.317\exp(-3.5h_w) = 0.362 + 0.317\exp[-3.5(2.0)] = 0.362$
Weir length = L_w = 42.5 in.
Volumetric liquid rate = q_L = 2,578(18.1)/[60(8.33)(59.5/62.4)] = 97.9 gpm

From Eq. (6-51), $h_l = \phi_e\left[h_w + C_l\left(\frac{q_L}{L_w\phi_e}\right)^{2/3}\right] = 0.381\left[2 + 0.362\left(\frac{97.9}{(42.5)0.381}\right)^{2/3}\right] = 1.22$ in. liq

From Eq. (6-55), with maximum bubble size = D_H = 3/16 inch = 0.00476 m and liquid density = 59.5 lb/ft^3 or 954 kg/m^3, and σ = 58 dyne/cm = 0.058 kg/s^2,
$h_\sigma = 6\sigma / g\rho_L D_{B_{max}} = 6(0.058)/(9.8)(954)(0.00476) = 0.0078$ m = 0.31 in. liquid
From Eq. (2), $h_t = h_d + h_l + h_\sigma$ = 1.35 + 1.22 + 0.31 = 2.88 inches liquid = 0.098 psi/tray.

(c) Applying the criterion of Eq. (6-68) to the top tray, $h_d + h_\sigma$ = 3.39 + 0.13 = 3.52 in., which is greater than h_l = 0.74 in. Therefore, weeping will not occur.
Applying the criterion of Eq. (6-68) to the bottom tray, $h_d + h_\sigma$ = 1.35 + 0.31 = 1.66 in., which is greater than h_l = 1.22 in. Therefore, weeping will not occur.

(d) From Fig. 6.28 for the top tray, with F_{LV} = 0.0192 and % flood = 73%, fractional entrainment = ψ = 0.11, which is fairly high.
From Fig. 6.28 for the bottom tray, with F_{LV} = 0.0473 and % flood = 39%, fractional entrainment = ψ = 0.0065, which is very low.

The fractional entrainment is defined as, $\psi = e/(L + e)$. Rearranging, entrainment rate = $e = \psi L/(1 - \psi)$.
At the top tray, e = 0.11(727)/(1 - 0.11) = 90 lbmol/h
At the bottom tray, e = 0.0065(2,578)/(1 - 0.0065) = 16.9 lbmol/h

(e) From Eqs. (6-70) and (6-72), the froth height in the downcomer = $h_{df} = (h_t + h_l + h_{da}) / 0.5$
Estimate the head loss for flow under the downcomer from Eq. (6-71). Area for flow under the downcomer apron = $A_{da} = L_w h_a$ = 42.5(2 - 0.5) = 63.8 in^2 = 0.433 ft^2

For the top tray, q_L = 59.4 gpm. $h_{da} = 0.03\left[\frac{59.4}{100(0.433)}\right]^2 = 0.056$ in. liquid

h_{df} = (4.26 + 0.74 + 0.056) / 0.5 = 10.1 in. liquid

For the bottom tray, q_L = 98.3 gpm. $h_{da} = 0.03\left[\frac{98.3}{100(0.433)}\right]^2 = 0.155$ in. liquid

h_{df} = (2.88 + 1.22 + 0.155) / 0.5 = 8.5 in. liquid

Exercise 7.49

Subject: Tray hydraulics for methanol-water separation.

Given: Data from Exercise 7.41, except that feed rate is increased by 30%.

Find: (a) Percent of flooding.
(b) Tray pressure drop in psi.
(c) Entrainment rate.
(d) Downcomer froth height.
Is operation acceptable or should packing be used in one or both sections?

Analysis: Use the material balance from Exercise 7.41. Make calculations at the top and bottom trays. But take into account the 30% increase in all flow rates.
(a) At the top of the column, the reflux rate is 1.3(0.947)(768) = 945 lbmol/h. The overhead vapor rate = 1.3[0.947(768) + 768] = 1,944 lbmol/h. Use the entrainment flooding correlation of Fig. 6.24, with densities from a simulation program, where the abscissa is,

$$F_{LV} = \frac{LM_L}{VM_G}\left(\frac{\rho_V}{\rho_L}\right)^{1/2} = \frac{945(30.9)}{1{,}944(30.9)}\left(\frac{0.0703}{47.2}\right)^{1/2} = 0.0192 \qquad (1)$$

From Fig. 6.24, for 24-inch tray spacing, $C_F = 0.38$ ft/s. Because $F_{LV} < 1$, $A_d/A = 0.1$.
$F_{HA} = 1.0$, $F_F = 1.0$, and since $\sigma = 20$ dynes/cm, $F_{ST} = 1.0$.
From Eq. (6-24), $C = F_{ST}F_FF_{HA}C_F = (1)(1)(1)(0.38) = 0.38$ ft/s
From Eq. (6-40), $U_f = C\left[(\rho_L - \rho_V)/\rho_V\right]^{1/2} = 0.38\left[(47.2 - 0.0703)/0.0703\right]^{1/2} = 9.84$ ft/s
From a rearrangement of Eq. (6-44), solving for the fraction of flooding,

$$f = \frac{4VM_V}{D^2U_f\pi(1 - A_d/A)\rho_V} = \frac{4(1{,}944/3{,}600)(30.9)}{6^2(9.84)(3.14)(1-0.1)(0.0703)} = 0.95 \text{ or } 95\%$$ Unacceptable!

At the bottom of the column, the boilup rate from Exercise 7.41 is 1.3(1.138)(1,209) = 1,789 lbmol/h. The liquid rate leaving the bottom tray = 1.3(1,376 + 1,201.9) = 3,351 lbmol/h. Use the entrainment flooding correlation of Fig. 6.24, with densities and molecular weights from a simulation program, where the abscissa is,

$$F_{LV} = \frac{LM_L}{VM_G}\left(\frac{\rho_V}{\rho_L}\right)^{1/2} = \frac{3{,}351(18.1)}{1{,}789(18.8)}\left(\frac{0.0408}{59.5}\right)^{1/2} = 0.0473$$

From Fig. 6.24, for 24-inch tray spacing, $C_F = 0.37$ ft/s. Because $F_{LV} < 1$, $A_d/A = 0.1$.
$F_{HA} = 1.0$, $F_F = 1.0$, and since $\sigma = 20$ dynes/cm, $F_{ST} = (58/20)^{0.2} = 1.24$
From Eq. (6-24), $C = F_{ST}F_FF_{HA}C_F = (1.24)(1)(1)(0.37) = 0.46$ ft/s
From Eq. (6-40), $U_f = C\left[(\rho_L - \rho_V)/\rho_V\right]^{1/2} = 0.46\left[(59.5 - 0.04)/0.0408\right]^{1/2} = 17.6$ ft/s
From a rearrangement of Eq. (6-44), solving for the fraction of flooding,

$$f = \frac{4VM_V}{D^2U_f\pi(1 - A_d/A)\rho_V} = \frac{4(1{,}789/3{,}600)(18.8)}{6^2(17.6)(3.14)(1-0.1)(0.0408)} = 0.51 \text{ or } 51\%$$

Exercise 7.49 (continued)

Analysis: (continued)

(b) Vapor pressure drop per tray is given by Eq. (6-49), $h_t = h_d + h_l + h_\sigma$ (2)

From Eq. (6-50), $h_d = 0.186\left(\frac{u_o^2}{C_o^2}\right)\left(\frac{\rho_V}{\rho_L}\right)$ (3)

Column area = $A = \pi D^2/4 = 3.14(6)^2/4 = 28.3$ ft^2

Take downcomer area = $A_d = 0.1(28.3) = 2.83$ ft^2

Bubbling area = $A_a = A - 2A_d = 28.3 - 2(2.83) = 22.6$ ft^2

Hole area = $A_h = 0.1(22.6) = 2.26$ ft^2

Consider first, the **conditions at the top of the column.**

From the continuity equation, $u_o = m/A_h\rho_V$ (4)

$u_o = (1{,}944/3{,}600)(30.9)/[(2.26)(0.0703)] = 105$ ft/s and $C_o = 0.73$

From Eq. (3), $h_d = 0.186\left(\frac{105^2}{0.73^2}\right)\left(\frac{0.0703}{47.2}\right) = 5.73$ inches of liquid

Superficial velocity based on bubbling area = $U_a = 105(2.26/22.6) = 10.4$ ft/s

From Eq. (6-53), $K_s = U_a\left(\frac{\rho_V}{\rho_L - \rho_V}\right)^{1/2} = 10.4\left(\frac{0.0703}{47.2 - 0.0703}\right)^{1/2} = 0.40$ ft/s

From Eq. (6-52), $\phi_e = \exp(-4.257K_s^{0.91}) = \exp[-4.257(0.40)^{0.91}] = 0.16$

From Eq. (6-54), $C_l = 0.362 + 0.317\exp(-3.5h_w) = 0.362 + 0.317\exp[-3.5(2.0)] = 0.362$

Weir length = $L_w = 42.5$ in.

Volumetric liquid rate = $q_L = 945(30.9)/[60(8.33)(47.2/62.4)] = 77.2$ gpm

From Eq. (6-51), $h_l = \phi_e\left[h_w + C_l\left(\frac{q_L}{L_w\phi_e}\right)^{2/3}\right] = 0.16\left[2 + 0.362\left(\frac{77.2}{(42.5)0.16}\right)^{2/3}\right] = 0.61$ in. liquid

From Eq. (6-55), with maximum bubble size = D_H = 3/16 inch = 0.00476 m and liquid density = 47.2 lb/ft^3 or 756 kg/m^3,

$h_\sigma = 6\sigma / g\rho_L D_{B_{\max}} = 6(20/1000)/(9.8)(756)(0.00476) = 0.0034$ m = 0.13 in. liquid

From Eq. (2), $h_t = h_d + h_l + h_\sigma = 5.73 + 0.61 + 0.13 = 6.47$ inches liquid = 0.175 psi/tray.

This is a very high pressure drop/tray.

Consider next, the **conditions at the bottom tray of the column**.

From the continuity equation, $u_o = m/A_h\rho_V$ (4)

$u_o = (1{,}789/3{,}600)(18.1)/[(2.26)(0.0408)] = 97.9$ ft/s and $C_o = 0.73$

From Eq. (3), $h_d = 0.186\left(\frac{97.9^2}{0.73^2}\right)\left(\frac{0.0408}{59.5}\right) = 2.28$ inches of liquid

Superficial velocity based on bubbling area = $U_a = 97.9(2.26/22.6) = 9.8$ ft/s

From Eq. (6-53), $K_s = U_a\left(\frac{\rho_V}{\rho_L - \rho_V}\right)^{1/2} = 9.8\left(\frac{0.0408}{59.5 - 0.0408}\right)^{1/2} = 0.255$ ft/s

From Eq. (6-52), $\phi_e = \exp(-4.257K_s^{0.91}) = \exp[-4.257(0.255)^{0.91}] = 0.293$

Exercise 7.49 (continued)

Analysis: (b) (continued)

From Eq. (6-54), $C_l = 0.362 + 0.317\exp(-3.5h_w) = 0.362 + 0.317\exp[-3.5(2.0)] = 0.362$

Weir length = L_w = 42.5 in.

Volumetric liquid rate = q_L = 3,351(18.1)/[60(8.33)(59.5/62.4)] =127 gpm

From Eq. (6-51), $h_l = \phi_e\left[h_w + C_l\left(\frac{q_L}{L_w\phi_e}\right)^{2/3}\right] = 0.293\left[2 + 0.362\left(\frac{127}{(42.5)0.293}\right)^{2/3}\right] = 1.08$ in. liq

From Eq. (6-55), with maximum bubble size = D_H = 3/16 inch = 0.00476 m and liquid density = 59.5 lb/ft^3 or 954 kg/m^3, and σ = 58 dyne/cm = 0.058 kg/s^2,

$h_\sigma = 6\sigma / g\rho_L D_{B_{max}} = 6(0.058) / (9.8)(954)(0.00476) = 0.0078$ m = 0.31 in. liquid

From Eq. (2), $h_t = h_d + h_l + h_\sigma$ =2.28 + 1.08 + 0.31 = 3.67 inches liquid = 0.125 psi/tray.

This pressure drop is a slightly on the high side.

(c) From Fig. 6.28 for the top tray, with F_{LV} = 0.0192 and % flood = 95%, fractional entrainment = ψ = 0.50, which is fairly high.

From Fig. 6.28 for the bottom tray, with F_{LV} = 0.0473 and % flood = 51%, fractional entrainment = ψ = 0.017, which is low.

The fractional entrainment is defined as, $\psi = e/(L + e)$. Rearranging, entrainment rate = $e = \psi L/(1 - \psi)$.

At the top tray, e = 0.50(945)/(1 - 0.50) = 945 lbmol/h, which is very excessive.

At the bottom tray, e = 0.017(3,351)/(1 - 0.017) = 58 lbmol/h

(d) From Eqs. (6-70) and (6-72), the froth height in the downcomer = $h_{df} = (h_t + h_l + h_{da}) / 0.5$

Estimate the head loss for flow under the downcomer from Eq. (6-71). Area for flow under the downcomer apron = $A_{da} = L_w h_a$ = 42.5(2 - 0.5) = 63.8 in^2 = 0.433 ft^2

For the top tray, q_L = 77.2 gpm. $h_{da} = 0.03\left[\frac{77.2}{100(0.433)}\right]^2 = 0.095$ in. liquid

h_{df} = (6.47 + 0.61 + 0.095) / 0.5 = 14.4 in. liquid

For the bottom tray, q_L = 128 gpm. $h_{da} = 0.03\left[\frac{128}{100(0.433)}\right]^2 = 0.262$ in. liquid

h_{df} = (3.67 + 1.08 + 0.262) / 0.5 = 10.0 in. liquid

The new operation is not acceptable in the rectifying section because % flooding is 95%, causing very high entrainment. Should retrofit that section with structured packing. Bottom section is operable with the trays if the higher pressure drop is acceptable.

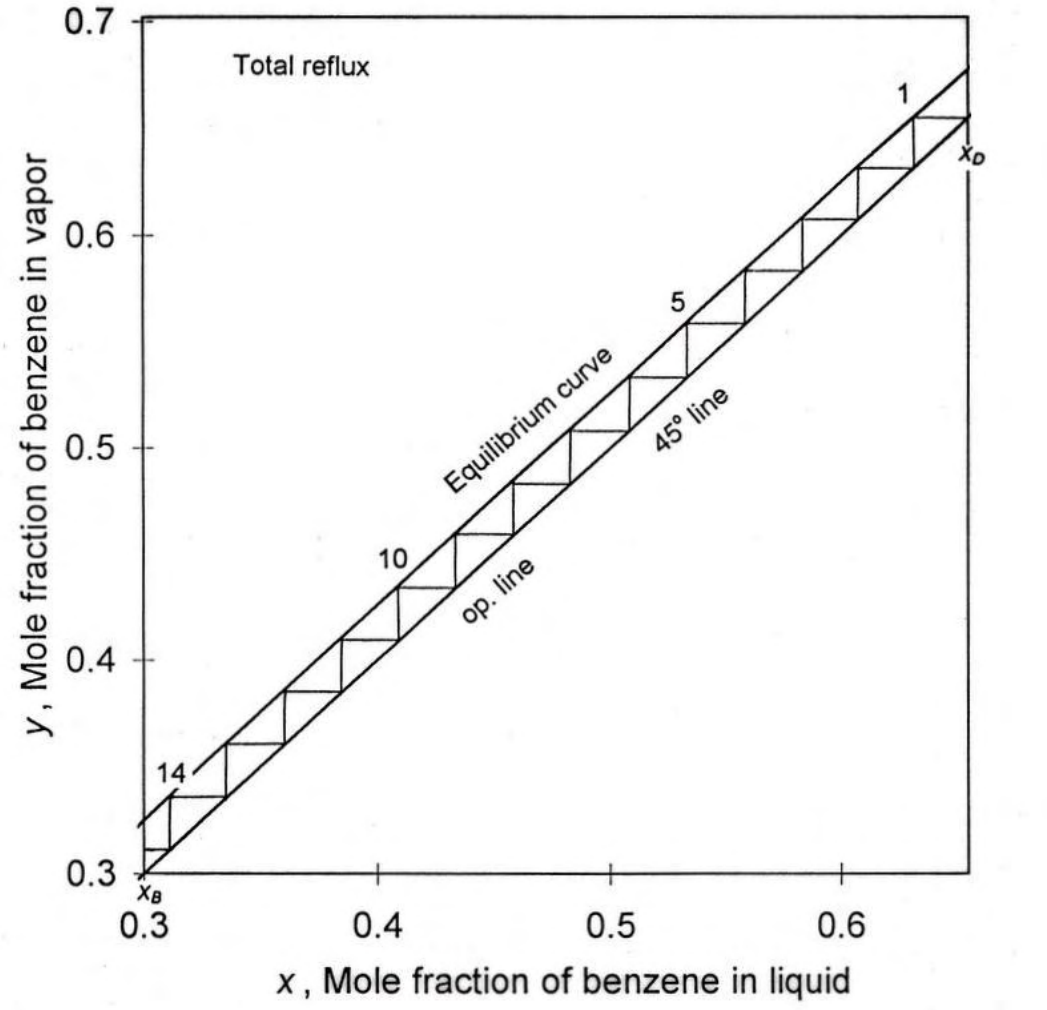
Exercise 7.50

Subject: Determination of HETP from experimental data for a packed column separating benzene and dichloroethane at total reflux.

Given: 10 feet of packing, with operation at 1 atm. Vapor-liquid equilibrium data in terms of benzene mole fractions. Measured benzene mole fractions are $x_D = 0.653$ and $x_B = 0.298$.

Find: HETP in inches. Limitations of the use of the HETP for design.

Analysis: In the plot below, the *y*-*x* equilibrium data and the operating line (45° line for total reflux condition) are plotted and equilibrium stages are stepped off between $x = 0.298$ and 0.653. The number of stages = $N_t = 14.4$. From Eq. (6-73), HETP = 10/14.4 = 0.7 ft. This value must be used with caution for design, because the HETP is a function of the *L*/*V* ratio. The value of 0.7 ft applies only to *L*/*V* =1.



Exercise 7.51

Subject: Design of a packed column for separation of a mixture of ethanol and water at 1 atm.

Given: Bubble-point feed of 10 mol% ethanol. Bottoms of 1 mol% ethanol and distillate of 80 mol% ethanol. Reflux ratio at 1.5 times minimum. Equilibrium data from Exercise 7.29.

Assumptions: Constant molar overflow.

Find: (a) Equilibrium stages above and below feed.
(b) Number of transfer units above and below the feed.
(c) Height of plate column for 18-inch tray spacing and 80% tray efficiency.
(d) Height of packing for H_{OG} = 1.2 ft.
(e) HTU from HTU for benzene-toluene system.

Analysis: By material balance, with a basis of 100 moles of feed,
Total material balance, $F = 100 = D + B$
Benzene material balance, $0.10F = 10 = 0.80D + 0.01B$
Solving these two equations, D = 11.39 moles and B = 88.61 moles.

(a) Below is the McCabe-Thiele diagram showing the equilibrium curve from the data of Exercise 7.29, a vertical q-line for the saturated liquid feed at x_F = 0.10, and the construction of the rectification section operating line for determining the minimum reflux ratio. The slope of that line is, (0.80 - 0.44)/(0.80 - 0.10) = 0.514 = L_{min}/V. From a rearrangement of Eq. (7-7),

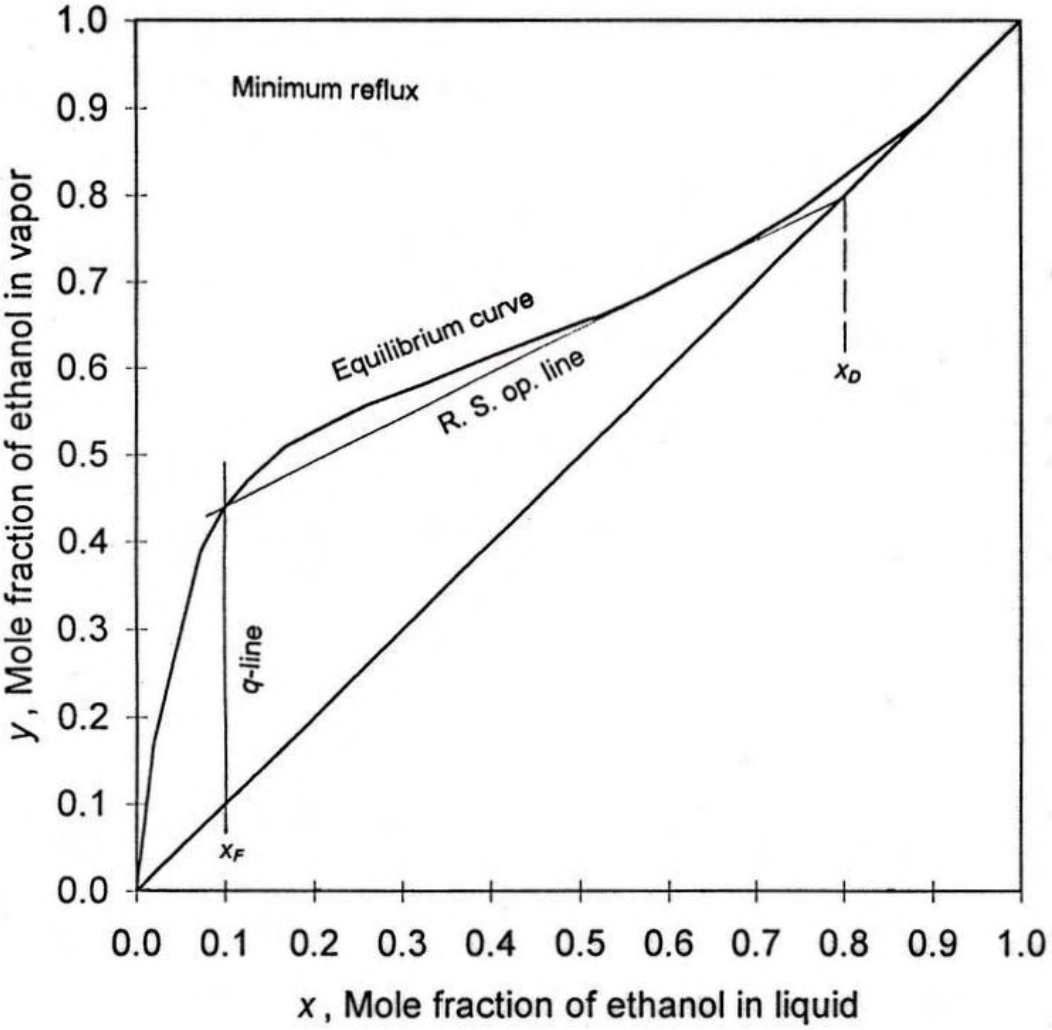
$$R_{min} = \frac{(L_{min}/V)}{1-(L_{min}/V)} = \frac{0.514}{1-0.514} = 1.058 \quad \text{and } R = 1.5\ R_{min} = 1.5(1.058) = 1.59$$

Slope of the rectification section operating line is, from Eq. (7-7), L/V = 1.59/(1 + 1.59) = 0.614.

In the McCabe-Thiele diagrams below, one for the higher concentration region and one for the lower concentration region, a rectification section operating line of this slope is drawn that passes through the 45° line at $x = x_D$ = 0.8. A stripping section operating line is drawn that extends from the intersection of the rectifying operating line and the q-line to the 45° line at $x = x_B$ = 0.01. The stages are stepped off, with the optimal feed stage location. The result is 3 equilibrium stages in the stripping section, including one for the partial reboiler, and 13.8 equilibrium stages in the rectifying section.

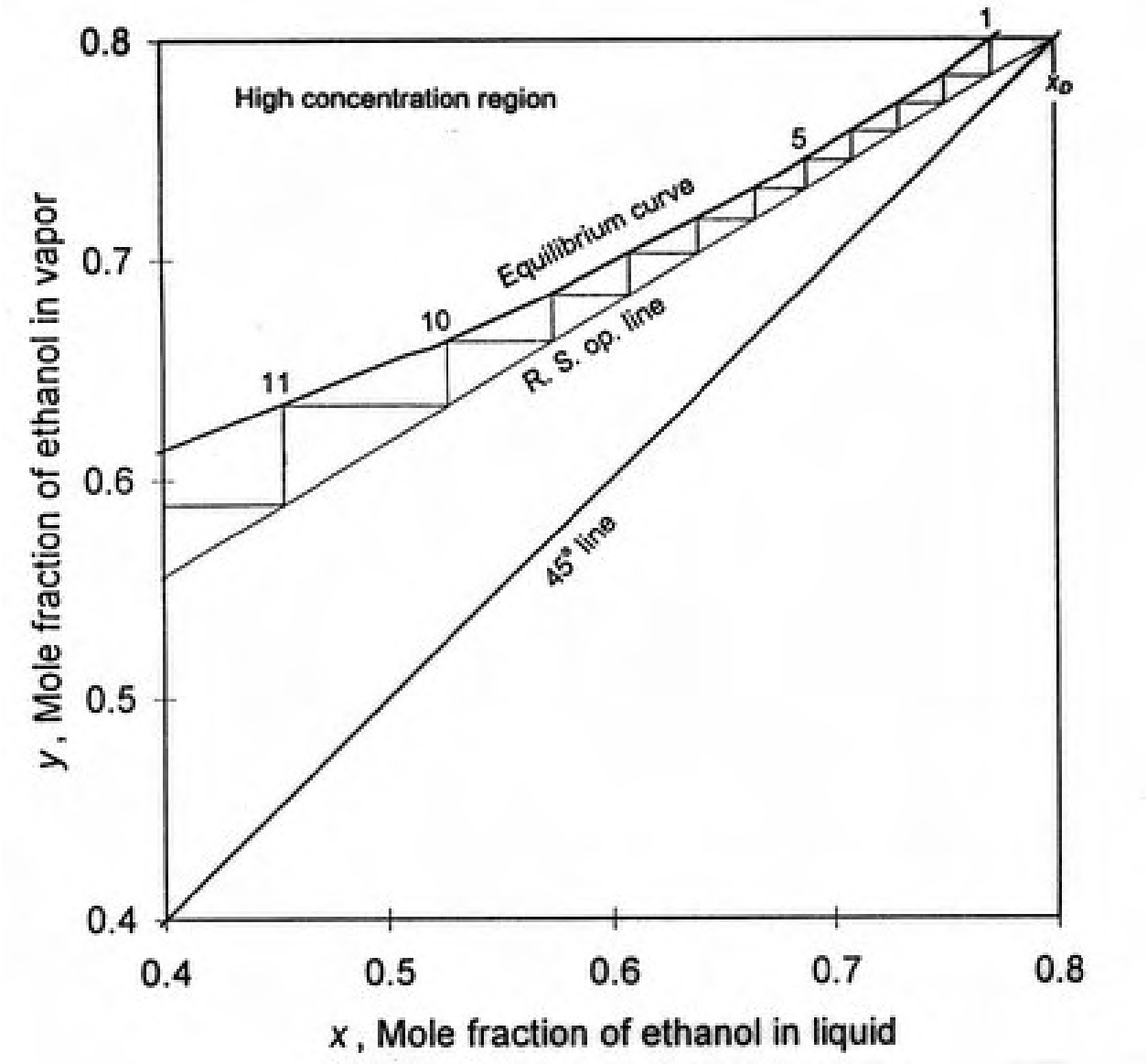
Exercise 7.51 (continued)

Analysis: (a) (continued)



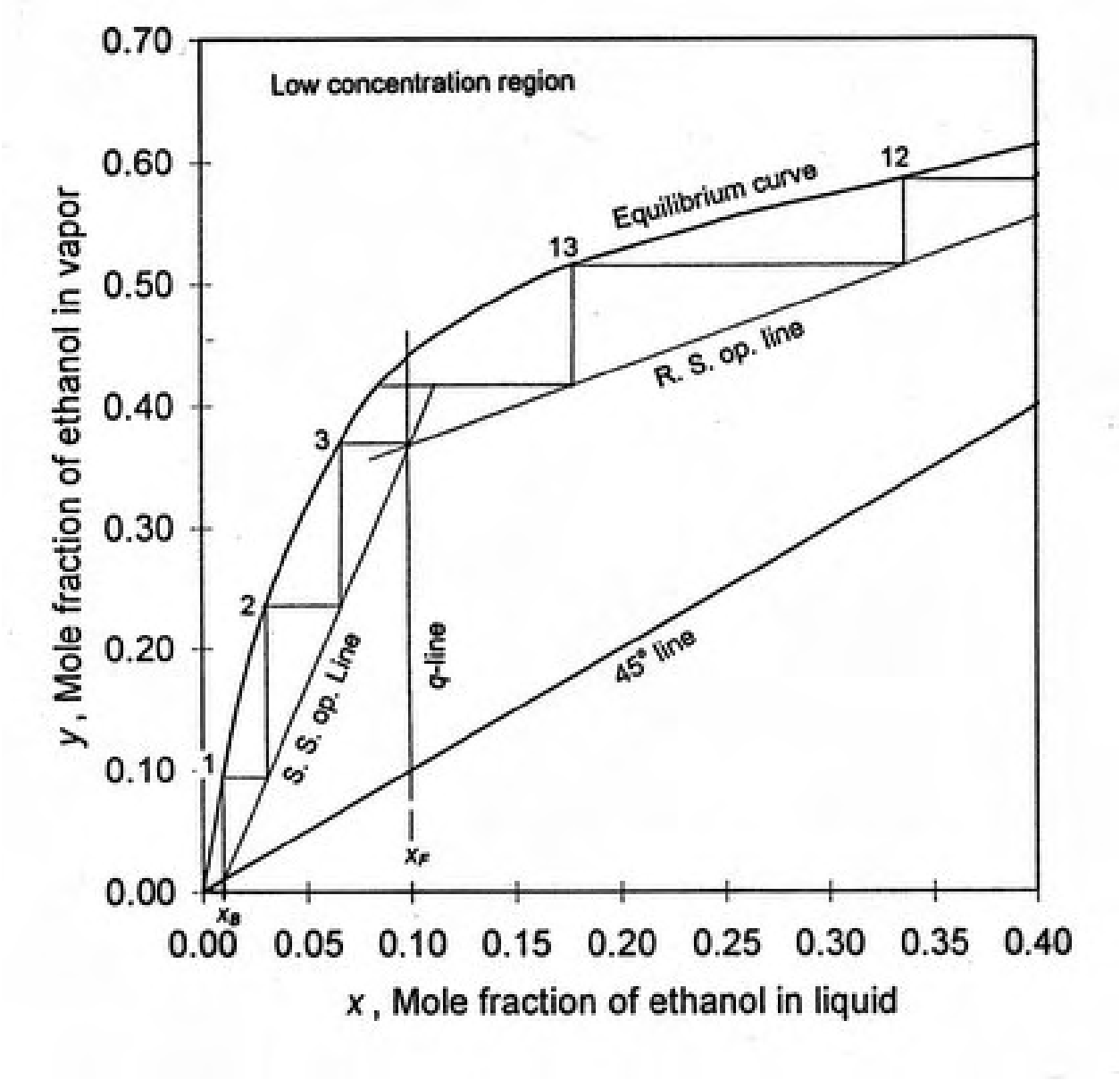
Exercise 7.51 (continued)

Analysis: (a) (continued)



Exercise 7.51 (continued)

Analysis: (a) (continued)



Exercise 7.51 (continued)

Analysis: (continued)

(b) Because the value of H_{OG} is given in part (d), calculate N_{OG} for each section, using from

Table 6.7 for EM diffusion, $N_{OG} = \int \frac{dy}{y^* - y}$

For the stripping section, the first stage is the partial reboiler. Therefore, from the McCabe-Thiele diagram, starting from Stage 2, the limits on y are $y = 0.09$ at $x = 0.03$ to $y = 0.37$ at $x = 0.10$.
Using the trapezoidal method to solve the integral,

$$(N_{OG})_{SS} = \sum \frac{\Delta y}{(y^* - y)} = \frac{(0.23 - 0.09)}{0.14} + \frac{(0.37 - 0.23)}{0.10} = 2.4$$

For the rectifying section, the limits on y are $y = 0.37$ at $x = 0.1$ to $y = 0.80$.
Using the trapezoidal method to solve the integral,

$$(N_{OG})_{RS} = \sum \frac{\Delta y}{(y^* - y)} = \frac{(0.42 - 0.37)}{0.084} + \frac{(0.665 - 0.42)}{0.063} + \frac{(0.80 - 0.665)}{0.017} = 12.4$$

(c) For 15.8 equilibrium stages at 80% tray efficiency, need 15.8/0.8 = 19.8 or 20 trays. If they are on 18-inch spacing, column height = 19(1.5) + 4 + 10 = 42.5 ft.

(d) For H_{OG} = 1.2 ft, packed height = 1.2(2.4 + 12.4) = 18 ft. Add 14 ft for disengagement at the top and sump at the bottom. Need 18 + 14 = 32 ft column.

(e) We would need data on individual values of H_L and H_G. From Eq. (6-132), H_L is proportional to $\left(\frac{1}{D_L}\right)^{1/2}$. Therefore, can ratio with the liquid diffusivities.

From Eq. (6-133), H_G is proportional to $\left(\frac{\rho_V}{\mu_V}\right)^{-3/4}\left(\frac{\mu_V}{\rho_V D_V}\right)^{-1/3}$.

Therefore, we can ratio off these properties. Then from Eq. (7.52),

$H_{OG} = H_G + mH_L$, where $m = dy/dx$, which varies over the equilibrium curve.

Exercise 7.52

Subject: Doubling plant capacity for distillation of methanol-water by adding a packed column.

Given: Conditions to duplicate those of Exercise 7.41. Design for 70% of flooding. Two packings to be considered: 1. 50-mm plastic NOR PAC rings and 2. Montz metal B1-300.

Assumptions: Constant molar overflow. Partial reboiler is an equilibrium stage.

Find: (a) Liquid holdup.
(b) Column diameter.
(c) H_{OG}.
(d) Packed height.
(e) Pressure drop.
Advantages of packed column over trayed column. Preferred packing.

Analysis: First, convert the performance data for feed and product flow rates and compositions from mass units into mole units, using molecular weights of 32.04 for methanol and 18.02 for water. The results are as follows:

	Flow rate, lbmol/h:			Mole fraction:		
Component	Feed	Distillate	Bottoms	Feed	Distillate	Bottoms
Methanol	709.1	702.7	6.4	0.360	0.915	0.0053
Water	1260.8	65.3	1195.5	0.640	0.085	0.9947
Total:	1969.9	768.0	1201.9	1.000	1.000	1.0000

The results of Exercise of 7.41 show that the observed reflux and boilup ratios (0.947 and 1.138, respectively) are consistent with the separation achieved. Therefore, at the top of the column, $L = RD = 0.947(768) = 727$ lbmol/h, and $V = L + D = 727 + 768 = 1{,}495$ lbmol/h.
At the bottom of the column,

$$\overline{V} = V_B B = 1.138(1{,}201.9) = 1{,}367.8 \text{ lbmol/h}, \text{ and } \overline{L} = \overline{V} + B = 1{,}367.8 + 1{,}201.9 = 2{,}569.7 \text{ lbmol/h}$$

Before computing liquid holdup, we need to compute column diameter.
(b) **<u>Column diameter based on conditions at the top of the column</u>,**
where $T = 154^{\circ}$F and $P = 14.7$ psia = 1 atm.
Use Figs. 6.36a, b, and c to compute flooding velocity, following Example 6.13.
From the ideal gas law, $\rho_V = PM_V/RT = (1)(30.9)/[0.730(154 + 460)] = 0.0689$ lb/ft^3
For the liquid, which is mainly methanol, use $\rho_L = 0.77$ g/cm^3 = 48 lb/ft^3 and $\mu_L = 0.35$ cP.
The abscissa in Fig. 6.36a = $X = \left(\frac{LM_L}{VM_V}\right)\left(\frac{\rho_V}{\rho_L}\right)^{1/2} = \frac{727(30.9)}{1495(30.9)}\left(\frac{0.0689}{48}\right)^{1/2} = 0.0184$

From Fig. 6.36a, Y at flooding = 0.21; from Fig. 6.36b, for $\rho_{water}/\rho_L = 1/0.77 = 1.3$, $f\{\rho_L\} = 1.6$; and from Fig. 6.36c, for $\mu_L = 0.35$ cP, $f\{\mu_L\} = 0.8$.
From Table 6.8, $F_P = 14$ for NOR PAC and $F_P = 33$ for Montz.

Exercise 7.52 (continued)

Analysis: (b) (continued)

From a rearrangement of the ordinate of Fig. 6.36a, $u_o^2 = Y\dfrac{g}{F_P}\left(\dfrac{\rho_{H_2O\,(L)}}{\rho_V}\right)\dfrac{1}{f\{\rho_L\}f\{\mu_L\}}$

For NOR PAC, $u_o^2 = 0.21\left(\dfrac{32.2}{14}\right)\left(\dfrac{62.4}{0.0689}\right)\dfrac{1}{1.6(0.8)} = 341\ (\text{ft/s})^2$ and $u_o = 18.5$ ft/s

For Montz, $u_o^2 = 0.21\left(\dfrac{32.2}{33}\right)\left(\dfrac{62.4}{0.0689}\right)\dfrac{1}{1.6(0.8)} = 145\ (\text{ft/s})^2$ and $u_o = 12.0$ ft/s

For fraction of flooding = $f = 0.7$, $u_V = u_o f = 18.5(0.7) = 13.0$ ft/s for NOR PAC,
$u_V = u_o f = 12.0(0.7) = 8.4$ ft/s for Montz.

From Eq. (6-103), column diameter = $D_T = \left(\dfrac{4VM_V}{fu_0\pi\rho_V}\right)^{1/2} = \left(\dfrac{4VM_V}{u_V\pi\rho_V}\right)^{1/2}$

For NORPAC, $D_T = \left[\dfrac{4(1495/3600)(30.9)}{13(3.14)(0.0689)}\right]^{1/2} = 4.3$ ft.

For Montz, $D_T = \left[\dfrac{4(1495/3600)(30.9)}{8.4(3.14)(0.0689)}\right]^{1/2} = 5.3$ ft

Column diameter based on conditions at the bottom of the column,
where $T = 207^\circ$F and $P = 15.5$ psia = 1.05 atm.
Use Figs. 6.36a, b, and c to compute flooding velocity, following Example 6.13.
From the ideal gas law, $\rho_V = PM_V/RT = (1.05)(18.1)/[0.730(207 + 460)] = 0.039$ lb/ft^3
For the liquid, which is mainly water, use $\rho_L = 1.00$ g/cm^3 = 62.4 lb/ft^3 and $\mu_L = 0.27$ cP.

The abscissa in Fig. 6.36a = $X = \left(\dfrac{LM_L}{VM_V}\right)\left(\dfrac{\rho_V}{\rho_L}\right)^{1/2} = \dfrac{2569.7(18.1)}{1367.8(18.1)}\left(\dfrac{0.039}{62.4}\right)^{1/2} = 0.047$

From Fig. 6.36a, Y at flooding = 0.17; from Fig. 6.36b, for $\rho_{water}/\rho_L = 1/1 = 1$, $f\{\rho_L\} = 1$;
and from Fig. 6.36c, for $\mu_L = 0.27$ cP, $f\{\mu_L\} = 0.77$.
From Table 6.8, $F_P = 14$ for NOR PAC and $F_P = 33$ for Montz.

From a rearrangement of the ordinate of Fig. 6.36a, $u_o^2 = Y\dfrac{g}{F_P}\left(\dfrac{\rho_{H_2O\,(L)}}{\rho_V}\right)\dfrac{1}{f\{\rho_L\}f\{\mu_L\}}$

For NOR PAC, $u_o^2 = 0.17\left(\dfrac{32.2}{14}\right)\left(\dfrac{62.4}{0.039}\right)\dfrac{1}{1(0.77)} = 812\ (\text{ft/s})^2$ and $u_o = 28.5$ ft/s

For Montz, $u_o^2 = 0.17\left(\dfrac{32.2}{33}\right)\left(\dfrac{62.4}{0.039}\right)\dfrac{1}{1(0.77)} = 345\ (\text{ft/s})^2$ and $u_o = 18.6$ ft/s

For fraction of flooding = $f = 0.7$, $u_V = u_o f = 28.5(0.7) = 20.0$ ft/s for NOR PAC,
$u_V = u_o f = 18.6(0.7) = 13.0$ ft/s for Montz.

From Eq. (6-103), column diameter = $D_T = \left(\dfrac{4VM_V}{fu_0\pi\rho_V}\right)^{1/2} = \left(\dfrac{4VM_V}{u_V\pi\rho_V}\right)^{1/2}$

Exercise 7.52 (continued)

Analysis: (b) (continued)

For NOR PAC, $D_T = \left[\dfrac{4(1367.8/3600)(18.1)}{20(3.14)(0.039)}\right]^{1/2} = 3.4$ ft.

For Montz, $D_T = \left[\dfrac{4(1367.8/3600)(18.1)}{13.0(3.14)(0.039)}\right]^{1/2} = 4.2$ ft

(a) For liquid holdup estimates, assume the column operates in the preloading region. Therefore, the holdup is independent of the gas rate. Follow Example 6.12. Pertinent packing characteristics from Table 6.8:

Packing	a, m^2/m^3	a, ft^2/ft^3	ε	C_h
NOR PAC	86.8	26.5	0.947	0.651
Montz	300	91.4	0.930	0.482

Use Eqs. (6-97) to (6-101), which requires calculating the liquid Reynolds and Froude numbers.

Liquid holdup based on conditions at the top of the column.

By the continuity equation, superficial liquid velocity is,

$u_L = LM_L/\rho_L S = (727/3600)(30.9)/\,[48(3.14)(D_T)^2/4] = 0.166/(D_T)^2$ ft/s

From Eq. (6-98), $N_{\mathrm{Re}_L} = \dfrac{u_L \rho_L}{\mu_L a} = \dfrac{(0.166/D_T^2)48}{(0.35)(0.000672)a} = \dfrac{33900}{D_T^2 a}$

From Eq. (6-99), $N_{\mathrm{Fr}_L} = \dfrac{u_L^2 a}{g} = \dfrac{(0.166/D_T^2)^2\, a}{32.2} = 0.000856\dfrac{a}{D_T^4}$

Packing	D_T, ft	u_L, ft/s	a, ft^2/ft^3	N_{Re_L}	N_{Fr_L}
NOR PAC	4.3	0.00898	26.5	69.2	6.63×10^{-5}
Montz	5.3	0.00591	91.4	13.2	9.91×10^{-5}

Since both values of $N_{\mathrm{Re}_L} > 5$, use Eq. (6-101), $a_h/a = 0.85 C_h N_{\mathrm{Re}_L}^{0.25} N_{\mathrm{Fr}_L}^{0.1}$

For NOR PAC, $a_h/a = 0.85(0.651)(69.2)^{0.25}(6.63\times10^{-5})^{0.1} = 0.61$

For Montz, $a_h/a = 0.85(0.482)(13.2)^{0.25}(9.91\times10^{-5})^{0.1} = 0.31$

From Eq. (6-97), the fractional liquid holdup is $h_L = \left(12\dfrac{N_{\mathrm{Fr}_L}}{N_{\mathrm{Re}_L}}\right)^{1/3}\left(\dfrac{a_h}{a}\right)^{2/3}$

For NOR PAC, $h_L = \left[(12)\dfrac{6.63\times10^{-5}}{69.2}\right]^{1/3}(0.61)^{2/3} = 0.0162$ m^3/m^3

For Montz, $h_L = \left[(12)\dfrac{9.91\times10^{-5}}{13.2}\right]^{1/3}(0.31)^{2/3} = 0.0241$ m^3/m^3

These liquid holdups at the top of the column are quite small.

Exercise 7.52 (continued)

Analysis: (a) (continued)

Liquid holdup based on conditions at the bottom of the column.

By the continuity equation, superficial liquid velocity is,

$u_L = LM_L/\rho_L S = (2570/3600)(18.1)/\,[62.4(3.14)(D_T)^2/4] = 0.264/(D_T)^2$ ft/s

From Eq. (6-98), $N_{\mathrm{Re}_L} = \dfrac{u_L \rho_L}{\mu_L a} = \dfrac{(0.264/D_T^2)62.4}{(0.27)(0.000672)a} = \dfrac{90800}{D_T^2 a}$

From Eq. (6-99), $N_{\mathrm{Fr}_L} = \dfrac{u_L^2 a}{g} = \dfrac{(0.264/D_T^2)^2 a}{32.2} = 0.00216\dfrac{a}{D_T^4}$

Packing	D_T, ft	u_L, ft/s	a, ft^2/ft^3	N_{Re_L}	N_{Fr_L}
NOR PAC	3.4	0.0228	26.5	296	4.28×10^{-4}
Montz	4.2	0.0150	91.4	56.3	6.39×10^{-4}

Since both values of N_{Re_L} are > 5, use Eq. (6-101), $a_h/a = 0.85 C_h N_{\mathrm{Re}_L}^{0.25} N_{\mathrm{Fr}_L}^{0.1}$

For NOR PAC, $a_h/a = 0.85(0.651)(296)^{0.25}(4.28\times10^{-4})^{0.1} = 1.057$

For Montz, $a_h/a = 0.85(0.482)(56.3)^{0.25}(6.39\times10^{-4})^{0.1} = 0.54$

From Eq. (6-97), the fractional liquid holdup is $h_L = \left(12\dfrac{N_{\mathrm{Fr}_L}}{N_{\mathrm{Re}_L}}\right)^{1/3}\left(\dfrac{a_h}{a}\right)^{2/3}$

For NOR PAC, $h_L = \left[(12)\dfrac{4.28\times10^{-4}}{69.2}\right]^{1/3}(1.057)^{2/3} = 0.0269$ m^3/m^3

For Montz, $h_L = \left[(12)\dfrac{6.39\times10^{-4}}{56.3}\right]^{1/3}(0.54)^{2/3} = 0.0341$ m^3/m^3

These liquid holdups at the bottom of the column are quite small.

(c) From Eq. (7.52), $H_{OG} = H_G + \left(\dfrac{mV}{L}\right)H_L$, where we must use the slope, m, of the equilibrium curve instead of a K-value because the equilibrium curve is curved.

At the top of the column:

Near a mole fraction, x_D , of 0.9, m = (0.9780 - 0.9359)/0.10 = 0.42

Estimate H_L from Eq. (6-132), using the following properties and parameters:

	NOR PAC	Montz
C_L	1.080	1.165
h_L, m^3/m^3	0.0162	0.0241
ε, m^3/m^3	0.947	0.930
u_L, ft/s	0.00898	0.00591
a, m^2/m^3	86.8	300
a_h, m^2/m^3	52.9	93

Exercise 7.52 (continued)

Analysis: (c) at the top of the column (continued)

Need an estimate of the diffusivity of methanol in water at high concentrations of methanol. From Example 3.7, the diffusivity of methanol in water at a mole fraction of 0.8 and 25°C is 1.5 x 10^{-5} cm^2/s. Use Eq. (3-39) to correct this for temperature to 170°F or 350 K and viscosity. For methanol, viscosity at 25°C (298 K) = 0.55 cP and at 350 K, viscosity = 0.32 cP. Therefore,

$$D_{\text{MeOH}} = 1.50\times10^{-5}\left(\frac{350}{298}\right)\left(\frac{0.55}{0.32}\right) = 3.0\times10^{-5}\ \text{cm}^2/\text{s}$$

From Eq. (6-132), for NOR PACK, using SI (instead of American Engineering) units,

$$H_L = \frac{1}{C_L}\left(\frac{1}{12}\right)^{1/6}\left[\frac{4h_L\varepsilon}{D_L a u_L}\right]^{1/2}\left(\frac{u_L}{a}\right)\left(\frac{a}{a_{Ph}}\right) = \frac{1}{1.08}\left(\frac{1}{12}\right)^{1/6}\left[\frac{4(0.0162)(0.947)}{(3.0\times10^{-9})(86.8)(0.00274)}\right]^{1/2}\left(\frac{0.00274}{86.8}\right)\left(\frac{a}{a_{Ph}}\right)$$

$$= 0.174\left(\frac{a}{a_{Ph}}\right)\ \text{m}$$

To compute (a_{Ph}/a), we need for the liquid phase, the Reynolds, Weber, and Froude numbers from equations (6-138), (6-139), and (6-140), respectively, based on the packing hydraulic diameter from (6-137).

$$d_h = \text{ packing hydraulic diameter} = 4\frac{\varepsilon}{a} = 4\left(\frac{0.947}{86.8}\right) = 0.0436\ \text{m} = 0.143\ \text{ft}$$

$$\text{Reynolds number} = N_{\text{Re}_L,h} = \frac{u_L d_h \rho_L}{\mu_L} = \frac{(0.00898)(0.143)(48)}{[(0.35)(0.000672)]} = 262$$

Take the surface tension of methanol at 154°F as σ = 17 dynes/cm = 0.001165 lb_f/ft or 0.001165(32.2) = 0.0375 lb_m/s^2

$$\text{Weber number} = N_{\text{We}_L,h} = \frac{u_L^2 \rho_L d_h}{\sigma} = \frac{(0.00898)^2\,(48)(0.143)}{0.0375} = 0.0148$$

$$\text{Froude number} = N_{\text{Fr}_L,h} = \frac{u_L^2}{g d_h} = \frac{(0.00898)^2}{32.2(0.143)} = 0.0000175$$

From (6-136), $\frac{a_{Ph}}{a} = 1.5(a d_h)^{-1/2}\left(N_{\text{Re}_L,h}\right)^{-0.2}\left(N_{\text{We}_L,h}\right)^{0.75}\left(N_{\text{Fr}_L,h}\right)^{-0.45}$

$$= 1.5[(86.8)(0.0436)]^{-1/2}(262)^{-0.2}(0.0148)^{0.75}(0.0000175)^{-0.45} = 1.485$$

Exercise 7.52 (continued)

Analysis: (c) at the top of the column (continued)

$$H_L = 0.174\left(\frac{1}{1.485}\right) = 0.117 \text{ m}$$

From Eq. (6-132), for Montz, using SI units,

$$H_L = \frac{1}{C_L}\left(\frac{1}{12}\right)^{1/6}\left[\frac{4h_L\varepsilon}{D_L a u_L}\right]^{1/2}\left(\frac{u_L}{a}\right)\left(\frac{a}{a_{Ph}}\right) = \frac{1}{1.165}\left(\frac{1}{12}\right)^{1/6}\left[\frac{4(0.0241)(0.930)}{(3.0\times10^{-9})(300)(0.00180)}\right]^{1/2}\left(\frac{0.00180}{300}\right)\left(\frac{a}{a_{Ph}}\right)$$

$$= 0.0253\left(\frac{a}{a_{Ph}}\right) \text{ m}$$

To compute (a_{Ph}/a), we need for the liquid phase, the Reynolds, Weber, and Froude numbers from equations (6-138), (6-139), and (6-140), respectively, based on the packing hydraulic diameter from (6-137).

$$d_h = \text{ packing hydraulic diameter} = 4\frac{\varepsilon}{a} = 4\left(\frac{0.930}{300}\right) = 0.0124 \text{ m} = 0.0407 \text{ ft}$$

$$\text{Reynolds number} = N_{\text{Re}_L,h} = \frac{u_L d_h \rho_L}{\mu_L} = \frac{(0.00591)(0.0407)(48)}{[(0.35)(0.000672)]} = 49.1$$

$$\text{Weber number} = N_{\text{We}_L,h} = \frac{u_L^2 \rho_L d_h}{\sigma} = \frac{(0.00898)^2(48)(0.407)}{0.0375} = 0.00421$$

$$\text{Froude number} = N_{\text{Fr}_L,h} = \frac{u_L^2}{g d_h} = \frac{(0.00898)^2}{32.2(0.0407)} = 0.0000615$$

$$\text{From (6-136), } \frac{a_{Ph}}{a} = 1.5(a d_h)^{-1/2}\left(N_{\text{Re}_L,h}\right)^{-0.2}\left(N_{\text{We}_L,h}\right)^{0.75}\left(N_{\text{Fr}_L,h}\right)^{-0.45}$$

$$= 1.5[(300)(0.0124)]^{-1/2}(49.1)^{-0.2}(0.00421)^{0.75}(0.0000615)^{-0.45} = 0.47$$

$$H_L = 0.0253\left(\frac{1}{0.47}\right) = 0.054 \text{ m}$$

Exercise 7.52 (continued)

Analysis: (c) at the top of the column (continued)

Now estimate the value of H_G from Eq. (6-133). Estimate the gas diffusivity from Eq. (3-36), where from Table 3.1, $\sum_V = 13.1$ for water, and $\sum_V = 15.9 + 4(2.31) + 6.11 = 31.2$ for methanol and molecular weights are 32 for methanol and 18 for water.

$$D_V = D_{AB} = \frac{0.00143T^{1.75}}{P\left[\frac{2}{(1/M_A)+(1/M_B)}\right]^{1/2}\left[\left(\sum_V\right)_A^{1/3}+\left(\sum_V\right)_B^{1/3}\right]^2}$$

$$= \frac{0.00143(350)^{1.75}}{(1)\left[\frac{2}{(1/18)+(1/32)}\right]^{1/2}\left[(13.1)^{1/3}+(31.2)^{1/3}\right]^2} = 0.28 \text{ cm}^2/\text{s}$$

Use the following additional properties and parameters, together with μ_ς = 1.1 x 10^{-2} cP and ρ_V = 0.0688 lb/ft^3, where from Eqs. (6-134) and (6-135), $N_{\text{Re}_V} = \frac{u_V \rho_V}{a\mu_V}$ and $N_{\text{Sc}_V} = \frac{\mu_V}{\rho_V D_V}$

	NOR PAC	Montz
C_V	0.322	0.422
u_V, m/s	3.96	2.56
$(N_{\text{Sc}})_V$	0.36	0.36
$(N_{\text{Re}})_V$	4,560	850

From Eq. (6-133), for NOR PAC, using SI units,

$$H_G = \frac{1}{C_V}(\varepsilon - h_L)^{1/2}\left(\frac{4\varepsilon}{a^4}\right)^{1/2}\left(N_{\text{Re}_V}\right)^{-3/4}\left(N_{\text{Sc}_V}\right)^{-1/3}\left(\frac{u_V a}{D_V a_{Ph}}\right)$$

$$= \frac{1}{0.322}(0.947-0.0162)^{1/2}\left[\frac{4(0.947)}{86.8^4}\right]^{1/2}(4{,}560)^{-3/4}(0.36)^{-1/3}\left[\frac{(3.96)(86.8)}{(0.28\times10^{-4})(71.2)}\right] = 0.34 \text{ m}$$

For Montz,

$$H_G = \frac{1}{0.422}(0.947-0.0241)^{1/2}\left[\frac{4(0.930)}{300^4}\right]^{1/2}(850)^{-3/4}(0.36)^{-1/3}\left[\frac{(2.56)(300)}{(0.28\times10^{-4})(78)}\right] = 0.16 \text{ m}$$

At the top of the column, vapor rate = V =1,495 lbmol/h and liquid rate = L = 727 lbmol/h. Therefore, mV/L = (0.42)(1,495)/(727) = 0.864

From Eq. (7.51), for NOR PAC, $H_{OG} = H_G + \left(\frac{mV}{L}\right)H_L = 0.34 + (0.864)(0.117) = 0.44$ m = 1.5 ft

Exercise 7.52 (continued)

Analysis: (c) at the top of the column (continued)

For Montz, $H_{OG} = H_G + \left(\frac{mV}{L}\right) H_L = 0.16 + (0.864)(0.054) = 0.21 \text{ m} = 0.68 \text{ ft}$

At the bottom of the column:

Near a mole fraction, x_B , of 0.005, m = 2.5

Estimate H_L from Eq. (6-123), using the following properties and parameters:

	NOR PAC	Montz
C_L	1.080	1.165
h_L, m^3/m^3	0.0269	0.0341
ε , m^3/m^3	0.947	0.930
u_L, ft/s	0.0228	0.0150
a, m^2/m^3	86.8	300
a_h, m^2/m^3	91.7	162

Need an estimate of the diffusivity of methanol in water at low concentrations of methanol. From Example 3.7, the diffusivity of methanol in water at infinite dilution at 25°C is 1.5 x 10^{-5} cm^2/s. Use Eq. (3-39) to correct this for temperature to 207°F or 370 K and viscosity. For water, viscosity at 25°C (298 K) = 0.90 cP and at 370 K, viscosity = 0.26 cP. Therefore,

$$D_{\text{MeOH}} = 1.50\times10^{-5}\left(\frac{370}{298}\right)\left(\frac{0.90}{0.26}\right) = 6.4\times10^{-5} \text{ cm}^2/\text{s}$$

From Eq. (6-132), for NOR PACK, using SI (instead of American Engineering) units,

$$H_L = \frac{1}{C_L}\left(\frac{1}{12}\right)^{1/6}\left[\frac{4h_L\varepsilon}{D_L a u_L}\right]^{1/2}\left(\frac{u_L}{a}\right)\left(\frac{a}{a_{Ph}}\right) = \frac{1}{1.08}\left(\frac{1}{12}\right)^{1/6}\left[\frac{4(0.0269)(0.947)}{(6.4\times10^{-9})(86.8)(0.0228)}\right]^{1/2}\left(\frac{0.0228}{86.8}\right)\left(\frac{a}{a_{Ph}}\right)$$

$$= 0.456\left(\frac{a}{a_{Ph}}\right) \text{ m}$$

To compute (a_{Ph}/a), we need for the liquid phase, the Reynolds, Weber, and Froude numbers from equations (6-138), (6-139), and (6-140), respectively, based on the packing hydraulic diameter from (6-137).

$$d_h = \text{ packing hydraulic diameter} = 4\frac{\varepsilon}{a} = 4\left(\frac{0.947}{86.8}\right) = 0.0436 \text{ m} = 0.143 \text{ ft}$$

$$\text{Reynolds number} = N_{\text{Re}_L,h} = \frac{u_L d_h \rho_L}{\mu_L} = \frac{(0.0228)(0.143)(62.4)}{[(0.27)(0.000672)]} = 1120$$

Exercise 7.52 (continued)

Analysis: (c) at the bottom of the column (continued)

Take the surface tension of water at 207°F as $\sigma = 60$ dynes/cm = 0.00411 lb_f/ft or 0.00411(32.2) = 0.132 lb_m/s^2

Weber number = $N_{We_L,h} = \dfrac{u_L^2 \rho_L d_h}{\sigma} = \dfrac{(0.0228)^2 (62.4)(0.143)}{0.132} = 0.035$

Froude number = $N_{Fr_L,h} = \dfrac{u_L^2}{g d_h} = \dfrac{(0.0228)^2}{32.2(0.143)} = 0.000113$

From (6-136), $\dfrac{a_{Ph}}{a} = 1.5(a d_h)^{-1/2} \left(N_{Re_L,h}\right)^{-0.2} \left(N_{We_L,h}\right)^{0.75} \left(N_{Fr_L,h}\right)^{-0.45}$

$$= 1.5\left[(86.8)(0.0436)\right]^{-1/2} (1120)^{-0.2} (0.035)^{0.75} (0.000113)^{-0.45} = 0.92$$

$H_L = 0.456 \left(\dfrac{1}{0.92}\right) = 0.50$ m

From Eq. (6-132), for Montz, using SI units,

$$H_L = \frac{1}{C_L}\left(\frac{1}{12}\right)^{1/6} \left[\frac{4 h_L \varepsilon}{D_L a u_L}\right]^{1/2} \left(\frac{u_L}{a}\right)\left(\frac{a}{a_{Ph}}\right) = \frac{1}{1.165}\left(\frac{1}{12}\right)^{1/6} \left[\frac{4(0.0341)(0.930)}{(6.4\times10^{-9})(300)(0.0150)}\right]^{1/2} \left(\frac{0.0150}{300}\right)\left(\frac{a}{a_{Ph}}\right)$$

$$= 0.0595 \left(\frac{a}{a_{Ph}}\right) \text{ m}$$

To compute (a_{Ph}/a), we need for the liquid phase, the Reynolds, Weber, and Froude numbers from equations (6-138), (6-139), and (6-140), respectively, based on the packing hydraulic diameter from (6-137).

$d_h =$ packing hydraulic diameter = $4\dfrac{\varepsilon}{a} = 4\left(\dfrac{0.930}{300}\right) = 0.0124$ m = 0.0407 ft

Reynolds number = $N_{Re_L,h} = \dfrac{u_L d_h \rho_L}{\mu_L} = \dfrac{(0.0150)(0.0407)(62.4)}{[(0.27)(0.000672)]} = 210$

Exercise 7.52 (continued)

Analysis: (c) at the bottom of the column (continued)

Weber number = $N_{\mathrm{We}_L,h} = \dfrac{u_L^2 \rho_L d_h}{\sigma} = \dfrac{(0.0150)^2\,(62.4)(0.407)}{0.132} = 0.0433$

Froude number = $N_{\mathrm{Fr}_L,h} = \dfrac{u_L^2}{g d_h} = \dfrac{(0.0150)^2}{32.2(0.0407)} = 0.000172$

From (6-136), $\dfrac{a_{Ph}}{a} = 1.5(a d_h)^{-1/2} \left(N_{\mathrm{Re}_L,h}\right)^{-0.2} \left(N_{\mathrm{We}_L,h}\right)^{0.75} \left(N_{\mathrm{Fr}_L,h}\right)^{-0.45}$

$= 1.5\left[(300)(0.0124)\right]^{-1/2} (210)^{-0.2} (0.0433)^{0.75} (0.000172)^{-0.45} = 1.25$

$H_L = 0.0595 \left(\dfrac{1}{1.25}\right) = 0.048$ m

Now estimate the value of H_G from Eq. (6-133). Estimate the gas diffusivity from Eq. (3-36), where from Table 3.1, $\sum_V = 13.1$ for water, and $\sum_V = 15.9 + 4(2.31) + 6.11 = 31.2$ for methanol and molecular weights are 32 for methanol and 18 for water.

$$D_V = D_{AB} = \frac{0.00143 T^{1.75}}{P\left[\dfrac{2}{(1/M_A)+(1/M_B)}\right]^{1/2} \left[\left(\sum_V\right)_A^{1/3} + \left(\sum_V\right)_B^{1/3}\right]^2}$$

$$= \frac{0.00143(370)^{1.75}}{(1)\left[\dfrac{2}{(1/18)+(1/32)}\right]^{1/2} \left[(13.1)^{1/3} + (31.2)^{1/3}\right]^2} = 0.31 \text{ cm}^2/\text{s}$$

Use the following additional properties and parameters, together with μ_V = 1.2 x 10^{-2} cP and ρ_V = 0.0370 lb/ft^3 , where from Eqs. (6-134) and (6-135), $N_{\mathrm{Re}_V} = \dfrac{u_V \rho_V}{a \mu_V}$ and $N_{\mathrm{Sc}_V} = \dfrac{\mu_V}{\rho_V D_V}$

	NOR PAC	**Montz**
C_V	0.322	0.422
u_V, m/s	6.10	3.96
$(N_{\mathrm{Sc}})_V$	0.65	0.65
$(N_{\mathrm{Re}})_V$	3,470	652

From Eq. (6-133), for NOR PAC,

Exercise 7.52 (continued)

Analysis: (c) at the bottom of the column (continued)

From Eq. (6-133), for NOR PAC, using SI units,

$$H_G = \frac{1}{C_V}(\varepsilon - h_L)^{1/2}\left(\frac{4\varepsilon}{a^4}\right)^{1/2}\left(N_{\mathrm{Re}_V}\right)^{-3/4}\left(N_{\mathrm{Sc}_V}\right)^{-1/3}\left(\frac{u_V a}{D_V a_{Ph}}\right)$$

$$= \frac{1}{0.322}(0.947-0.0269)^{1/2}\left[\frac{4(0.947)}{86.8^4}\right]^{1/2}(3,470)^{-3/4}(0.65)^{-1/3}\left[\frac{(6.10)(86.8)}{(0.34\times10^{-4})(44.2)}\right] = 0.69 \text{ m}$$

For Montz,

$$H_G = \frac{1}{0.422}(0.947-0.0341)^{1/2}\left[\frac{4(0.930)}{300^4}\right]^{1/2}(652)^{-3/4}(0.65)^{-1/3}\left[\frac{(3.96)(300)}{(0.34\times10^{-4})(207)}\right] = 0.073 \text{ m}$$

At the bottom of the column, vapor rate = V =1,368 lbmol/h and liquid rate = L = 2,570 lbmol/h. Therefore, mV/L = (2.50)(1,368)/(2,570) = 1.33

From Eq. (7.51), for NOR PAC, $H_{OG} = H_G + \left(\frac{mV}{L}\right)H_L = 0.69 + (1.33)(0.50) = 1.36$ m $= 4.4$ ft

For Montz, $H_{OG} = H_G + \left(\frac{mV}{L}\right)H_L = 0.073 + (1.33)(0.048) = 0.14$ m $= 0.45$ ft

(d) The packed height is given by Eq. (6-127), $l_T = H_{OG}N_{OG}$

Calculate N_{OG} for each section, using from Table 6.7 for EM diffusion, $N_{OG} = \int \frac{dy}{y^* - y}$

Apply this equation to the rectifying section and to the stripping section, using the McCabe-Thiele diagrams developed in Exercise 7.41.

For the rectifying section, the limits on y from the feed to the distillate are 0.64 to 0.915. The difference, y^*-y is almost constant at an average value of approximately 0.065. Therefore, $(N_{OG})_{RS} = \Delta y/(y^*-y)$ = (0.915-0.64)/0.065 = 4.2. Therefore,

Packed height for NOR PAC = (1.5)(4.2) = 6.3 ft

Packed height for Montz = (0.68)(4.2) = 2.9 ft

For the stripping section, after accounting for the partial reboiler, the limits on y from the bottom to the feed are 0.05 to 0.68. The difference, y^*-y varies from 0.12 at y = 0.05, to 0.23 at y = 0.17, to 0.19 at y = 0.40, to 0.09 at y = 0.59, to 0.03 at y = 0.68 Using the trapezoidal method to solve the integral,

$$\left(N_{OG}\right)_{RS} = \sum \frac{\Delta y}{(y^*-y)} = \frac{(0.17-0.05)}{0.175} + \frac{(0.40-0.17)}{0.21} + \frac{(0.59-0.40)}{0.14} + \frac{(0.68-0.59)}{0.06} = 4.6$$

Exercise 7.52 (continued)

Analysis: (d) (continued)

Packed height for NOR PAC = (4.4)(4.6) = 20.2 ft
Packed height for Montz = (0.45)(4.6) = 2.1 ft

The total packed height for both sections are:
6.3 + 20.2 = 26.5 ft for NOR PAC
2.9 + 2.1 = 5.0 ft for Montz
However, these heights are approximate because they are based on values of H_{OG} that are assumed constant over the packed sections, which is not the case because m varies.

(e) Compute pressure drops for the packed sections from the correlation of Billet and Schultes. The pressure drop per unit height of packed bed is given by Eq. (6-115),

$$\frac{\Delta P}{l_T} = \left(\frac{\Delta P_o}{l_T}\right)\left(\frac{\varepsilon - h_L}{\varepsilon}\right)^{3/2} \exp\left[\frac{13300}{a^{3/2}}\left(N_{\mathrm{Fr}_L}\right)^{1/2}\right] \qquad (1)$$

This equation will be used for each packing in each section.

From Eq. (6-110), $$\frac{\Delta P_o}{l_T} = \Psi_o \frac{a}{\varepsilon^3}\frac{u_V^2 \rho_V}{2 g_c}\frac{1}{K_W} \qquad (2)$$

The required packing parameters are as follows from Table 6.8 and above:

	NOR PAC	Montz
F_P, ft^2/ft^3	14	33
a, m^2/m^3	86.8	300
ε, m^3/m^3	0.947	0.930
C_h	0.651	0.482
C_p	0.350	0.295

From Eq. (6-112), $D_P = 6\left(\frac{1-\varepsilon}{a}\right) = 6\left(\frac{1-0.947}{86.8}\right) = 0.00366$ m or 0.012 ft for NOR PAC

$$D_P = 6\left(\frac{1-\varepsilon}{a}\right) = 6\left(\frac{1-0.930}{300}\right) = 0.0014 \text{ m or } 0.00459 \text{ ft for Montz}$$

Rectifying section of the column:
For NOR PAC , column diameter = D_T = 4.3 ft

From Eq. (6-111), $\frac{1}{K_W} = 1 + \frac{2}{3}\left(\frac{1}{1-\varepsilon}\right)\frac{D_P}{D_T} = 1 + \frac{2}{3}\left(\frac{1}{1-0.947}\right)\frac{0.012}{4.3} = 1.035$

Therefore, K_W = 1/1.035 = 0.966

Exercise 7.52 (continued)

Analysis: (e) (continued)

For Montz, column diameter = D_T = 5.3 ft

From Eq. (6-111), $\frac{1}{K_W} = 1 + \frac{2}{3}\left(\frac{1}{1-\varepsilon}\right)\frac{D_P}{D_T} = 1 + \frac{2}{3}\left(\frac{1}{1-0.930}\right)\frac{0.00459}{5.3} = 1.008$

Therefore, K_W = 1/1.008 = 0.992

Superficial gas velocity at 70% of flooding from above = 13 ft/s for NOR PAC.
Superficial gas velocity at 70% of flooding from above = 8.4 ft/s for Montz
Gas viscosity = 0.011 cP and gas density = 0.0688 lb/ft^3.

From Eq. (6-114), for NOR PAC,

$$N_{\mathrm{Re}_V} = \frac{u_V D_P \rho_V}{(1-\varepsilon)\mu_V} K_W = \frac{(13)(0.012)(0.0688)}{(1-0.947)(0.011)(0.000672)}(0.966) = 26,500$$

For Montz,

$$N_{\mathrm{Re}_V} = \frac{(8.4)(0.00459)(0.0688)}{(1-0.930)(0.011)(0.000672)}(0.992) = 5,090$$

From Eq. (6-113), for NOR PAC,

$$\Psi_o = C_p\left(\frac{64}{N_{\mathrm{Re}_V}} + \frac{1.8}{N_{\mathrm{Re}_V}^{0.08}}\right) = 0.350\left(\frac{64}{26,500} + \frac{1.8}{26,500^{0.08}}\right) = 0.280$$

For Montz,

$$\Psi_o = 0.295\left(\frac{64}{5,090} + \frac{1.8}{5,090^{0.08}}\right) = 0.272$$

From Eq. (2), for NOR PAC,

$$\frac{\Delta P_o}{l_T} = \Psi_o \frac{a}{\varepsilon^3}\frac{u_V^2 \rho_V}{2g_c}\frac{1}{K_W} = 0.280\frac{86.8(0.3048)}{0.947^3}\left[\frac{13^2(0.0688)}{2(32.2)}\right]\frac{1}{0.966} = 1.63 \text{ lbf/ft}^3 \text{ or } 0.0113 \text{ psi/ft}$$

For Montz,

$$\frac{\Delta P_o}{l_T} = 0.272\frac{300(0.3048)}{0.930^3}\left[\frac{8.4^2(0.0688)}{2(32.2)}\right]\frac{1}{0.992} = 2.35 \text{ lbf/ft}^3 \text{ or } 0.0163 \text{ psi/ft}$$

From Eq. (1), for NOR PAC, with h_L = 0.0162 m^3/m^3 and liquid Froude number = 6.63x10^{-5}

$$\frac{\Delta P}{l_T} = 0.0113\left(\frac{0.947-0.0162}{0.947}\right)^{1.5}\exp\left[\frac{13300}{86.8^{3/2}}\left(6.63\times10^{-5}\right)^{1/2}\right] = 0.0126 \text{ psi/ft}$$

Exercise 7.52 (continued)

Analysis: (e) Rectifying section (continued)

From Eq. (1), for Montz, with $h_L = 0.0241$ m^3/m^3 and liquid Froude number =9.91x10^{-5}

$$\frac{\Delta P}{l_T} = 0.0163\left(\frac{0.930-0.0241}{0.930}\right)^{1.5} \exp\left[\frac{13300}{300^{3/2}}\left(9.91\times10^{-5}\right)^{1/2}\right] = 0.0161 \text{ psi/ft}$$

Stripping section of the column:

For NOR PAC , column diameter = D_T = 3.4 ft

From Eq. (6-111), $\frac{1}{K_W} = 1+\frac{2}{3}\left(\frac{1}{1-\varepsilon}\right)\frac{D_P}{D_T} = 1+\frac{2}{3}\left(\frac{1}{1-0.947}\right)\frac{0.012}{3.4} = 1.044$

Therefore, K_W = 1/1.044 = 0.957

For Montz, column diameter = D_T = 4.2 ft

From Eq. (6-102), $\frac{1}{K_W} = 1+\frac{2}{3}\left(\frac{1}{1-\varepsilon}\right)\frac{D_P}{D_T} = 1+\frac{2}{3}\left(\frac{1}{1-0.930}\right)\frac{0.00459}{4.2} = 1.010$

Therefore, K_W = 1/1.010 = 0.990

Superficial gas velocity at 70% of flooding from above = 20 ft/s for NOR PAC.
Superficial gas velocity at 70% of flooding from above = 13 ft/s for Montz
Gas viscosity = 0.012 cP and gas density = 0.0370 lb/ft^3.

From Eq. (6-114), for NOR PAC,

$$N_{\mathrm{Re}_V} = \frac{u_V D_P \rho_V}{(1-\varepsilon)\mu_V} K_W = \frac{(20)(0.012)(0.0370)}{(1-0.947)(0.012)(0.000672)}(0.957) = 19,900$$

For Montz,

$$N_{\mathrm{Re}_V} = \frac{(13)(0.00459)(0.0370)}{(1-0.930)(0.012)(0.000672)}(0.990) = 3,870$$

From Eq. (6-113), for NOR PAC,

$$\Psi_o = C_p\left(\frac{64}{N_{\mathrm{Re}_V}} + \frac{1.8}{N_{\mathrm{Re}_V}^{0.08}}\right) = 0.350\left(\frac{64}{19,900} + \frac{1.8}{19,900^{0.08}}\right) = 0.287$$

For Montz,

$$\Psi_o = 0.295\left(\frac{64}{3,870} + \frac{1.8}{3,870^{0.08}}\right) = 0.279$$

Exercise 7.52 (continued)

Analysis: (e) Stripping section (continued)

From Eq. (2), for NOR PAC,

$$\frac{\Delta P_o}{l_T} = \Psi_o \frac{a}{\varepsilon^3}\frac{u_V^2 \rho_V}{2g_c}\frac{1}{K_W} = 0.287\frac{86.8(0.3048)}{0.947^3}\left[\frac{20^2(0.0370)}{2(32.2)}\right]\frac{1}{0.957} = 2.15 \text{ lbf/ft}^3 \text{ or } 0.0149 \text{ psi/ft}$$

For Montz,

$$\frac{\Delta P_o}{l_T} = 0.279\frac{300(0.3048)}{0.930^3}\left[\frac{8.4^2(0.0370)}{2(32.2)}\right]\frac{1}{0.990} = 3.11 \text{ lbf/ft}^3 \text{ or } 0.0216 \text{ psi/ft}$$

From Eq. (1), for NOR PAC, with $h_L = 0.0269$ m^3/m^3 and liquid Froude number = $4.28\text{x}10^{-4}$

$$\frac{\Delta P}{l_T} = 0.0149\left(\frac{0.947-0.0269}{0.947}\right)^{3/2}\exp\left[\frac{13300}{300^{3/2}}\left(4.28\times10^{-4}\right)^{1/2}\right] = 0.0150 \text{ psi/ft}$$

From Eq. (1), for Montz, with $h_L = 0.0341$ m^3/m^3 and liquid Froude number = $6.39\text{x}10^{-4}$

$$\frac{\Delta P}{l_T} = 0.0216\left(\frac{0.930-0.0341}{0.930}\right)^{1.5}\exp\left[\frac{13300}{300^{3/2}}\left(6.39\times10^{-4}\right)^{1/2}\right] = 0.0218 \text{ psi/ft}$$

Summary of Results:

	NOR PAC	Montz
Column diameter, ft:		
Rectifying section	4.3	5.3
Stripping section	3.4	4.2
Packed height, ft		
Rectifying section	6.3	2.9
Stripping section	20.2	2.1
Total	26.5	5.0
Pressure drop, psi	0.38	0.093

From these results, the column diameter for NOR PAC would be 4.5 ft without swaging.
The column diameter for Montz would be 5.5 ft without swaging.
The column height for NOR PAC, allowing 4 ft for disengagement, 2 ft for feed entry, and 10 ft for sump at the bottom would be 42.5 ft or say 43 ft.
Similarly, the column height for Montz would be 21 ft.

Exercise 7.52 (continued)

Analysis: Summary (continued)

The above may be compared with the existing plate column of Exercise 7.41:

	Plate column	NOR PAC	Montz
Column diameter, ft	6.0	4.5	5.5
Column height, ft	36	43	21
Pressure drop, psi	0.8	0.38	0.093

The packed columns are smaller in diameter, the NOR PAC column significantly smaller. The Montz structure packing column is shorter in height and has much less pressure drop. The NOR PAC rings random packing column is taller and has significantly more pressure drop than the column with Montz packing. The pressure drop is not critical. Because of the much higher cost for Montz packing and the much smaller diameter for the NOR PAC column, it is probable that economics would favor the NOR PAC column.

Exercise 7.53

Subject: Distillation of a mixture of benzene and toluene in a packed column.

Given: Conditions in Example 7.1, but using 50-mm Hiflow rings at 70% of flooding.

Assumptions: Constant molar overflow. Partial reboiler is an equilibrium stage.

Find: (a) Liquid holdup.
(b) Column diameter.
(c) H_{OG}.
(d) Packed height.
(e) Pressure drop.
Advantages of packed column over trayed column.

Analysis:
At the top of the column, $L = RD$ =1.59(275) = 437 lbmol/h, and $V = L + D$ = 437 + 275 = 712 lbmol/h. At the bottom of the column, for constant molar overflow and 61.1 mol% feed vapor, $\overline{V} = 712 - 0.611(450) = 437$ lbmol / h, and $\overline{L} = \overline{V} + B = 437 + 175 = 612$ lbmol / h
Before computing liquid holdup, we need to compute column diameter.

(b) **<u>Column diameter based on conditions at the top of the column</u>,**
where T = 180°F and P = 14.7 psia = 1 atm.
Use Figs. 6.36a, b, and c to compute flooding velocity, following Example 6.13.
From the ideal gas law, $\rho_V = PM_V/RT$ = (1)(78.8)/[0.730(180 + 460)] = 0.171 lb/ft^3
For the liquid, which is mainly benzene, use ρ_L = 50.6 lb/ft^3 and μ_L = 0.31 cP.

The abscissa in Fig. 6.36a = $X = \left(\frac{LM_L}{VM_V}\right)\left(\frac{\rho_V}{\rho_L}\right)^{1/2} = \frac{437(79.4)}{712(78.8)}\left(\frac{0.171}{50.6}\right)^{1/2} = 0.0376$

From Fig. 6.36a, Y at flooding = 0.17; from Fig. 6.36b, for ρ_{water}/ρ_L = 62.4/50.6 = 1.23, $f\{\rho_L\}$ = 1.5; and from Fig. 6.36c, for μ_L = 0.31 cP, $f\{\mu_L\}$ = 0.8.
From Table 6.8, F_P = 16 for 50-mm Hiflow rings.
From a rearrangement of the ordinate of Fig. 6.36a,

$$u_o^2 = Y\frac{g}{F_P}\left(\frac{\rho_{H_2O\,(L)}}{\rho_V}\right)\frac{1}{f\{\rho_L\}f\{\mu_L\}} = 0.17\left(\frac{32.2}{16}\right)\left(\frac{62.4}{0.171}\right)\frac{1}{1.23(0.8)} = 127 \text{ (ft/s)}^2 \text{ and } u_o = 11.2 \text{ ft/s}$$

For fraction of flooding = f = 0.7, $u_V = u_o f$ = 11.2(0.7) = 7.84 ft/s.
From Eq. (6-103), column diameter is,

$$D_T = \left(\frac{4VM_G}{fu_0\pi\rho_G}\right)^{1/2} = \left(\frac{4VM_G}{u_G\pi\rho_G}\right)^{1/2} = \left[\frac{4(712/3600)(78.8)}{7.84(3.14)(0.171)}\right]^{1/2} = 3.8 \text{ ft.}$$

Exercise 7.53 (continued)

Analysis: (b) (continued)

Column diameter based on conditions at the bottom of the column,

where $T = 227^{\circ}$F and $P = 14.7$ psia = 1 atm.

Use Figs. 6.36a, b, and c to compute flooding velocity, following Example 6.13.

From the ideal gas law, $\rho_V = PM_V/RT = (1)(90.6)/[0.730(227 + 460)] = 0.181$ lb/ft^3

For the liquid, which is mainly benzene, use $\rho_L = 48.7$ lb/ft^3 and $\mu_L = 0.25$ cP.

The abscissa in Fig. 6.36a = $X = \left(\frac{LM_L}{VM_V}\right)\left(\frac{\rho_V}{\rho_L}\right)^{1/2} = \frac{612(90.6)}{437(91.5)}\left(\frac{0.181}{48.7}\right)^{1/2} = 0.085$

From Fig. 6.36a, Y at flooding = 0.12; from Fig. 6.36b, for $\rho_{water}/\rho_L = 62.4/48.7 = 1.28$, $f\{\rho_L\} = 1.5$; and from Fig. 6.36c, for $\mu_L = 0.25$ cP, $f\{\mu_L\} = 0.78$.

From Table 6.8, $F_P = 16$ for 50-mm Hiflow rings.

From a rearrangement of the ordinate of Fig. 6.36a,

$$u_o^2 = Y\frac{g}{F_P}\left(\frac{\rho_{H_2O\,(L)}}{\rho_V}\right)\frac{1}{f\{\rho_L\}f\{\mu_L\}} = 0.12\left(\frac{32.2}{16}\right)\left(\frac{62.4}{0.181}\right)\frac{1}{1.50(0.78)} = 71 \text{ (ft/s)}^2 \text{ and } u_o = 8.43 \text{ ft/s}$$

For fraction of flooding = $f = 0.7$, $u_V = u_o f = 8.43(0.7) = 5.9$ ft/s.

From Eq. (6-103), column diameter is,

$$D_T = \left(\frac{4VM_V}{fu_0\pi\rho_V}\right)^{1/2} = \left(\frac{4VM_V}{u_V\pi\rho_V}\right)^{1/2} = \left[\frac{4(437/3600)(90.6)}{5.9(3.14)(0.181)}\right]^{1/2} = 3.6 \text{ ft.}$$

(a) For liquid holdup estimates, assume the column operates in the preloading region. Therefore, the holdup is independent of the gas rate. Follow Example 6.12. Pertinent packing characteristics from Table 6.8 are $a = 92.3$ m^2/m^3 = 28.1 ft^2/ft^3, $\varepsilon = 0.977$, and $C_h = 0.876$

Use Eqs. (6-97) to (6-101), which requires calculating the liquid Reynolds and Froude numbers.

Liquid holdup based on conditions at the top of the column.

By the continuity equation, superficial liquid velocity is,

$u_L = LM_L/\rho_L S = (437/3600)(79.9)/[50.6(3.14)(3.8)^2/4] = 0.0168$ ft/s

From Eq. (6-98), $N_{Re_L} = \frac{u_L\rho_L}{\mu_L a} = \frac{(0.0168)50.6}{(0.31)(0.000672)28.1} = 145$

From Eq. (6-99), $N_{Fr_L} = \frac{u_L^2 a}{g} = \frac{(0.0168)^2\,28.1}{32.2} = 2.46\times10^{-4}$

Since $N_{Re} > 5$, use Eq. (6-101),

$$a_h/a = 0.85C_h N_{Re_L}^{0.25} N_{Fr_L}^{0.1} = 0.85(0.876)(145)^{0.25}(2.46\times10^{-4})^{0.1} = 1.12$$

Exercise 7.53 (continued)

Analysis: (a) top of the column (continued)
From Eq. (6-97), the fractional liquid holdup is,

$$h_L = \left(12\frac{N_{\mathrm{Fr}_L}}{N_{\mathrm{Re}_L}}\right)^{1/3}\left(\frac{a_h}{a}\right)^{2/3} = \left[(12)\frac{2.46\times10^{-4}}{145}\right]^{1/3}(1.12)^{2/3} = 0.0294 \text{ m}^3/\text{m}^3$$

Liquid holdup based on conditions at the bottom of the column.
By the continuity equation, superficial liquid velocity is,
$u_L = LM_L/\rho_L S = (612/3600)(90.6)/\,[50.6(3.14)(3.6)^2/4] = 0.0299$ ft/s

From Eq. (6-98), $N_{\mathrm{Re}_L} = \dfrac{u_L\rho_L}{\mu_L a} = \dfrac{(0.0299)48.7}{(0.25)(0.000672)28.1} = 308$

From Eq. (6-99), $N_{\mathrm{Fr}_L} = \dfrac{u_L^2 a}{g} = \dfrac{(0.0299)^2\,28.1}{32.2} = 7.80\times10^{-4}$

Since $N_{\mathrm{Re}} > 5$, use Eq. (6-101),

$$a_h/a = 0.85C_h N_{\mathrm{Re}_L}^{0.25} N_{\mathrm{Fr}_L}^{0.1} = 0.85(0.876)(308)^{0.25}(7.80\times10^{-4})^{0.1} = 1.52$$

From Eq. (6-97), the fractional liquid holdup is,

$$h_L = \left(12\frac{N_{\mathrm{Fr}_L}}{N_{\mathrm{Re}_L}}\right)^{1/3}\left(\frac{a_h}{a}\right)^{2/3} = \left[(12)\frac{7.80\times10^{-4}}{308}\right]^{1/3}(1.52)^{2/3} = 0.0412 \text{ m}^3/\text{m}^3$$

(c) From Eq. (7.51), $H_{OG} = H_G + \left(\dfrac{mV}{L}\right)H_L$, where we must use the slope, m, of the equilibrium curve instead of a K-value because the equilibrium curve is curved.

At the top of the column:

Estimate H_L from Eq. (6-132), using the following properties and parameters:
$C_L = 1.168$, $h_L = 0.0294$ m^3/m^3, $\varepsilon = 0.977$, and $u_L = 0.00512$ m/s.
We need an estimate of the diffusivity of benzene in toluene at high concentrations of benzene. Because these two components form a nearly ideal solution, assume that this diffusivity is equal to that of toluene (A) at infinite dilution in benzene (B), as estimated from the Eq. (3-42), using Table 3.3 and Table 3.2. In this equation, $T = 180^\circ$F = 356 K, $\mathscr{R}_B = 205.3$, $\mathscr{R}_A = 245.5$, $\mu_B = 0.32$ cP, and $v_B = 6(14.8)+6(3.7) - 15 = 96$

$$D_L = D_{AB} = 1.55\times10^{-8}\frac{T^{1.29}(P_B^{0.5}/P_A^{0.5})}{\mu_B^{0.92}v_B^{0.23}} = 1.55\times10^{-8}\frac{355^{1.29}(205.3^{0.5}/245.5^{0.42})}{0.32^{0.92}96^{0.23}} = 4.28\times10^{-5} \text{ cm}^2/\text{s}$$

Exercise 7.53 (continued)

Analysis: (c) top of the column (continued)
From Eq. (6-132),

$$H_L = \frac{1}{C_L}\left(\frac{1}{12}\right)^{1/6}\left[\frac{4h_L\varepsilon}{D_L a u_L}\right]^{1/2}\left(\frac{u_L}{a}\right)\left(\frac{a}{a_{Ph}}\right) = \frac{1}{1.168}\left(\frac{1}{12}\right)^{1/6}\left[\frac{4(0.0294)(0.977)}{(4.28\times10^{-9})(92.3)(0.00512)}\right]^{1/2}\left(\frac{0.00512}{92.3}\right)\left(\frac{a}{a_{Ph}}\right)$$

$$= 0.24\left(\frac{a}{a_{Ph}}\right) \text{ m}$$

To compute (a_{Ph}/a), we need for the liquid phase, the Reynolds, Weber, and Froude numbers from equations (6-138), (6-139), and (6-140), respectively, based on the packing hydraulic diameter from (6-137).

$$d_h = \text{ packing hydraulic diameter} = 4\frac{\varepsilon}{a} = 4\left(\frac{0.977}{92.3}\right) = 0.0423 \text{ m} = 0.139 \text{ ft}$$

$$\text{Reynolds number} = N_{\text{Re}_L,h} = \frac{u_L d_h \rho_L}{\mu_L} = \frac{(0.0168)(0.139)(50.6)}{[(0.31)(0.000672)]} = 567$$

Take the surface tension of benzene at 180°F as $\sigma = 21$ dynes/cm = 0.00144 lb_f/ft or $0.00144(32.2) = 0.0464$ lb_m/s^2

$$\text{Weber number} = N_{\text{We}_L,h} = \frac{u_L^2 \rho_L d_h}{\sigma} = \frac{(0.0168)^2(50.6)(0.139)}{0.0464} = 0.0428$$

$$\text{Froude number} = N_{\text{Fr}_L,h} = \frac{u_L^2}{g d_h} = \frac{(0.0168)^2}{32.2(0.139)} = 0.0000631$$

$$\text{From (6-136), } \frac{a_{Ph}}{a} = 1.5(a d_h)^{-1/2}\left(N_{\text{Re}_L,h}\right)^{-0.2}\left(N_{\text{We}_L,h}\right)^{0.75}\left(N_{\text{Fr}_L,h}\right)^{-0.45}$$

$$= 1.5\left[(92.3)(0.0423)\right]^{-1/2}(567)^{-0.2}(0.0428)^{0.75}(0.0000631)^{-0.45} = 1.56$$

$$H_L = 0.24\left(\frac{1}{1.56}\right) = 0.154 \text{ m}$$

Exercise 7.53 (continued)

Analysis: (c) at the top of the column (continued)

Now estimate the value of H_G from Eq. (6-133). Estimate the gas diffusivity from Eq. (3-36), where from Table 3.1,
$\sum_V = 6(15.9+2.31)-18.3 = 90.96$ for benzene, and $\sum_V = 7(15.9+2.31)+2.31-18.3 = 111.5$ for toluene and molecular weights are 787 for benzene and 92 for toluene.

$$D_G = D_{AB} = \frac{0.00143T^{1.75}}{P\left[\frac{2}{(1/M_A)+(1/M_B)}\right]^{1/2}\left[\left(\sum_V\right)_A^{1/3}+\left(\sum_V\right)_B^{1/3}\right]^2}$$

$$= \frac{0.00143(355)^{1.75}}{(1)\left[\frac{2}{(1/78)+(1/92)}\right]^{1/2}\left[(90.96)^{1/3}+(111.5)^{1/3}\right]^2} = 0.052 \text{ cm}^2/\text{s}$$

Use the following additional properties and parameters, together with $\mu_V = 0.0091$ cP and $\rho_V =$ 0.171 lb/ft^3, where from Eq. (6-134), $N_{\text{Re}_V} = \frac{u_V\rho_V}{a\mu_V} = \frac{(7.84)(0.171)}{(28.1)(0.0091)(0.000672)} = 7{,}800$

From (6-135) $N_{\text{Sc}_V} = \frac{\mu_V}{\rho_V D_V} = \frac{(0.0091)(0.000672)}{(0.171)\left[\frac{0.052}{(2.54)^2(12)^2}\right]} = 0.639$

From Eq. (6-133), with $C_V = 0.408$ from Table 6.8,

$$H_G = \frac{1}{C_V}(\varepsilon - h_L)^{1/2}\left(\frac{4\varepsilon}{a^4}\right)^{1/2}\left(N_{\text{Re}_V}\right)^{-3/4}\left(N_{\text{Sc}_V}\right)^{-1/3}\left(\frac{u_V a}{D_V a_{Ph}}\right)$$

$$= \frac{1}{0.408}(0.977-0.0273)^{1/2}\left[\frac{4(0.977)}{92.3^4}\right]^{1/2}(7{,}800)^{-3/4}(0.639)^{-1/3}\left[\frac{(2.39)(92.3)}{(0.052\times10^{-4})(144)}\right] = 0.23 \text{ m}$$

At the top of the column, vapor rate = V =712 lbmol/h and liquid rate = L = 437 lbmol/h.
Therefore, V/L = (712)/(437) = 1.63

<u>At the bottom of the column</u>:

Near a mole fraction, x_B, of 0.05, m = 2.1

Need an estimate of the liquid diffusivity of benzene in toluene at low concentrations of benzene. At the bottom, temperature = 227°F = 382 K and liquid viscosity = 0.25 cP. This time, benzene is component A and toluene is B. From Eq. (3-42),

$$D_L = D_{\text{AB}} = 1.55\times10^{-8}\frac{T^{1.29}(\text{P}_\text{B}^{0.5}/\text{P}_\text{A}^{0.5})}{\mu_\text{B}^{0.92}v_\text{B}^{0.23}} = 1.55\times10^{-8}\frac{382^{1.29}(245.5^{0.5}/205.3^{0.42})}{0.25^{0.92}118.2^{0.23}} = 6.64\times10^{-5}$$

Exercise 7.53 (continued)

Analysis: (c) bottom of the column (continued)
From Eq. (6-132), using SI units

$$H_L = \frac{1}{C_L}\left(\frac{1}{12}\right)^{1/6}\left[\frac{4h_L\varepsilon}{D_L a u_L}\right]^{1/2}\left(\frac{u_L}{a}\right)\left(\frac{a}{a_{Ph}}\right)$$

$$= \frac{1}{1.168}\left(\frac{1}{12}\right)^{1/6}\left[\frac{4(0.0312)(0.977)}{(6.64\times10^{-9})(92.3)(0.00911)}\right]^{1/2}\left(\frac{0.00911}{92.3}\right)\left(\frac{a}{a_{Ph}}\right) = 0.26\left(\frac{a}{a_{Ph}}\right) \text{ m}$$

To compute (a_{Ph}/a), we need for the liquid phase, the Reynolds, Weber, and Froude numbers from equations (6-138), (6-139), and (6-140), respectively, based on the packing hydraulic diameter from (6-137).

$$d_h = \text{ packing hydraulic diameter} = 4\frac{\varepsilon}{a} = 4\left(\frac{0.977}{92.3}\right) = 0.0423 \text{ m} = 0.139 \text{ ft}$$

$$\text{Reynolds number} = N_{\text{Re}_L,h} = \frac{u_L d_h \rho_L}{\mu_L} = \frac{(0.0299)(0.139)(48.7)}{[(0.25)(0.000672)]} = 1205$$

Take the surface tension of toluene at 227°F as σ = 18 dynes/cm = 0.00123 lb_f/ft or 0.00123(32.2) = 0.0397 lb_m/s^2

$$\text{Weber number} = N_{\text{We}_L,h} = \frac{u_L^2 \rho_L d_h}{\sigma} = \frac{(0.0299)^2 (48.7)(0.139)}{0.0397} = 0.152$$

$$\text{Froude number} = N_{\text{Fr}_L,h} = \frac{u_L^2}{g d_h} = \frac{(0.0299)^2}{32.2(0.139)} = 0.000200$$

$$\text{From (6-136), } \frac{a_{Ph}}{a} = 1.5(a d_h)^{-1/2}\left(N_{\text{Re}_L,h}\right)^{-0.2}\left(N_{\text{We}_L,h}\right)^{0.75}\left(N_{\text{Fr}_L,h}\right)^{-0.45}$$

$$= 1.5[(92.3)(0.0423)]^{-1/2}(1205)^{-0.2}(0.152)^{0.75}(0.000200)^{-0.45} = 2.07$$

$$H_L = 0.26\left(\frac{1}{2.07}\right) = 0.126 \text{ m}$$

Exercise 7.53 (continued)

Analysis: (c) bottom of the column (continued)

Now estimate the value of H_G from Eq. (6-133). Estimate the gas diffusivity from Eq. (3-36), by ratio from the value above for the top of the column,

$$D_V = 0.052(382/354)^{1.75} = 0.059 \text{ cm}^2/\text{s}$$

Use the following additional properties and parameters, together with $\mu_V = 0.0092$ cP and $\rho_V =$ 0.179 lb/ft^3, where from Eq. (6-134), $N_{\text{Re}_V} = \dfrac{u_V \rho_V}{a\mu_V} = \dfrac{(5.9)(0.181)}{(28.1)(0.0092)(0.000672)} = 6{,}150$

From (6-135),) $N_{\text{Sc}_V} = \dfrac{\mu_V}{\rho_V D_V} = \dfrac{(0.0092)(0.000672)}{(0.181)\left[\dfrac{0.059}{(2.54)^2(12)^2}\right]} = 0.54$

From Eq. (6-133),

$$H_G = \frac{1}{C_V}(\varepsilon - h_L)^{1/2}\left(\frac{4\varepsilon}{a^4}\right)^{1/2}\left(N_{\text{Re}_V}\right)^{-3/4}\left(N_{\text{Sc}_V}\right)^{-1/3}\left(\frac{u_V a}{D_V a_{Ph}}\right)$$

$$= \frac{1}{0.408}(0.977 - 0.0412)^{1/2}\left[\frac{4(0.977)}{92.3^4}\right]^{1/2}(6{,}150)^{-3/4}(0.54)^{-1/3}\left[\frac{(1.80)(92.3)}{(0.059\times10^{-4})(191)}\right] = 0.14 \text{ m}$$

At the bottom of the column, vapor rate = V =437 lbmol/h and liquid rate = L = 612 lbmol/h. Therefore, V/L = (437)/(612) = 0.714

From Eq. (7.51), $H_{OG} = H_G + \left(\dfrac{mV}{L}\right)H_L$

Therefore, values of H_{OG} depend on the slope of the equilibrium line, which varies widely from the top of the column to the bottom. At the top, assuming H_G and H_L are constant,

$$H_{OG} = H_G + \left(\frac{mV}{L}\right)H_L = 0.23 + 1.63(0.154)\ m = 0.23 + 0.25\ m$$

At the bottom, assuming H_G and H_L are constant,

$$H_{OG} = H_G + \left(\frac{mV}{L}\right)H_L = 0.14 + 0.714(0.126)\ m\ = 0.14 + 0.09\ m$$

(d) The packed height is given by Eq. (6-127), $l_T = H_{OG}N_{OG}$ = HETP N_t

Apply these equations in a stage-by-stage fashion, using the equilibrium stages in Fig. 7.15. For each stage, convert the value of H_{OG} to HETP with Eq. (7.53) as in Table 7.7 for Example 7.9,

$$\text{HETP} = H_{OG}\ \ln\lambda/(\lambda - 1)$$

Exercise 7.53 (continued)

Analysis: (d) (continued)

Using a spreadsheet, the following results are obtained:

Rectifying Section:

Stage	m	$\lambda = mV/L$	H_{OG}, m	HETP, m
1	0.47	0.77	0.35	0.39
2	0.53	0.86	0.36	0.39
3	0.61	0.99	0.38	0.38
4	0.67	1.09	0.40	0.38
5	0.72	1.17	0.41	0.38
6	0.80	1.30	0.43	0.38
Total height =		2.31 m		

Stripping Section:

Stage	m	$\lambda = mV/L$	H_{OG}, m	HETP, m
7	0.90	0.64	0.22	0.27
8	0.98	0.70	0.23	0.27
9	1.15	0.82	0.24	0.27
10	1.40	1.00	0.27	0.27
11	1.70	1.21	0.29	0.27
12	1.90	1.36	0.31	0.27
0.2 of 13	2.20	1.57	0.34	0.2*0.27 = 0.05
Total height =		1.67 m		

Note that although H_{OG} varies significantly with stage in both sections, HETP does not.
The total packed height = 2.31 + 1.67 = 3.98 m or 13.1 ft.

(e) Compute pressure drops for the packed sections from the correlation of Billet and Schultes.
The pressure drop per unit height of packed bed is given by Eq. (6-115),

$$\frac{\Delta P}{l_T} = \left(\frac{\Delta P_o}{l_T}\right)\left(\frac{\varepsilon - h_L}{\varepsilon}\right)^{1.5} \exp\left[\frac{13300}{a^{3/2}}\left(N_{\mathrm{Fr}_L}\right)^{1/2}\right] \qquad (1)$$

This equation will be used in each section.

From Eq. (6-110), $$\frac{\Delta P_o}{l_T} = \Psi_o \frac{a}{\varepsilon^3}\frac{u_o^2 \rho_G}{2 g_c}\frac{1}{K_W} \qquad (2)$$

The required packing parameters are as follows from Table 6.8 and above:
$F_P = 16\ \mathrm{ft^2/ft^3}$, $a = 92.3\ \mathrm{m^2/m^3}$, $\varepsilon = 0.977\ \mathrm{m^3/m^3}$, $C_h = 0.876$, and $C_p = 0.421$

Exercise 7.53 (continued)

Analysis: (e) (continued)

From Eq. (6-112), $D_P = 6\left(\frac{1-\varepsilon}{a}\right) = 6\left(\frac{1-0.977}{92.3}\right) = 0.00150\,\text{m}$ or 0.0049 ft

Rectifying section of the column:

Column diameter = $D_T = 3.8$ ft

From Eq. (6-111), $\frac{1}{K_W} = 1 + \frac{2}{3}\left(\frac{1}{1-\varepsilon}\right)\frac{D_P}{D_T} = 1 + \frac{2}{3}\left(\frac{1}{1-0.977}\right)\frac{0.0049}{3.8} = 1.037$

Therefore, $K_W = 1/1.037 = 0.964$

Superficial gas velocity at 70% of flooding from above = 7.84 ft/s
Gas viscosity = 0.0091 cP and gas density = 0.171 lb/ft^3.

From Eq. (6-114), $N_{\text{Re}_V} = \frac{u_V D_P \rho_V}{(1-\varepsilon)\mu_V} K_W = \frac{(7.84)(0.0049)(0.171)}{(1-0.977)(0.0091)(0.000672)}(0.964) = 45{,}000$

From Eq. (6-113), $\Psi_o = C_p\left(\frac{64}{N_{\text{Re}_V}} + \frac{1.8}{N_{\text{Re}_V}^{0.08}}\right) = 0.421\left(\frac{64}{45{,}000} + \frac{1.8}{45{,}000^{0.08}}\right) = 0.322$

From Eq. (2), $\frac{\Delta P_o}{l_T} = 0.322\frac{92.3(0.3048)}{0.977^3}\left[\frac{7.84^2(0.171)}{2(32.2)}\right]\frac{1}{0.977} = 1.62$ lbf/ft^3 or 0.0113 psi/ft

From Eq. (1), with $h_L = 0.0294$ m^3/m^3 and liquid Froude number = 2.46 x 10^{-4}

$$\frac{\Delta P}{l_T} = 0.0113\left(\frac{0.977-0.0294}{0.977}\right)^{3/2}\exp\left[\frac{13300}{92.3^{3/2}}\left(2.46\times10^{-4}\right)^{1/2}\right] = 0.0137 \text{ psi/ft}$$

Stripping section of the column:

Column diameter = $D_T = 3.6$ ft

From Eq. (6-102), $\frac{1}{K_W} = 1 + \frac{2}{3}\left(\frac{1}{1-\varepsilon}\right)\frac{D_P}{D_T} = 1 + \frac{2}{3}\left(\frac{1}{1-0.977}\right)\frac{0.0049}{3.6} = 1.039$

Therefore, $K_W = 1/1.039 = 0.962$

Superficial gas velocity at 70% of flooding from above = 5.9 ft/s
Gas viscosity = 0.0092 cP and gas density = 0.179 lb/ft^3.

Exercise 7.53 (continued)

Analysis: (e) Stripping section (continued)

From Eq. (6-105), $N_{\mathrm{Re}_V} = \dfrac{u_V D_P \rho_V}{(1-\varepsilon)\mu_V} K_W = \dfrac{(5.9)(0.0049)(0.179)}{(1-0.977)(0.0092)(0.000672)}(0.962) = 35{,}000$

From Eq. (6-104), $\Psi_o = C_p\left(\dfrac{64}{N_{\mathrm{Re}_V}} + \dfrac{1.8}{N_{\mathrm{Re}_V}^{0.08}}\right) = 0.421\left(\dfrac{64}{35{,}000} + \dfrac{1.8}{35{,}000^{0.08}}\right) = 0.329$

From Eq. (2),

$$\frac{\Delta P_o}{l_T} = 0.329\frac{92.3(0.3048)}{0.977^3}\left[\frac{5.9^2(0.179)}{2(32.2)}\right]\frac{1}{0.962} = 1.0 \text{ lbf/ft}^3 \text{ or } 0.0069 \text{ psi/ft}$$

From Eq. (1), with $h_L = 0.0412$ m^3/m^3 and liquid Froude number = 7.80 x 10^{-4}

$$\frac{\Delta P}{l_T} = 0.0069\left(\frac{0.977-0.0412}{0.977}\right)^{3/2} \exp\left[\frac{13300}{92.3^{3/2}}\left(7.80\times10^{-4}\right)^{1/2}\right] = 0.0098 \text{ psi/ft}$$

From these results, the column diameter would be 4.0 ft without swaging. Take the packed height as 14 ft. The column height, allowing 4 ft for disengagement, 2 ft for feed entry, and 10 ft for sump at the bottom would be 30 ft.

The total pressure drop is: (2.31/0.3048)(0.0069) + (1.67/0.3048)(0.0098) = 0.11 psi.

For the plate column of Example 7.1, with 12.2 equilibrium stages, take tray efficiency = 80%. Therefore, need 16 trays, with a column height of 44 ft. Take a pressure drop of 0.08 psi/tray, giving a total pressure drop of 18(0.08) = 1.44 psi. The column diameter is estimated to be 4.5 ft.

The following summarizes the comparison. with the plate column of Exercise 7.1:

	Plate column	**Packed column**
Column diameter, ft	4.5	4.0
Column height, ft	44	30
Pressure drop, psi	1.44	0.11

The packed column is very competitive with the plate column.

Exercise 7.54

Subject: Determining compositions and energy requirements for a mixture of nC_6 and nC_8 with an enthalpy-concentration diagram for 101 kPa.

Given: Enthalpy-concentration diagram in Fig. 7.37.

Find: (a) Composition of vapor at bubble-point for 30 mol% nC_6.
(b) Energy to vaporize 60 mol% of a mixture initially at 100°F with 20 mol% nC_6 .
(c) Vapor and liquid compositions resulting from part (b).

Analysis: (a) In Fig. 7.37, below, the bubble point for 30 mol% nC_6 in nC_8 is shown as point B, which corresponds to a temperature of 211°F. An equilibrium tie line is drawn from point B to point M at the intersection with the saturated vapor line. The vapor composition at point M is 69 mol% nC_6 and 31 mol% nC_8.

(b) From Fig. 7.37, reproduced below, the enthalpy of the initial mixture of 20 mol% nC_6 at 100°F, shown at point G, is 6,500 Btu/lbmol = H_G . A vertical line is drawn upward from point G until it reaches the point E, located on the dashed tie line between the saturated liquid and saturated vapor curves, at a point that is 60% of the way from the saturated liquid curve to the saturated vapor curve. The enthalpy of the two-phase mixture at point E is 23,000 Btu/lbmol = H_E. Therefore, the energy required = $Q = H_E - H_G$ = 23,000 - 6,500 = 16,500 Btu/lbmol.

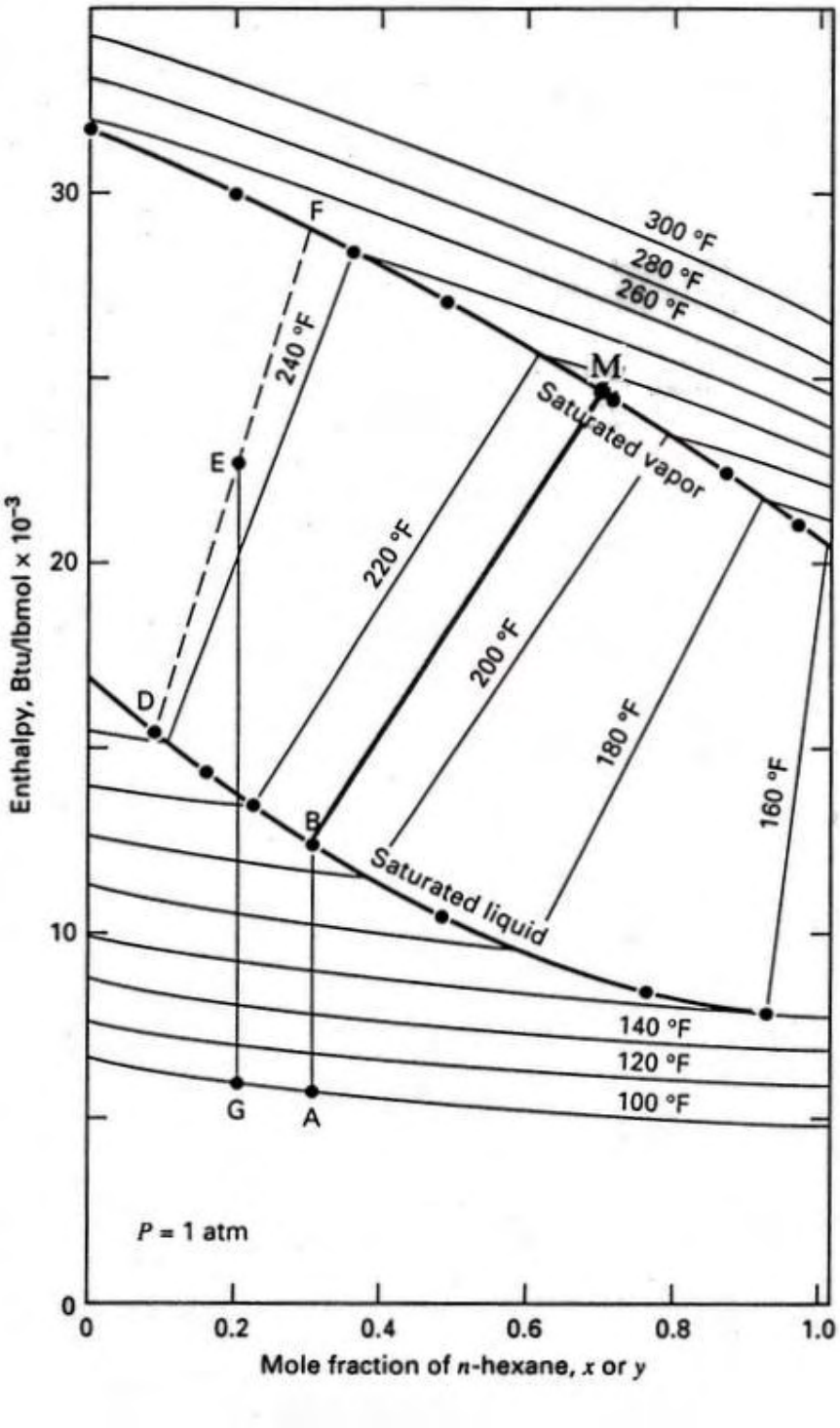
(c) From the reproduction of Fig. 7.37 below, the equilibrium liquid phase composition is at point D, which is 7.5 mol% nC_6 , while the equilibrium vapor composition is at point F, which is 28.5 mol% nC_6 . Checking this by material balance on nC_6 , for a basis of 100 lbmoles of mixture:

0.20(100) = 20 lbmoles
0.075(40) + 0.285(60) = 20.1 lbmoles

This is a reasonably good check.

Exercise 7.54 (continued)

Analysis: (continued)



Exercise 7.55

Subject: Determining compositions and energy requirements for a mixture of nC_6 and nC_8 with an enthalpy-concentration diagram for 101 kPa.

Given: Enthalpy-concentration diagram in Fig. 7.37.

Find: (a) Temperature and compositions of liquid and vapor, where F_1 = 950 lb/h of 30 mol% nC_6 at 180°F is adiabatically mixed with F_2 = 1,125 lb/h of 80 mol% nC_6 at 240°F.

(b) Energy and resulting phase compositions when a mixture of 60 mol% nC_6 at 260°F is cooled and partially condensed to 200°F.

(c) Compositions and relative amounts of the two phases when the equilibrium vapor from part (b) is further cooled to 180°F.

Analysis: (a) In Fig. 7.37, reproduced on the next page, the two feeds before mixing are shown at F_1 and F_2. When these two feeds are adiabatically mixed, the resulting two-phase mixture contains the following, where it is necessary to convert mass to moles.

Component	nC_6	nC_8	Total
MW	86.11	114.14	
Feed F_1 :			
lb	232	718	950
lbmol	2.69	6.29	8.98
Feed F_2 :			
lb	845	280	1,125
lbmol	9.81	2.45	12.26
Total feeds:			
lbmol	12.5	8.74	21.24
mole fraction	0.5885	0.4115	100

Based on the mole fractions of the combined feed, point M, the adiabatic mixing point is located in Fig.7.37 on the next page. By coincidence the mixing line connecting the two feeds is also a tie line for a temperature of 204°F. The equilibrium vapor is located at point V, while the equilibrium liquid is located at point L. The equilibrium vapor has a mole fraction of 0.75 for nC_6 and 0.25 for nC_8. The equilibrium liquid has a mole fraction of 0.35 for nC_6 and 0.65 for nC_8.

Although not requested, the moles of equilibrium vapor and liquid can be determined by material balances. By total material balance,

$$F_1 + F_2 = 21.24 = V + L \qquad (1)$$

By material balance on n-hexane,

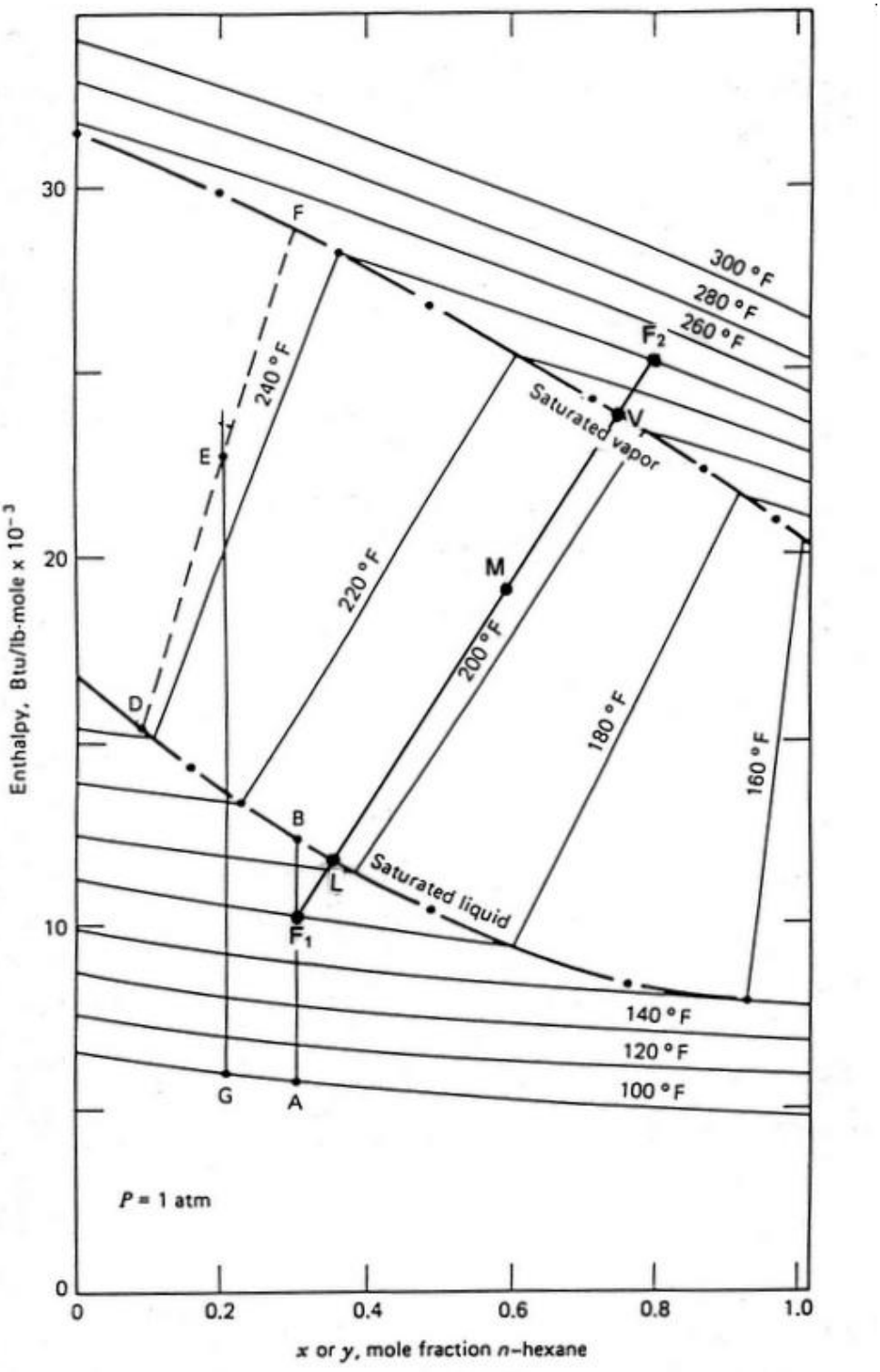
$$12.5 = 0.75V + 0.35L \qquad (2)$$

Solving Eqs. (1) and (2), V = 12.68 lbmol and L = 8.56 lbmol

The molar % vaporized = 12.69/21.24 x 100% = 59.7%. This is consistent with the value obtained by the inverse lever arm rule on the diagram on the next page.

Exercise 7.55 (continued)

Analysis: (a) (continued)



Exercise 7.55 (continued)

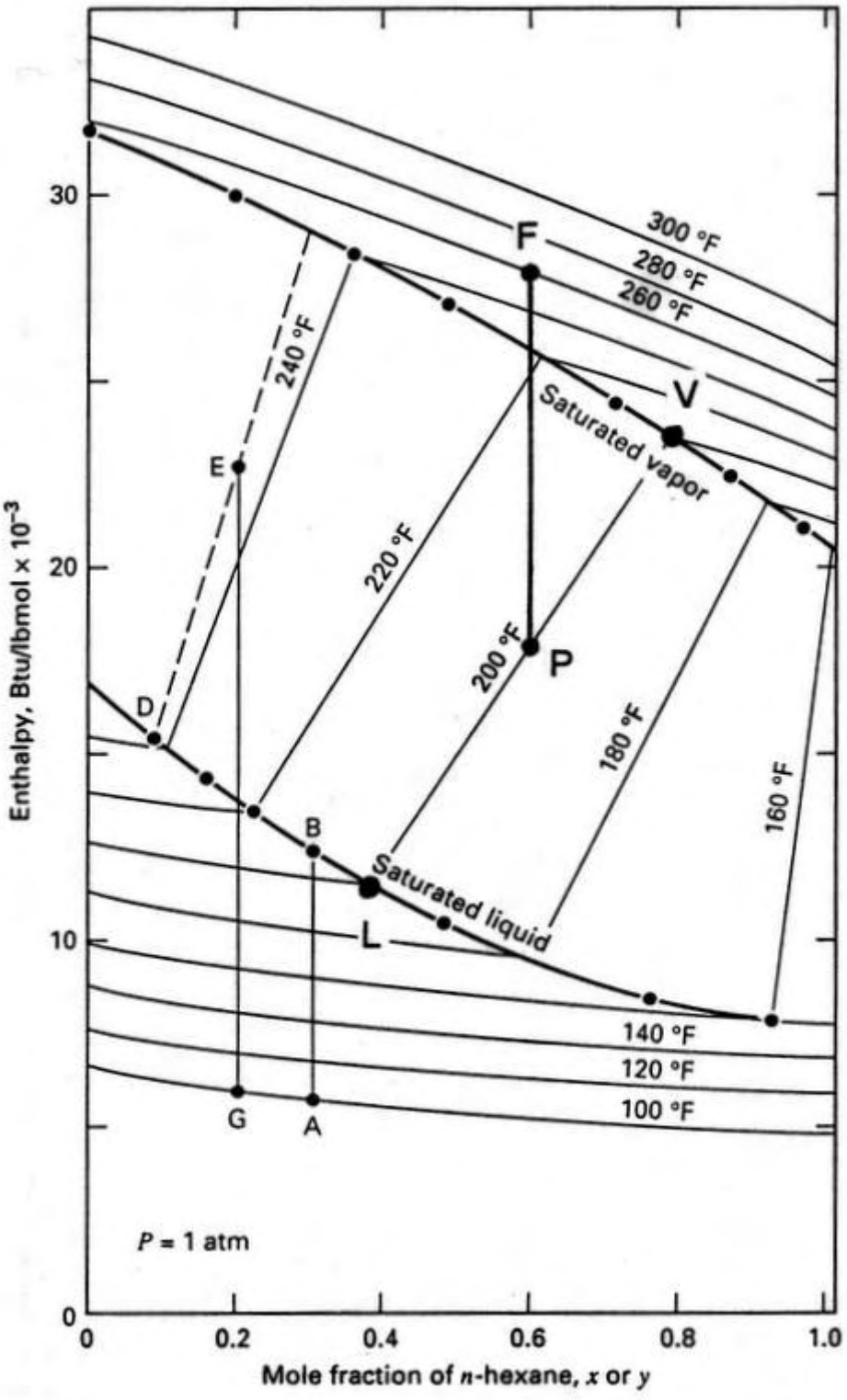
Analysis: (continued)

(b) From the diagram below, the enthalpy of the feed, F , of 60 mol% nC_6 at 260°F is equal to H_F = 27,700 Btu/lbmol. Upon cooling, the point P, in the two-phase region, is reached at 200°F. From the tie line through point P, the equilibrium vapor and liquid phases are shown at points V and L. The enthalpy of the two-phase mixture at point P = H_P = 17,700 Btu/lbmol. Therefore, the energy that must be removed = Q = 27,700 - 17,700 = 10,000 Btu/lbmol mixture. The composition of the equilibrium vapor at point V is 77 mol% nC_6. The composition of equilibrium liquid at point L is 38 mol% nC_6 . The amounts of vapor and liquid can be obtained by material balances or by the inverse lever arm rule using the plot below. By the latter, the molar percent vapor = 53%.

(c) In the diagram below, the equilibrium vapor from part (b), shown at F, is cooled to 180°F to point M in the two-phase region. This mixture splits into equilibrium vapor, V, and equilibrium liquid, L. The composition of V is 92 mol% nC_6. The composition of L is 60 mol% nC_6. By the lever arm rule, the mole % of equilibrium vapor = 60%.

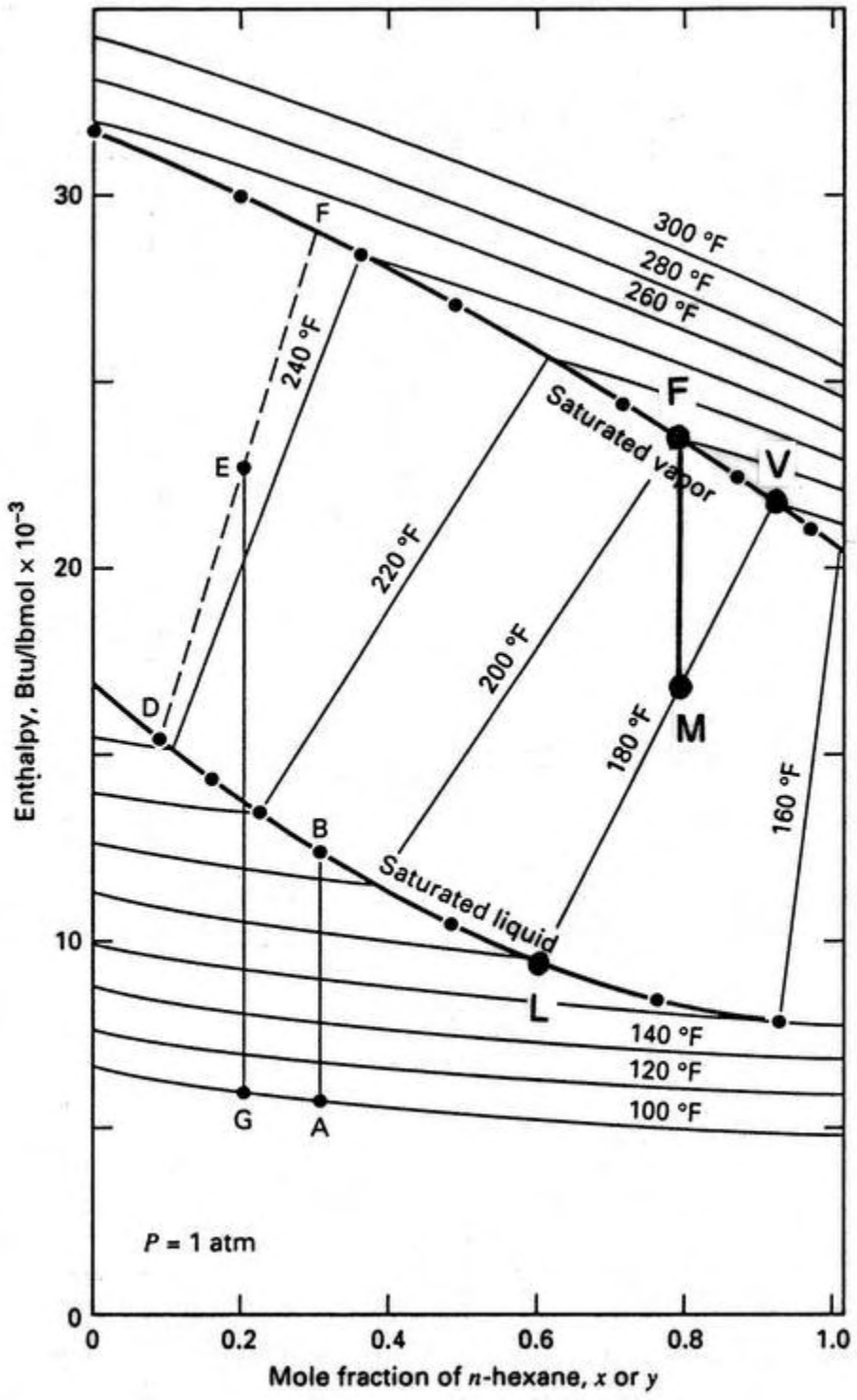
Exercise 7.55 (continued)

Analysis: (b) (continued)



Exercise 7.55 (continued)

Analysis: (c) (continued)



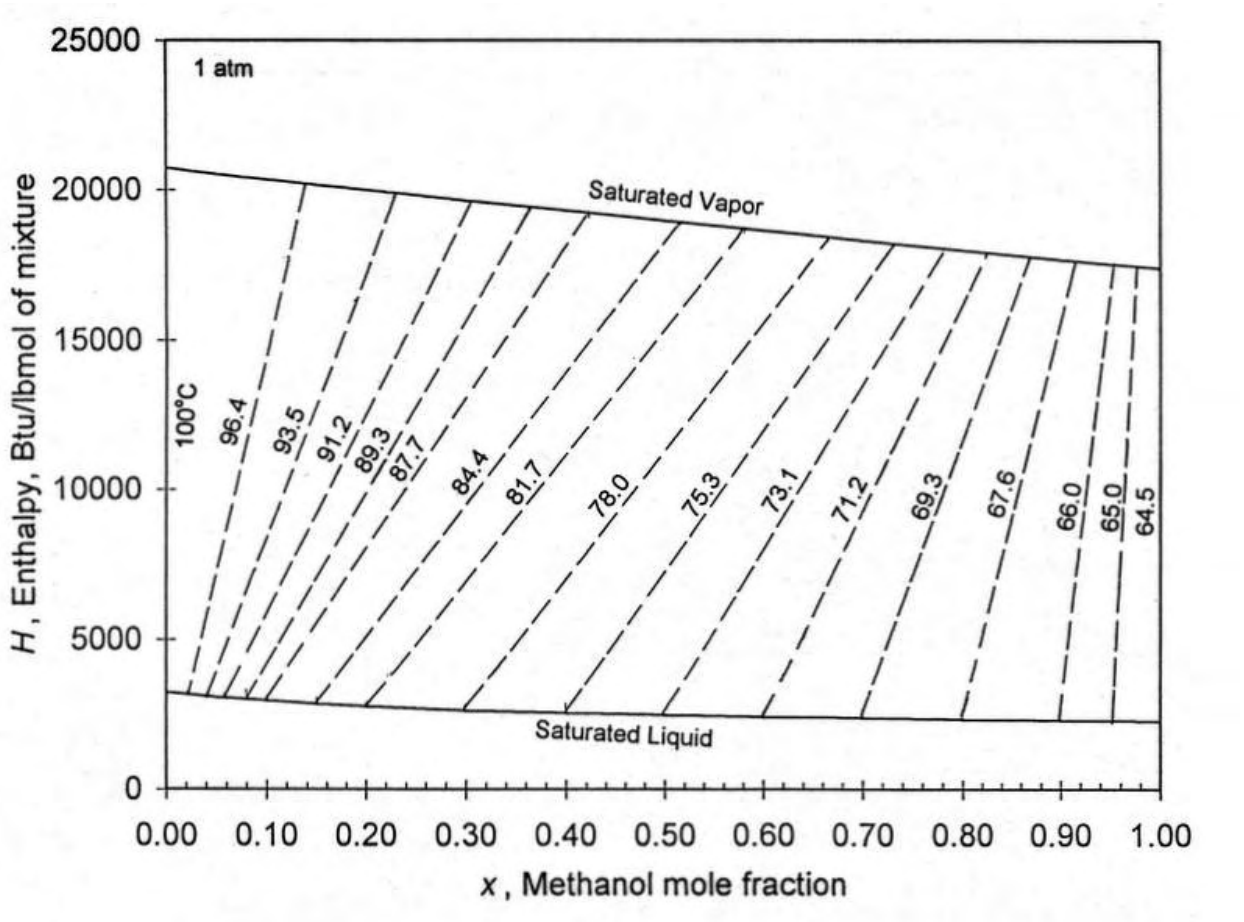
Exercise 7.56

Subject: Development of an enthalpy-concentration diagram for methanol-water at 1 atm. Use of diagram to obtain minimum stages.

Given: Enthalpy and vapor-liquid equilibrium data in Table 7.8. Feed of 100 lbmol/h containing 60 mol% methanol. Liquid distillate to contain 98 mol% methanol. Liquid bottoms to contain 96 mol% water.

Find: (a) Enthalpy-concentration diagram.
(b) Minimum number of stages.
(c) Temperatures of distillate and bottoms.

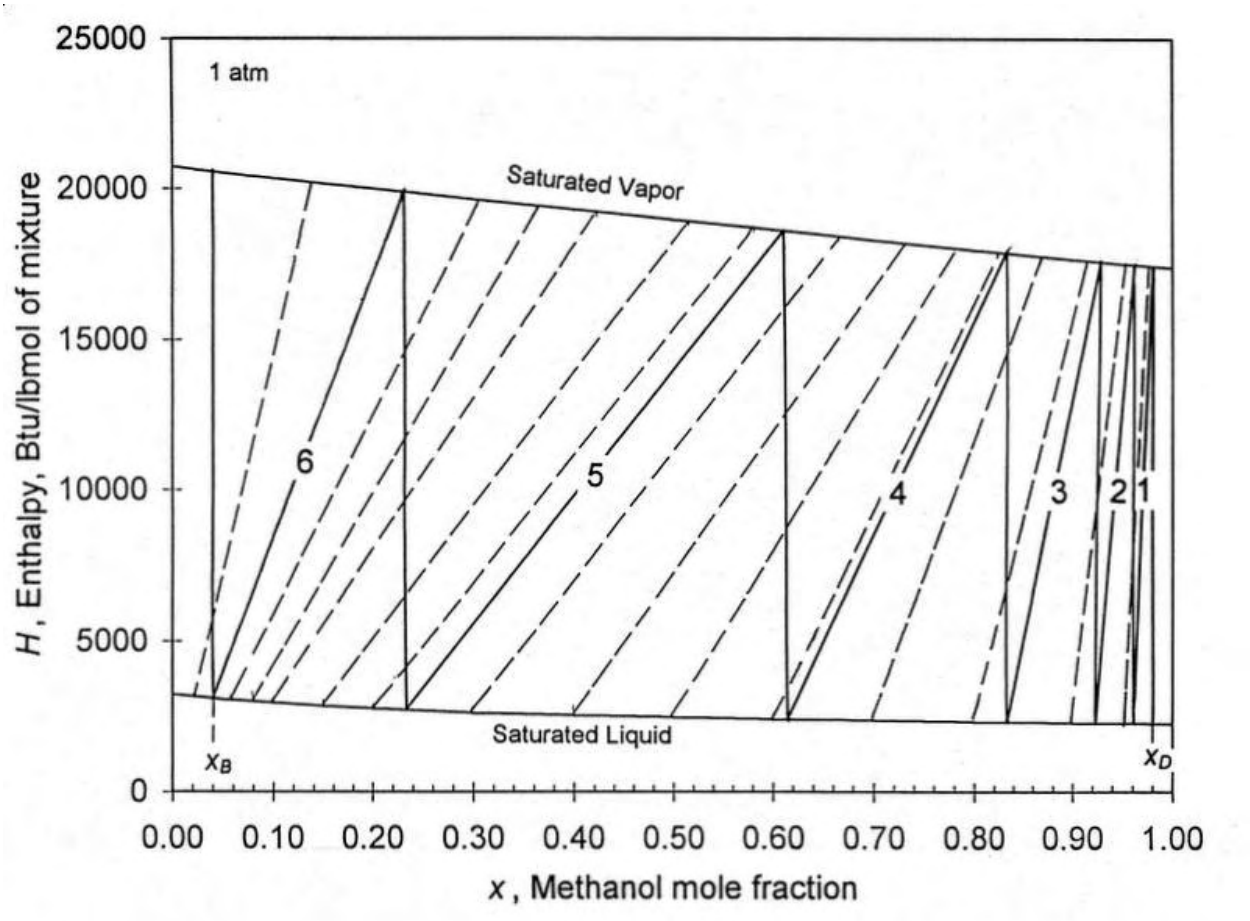
Analysis: (a) Use a spreadsheet to plot an enthalpy-concentration diagram, using the supplied data. The result is shown below, where the dashed lines are tie lines for the vapor-liquid equilibrium compositions at the temperatures indicated and a pressure of 1 atm.



Exercise 7.56 (continued)

Analysis: (continued)

(b) and (c) For the condition of total reflux, passing vapor and liquid streams have the same compositions and are saturated vapor and liquid, respectively. Therefore, while vapor and liquid streams at equilibrium are related by tie lines extending from the saturated liquid curve to the saturated vapor curve, passing vapor and liquid streams are related by vertical operating lines extending from the saturated liquid curve to the saturated vapor curve. By alternating between the equilibrium and operating lines, from the bottoms composition to the distillate composition, the minimum number of stages is determined by the number of tie lines used, as shown in the diagram below for the example of a methanol bottoms mole fraction of 0.04 and a methanol distillate mole fraction of 0.98, where the construction lines are solid lines and the equilibrium lines are numbered from the top. The minimum number of stages is seen to be 6. The value is independent of the feed condition because at total reflux, there is no feed. The temperature of the bottoms is 93.5°C. The temperature of the distillate is 64.7°C



Exercise 8.1

Subject: Extraction vs. Distillation.

Given: Dilute mixture of benzoic acid in water.

Find: Why liquid-liquid extraction is the preferred separation method.

Analysis: At 1 atm, the boiling point of benzoic acid is 249.2^{O}C. Thus, if a dilute solution of benzoic acid and water is distilled, a large amount of water, with its very high heat of vaporization (about 1,000 Btu/lb) must be vaporized, even though the relative volatility, α, is large and the separation is easy. L/L extraction can be used with a solvent like methyl isobutyl ketone, MIBK, which has a normal boiling point of 119^{o}C and can be easily recovered from the benzoic acid by distillation and then recycled [see Trans. AIChE, 42, 331 (1946).

Exercise 8.2

Subject: Liquid-Liquid Extraction vs. Distillation.

Given: Dilute mixture of formic acid in water.

Find: Why liquid-liquid extraction is the preferred separation method.

Analysis: At 1 atm, the boiling point of formic acid is 100.6^{o}C, almost identical to the normal boiling point of water. A maximum-boiling azeotrope is formed at 107.1^{o}C with 43.3 mol% water. Thus, it is impossible to separate formic acid from water at 1 atm by ordinary distillation. L/L extraction can be used with chloroform as the solvent to extract formic acid [see J. Chem. Eng. Data, 5, 301 (1960) and J. Chem. Eng. Data, 4, 42 (1959)]. Tetrahydrofuran can also be used as the solvent.

Exercise 8.3

Subject: Selection of extraction device.

Given: Liquid-liquid extraction of acetic acid from water by ethyl acetate. Fig. 8.8 for selecting extraction equipment.

Find: Adequacy of the RDC. Other types of adequate extractors.

Analysis: In the process of Fig. 8.1 for the L/L extraction of acetic acid from water by ethyl acetate, 6 equilibrium stages are needed. Pertinent properties are:
$\mu < 1$ cP, $\Delta\rho = 0.08$ g/cm^3, $\sigma_I > 30$ dyne/cm
Need stainless steel equipment. Assume no emulsion formation. Have large flow rates.
Assume water-rich phase has a density of 1,000 kg/m^3.
Assume ethyl acetate-rich phase has a density of 900 kg/m^3.
Feed rate = 30,300 lb/h or 13,700 kg/h
Solvent rate = 71,100 lb/h or 32,300 kg/h
Total volumetric throughput = 13,700/1,000 + 32,300/900 = 49.6 m^3/h
In Fig. 8.8, this throughput is on the border line.
Use a mixer-settler battery or any kind of a mechanically assisted column.

Exercise 8.4

Subject: Extraction devices.

Given: ARD and RDC.

Find: Advantages and disadvantages of each device.

Analysis:

RDC:

A great deal of experience exists.
Hundreds of units have been installed.
Can easily remove agitator assembly shaft.
Easily fabricated and assembled.

ARD:

Get reduced back-mixing.
Can not easily remove agitator assembly shaft.
More complex unit to fabricate and assemble.

Exercise 8.5

Subject: Selection of extraction devices.

Given: Cascade of mixer-settler units.

Find: Conditions for selection of this device.

Analysis: Mixer-settler units are preferred for:

1. Less than 5 equilibrium stages.
2. Low head room, if much floor space is available.
3. Easy scale-up and certain performance.
4. Wide ratio of feed-to-solvent flow rates.

Exercise 8.6

Subject: Selection of extraction device

Given: 4,000 bbl/day of petroleum reformate. 5 volumes of diethyleneglycol to extract aromatics from the paraffins in one volume of reformate. 8 theoretical stages.

Find: Preferred type of extractor using Tables 8.2 and 8.3, with Fig. 8.8.

Analysis: Total throughput is 4,000 + 5(4,000) = 24,000 bbl/day.
Assume 42 gal/bbl, which is equivalent to 0.159 m^3/bbl.
Then throughput = 24,000(0.159)/24 = 159 m^3/h

From Fig. 8.8, consider RDC, ARD, Kuhni, or Lurgi extractors.

Exercise 8.7

Subject: Selection of extraction solvents.

Given: The following mixtures:

(a) water - ethyl alcohol
(b) water - aniline
(c) water - acetic acid

Find: A possible solvent for each mixture and the resulting solute.

Analysis: Use Table 8.4, where the minus sign designates a suitable solvent group.

(a) water - ethyl alcohol:

Solute	Solute group	Desired solvent group	Possible solvent
water	Group 2	Group 1	no solvent to extract water
ethyl alcohol	Group 2	Group 1	n-butanol

(b) water - aniline:

Solute	Solute group	Desired solvent group	Possible solvent
water	Group 2	Group 1	no solvent to extract water
aniline	Assume Group 5 with amine group controlling	Groups 1 and 6	trichloroethane

(c) water - acetic acid:

Solute	Solute group	Desired solvent group	Possible solvent
water	Group 2	Group 1	no solvent to extract water
acetic acid	Group 1	Groups 2,3.4.5	2 - 1-butanol 3 - diisobutyl ketone 4 - methyl acetate 5 - isopropyl ether

Note that it is very difficult to find a solvent to extract water from organic compounds. For that separation, adsorption may be preferred. Also, distillation is possible if the water is the more volatile component.

Exercise 8.8

Subject: Selection of extraction solvents.

Given: The following mixtures with solute first:

(a) acetone - ethylene glycol
(b) toluene - n-heptane
(c) ethyl alcohol - glycerine

Find: Suitable solvents

Analysis: Use Table 8.4, where the minus sign designates a suitable solvent group.

(a) acetone - ethylene glycol:

Component	Group	Desired solvent group	Possible solvent
acetone (solute)	3	1 and 6	trichloroethane
ethylene glycol	2	1	

(b) toluene - n-heptane:

Component	Group	Desired solvent group	Possible solvent
toluene (solute)	7	maybe 3,5,6	aniline
n-heptane	8	none	

(c) ethyl alcohol - glycerine:

Component	Group	Desired solvent group	Possible solvent
ethyl alcohol (solute)	2	1	
glycerine		1	

Table 8.4 does not give a choice. From Section 15 of Perry's Handbook, possible solvents are benzene and carbon tetrachloride.

Exercise 8.9

Subject: Characteristics of the extraction of acetic acid (A) from a dilute solution in water (C), with ethyl acetate (S) at 25°C.

Given: Values or estimates of values of $(K_A)_D$, $(K_C)_D$, $(K_S)_D$, and β_{AC}.

Find: If the system exhibits (a) high selectivity, (b) high solvent capacity, and (c) ease of recovery of solvent. A better solvent.

Analysis: Use CHEMCAD with UNIFAC for LLE to obtain typical mass fraction compositions for two liquid phases in equilibrium at 25°C and 1 atm. The LLVF three-phase flash model gives the following results:

Mass fractions:

Component	Feed	Extract	Raffinate
acetic acid (A)	0.0588	0.0595	0.0564
water (C)	0.2353	0.0332	0.9242
ethyl acetate (S)	0.7059	0.9073	0.0194

Define K_D = mass fraction in extract phase/mass fraction in raffinate phase.
$(K_A)_D$ = 0.0595/0.0564 = 1.055
$(K_C)_D$ = 0.0332/0.9242 = 0.036
$(K_S)_D$ = 0.9073/0.0194 = 46.8
$\beta_{AC} = (K_A)_D / (K_C)_D$ = 1.055/0.036 = 29.3

(a) The value of β_{AC} is high, indicating a high selectivity.
(b) The value of $(K_A)_D$ is not high, indicating a solvent capacity that is not high.
(c) Since $(K_S)_D$ is high and $(K_C)_D$ is low, recovery of solvent is relatively easy.
A better solvent should be sought because ethyl acetate does not have a high capacity. From the results of Exercise 8.7, four other solvents are selected. Again using CHEMCAD, the following results are obtained for distribution coefficients and relative selectivity:

Solvent	β_{AC}	$(K_A)_D$	$(K_S)_D$	$(K_C)_D$
ethyl acetate	29.3	1.055	46.8	0.036
1-butanol	4.43	1.187	8.76	0.268
diisobutyl ketone	94.8	0.365	1710	0.00385
methyl acetate	12.8	1.470	6.50	0.115
diisopropyl ether	102.7	0.453	516	0.00441

No solvent meets all four criteria. Ethyl acetate may be the compromise. No solvent has a high capacity.

Exercise 8.10

Subject: Estimation of interfacial tension.

Given: Composition of a ternary mixture.

Find: Method for estimating the interfacial tension from the values of surface tension in air for each component in the mixture.

Analysis: Antonoff's rule can be used to compute the interfacial tension for two liquid phases, I and II, in equilibrium,

$$\sigma_i = \left| (\sigma_{II})_{\text{in air}} - (\sigma_I)_{\text{in air}} \right|$$

This equation, which is discussed in,

1. J. Russ. Phys. Chem. Soc., 39, 342 (1907).
2. Hart, Duga, Res./Devel., 16 (9), 46 (1965).

requires values of the multicomponent surface tensions of each phase [see Reid, Prausnitz, and Poling, "The Properties of Liquids and Gases", 4th ed. (1986)].

Exercise 8.11

Subject: Extraction of acetone (A) from water (C) by 1,1,2-trichloroethane (S) at 25°C

Given: 1,000 kg/h of 45 wt% A in C. Liquid-liquid equilibrium data. 10 wt% A in raffinate.

Find: Using Hunter-Nash method with an equilateral triangle diagram.
(a) Minimum flow rate of S.
(b) Number of equilibrium stages for solvent rate of 1.5 times minimum.
(c) Flow rate and composition of each stream leaving each stage.

Analysis: Using the given equilibrium data in weight fractions, the triangular diagram is shown on the next page, where a solid line is used for the equilibrium curve and dashed lines are used for the tie lines, only three of which are given. Additional tie-line locations can be made using either of the two techniques illustrated in Fig. 8.16.

(a) The minimum solvent flow rate corresponds to an infinite number of equilibrium stages. To determine this minimum: (1) Points are plotted on the triangular diagram for the given compositions of the solvent, S (pure S), feed, F (45 wt% A, 55 wt% C), and raffinate, R_N (10 wt% A on the equilibrium curve), followed by drawing an operating line through the points S and R_N and extending it only to the right because the tie lines slope down from left to right; (2) Because the pinch region, where equilibrium stages crowd together, may occur anywhere, additional potential operating lines are drawn through the tie lines extended to the right until they cross the operating line at the solvent end, drawn in (1), where these intersections for four tie lines (the three given and one other that extends through the feed point) are denoted P_1, P_2, P_3, and P_4; (3) The intersection point farthest from the triangular diagram is the one used to determine the minimum solvent rate, where here it is $P_1 = P_{\min}$, corresponding to a pinch point at the feed end of the cascade; (4) An operating line is drawn from P_1 through F to the determine the extract E_1, followed by drawing lines from $E_!$ to R_N and from S to F, with the intersection of these two lines determining the mixing point, M. The wt% A at the mixing point is 36.5%. From Eq. (8-10),

$$\frac{S_{\min}}{F} = \frac{(x_A)_F - (x_A)_M}{(x_A)_M - (x_A)_S} = \frac{0.45 - 0.365}{0.365 - 0.0} = 0.233$$

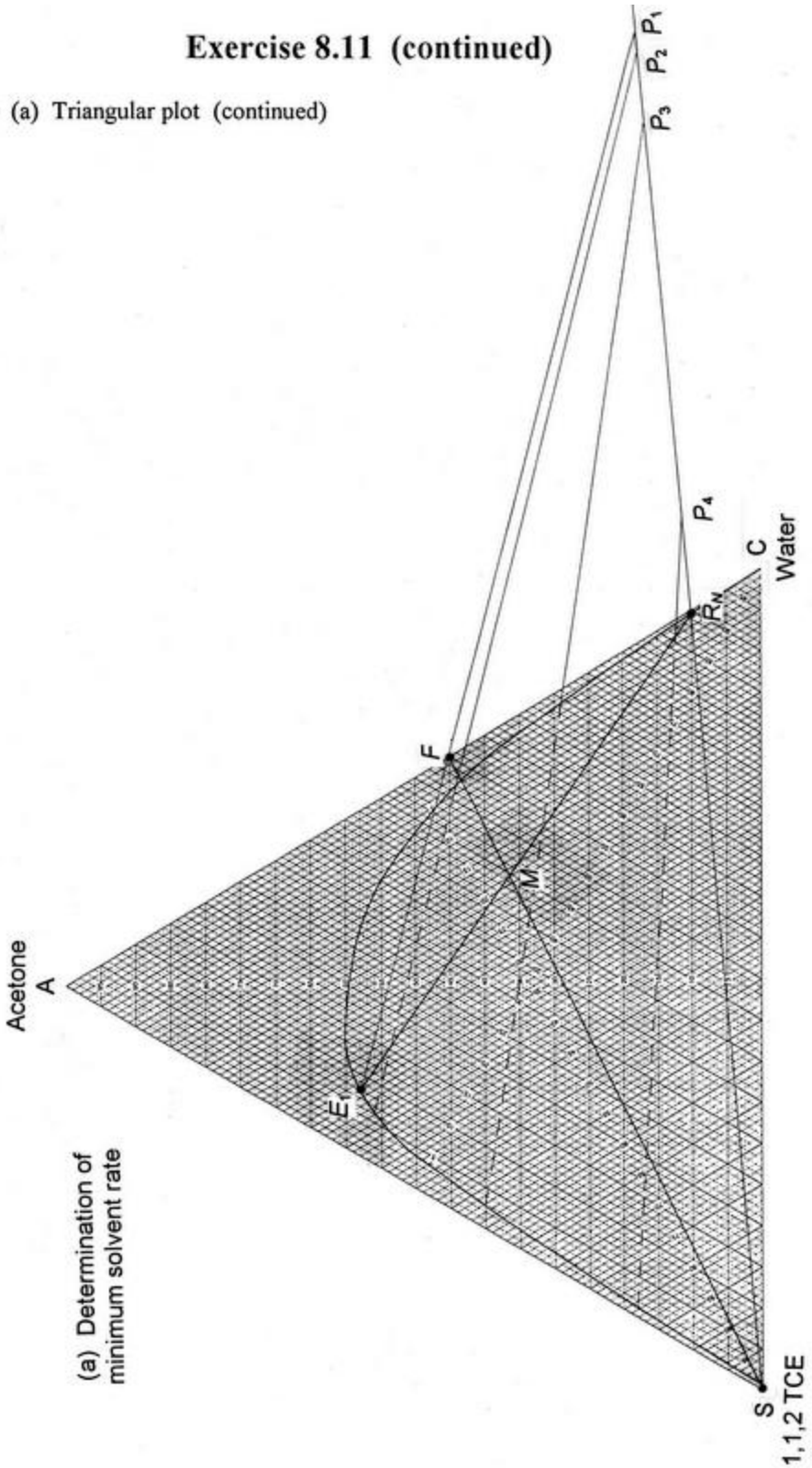
Therefore, $S_{\min} = 0.233F = 0.233(1{,}000) = 233$ kg/h

(b) Solvent rate = 1.5 $S_{\min}$ = 1.5(233) = 350 kg/h

With this rate, the total (feed + solvent) component flow rates becomes: A = 450 kg/h, C = 550 kg/h, and S = 350 kg/h, giving a total of 1,350 kg/h. Thus, the mixing point is at $(x_A)_M$ = 450/1,350 = 0.333, $(x_C)_M$ = 550/1,350 = 0.408, and $(x_S)_M$ = 350/1,350 = 0.259. This point is plotted as M on the second triangular diagram on a following page. A line from R_N through M to an intersection with the equilibrium curve determines the extract point E_1, as illustrated in Fig. 8.14. The operating point P is now determined, as in Fig. 8.17, by finding the intersection of lines drawn through S and R_N, and through F and E_1. The number of equilibrium stages is now stepped off, as in Fig. 8.17, giving a value of N_t slightly greater than 5.

Exercise 8.11 (continued)

Analysis: (a) Triangular plot (continued)



(a) Determination of minimum solvent rate

Exercise 8.11 (continued)

Analysis: (continued)

(c) First compute the two product flow rates, using the following product compositions read from the plot:

Mass fractions:

Component	Acetone	Water	1,1,2 TCE
Feed	0.450	0.550	0.000
Solvent	0.000	0.000	1.000
Raffinate	0.100	0.895	0.005
Extract	0.509	0.040	0.451

By overall total material balance, $F + S = 1{,}000 + 350 = 1{,}350 = R_N + E_1$ 1)

By overall acetone balance, $0.45F = 450 = 0.100R_N + 0.509E_1$ (2)

Solving Eqs. (1) and (2) simultaneously, $E_1 = 770$ kg/h and $R_N = 580$ kg/h

The composition of each stream leaving each stage can be read from the right-triangle plot prepared in part (b). Let x be mass fraction in the raffinate and y be mass fraction in the extract. The stages are arbitrarily numbered from the feed end. The flow rate of each stream leaving each stage is best obtained by total material balances around groups of stages and the inverse lever arm rule, using the operating lines as. A total balance for the first n-1 stages is:

$$F + E_n = 1{,}000 + E_n = R_{n-1} + E_1 = R_{n-1} + 770$$

or

$$R_{n-1} - E_n = 1{,}000 - 770 = 230 \qquad (3)$$

By the inverse lever arm rule with the right-triangle diagram,

$$\frac{R_{n-1}}{E_n} = \frac{\overline{E_n P}}{\overline{R_{n-1} P}} \qquad (4)$$

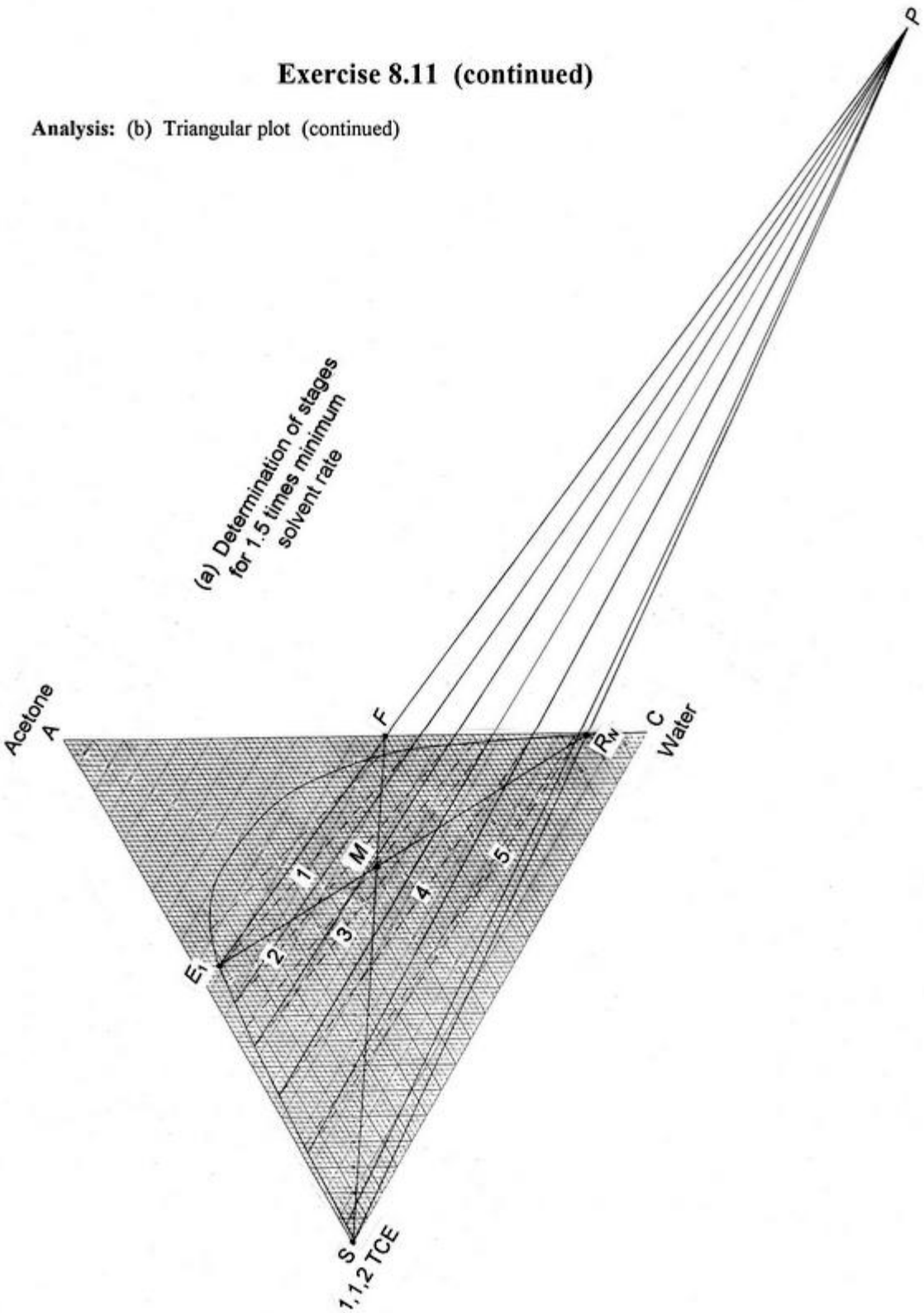
where the lines are measured from the right-triangle diagram.

Eqs. (3) and (4) are solved simultaneously for R_{n-1} and E_n for $n = 2$ to 6. The following results are obtained:

	Raffinate:			Extract:			kg/h:	
Stage	x_A	x_C	x_S	y_A	y_C	y_S	R	E
1	0.390	0.581	0.029	0.509	0.040	0.451	935	770
2	0.325	0.651	0.024	0.440	0.033	0.537	822	706
3	0.260	0.724	0.016	0.360	0.024	0.616	738	592
4	0.190	0.800	0.010	0.270	0.017	0.713	656	508
5	0.100	0.895	0.005	0.165	0.011	0.824	580	426

Exercise 8.11 (continued)

Analysis: (b) Triangular plot (continued)



Exercise 8.12

Subject: Extraction of acetone (A) from water (C) by 1,1,2-trichloroethane (S) at 25°C

Given: 1,000 kg/h of 45 wt% A in C. Liquid-liquid equilibrium data. 10 wt% A in raffinate.

Find: Using a right triangle diagram.
(a) Minimum flow rate of S.
(b) Number of equilibrium stages for solvent rate of 1.5 times minimum.
(c) Flow rate and composition of each stream leaving each stage.

Analysis: Using the given equilibrium data in weight fractions, the right-triangle diagram is shown on the next page, where a solid line is used for the equilibrium curve and dashed lines are used for the tie lines, only three of which are given. Additional tie-line locations can be made using either of the two techniques illustrated in Fig. 8.16.

(a) The minimum solvent flow rate corresponds to an infinite number of equilibrium stages. To determine this minimum: (1) Points are plotted on the triangular diagram for the given compositions of the solvent, S (pure S), feed, F (45 wt% A, 55 wt% C), and raffinate, R_N (10 wt% A on the equilibrium curve), followed by drawing an operating line through the points S and R_N and extending it only to the right because the tie lines slope down from left to right; (2) Because the pinch region, where equilibrium stages crowd together, may occur anywhere, additional potential operating lines are drawn through the tie lines extended to the right until they cross the operating line at the solvent end, drawn in (1), where these intersections for four tie lines (the three given and one other that extends through the feed point) are denoted P_1, P_2, P_3, and P_4; (3) The intersection point farthest from the triangular diagram is the one used to determine the minimum solvent rate, where here it is $P_1 = P_{\min}$, corresponding to a pinch point at the feed end of the cascade; (4) An operating line is drawn from P_1 through F to the determine the extract E_1, followed by drawing lines from $E_!$ to R_N and from S to F, with the intersection of these two lines determining the mixing point, M. The wt% A at the mixing point is 36.5%. From Eq. (8-10),

$$\frac{S_{\min}}{F} = \frac{(x_A)_F - (x_A)_M}{(x_A)_M - (x_A)_S} = \frac{0.45 - 0.365}{0.365 - 0.0} = 0.233$$

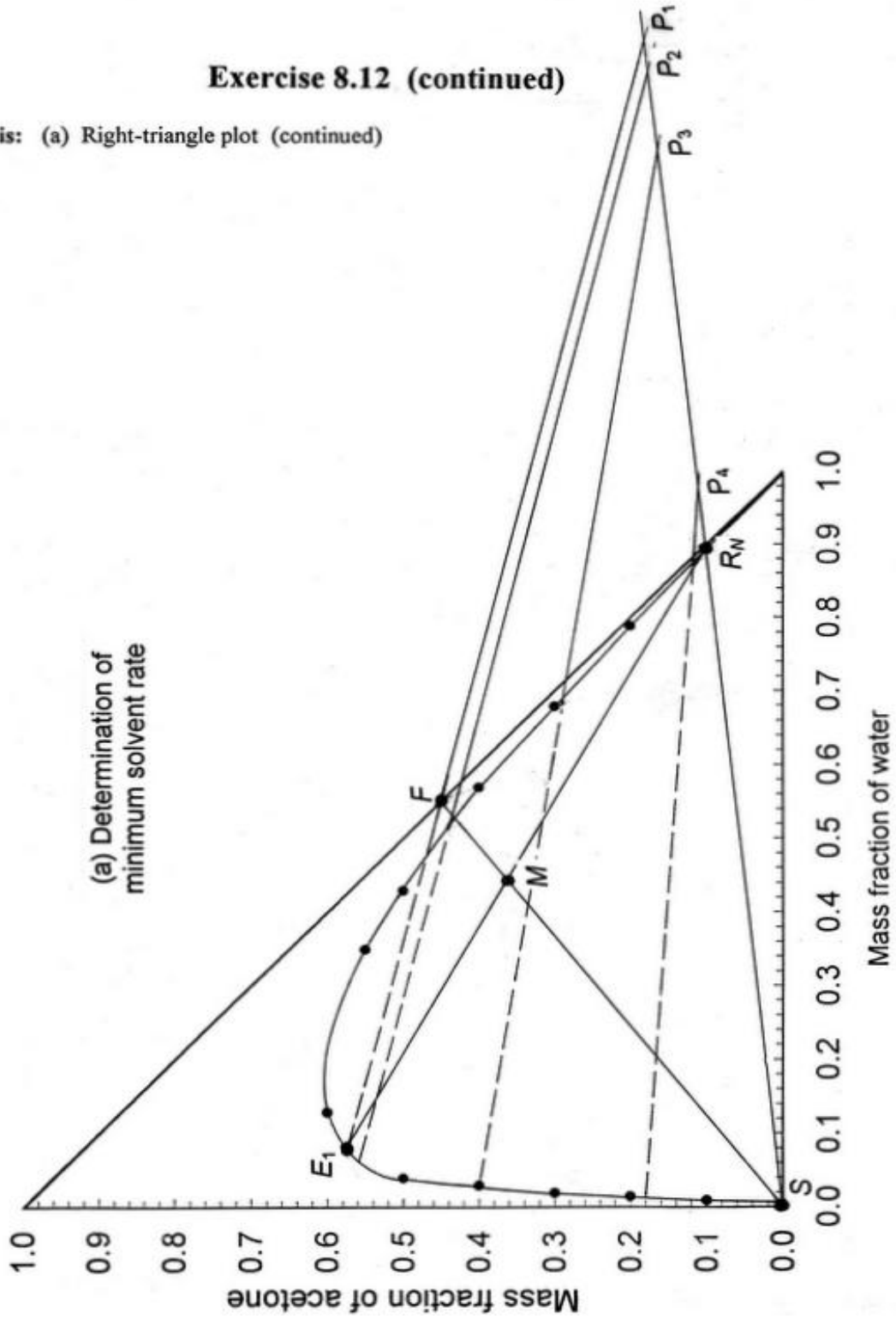
Therefore, $S_{\min} = 0.233F = 0.233(1{,}000) = 233$ kg/h

(b) Solvent rate = 1.5 $S_{\min}$ = 1.5(233) = 350 kg/h

With this rate, the total (feed + solvent) component flow rates becomes: A = 450 kg/h, C = 550 kg/h, and S = 350 kg/h, giving a total of 1,350 kg/h. Thus, the mixing point is at $(x_A)_M$ = 450/1,350 = 0.333, $(x_C)_M$ = 550/1,350 = 0.408, and $(x_S)_M$ = 350/1,350 = 0.259. This point is plotted as M on the second triangular diagram on a following page. A line from R_N through M to an intersection with the equilibrium curve determines the extract point E_1, as illustrated in Fig. 8.14. The operating point P is now determined, as in Fig. 8.17, by finding the intersection of lines drawn through S and R_N, and through F and E_1. The number of equilibrium stages is now stepped off, as in Fig. 8.17, giving a value of just slightly greater than $N_t = 5$.

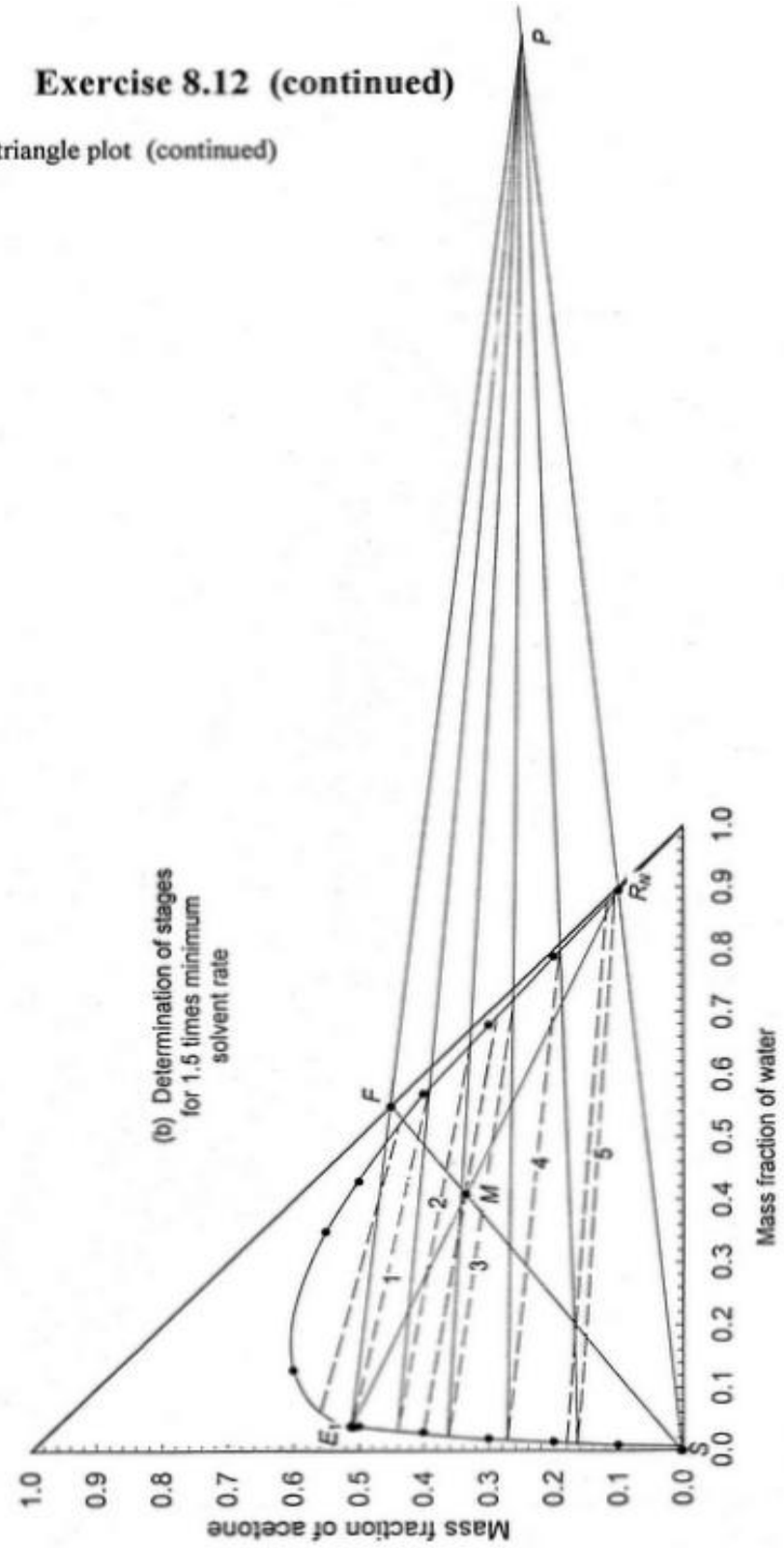
Exercise 8.12 (continued)

Analysis: (a) Right-triangle plot (continued)



Exercise 8.12 (continued)

Analysis: (b) Right-triangle plot (continued)



Exercise 8.12 (continued)

Analysis: (continued)

(c) First compute the two product flow rates, using the following product compositions read from the plot:

Mass fractions:

Component	Acetone	Water	1,1,2 TCE
Feed	0.450	0.550	0.000
Solvent	0.000	0.000	1.000
Raffinate	0.100	0.895	0.005
Extract	0.509	0.040	0.451

By overall total material balance, $F + S = 1{,}000 + 350 = 1{,}350 = R_N + E_1$ 1)

By overall acetone balance, $0.45F = 450 = 0.100R_N + 0.509E_1$ (2)

Solving Eqs. (1) and (2) simultaneously, $E_1 = 770$ kg/h and $R_N = 580$ kg/h

The composition of each stream leaving each stage can be read from the right-triangle plot prepared in part (b). Let x be mass fraction in the raffinate and y be mass fraction in the extract. The stages are arbitrarily numbered from the feed end. The flow rate of each stream leaving each stage is best obtained by total material balances around groups of stages and the inverse lever arm rule, using the operating lines. A total balance for the first n-1 stages is:

$$F + E_n = 1{,}000 + E_n = R_{n-1} + E_1 = R_{n-1} + 770$$

or

$$R_{n-1} - E_n = 1{,}000 - 770 = 230 \qquad (3)$$

By the inverse lever arm rule with the right-triangle diagram,

$$\frac{R_{n-1}}{E_n} = \frac{\overline{E_n P}}{\overline{R_{n-1} P}} \qquad (4)$$

where the lines are measured from the right-triangle diagram.

Eqs. (3) and (4) are solved simultaneously for R_{n-1} and E_n for $n = 2$ to 6. The following results are obtained:

	Raffinate:			Extract:			kg/h:	
Stage	x_A	x_C	x_S	y_A	y_C	y_S	R	E
1	0.390	0.581	0.029	0.509	0.040	0.451	935	770
2	0.325	0.651	0.024	0.440	0.033	0.537	822	706
3	0.260	0.724	0.016	0.360	0.024	0.616	738	592
4	0.190	0.800	0.010	0.270	0.017	0.713	656	508
5	0.100	0.895	0.005	0.165	0.011	0.824	580	426

Exercise 8.13

Subject: Extraction of isopropanol (A) from diisopropylether (C) by water (S) at 25°C.

Given: Feed containing 45 wt% A, 50 wt% C, and 5 wt% S. Raffinate to contain 2.5 wt% A. Extract to contain 20 wt% A. Liquid-liquid equilibrium data.

Find: Using Varteressian-Fenske method with a McCabe-Thiele diagram, find the number of theoretical stages. Can an extract of 25 wt% A be obtained?

Analysis: Because the wt% of the solute, A, in both the raffinate and extract are given, the solvent rate must be determined. Do this first by constructing a right-triangle diagram from the equilibrium tie line and phase boundary data. As shown on the next page, for a diagram that does not show the tie lines, points on the diagram are placed for: the feed, F, (45 wt% A, 50 wt% C, and 5 wt% S); the solvent, S, (100% S); the raffinate, R, (2.5 wt% A on the phase boundary line); and the extract, E, (20 wt% A on the phase boundary line). The mixing point, M, is determined by the intersection of lines drawn from: (1) F to S and (2) R to E. The ratio of solvent to feed is given by the inverse lever arm rule as the ratio of line length MF to line length MS, which equals 1.67. Take a basis of 100 kg/h of feed. Then the solvent rate is 1.67(100) = 167 kg/h. The flow rates of raffinate and extract are obtained from an overall total material balance and an overall material balance for A:

$$F + S = 100 + 167 = 267 = R + E \qquad (1)$$

$$(x_A)_F F + (x_A)_S S = 0.45(100) + 0 = 45 = (x_A)_R R + (x_A)_E E = 0.025R + 0.20E \qquad (2)$$

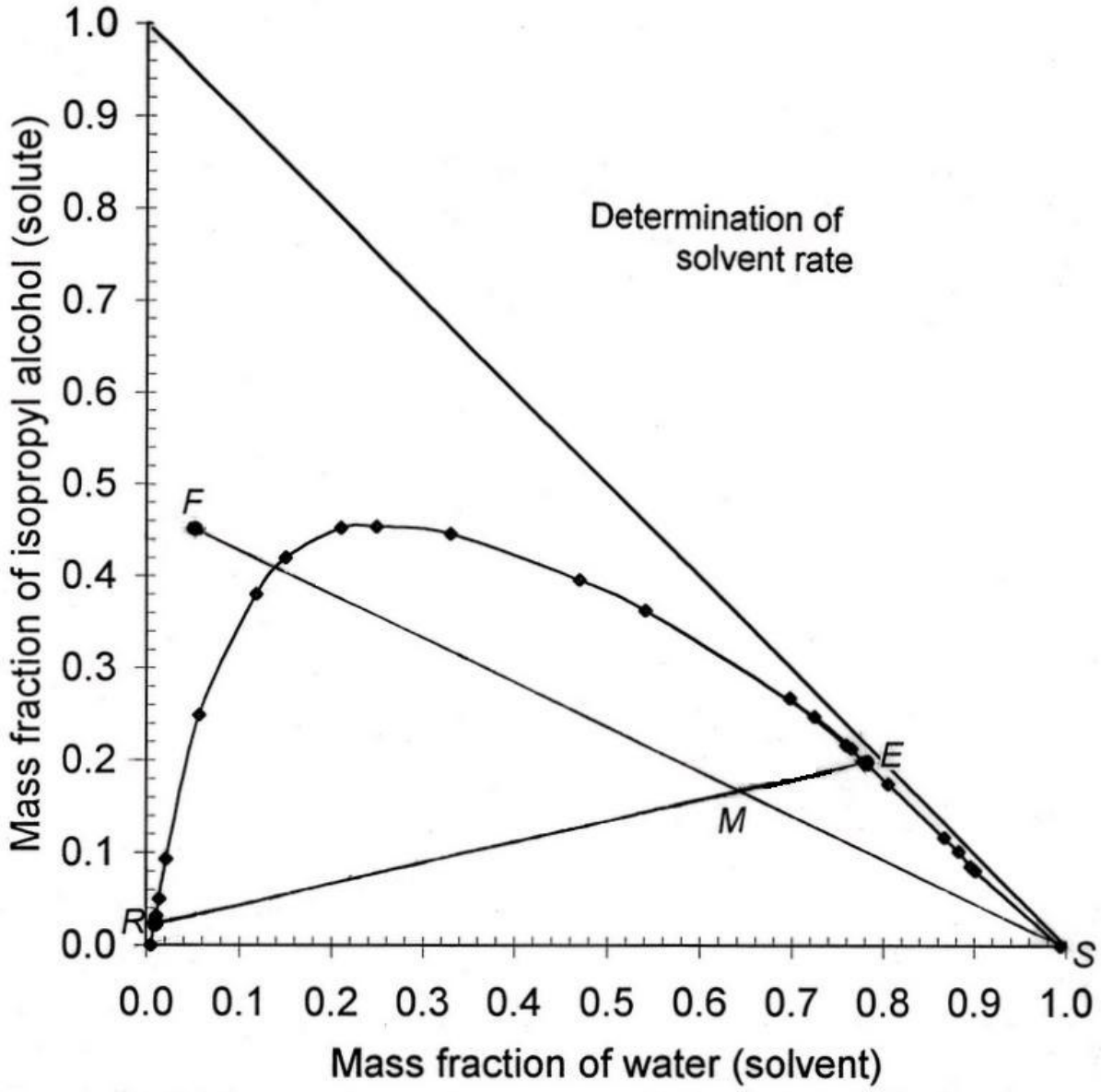
Solving Eqs. (1) and (2) simultaneously, R = 48 kg/h and E = 219 kg/h. The resulting overall material balance is as follows, where raffinate and extract compositions are read from the phase boundary curve.

Component	Feed	Solvent	Raffinate	Extract
Isopropyl alcohol (A)	45.0	0.0	1.20	43.80
Diisopropyl ether (C)	50.0	0.0	46.28	3.72
Water (S)	5.0	167.0	0.52	171.48
Total	100.0	167.0	48.00	219.00

To determine the number of equilibrium stages for the above solvent rate and material balance, using the Varteressian-Fenske method with a McCabe-Thiele diagram, an equilibrium curve and an operating curve are needed in a McCabe-Thiele plot of mass fraction of alcohol in the extract against the mass fraction of alcohol in the raffinate, as illustrated for a different system in Fig. 8.25. The equilibrium curve is determined from the equilibrium tie-line data, shown in a right triangle diagram below and obtained directly from the statement of the exercise. These equilibria data are tabulated below. The operating curve is determined by first determining the operating point, P, as illustrated in Fig. 8.15, followed by drawing arbitrary straight lines through that point

Exercise 8.13 (continued)

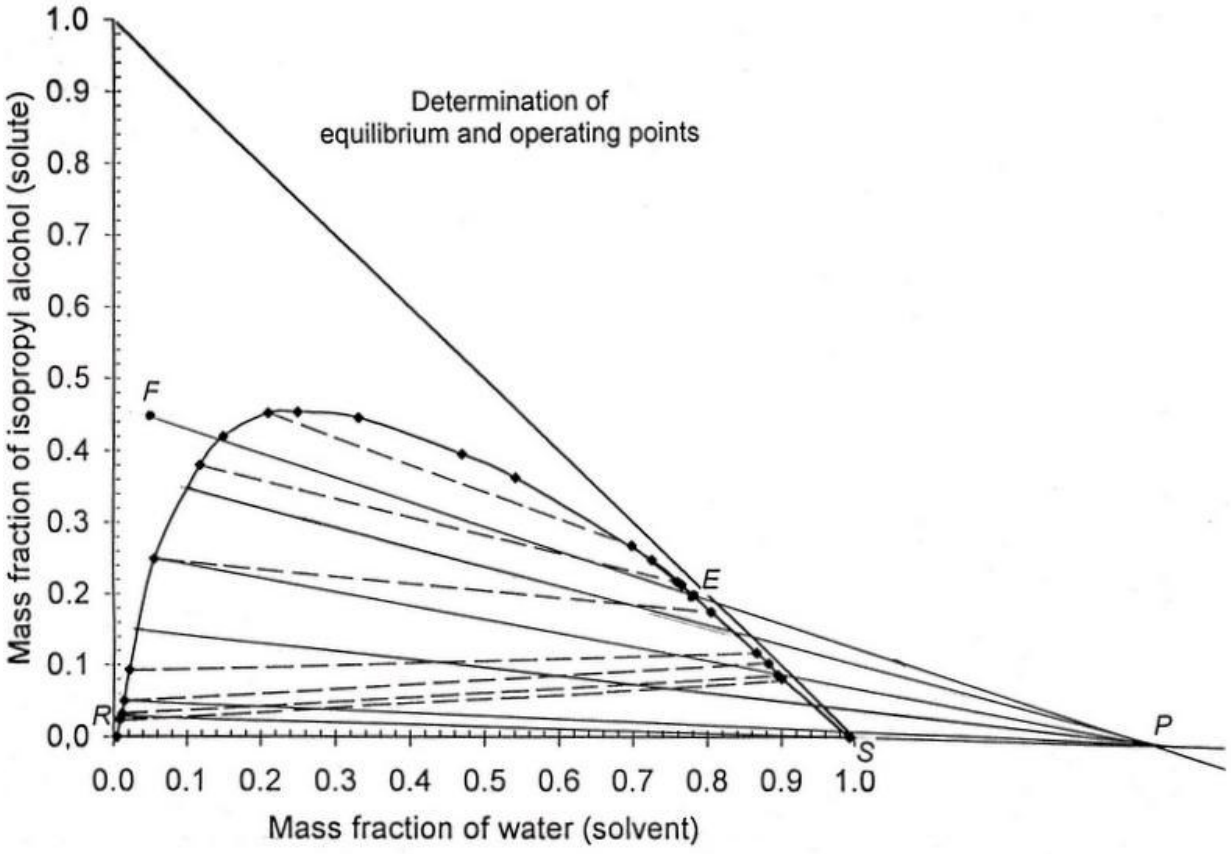
Analysis: (continued)



Exercise 8.13 (continued)

Analysis: (continued)

to give corresponding extract and raffinate compositions from intersections with the phase boundary curve, as illustrated in Fig. 8.21c. Several such operating lines are shown on the right-triangle diagram below. The operating points used to draw the operating curve on the McCabe-Thiele are tabulated below.



The points for the equilibrium curve are:

Mass fraction alcohol in Extract	Mass fraction alcohol in Raffinate
0.081	0.024
0.102	0.050
0.117	0.093
0.175	0.249
0.217	0.380
0.268	0.452

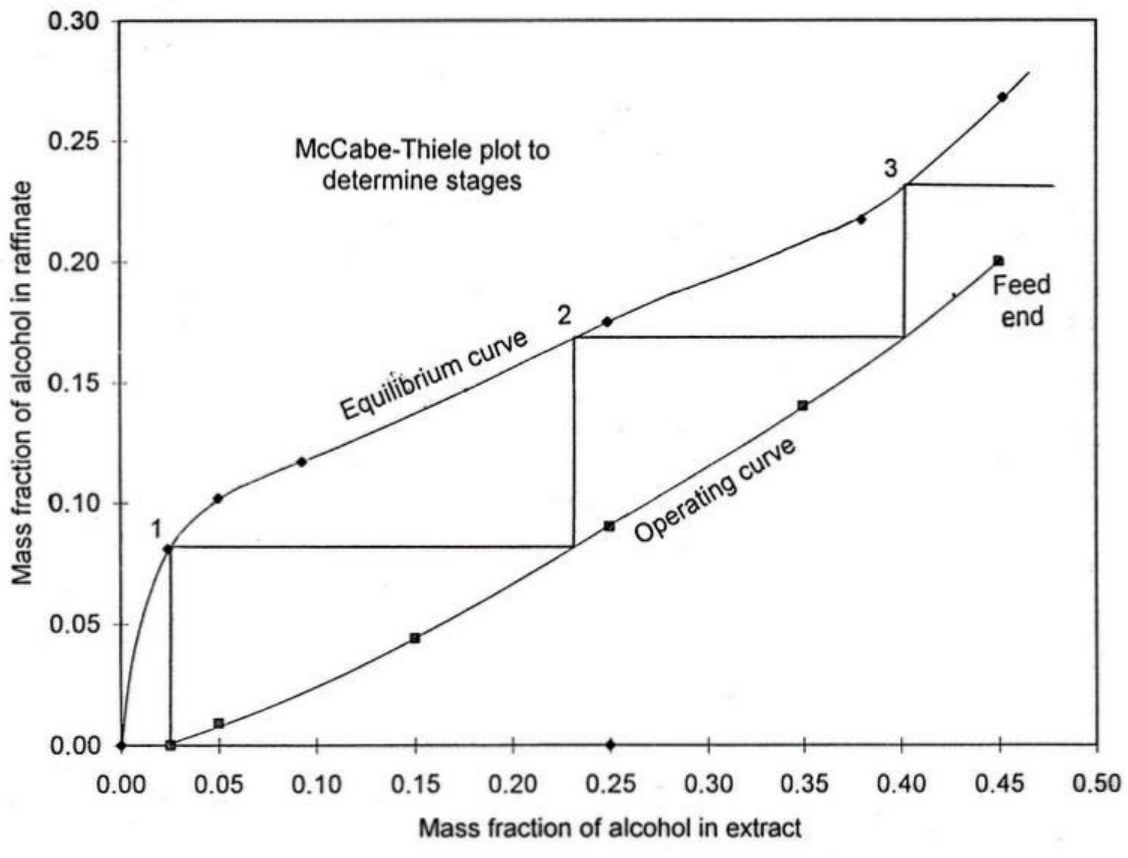
Exercise 8.13 (continued)

Analysis: (continued)

The determined points for the operating curve are:

Mass fraction alcohol in Extract	Mass fraction alcohol in Raffinate
0.000	0.025
0.009	0.050
0.044	0.150
0.095	0.250
0.150	0.350
0.200	0.450

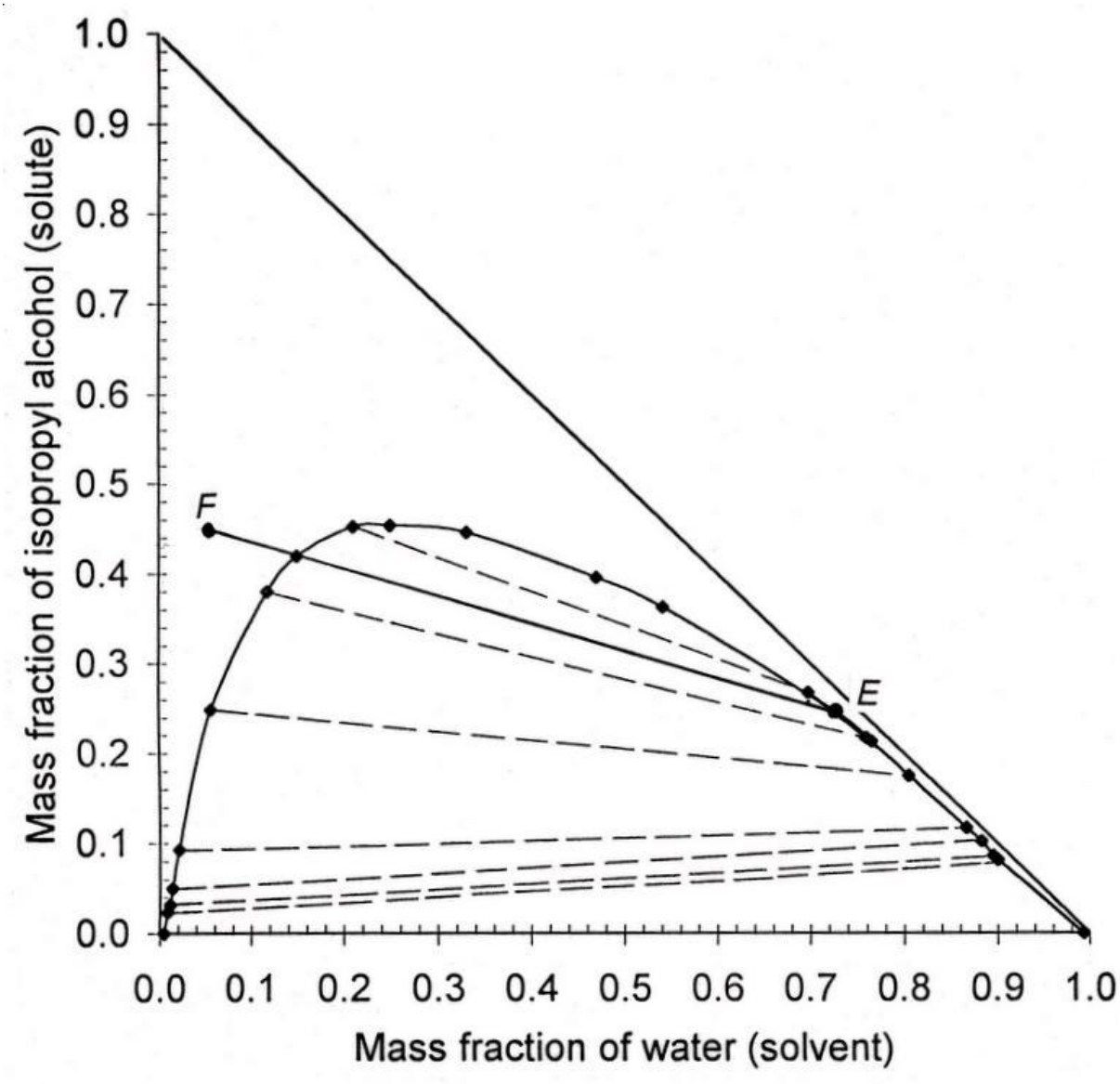
These points are plotted in the McCabe-Thiele diagram below, where the stages are stepped off as illustrated in Fig. 8.25. The result is 2.5 equilibrium stages.



Exercise 8.13 (continued)

Analysis: (continued)

To determine if an extract of 25 wt% A can be obtained, as shown in the diagram below, the feed and desired extract points are plotted as *F* and *E*, respectively, with a straight operating line drawn between the two points. Since that line appears to be coincident with an equilibrium tie line, the extract could be obtained, but only with an infinite number of stages. An extract with an alcohol content of greater than 25 wt% A is impossible because the operating line would have a slope less than an overlapping tie line, making it impossible to step off stages in the right direction.



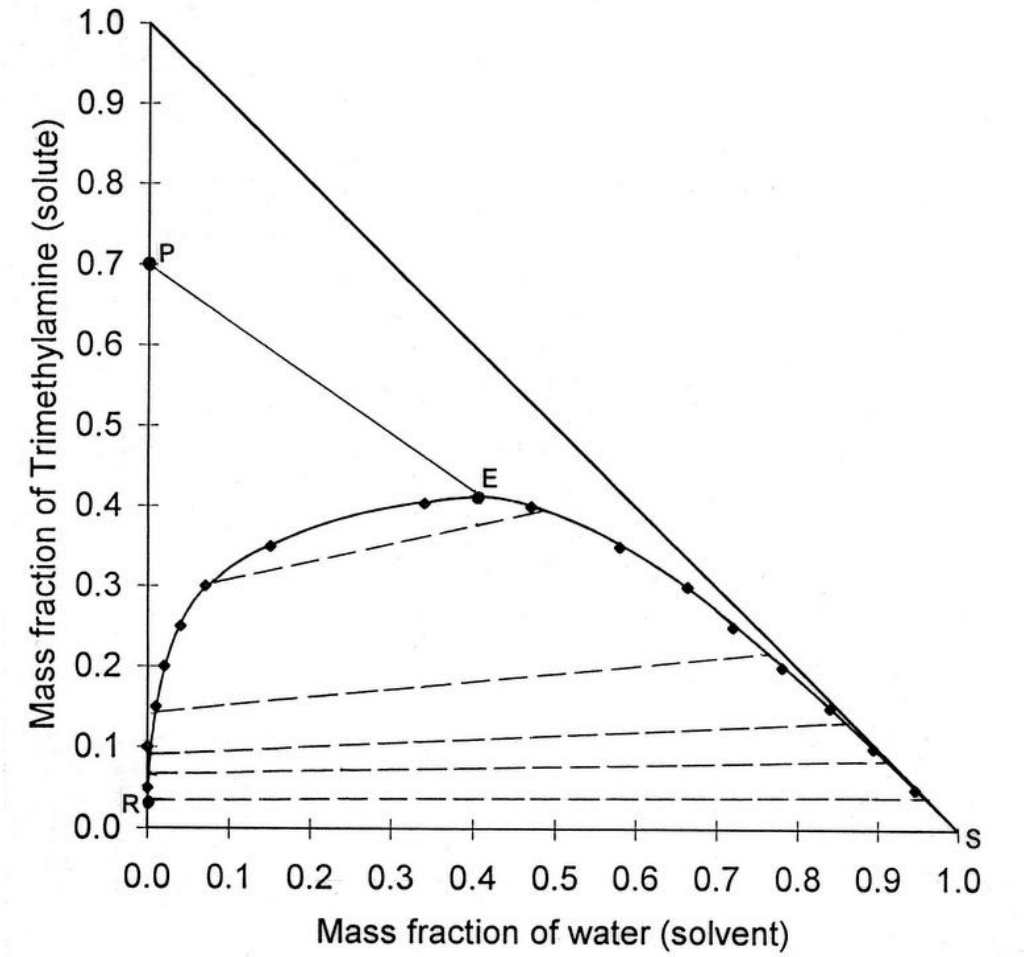
Exercise 8.14

Subject: Extraction of trimethylamine (TMA) from benzene (C) with water (S).

Given: Three equilibrium stages. Solvent-free extract to contain 70 wt% TMA. Solvent-free raffinate to contain 3 wt% TMA. Liquid-liquid equilibrium data.

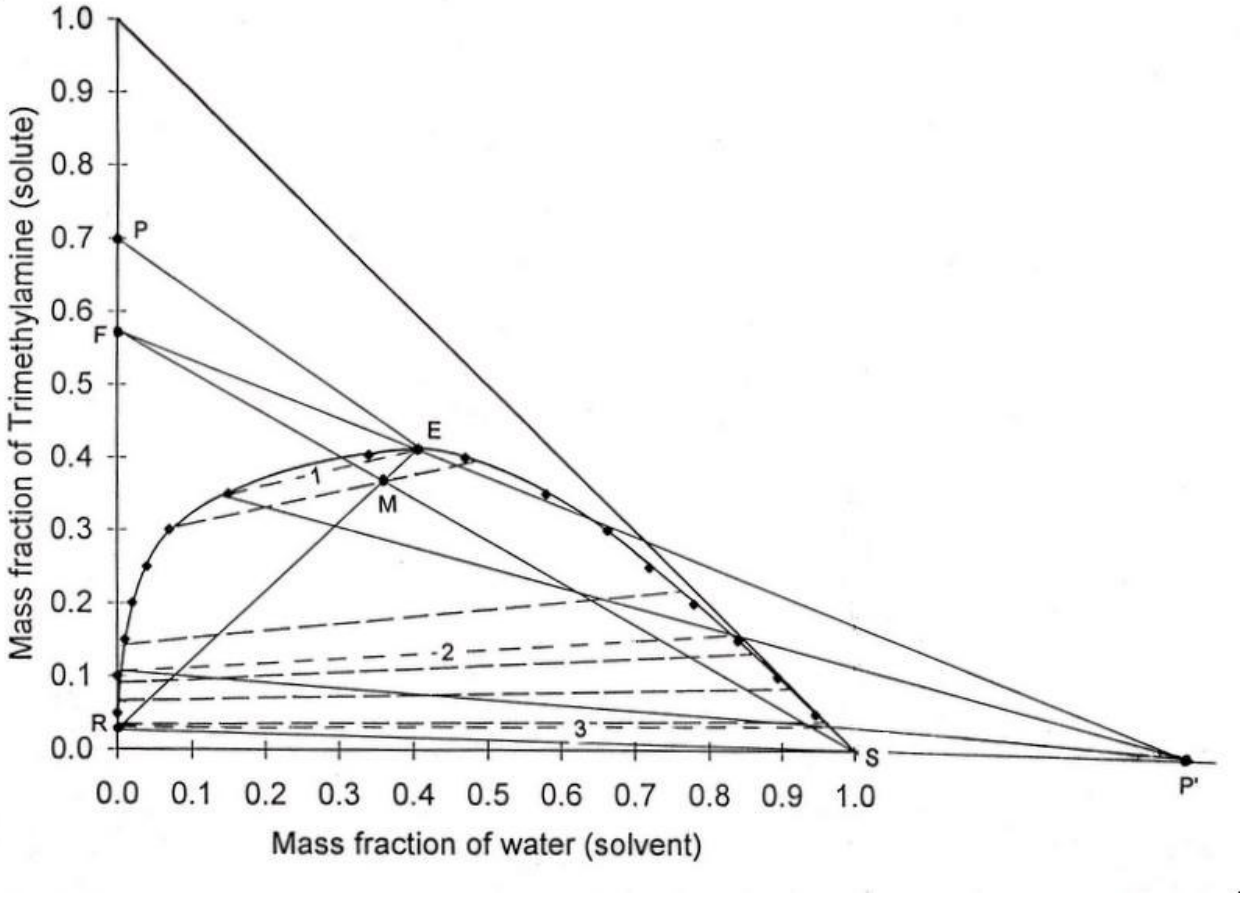
Find: Using the Hunter-Nash method with a right-triangle diagram, find feed composition and water-to-feed ratio.

Analysis: The given phase boundary liquid compositions and the equilibrium liquid-liquid compositions (as dashed tie lines) are plotted on the right-triangle diagram below. Included on the diagram are the final extract and raffinate compositions. The final extract composition is obtained by locating a point, P, for 70 wt% TMA, 30 wt% benzene, and 0% water (given solvent-free composition), and drawing a straight line from P toward the point S (pure water) to where the line intersects the phase boundary. This is point E for the extract. In a similar manner, the raffinate composition, R, is determined.



Exercise 8.14 (continued)

On a second diagram, shown below, a trial and error procedure is used to find the operating point, P' , that will result in the stepping off of three equilibrium stages, as illustrated in Fig. 8.19, to obtain the specified final extract and final raffinate. The final trial is shown on the diagram, where M is the mixing point for extract + raffinate, and for feed + solvent. Assuming water-free feed, the resulting feed composition is at F, with 57.5 wt% TMA and 42.5 wt% benzene. The ratio of mass of solvent to mass of feed is given by the ratio of line lengths = line FM/line MS = 0.56.



Exercise 8.15

Subject: Extraction of diphenylhexane (DPH) from docosane (C) with furfural (U) at 45 and 80°C

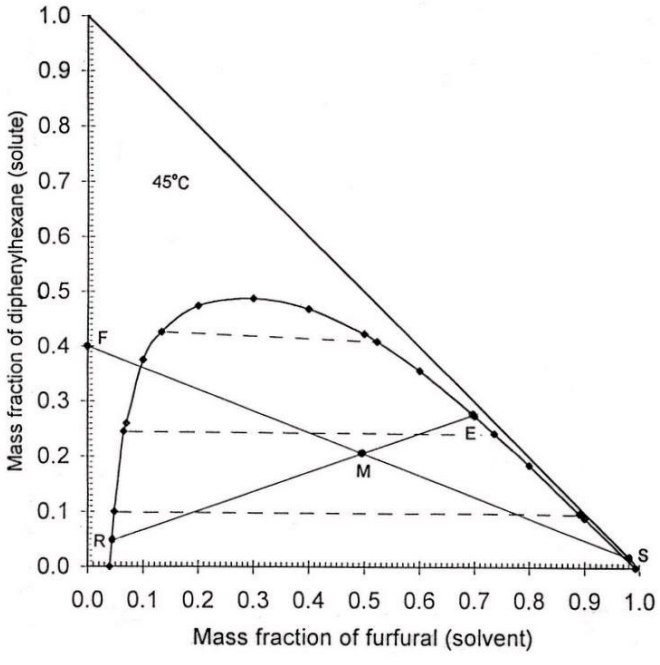
Given: Feed, F, of 500 kg/h of 40 wt% DPH in C. 500 kg/h of solvent, S, containing 98 wt% U and 2 wt% DPH. Raffinate to contain 5 wt% DPH. Liquid-liquid equilibrium data.

Find: Number of theoretical stages. DPH in kg/h in the extract.

Analysis:

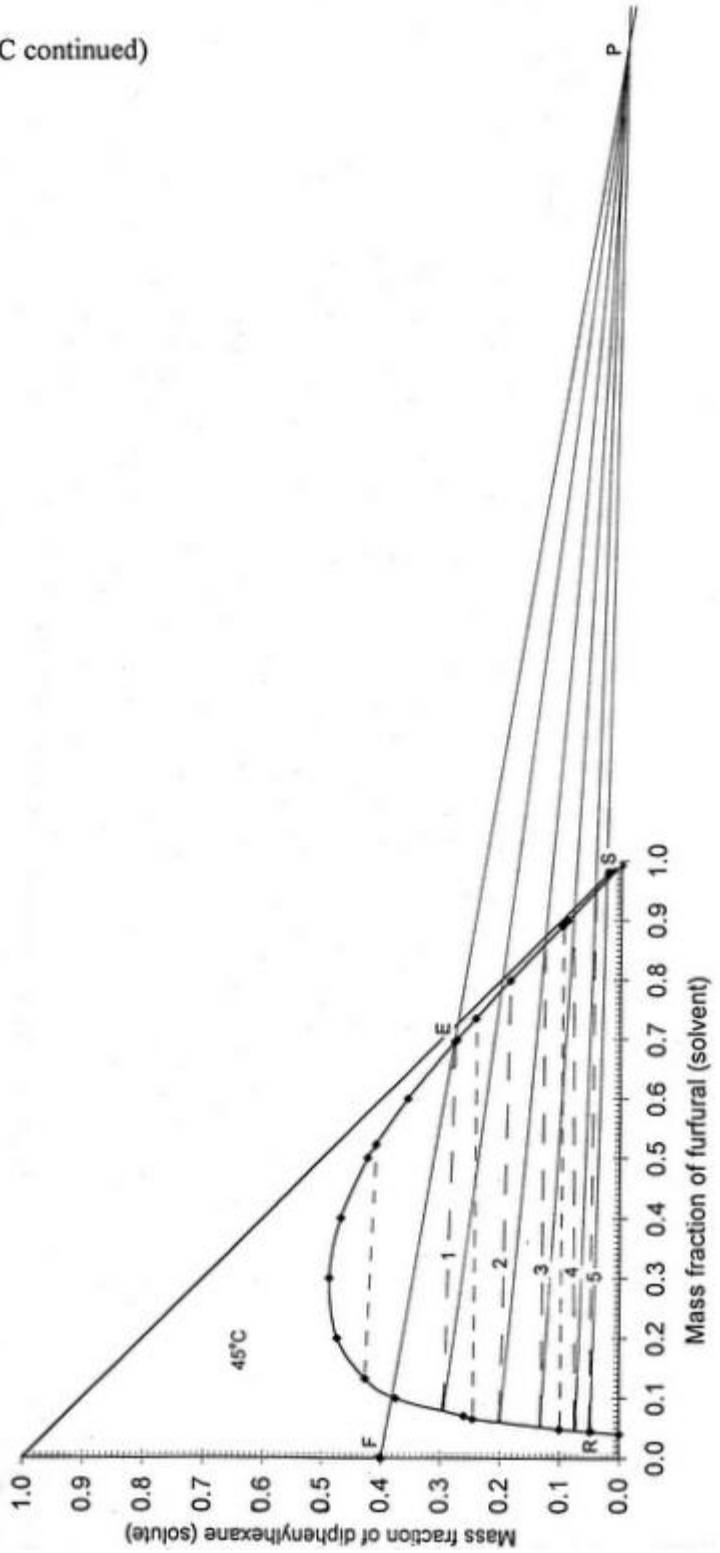
Case of 45°C: The given liquid-liquid equilibrium data are plotted in the right-triangle diagram below. Included on the diagram are composition points F for the feed, R for the raffinate on the equilibrium curve, and S for the solvent. A straight line extends from point F to point S. Because the mass flow rates of the feed and solvent are equal, the mixing point, M, is located at the midpoint of this line. Another straight line extends from point R to point M, and then to an intersection with the equilibrium curve at point E, which is the final extract. Using the inverse lever-arm rule on line RME, the mass ratio of R to E is 0.445. Combining this with an overall material balance: $F + S = 500 + 500 = 1{,}000 = R + E$

gives $R = 308$ kg/h and $E = 692$ kg/h. From the diagram, the mass fraction of DPH in the extract is 0.281. Therefore, the DPH in the extract is 0.281(692) = 194.5 kg/h, which is 92.6% of the total DPH entering the extractor. On the following page, the equilibrium stages are stepped on another right triangle diagram, as in Fig. 8.17, by determining the operating point P from extensions of lines drawn through points F and E, and S and R, followed by alternating between operating lines and equilibrium tie lines. The result is 5 equilibrium stages.



Exercise 8.15 (continued)

Analysis: (case of 45°C continued)

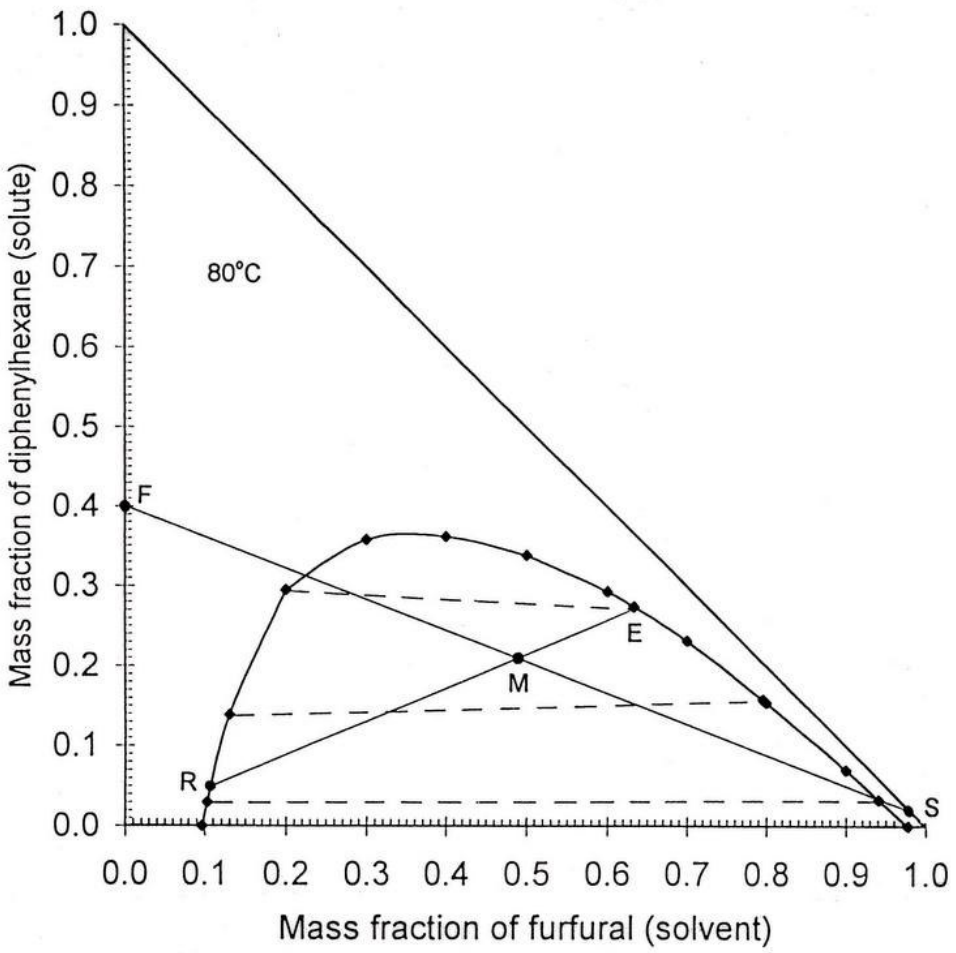


Exercise 8.15 (continued)

Analysis:

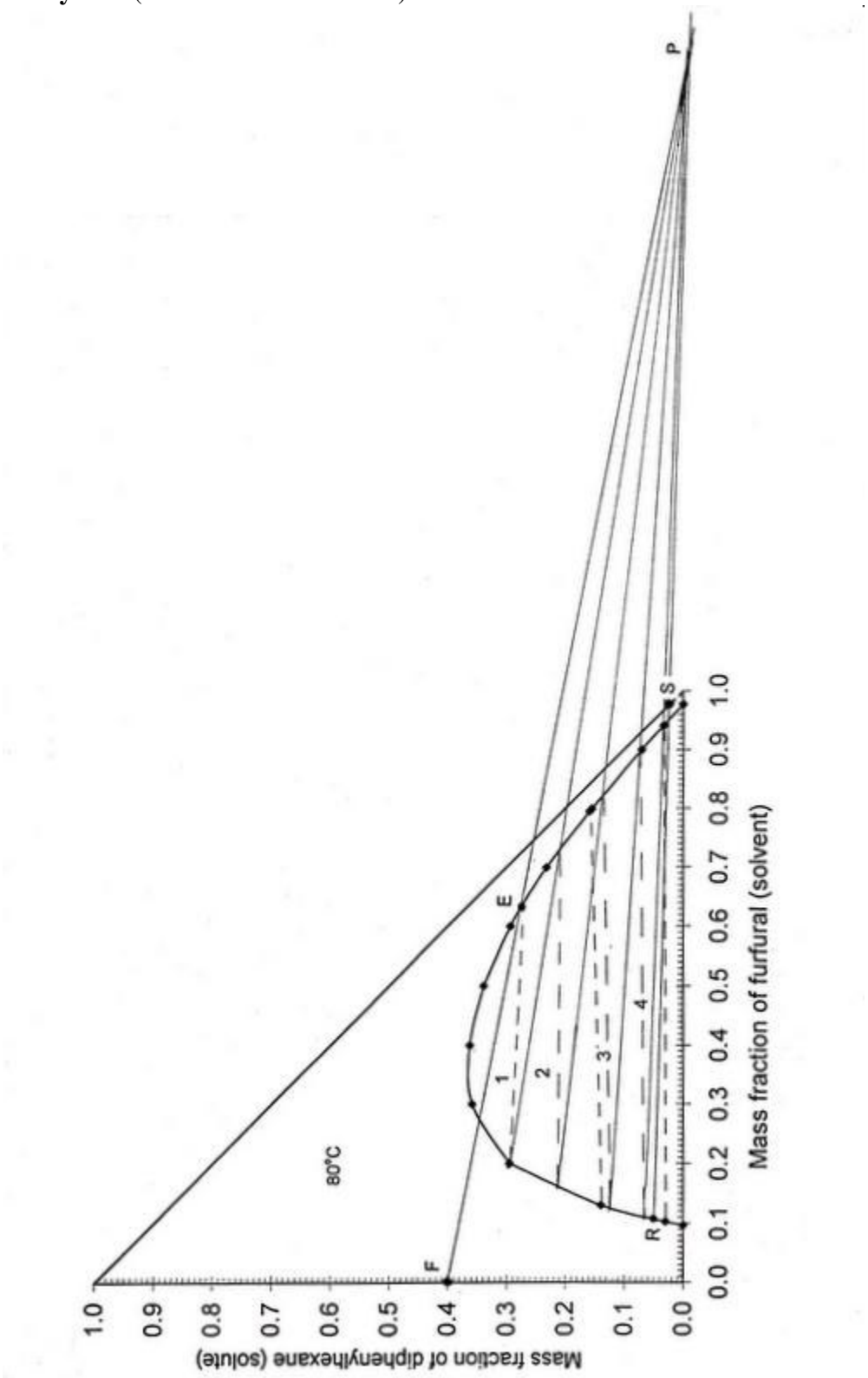
Case of 80°C: The given liquid-liquid equilibrium data are plotted in the right-triangle diagram below. Included on the diagram are composition points F for the feed, R for the raffinate on the equilibrium curve, and S for the solvent. A straight line extends from point F to point S. Because the mass flow rates of the feed and solvent are equal, the mixing point, M, is located at the midpoint of this line. Another straight line extends from point R to point M, and then to an intersection with the equilibrium curve at point E, which is the final extract. Using the inverse lever-arm rule on line RME, the mass ratio of R to E is 0.383. Combining this with an overall material balance: $F + S = 500 + 500 = 1{,}000 = R + E$

gives $R = 277$ kg/h and $E = 723$ kg/h. From the diagram, the mass fraction of DPH in the extract is 0.271. Therefore, the DPH in the extract is 0.271(723) = 195.9 kg/h, which is 93.3% of the total DPH entering the extractor. On the following page, the equilibrium stages are stepped on another right triangle diagram, as in Fig. 8.17, by determining the operating point P from extensions of lines drawn through points F and E, and S and R, followed by alternating between operating lines and equilibrium tie lines. The result is 4+ equilibrium stages.



Exercise 8.15 (continued)

Analysis: (case of 80°C continued)



Exercise 8.16

Subject: Selection of extraction method.

Given: Four ternary systems in Fig. 8.43. Diagrams 1, 2, 4 are Type I. Diagram 3 is Type II.

Find: Method for most economical process for each system. Methods are:
(a) Countercurrent extraction (CE).
(b) CE with extract reflux (ER).
(c) CE with raffinate reflux (RR).
(d) CE with ER and RR.

Analysis: Note that y_1 is the composition of the extract.
Raffinate reflux (RR) is of little value, so don't use it.

For Type I diagrams, extract reflux is rarely useful.

All three Type I diagrams exhibit solutropy, making it almost impossible to obtain a good separation.

The Type II diagram uses a poor solvent, making the use of extract reflux questionable.

Summary: Use CE for all four systems. However, better solvents should be sought for all four systems.

Exercise 8.17

Subject: Stage requirements for extraction of acetone (A) from two feeds, of different composition of acetone (A) and water (C), with a solvent of 1,1,2 - trichloroethane (S).

Given: Feed F of 7,500 kg/h containing 50 wt% A in C. Second feed F' of 7,500 kg/h containing 25 wt% A in C. Solvent of 5,000 kg/h of S. Raffinate to contain 10 wt% A. Liquid-liquid equilibrium data from Exercise 8.11.

Find: Number of equilibrium stages and feed locations, using a right-triangle diagram.

Analysis: Because the flow rates and compositions of both feeds and the solvent are given, the mixing point, M, can be computed, with the following results:

	kg/h:			
Component	**Feed, F**	**Feed, F'**	**Solvent, S**	**Mixing point, M**
Acetone	3,750	1,875	0	5,625
Water	3,750	5,625	0	9,375
Trichloroethane	0	0	5,000	5,000
Total:	7,500	7,500	5,000	20,000

Thus, the composition of the mixing point is 28.125 wt% A, 46.875 wt% C, and 25.0 wt% S. This is shown below on the right-triangle equilibrium diagram. Also shown is the composition of the raffinate, R, on the equilibrium curve and corresponding to 10 wt% A. A straight line extending from R, through M, to its intersection with the equilibrium curve, establishes the extract composition at point E, as shown in the diagram below.
The compositions of the raffinate and extract are thus determined from the diagram to be:

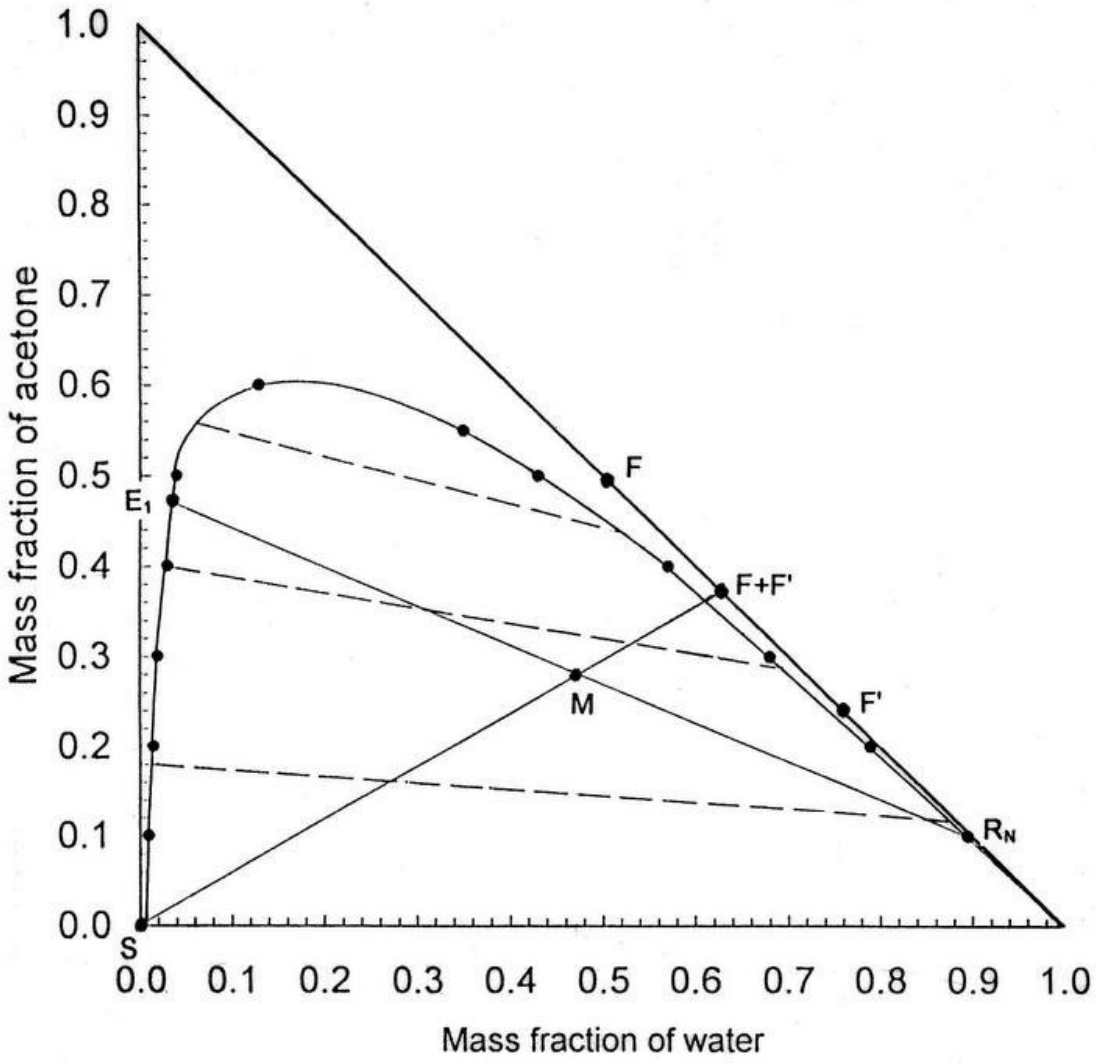
Composition	**Raffinate, wt%**	**Extract, wt%**
Acetone	10.0	46.5
Water	89.5	3.7
Trichloroethane	0.5	49.8
Total:	100.0	100.0

By component material balances or the inverse lever-arm rule, using the mixing point, the raffinate rate is 10,060 kg/h, the extract rate is 9,940 kg/h.

Because the two feeds differ in composition, they should not be mixed before entering the cascade, but should enter separately at different stages. Note that feed F' has a composition closer to the final raffinate, leaving from stage *N*, than feed F. Therefore, feed F' should be fed to an intermediate stage, *m*, and feed F should be fed to stage 1, from which the final extract leaves. Feed F' should enter at that stage, *m*, where it matches most closely the intermediate raffinate entering stage *m*. In the diagram on the next page, two operating points are shown, P_1 and P_2.

Exercise 8.17 (continued)

Analysis: (continued)



Point P_1 is used to step off stages from *m* to *N*, based on a material balance for the entire cascade, because both F and F' move in the direction toward the final raffinate. Thus, the material balance is: $F + F' + S = E_1 + R_N = M$

Rearranging for passing streams, $F + F' - E_1 = R_N - S = P_1$ (1)

Straight lines drawn through $(F + F_1)$ and E_1, and through R_N and S, intersect at the operating point P_1.

For stages 1 through *m*-1, the material balance is: $F + E_m = R_{m-1} + E_1$

Rearranging for passing streams, $F - E_1 = R_{m-1} - E_m = P_2$ (2)

Substituting Eq. (2) into Eq. (1), $P_2 + F' = R_N - S = P_1$ (3)

Exercise 8.17 (continued)

Analysis: (continued)

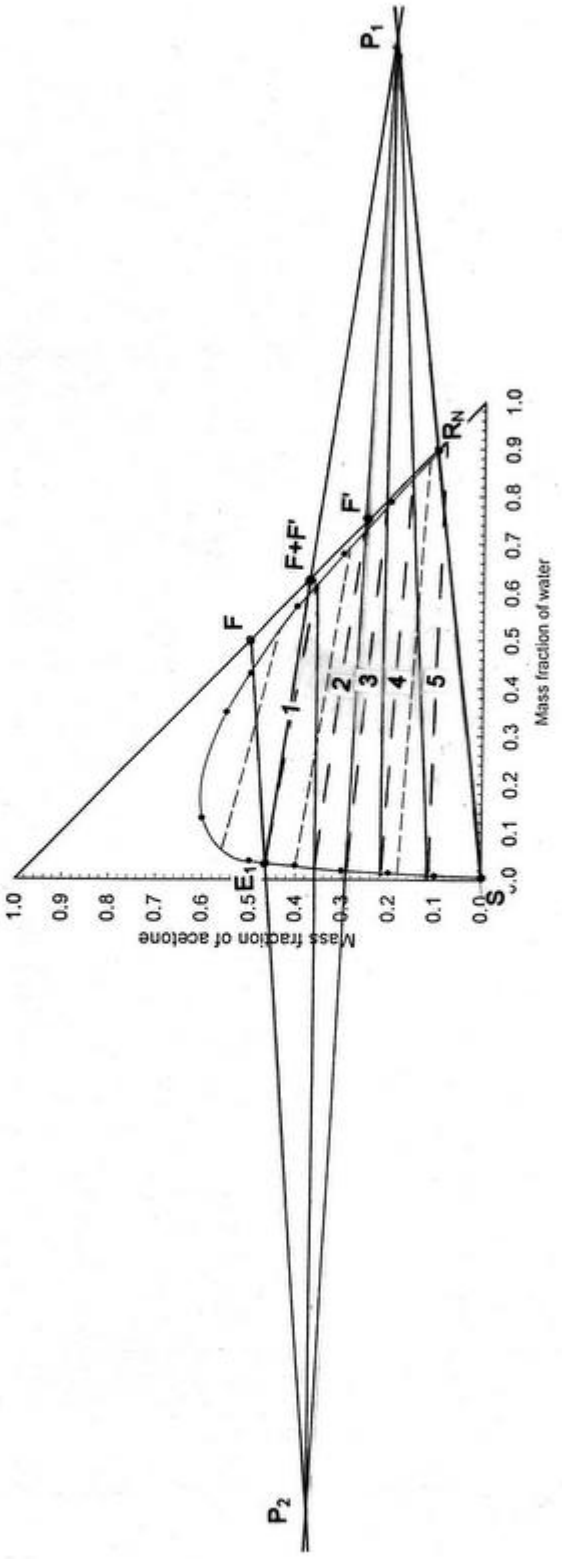
Therefore, operating point P_2 is obtained by the intersection of straight lines drawn through F and E_1, and through P_1 and F'.

The constructions to obtain P_1 and P_2 are shown on the next page. Note that for this system, P_1 and P_2 are on opposite sides of the triangular diagram.

The equilibrium stages are stepped off starting with P_2 from stage 1 at the end where the final extract, E_1, is produced. By a tie line, E_1 is in equilibrium with R_1. An operating line connecting R_1 with P_2 gives E_2. The stepping off, using P_2, is continued until R_2 is reached, which is very close to the composition of F'. Therefore, F' is fed to stage 2. The remaining stages are stepped off using P_1 until final raffinate R_N is reached. The total number of stages is almost 5.
Thus, feed F is fed to stage 1 and feed F' is fed to stage 2 of a cascade with almost 5 stages.

Exercise 8.17 (continued)

Analysis: (continued)



Exercise 8.18

Subject: Extraction of trimethylamine (T) from benzene (B) with water (W) in a three-equilibrium stage liquid-liquid extractor shown in Fig. 8.44.

Given: Feed of 10,000 kg/h of 40 wt% B and 60 wt% T. Fresh solvent is sent to each of the stages. The solvent flow rate to stage 3, call it S_3, is 5,185 kg/h. In Fig. 8.44, V_1 is to contain 76 wt% T on a solvent-free basis, and L_3 is to contain 3 wt% T on a solvent-free basis. Equilibrium data are given in Exercise 8.14.

Find: Using an equilateral-triangle diagram, determine the solvent flow rates to stages 1 and 2.

Analysis: The triangular diagram is shown on a following page. Since the extract, V_1, is given on a solvent-free basis, its complete composition is obtained by the intersection with the equilibrium curve of a line drawn from the point (76 wt% T and 24 wt% B) to the 100% W point. Similarly, the composition of the raffinate, L_3, is obtained by the intersection with the equilibrium curve of a line drawn from the point (3 wt% T and 97 wt% B) to the 100% W point. The resulting compositions of the final raffinate, L_3, and the final extract, V_1, are as follows:

Component	Raffinate, L_3, wt%	Extract, V_1, wt%
T	3.0	39.5
B	97.0	12.5
W	0.0	48.0
Total	100.0	100.0

Using these compositions, determine the flow rates of final raffinate and final extract by solving material balances for T and B:

T balance: $0.03\ L_3 + 0.395\ V_1 = 6{,}000$

B balance: $0.97\ L_3 + 0.125\ V_1 = 4{,}000$

Solving, $L_3 = 2{,}188$ kg/h and $V_1 = 15{,}020$ kg/h

By an overall total material balance, the total solvent water rate is:

$$S_3 + S_1 + S_2 = L_3 + V_1 - F = 2{,}188 + 15{,}020 - 10{,}000 = 7{,}208 \text{ kg/h}$$

where S_3 = Solvent in Fig. 8.44, which enters from the right into stage 3.

Because S_3 is given as 5,185 kg/h, $S_1 + S_2 = 7{,}208 - 5{,}185 = 2{,}023$ kg/h

From the above results, the overall mass balance is as follows in flow rates in kg/h:

Component	Feed	Solvent, S_3	L_3	V_1	$S_1 + S_2$
T	6,000	0	66	5,934	0
B	4,000	0	2,122	1,878	0
W	0	5,185	0	7,208	2,023
Total	10,000	5,185	2,188	15,020	2,023

Exercise 8.18 (continued)

Analysis: (continued)

The next step is to determine the separate values for S_1 and S_2. Because fresh solvent enters all three stages, instead of one operating point, P, there will be three operating points, designated here as P_1, P_2, and P_3. Referring to Fig. 8.44, let the operating point to the right of stage 3 be P_3. Therefore, from (8-5),

$$P_3 = S_3 - L_3 = 5{,}185 - 2{,}188 = 2{,}997 \text{ kg/h}$$

This operating point is located along a line from L_3 through solvent, S_3 to the right of the triangular diagram, as shown on the next page. This operating point is also common to the passing streams, V_3 and L_2 to the left of Stage 3 in Fig. 8.44. That is, $P_3 = V_3 - L_2 = 2{,}997$ kg/h. Using the following compositions from Fig. 8.44 and material balances, the following values are obtained for V_3 and L_2:

Component	Wt % in V_3	Flow in V_3, kg/h	Wt% in L_2	Flow in L_2, kg/h
T	4.05	219	11.75	285
B	0.35	19	88.22	2,141
W	95.60	5,186	0.03	1
Total	100.00	5,424	100.00	2,427

The location of P_3 is obtained by measurement, using a ratio, similar to (8-6),

$$\frac{\overline{L_3P_3}}{\overline{SP_3}} = \frac{L_3+P_3}{L_3} = \frac{S_3}{L_3} = \frac{5{,}185}{2{,}188} = 2.37 \text{ or } \frac{\overline{L_3S}}{\overline{L_3P_3}} = \frac{2.37-1.00}{2.37} = 0.578$$

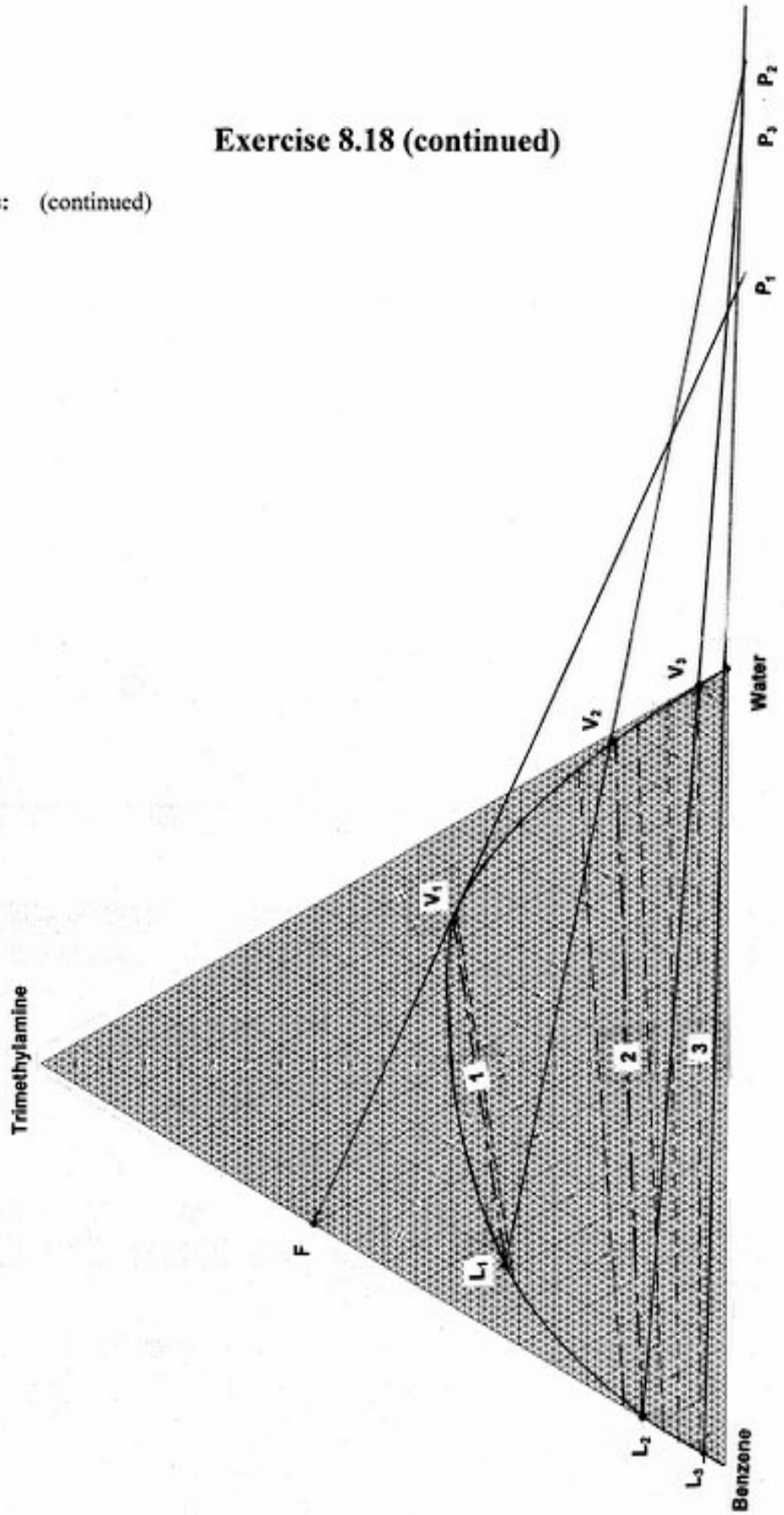
Using this ratio, with the measured length of $\overline{L_3S}$, the point P_3 is located as shown on the triangular plot below. In Fig. 8.44, the point V_3 is in equilibrium with L_3 and, therefore, is located at the end of a tie line drawn from L_3. V_3 operates with L_2, where L_2 is the intersection on the equilibrium curve of an extended line through V_3 and, again, P_3.
From the triangular diagram, the composition of V_2 is obtained from a tie line with L_2, and the composition of L_1 is obtained from a tie line with V_1. The results are as follows, including the results of material balances around stage 1, with flows in kg/h

Component	L_1, wt%	Flow in L_1, kg/h	V_2, wt%	Flow in V_2, kg/h	Flow in S_1, kg/h
T	32	1,199	16.7	1,133	0
B	59	2,210	1.3	88	0
W	9	337	82.0	5,562	1,983
Total	100	3,746	100.0	6,783	1,983

Since $S_1 = 1{,}983$ kg/h and, from above, $S_1 + S_2 = 2{,}023$, $S_2 = 2{,}023 - 1{,}983 = 40$ kg/h.

Exercise 8.18 (continued)

Analysis: (continued)



Exercise 8.19

Subject: Analysis of a multiple-feed countercurrent extraction cascade shown in Fig. 8.45.

Given: Feed F' contains solvent and solute. Feed F'' contains unextracted raffinate and solute.

Find: Equations to establish the three reference (operating) points on a right-triangle graph.

Analysis: Referring to Fig. 8.45, let:

P' be the operating point from the left side of stage 1 to between stages m-1 and m.

P'' be the operating point from between stages m and m+1 to between stages p-1 and p.

P''' be the operating point from between stages p and p+1 to the right side of stage n.

The equations for locating these three operating points are obtained by combining total material balance equations as follows, using the nomenclature of Fig. 8.45:

Overall material balance: Mixing point $= M = L_0 + F' + F'' + V_{n+1} = V_1 + L_n$ (1)

Material balance around stage m: $F' + V_{m+1} + L_{m-1} = V_m + L_m$ (2)

Material balance around stage p: $F'' + V_{p+1} + L_{p-1} = V_p + L_p$ (3)

Operating point P': $P' = V_1 - L_0 = \ldots\ldots = V_m - L_{m-1}$ (4)

Operating point P'': $P'' = V_{m+1} - L_m = \ldots\ldots = V_p - L_{p-1}$ (5)

Operating point P''': $P''' = V_{p+1} - L_p = \ldots\ldots = V_{n+1} - L_n$ (6)

From Eqs. (1) and (4): $V_1 - L_0 = M - (L_0 + L_n) = M - J = P'$ (7)

where $J = (L_0 + L_n)$

Locate J by the inverse lever arm rule, $\dfrac{\overline{JL_n}}{\overline{JL_0}} = \dfrac{L_0}{L_n}$ (8)

Then operating point P' is the intersection of lines through V_1 and L_0, and through M and J

Operating point P'' is obtained by combining Eqs. (2) and (5) to give:

$$P'' = V_{m+1} - L_m = V_m - L_{m-1} - F' = P' - F' \quad (9)$$

Operating point P''' is obtained by combining Eqs. (3) and (6) to give:

$$P''' = V_p - L_{p-1} - F'' = P'' - F'' = P' - (F' + F'') = P' - K \quad (10)$$

where $K = (F' + F'')$

Locate K by the inverse lever arm rule, $\dfrac{\overline{KF'}}{\overline{KF''}} = \dfrac{F''}{F'}$ (11)

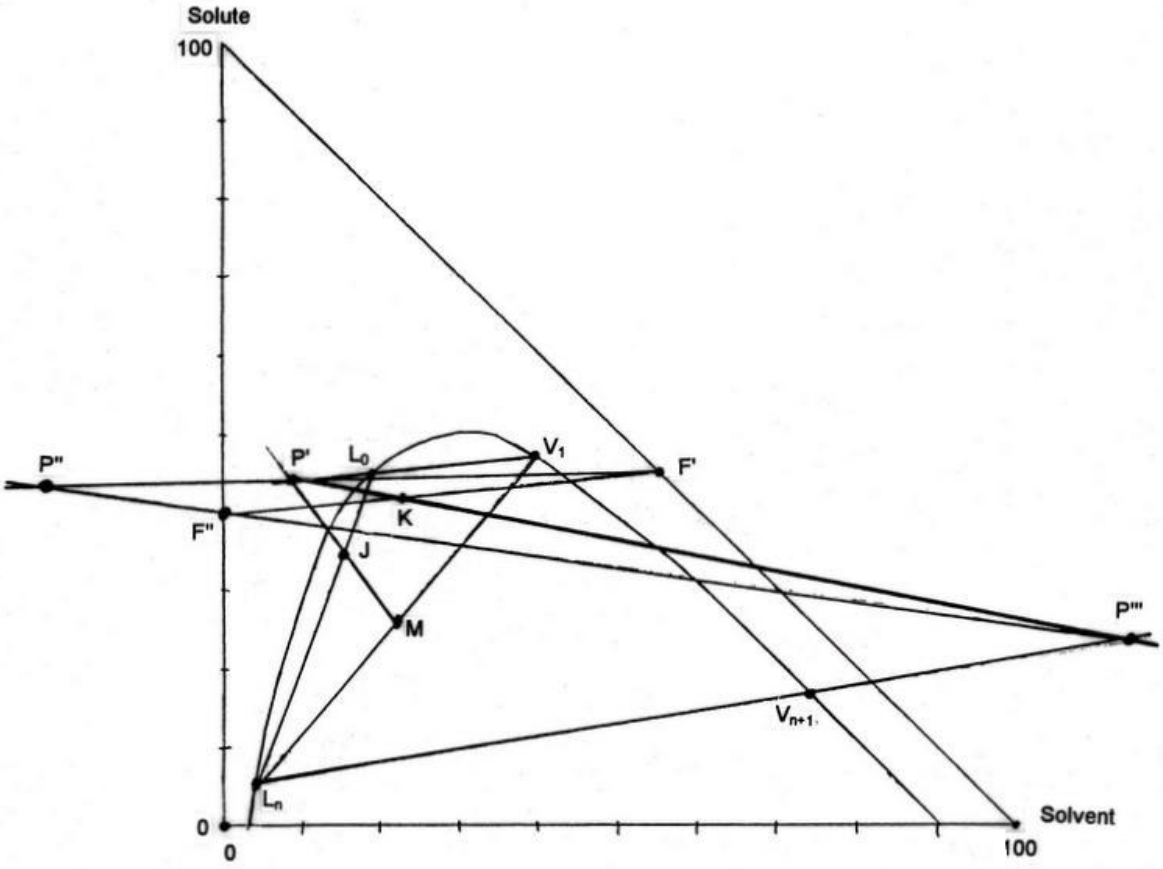
Then operating point P''' is the intersection of lines through V_{n+1} and L_n, and through P' and K

Operating point P''' is the intersection of lines through P' and F', and through P''' and F''

These constructions are illustrated in the right-triangle diagram on the next page.

Exercise 8.19 (continued)

Analysis: (continued)



Exercise 8.20

Subject: Extraction of methylcyclohexane (MCH) from n-heptane (C) with aniline (S) at 25°C in a countercurrent-stage extractor.

Given: Feed of 50 wt% MCH in C. On a solvent-free basis, extract contains 95 wt% MCH and raffinate contains 5 wt% MCH. Reflux at both ends as in Fig. 8.26a. Minimum extract reflux ratio = 3.49. Equilibrium data in Exercise 8.22.

Find: With a right-triangle diagram:

(a) Raffinate reflux ratio.

(b) Amount of aniline that must be removed by solvent removal at the top of the extractor, as shown in Fig. 8.26a.

(c) Amount of solvent that must be added to the mixer at the bottom of the extractor, as shown in Fig. 8.26a.

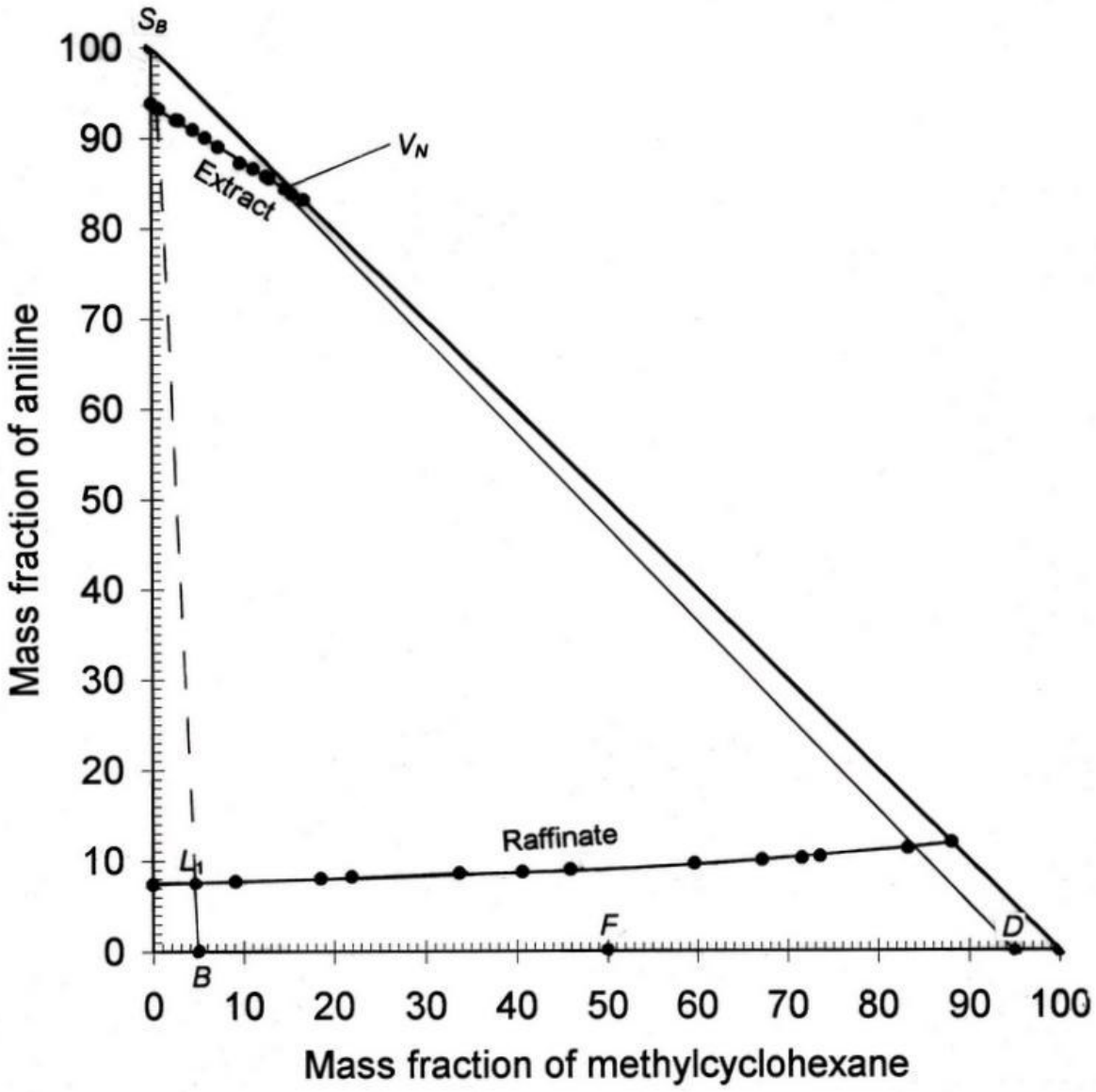
Analysis: The liquid-liquid phase equilibrium data are given, for each phase, as mass % MCH on an aniline-free basis, and mass of aniline per mass of aniline-free mixture. To plot the data on a triangular diagram, it is necessary to convert the equilibrium data to mass % for each of the three components. For example, when the HC-rich layer contains 9.9 wt% MCH on an aniline-free basis and 0.0836 lb aniline per lb aniline-free mixture, we have for 1 lb of aniline-free mixture:
0.099 lb MCH, 0.901 lb n-heptane, and 0.0836 lb aniline, for a total of 1.0836 lb. The corresponding mass % values are: MCH 9.14 wt%, n-heptane 83.15 wt%, and aniline 7.71 wt%. Calculations for the other equilibrium compositions given in the table accompanying Exercise 8.22 are summarized in the following table:

Hydrocarbon-rich layer:				Aniline-rich layer:		
Wt% MCH	Wt% nC_7	Wt% Aniline		Wt% MCH	Wt% nC_7	Wt% Aniline
0.00	92.60	7.40		0.00	6.20	93.80
9.14	83.15	7.71		0.80	5.99	93.21
18.58	73.41	8.01		2.70	5.30	92.00
21.94	69.85	8.21		3.00	5.11	91.89
33.73	57.68	8.59		4.61	4.50	90.89
40.63	50.68	8.69		6.00	4.00	90.00
45.96	45.05	8.99		7.40	3.60	89.00
59.66	30.74	9.60		9.80	2.98	87.22
67.14	22.86	10.00		11.32	2.11	86.57
71.58	18.23	10.19		12.69	1.60	85.71
73.57	16.04	10.39		13.10	1.39	85.51
83.30	5.41	11.29		15.59	0.62	83.79
88.11	0.00	11.89		16.89	0.00	83.11

The triangular liquid-liquid equilibrium diagram is given on the next page. Referring to Fig. 8.26a, compositions of feed, *F*, solvent-free extract, *D*, and solvent-free raffinate, *B*, are plotted.

Exercise 8.20 (continued)

Analysis: (continued)



Exercise 8.20 (continued)

Analysis: (continued)

By construction on the triangular diagram on the previous page, the compositions of the solvent-containing extract, V_N , and the solvent-containing raffinate, L_1 , are determined as intersections of straight lines (drawn from the solvent-free points toward the 100% solvent point, S_B) with the equilibrium curve. The wt% compositions of these points are read from the diagram to be:

	Wt%:	
Component	Extract, V_N	Raffinate, L_1
Aniline, S	84.0	7.5
n-Heptane, C	1.0	88.0
Methylcyclohexane, MCH	15.0	4.5
Total:	100.0	100.0

Take a basis of 1,000 kg/h of feed and make material balances for the minimum extract reflux condition. Because the feed is 50 wt% MCH and 50 wt% C, and the two solvent-free product compositions are symmetrical with respect to MCH and C, the solvent-free material balance is quickly determined to be:

	kg/h:		
Component	Feed, F	Extract, D	Raffinate, B
n-Heptane, C	500	25	475
Methylcyclohexane, MCH	500	475	25
Total:	1,000	500	500

(b) Assume the given minimum extract reflux ratio = 3.49 = L_R/D in Fig. 8.36a.
Then, L_R = 3.49(500) = 1,745 kg/h. Therefore, the flow rate of solvent-free extract in stream V_N = 1,745 + 500 = 2,245 kg/h. But, from above, this stream contains 84 wt% aniline solvent. Therefore, the flow rate of aniline in stream V_N = (84/16)(2,245) = 11,790 kg/h. This is the flow rate of aniline that must be removed by the separator at the top of the cascade.

(c) From above, the raffinate L_1 leaving at the bottom of the cascade is 7.5 wt% aniline. Therefore, aniline flow rate in B is (7.5/92.5)(500) = 40 kg/h and B = 540 kg/h
The entering solvent rate S_B is, therefore, 40 + 11,790 = 11,830 kg/h. This is the amount of fresh solvent that must be added to the mixer at the bottom of the column.

(a) Referring to Fig. 8.36a, define the raffinate reflux ratio as (L_1 - B)/B. Because the cascade is operating at minimum reflux, assume infinite stages so that V_B is in equilibrium with L_1. From the triangular diagram on the previous page, the composition of V_B is obtained by the dashed tie line from L_1, which gives 93.5 wt% aniline. A total material balance around the bottom Mixer gives:
$S_B - B$ = 11,830 - 540 = 11, 290 = $V_B - L_1$. An aniline balance around the bottom Mixer gives:
11,830 - 40 = 0.935V_B - 0.075L_1 . Solving these two equations gives L_1 = 1,435 kg/h.
Therefore, the raffinate reflux ratio = (1,435 - 540)/540 = 1.66.

Exercise 8.21

Subject: Liquid-liquid extraction of hafnium from zirconium in an aqueous nitric acid solution, using tributyl phosphate (TBP) as the solvent

Given: A flowsheet in Fig. 8.46 for a process comprised of 14 equilibrium stages and a solvent stripping unit. Feed consisting of 1.0 L/h of 5.10 N HNO_3, containing 127 g of dissolved Hf and Zr oxides per liter, including 22,000 ppm by wt. Hf, enters Stage 5. Stages 5 to 14 constitute an extraction section. TBP enters Stage 14. Scrubbing water enters Stage 1, with Stages 1 to 4 constituting a scrubbing section. Aqueous raffinate is removed from Stage 14. Organic-rich extract leaving Stage 1 enters the Stripping Unit, which recovers the TBP for recycle by stripping with fresh water. The aqueous product from stripping leaves the process. Stagewise data for the distribution of both Hf and Zr between TBP (containing nitric acid) and aqueous nitric acid.

Assumptions: The 22,000 ppm of Hf refers to a basis of Hf plus Zr, not to the total feed.

Find: (a) A material balance.
(b) A check on consistency of the given data.
(c) Advantages of the process. Need for all stages.

Analysis:

(a) and (b) The molecular weights of the components involved are:

Component	Molecular weight
Hf	178.6
Zr	91.22
HfO_2	210.60
ZrO_2	123.22
HNO_3	63.01

From the CRC Handbook, the density of aqueous 5.1 N HNO_3 = 1.166 g/cm^3
Neglect the effect of dissolved oxides on this density.
1.0 L/h = 1,000 cm^3/L. Therefore, in the feed have 1,166 g/h of combined HNO_3 and H_2O.
For 5.1 N HNO_3 = 5.1 mol/L of HNO_3, have 5.1(63.01) = 321.4 g/h HNO_3 in the feed.
Therefore, the H_2O in the feed = 1,166 - 321.4 = 844.6 g/h.
Since the feed includes 127 g/h of combined Hf and Zr oxides, the total feed flow rate = 1,166 + 127 = 1,293 g/h. Since the feed contains 22,000 parts of Hf per 1,000,000 parts of Zr, we have: (22,000/1,000,000 = 0.022 g Hf/g Zr. This corresponds to 0.022(210.6/178.6)/(123.22/91.22) = 0.0192 g HfO_2/g ZrO_2. Thus, of the 127 g/h of oxides, we have 127(0.0192/1.0192) = 2.39 g/h of HfO_2 and 127 - 2.39 = 124.61 g/h of ZrO_2. In summary, the feed contains:

Component	g/h	g/L	mol/L
HfO_2	2.39	2.39	0.0194
ZrO_2	124.61	124.61	0.5917
HNO_3	321.4	321.4	5.1
H_2O	884.6	884.6	49.1
Total:	1,293.0	1,293.0	

Exercise 8.21 (continued)

Analysis: (continued)

HfO_2 balance: From the given Stagewise Analyses table, the aqueous phase leaving Stage 14 is the final raffinate and contains 3.54 g total oxides /L and g Hf/g Zr = 0.72. Therefore, g HfO_2/g ZrO_2 = 0.72(210.6/178.6)/(123.22/91.22) = 0.6285. Then, g HfO_2/L = 3.54(0.6285/1.6285) = 1.366 g HfO_2/L and g ZrO_2/L = 3.54 - 1.366 = 2.174.
From the Stagewise Analyses table, it appears that the concentration of Hf in the extract leaving Stage 1 is negligible. Therefore, all of the HfO_2 entering in the feed exits in the raffinate. Therefore, with a feed of , Q_F, of 1 L/h with 2.39 g/L of HfO_2 and a raffinate with 1.366 g/L HfO_2, the volumetric flow rate of raffinate = 1.0(2.39/1.366) = 1.75 L/h = Q_R .
Total oxide balance: All of the oxides in the feed leave in either the raffinate from Stage 14 or the aqueous product (stripped extract, E) from the Stripper. Using the Stagewise Analyses table, a total oxide material balance gives: $127Q_F = 3.54Q_R + 76.4Q_E$,
where Q_F = 1.0 L/h and Q_R = 1.75 L/h.
Therefore, solving, Q_E = [127 - 3.54(1.75)]/76.4 = 1.58 L/h of stripped extract, which contains 76.4 g ZrO_2/L.
Total balance: Assume that the total volume flows in = total volume flows out. Let Q_{ST} = volumetric flow rate of stripping water, and Q_{SC} = volumetric flow rate of scrubbing water. Then a volumetric flow balance gives: $Q_{ST} + Q_{SC} = Q_E + Q_R - Q_F$ = 1.58 + 1.75 - 1.0 = 2.33 L/h.
Nitric acid balance: The Stagewise Analyses data around Stage 1 indicate that the scrubbing water contains HNO_3. Let x = mol/L of HNO_3 in the scrubbing water, but assume no HNO_3 in the stripping water. An overall nitric acid balance gives: $5.1(1) + xQ_{SC} = 2.56Q_R + 3.96Q_E$.
Therefore, xQ_{SC} = [2.56(1.75) + 3.96(1.58) - 5.1] = 5.64 mol/h = HNO_3 entering in scrub water.
Total balance around stripper: $Q_{ST} + Q_1 = Q_E + Q_S = 1.58 + Q_S$ (1)
HNO_3 balance around stripper: Using the Stagewise Analyses table,

$$1.95Q_1 + 0 = 3.96(1.58) + 0.65Q_s = 6.26 + 0.65Q_s \quad (2)$$

Oxide balance around stripper: Using the Stagewise Analyses table,

$$22.2Q_1 = 76.4(1.58) = 120.7 \text{ g/h of } ZrO_2$$

Therefore, solving, Q_1 = 120.7/22.2 = 5.44 L/h. From Eq. (2),

$$Q_S = [1.95(5.44) - 6.26]/0.65 = 6.69 \text{ L/h}$$

From Eq. (1), Q_{ST} = 1.58 + 6.69 - 5.44 = 2.83 L/h
From above, $Q_{ST} + Q_{SC}$ = 2.33. Therefore, this results in an impossible negative Q_{SC} .
The data are inconsistent, at least for the Hf/Zr ratio in the final raffinate. This error has a significant effect on the volumetric flow rate of the raffinate, which then affects other flow rates.

(c) The extractor as shown removes almost all of the ZrO_2 and is, therefore, effective. However, the Hf/Zr ratio in the aqueous phase, as shown in the Stagewise Analyses table, decreases, rather than increases, in Stages 13 and 14. This indicates the need for more nitric acid in the recycle solvent. Also, Stages 1 and 2 appear to do little extraction and might be eliminated.

Exercise 8.22

Subject: Extraction of diphenylhexane (DPH) from docosane (C) with furfural (U) at 45°C in a continuous, countercurrent, multistage liquid-liquid extraction system.

Given: Feed, F, of 5,000 kg/h of 65 wt% DPH, 28 wt% C, and 7 wt% U. Solvent is pure U. Raffinate to contain 12 wt% DPH. Liquid-liquid equilibrium data from Exercise 8.15.

Find: (a) Minimum solvent flow rate.
(b) Flow rate and composition of extract at minimum solvent rate.
(c) Number of equilibrium stages at a solvent rate of 1.5 times the minimum.

Analysis:

The given liquid-liquid equilibrium data at 45°C are plotted in the right-triangle diagram below. Included on the diagram are composition points F for the feed, R_N for the raffinate on the equilibrium curve, and S for the solvent.

(a) To find the minimum solvent flow rate, S_{min} , corresponding to an infinite number of equilibrium stages, A straight line is drawn on the diagram below that joins points R_N and S and extends to either side of the diagram. Similar lines are extended from the tie lines to where they intersect the first line. The construction is similar to Figure 8.18. For this exercise the intersection points are closest to the raffinate side as they are in Figure 8.18. Therefore the intersection farthest away corresponds to $S_{min.}$ and locates the composition of the final extract, E_1. From either the inverse lever-arm rule or a mass balance, the minimum solvent rate = 2,190 kg/h.

b) From the diagram, the composition of the extract is:

2 wt% docosane
28 wt% DPH
70 wt% furfural

The composition of the raffinate is:

83 wt% docosane
12 wt% DPH
5 wt% furfural

The total flow rate of extract + raffinate = feed + min. solvent = 5,000 + 2,190 = 7,190 kg/h
Using the inverse lever-arm rule or mass balances, E_1 = 3,355 kg/h and R_N = 3,835 kg/h

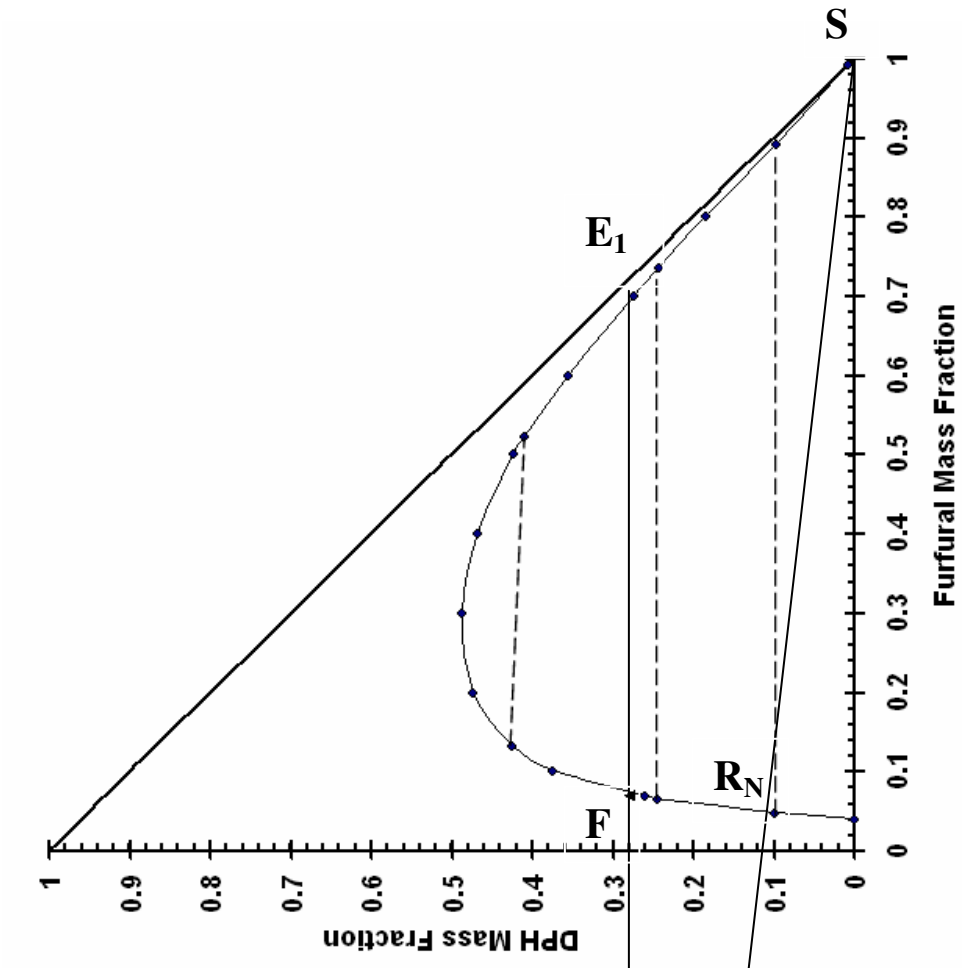
(c) The solvent rate for finite stages = 1.5 S_{min} = 1.5(2,190) = 3,285 kg/h. The mixing point for this rate is at a composition of:

DPH: 0.28(5,000)/(5,000 + 3,285) = 0.169 or 16.9 wt%
Furfural: [0.07(5,000) + 3,285]/(5,000 + 3,285) = 0.439 or 43.9 wt%

The second figure below shows the new extract point for this solvent rate and a mixing point. The operating point, P, is the intersection of the two lines, from through R_N and S; the other through F and E_1. The point is not shown because far to the left off the page. However, using that point and alternating between operating lines and equilibrium tie lines, as in Figure 8.17, only 2 equilibrium stages are required to move from E_1 to R_N .

Exercise 8.22 (continued)

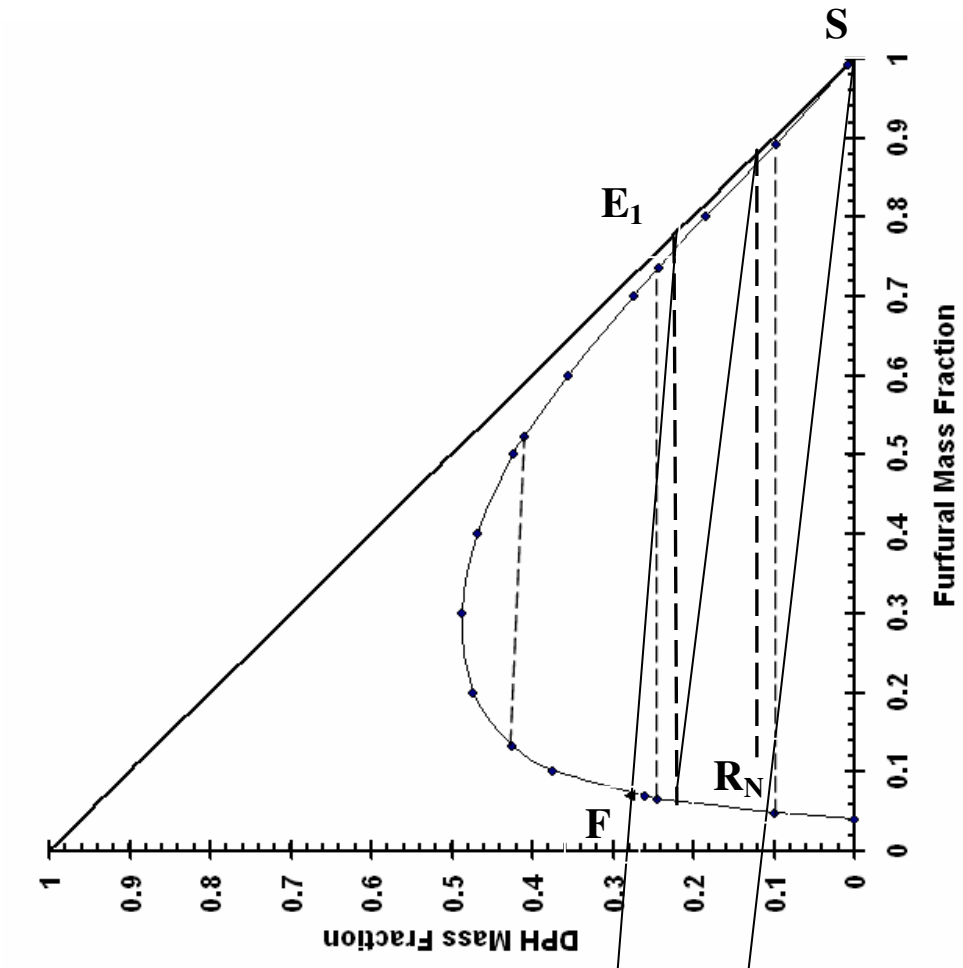
Analysis: (a) and (b)



P_{min} is further down

Exercise 8.22 (continued)

Analysis: (a) and (b)



P is further down

Exercise 8.23

Subject: Extraction of diphenylhexane (DPH) from docosane (C) with furfural (U) at 45°C in a single-stage and a continuous, countercurrent, multistage liquid-liquid extraction system.

Given: Feed, F, of 1,000 kg/h of 20 wt% DPH and 80 wt% docosane. Solvent is pure furfural. . Liquid-liquid equilibrium data from Exercise 8.15.

Find: (a) For a single equilibrium stage, the compositions and flow rates of extract and raffinate for solvent rates of 100, 1,000, and 10,000 kg/h.

(b) Minimum solvent flow rate to form two liquid phases.

(c) Maximum solvent flow rate to form two liquid phases.

(d) For two countercurrent-flow equilibrium stages, the compositions and flow rates of extract and raffinate for a solvent flow rate of 2,000 kg/h.

Analysis:

(a) First, calculate the composition of the mixing point for each solvent flow rate, noting that the feed is 800 kg/h of docosane and 200 kg/h of DPH.

Solvent flow rate, kg/h	100	1,000	10,000
Feed + Solvent, kg/h	1,100	2,000	11,000
Wt% DPH	0.182	0.100	0.0182
Wt% Furfural	0.091	0.500	0.910

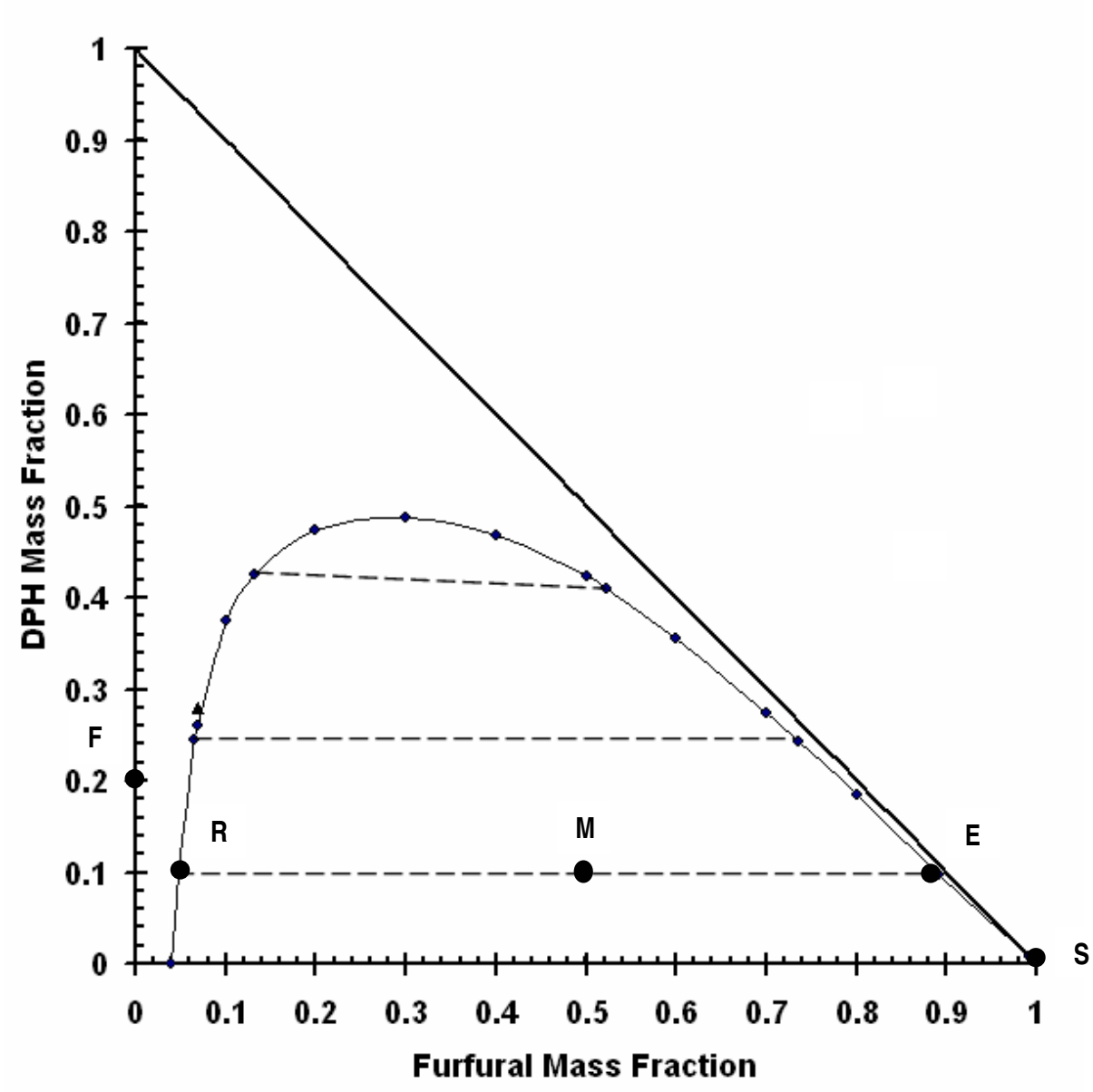
These three mixing points can be plotted on the triangular phase diagram shown below. Then a tie line is drawn through each mixing point. The intersections of the tie lines with the bimodal curve give the following compositions from a single equilibrium stage, in the manner of Figure 4.16, for each of the three cases:

Solvent flow rate, kg/h	100	1,000	10,000
Raffinate composition, wt%:			
DPH	18.2	10.1	2.1
Furfural	5.7	4.9	4.2
Docosane	76.1	85.0	93.7
Extract composition, wt%			
DPH	18.0	9.9	1.9
Furfural	80.5	1.1	98.0
Docosane	1.5	89.0	0.1

Exercise 8.23 (continued)

Analysis: (a) continued:

The following diagram shows the construction for a solvent rate of 1,000 kg/h.



Exercise 8.23 (continued)

Analysis: (a) continued:

Next, mass balances can be used to compute the flow rates of the raffinate and the extract for each of the three cases, as follows.

Case 1. Solvent flow rate = 100 kg/h

DPH mass balance: $0.182\,R + 0.180\,E = 200$

Total mass balance: $R + E = F + S = 1{,}000 + 100 = 1{,}100$

Solving, $R = 1{,}000$ kg/h and $E = 100$ kg/h

Case 2 Solvent flow rate = 1,000 kg/h

DPH mass balance: $0.101\,R + 0.099\,E = 200$

Total mass balance: $R + E = F + S = 1{,}000 + 1{,}000 = 2{,}000$

Solving, $R = 1{,}000$ kg/h and $E = 1{,}000$ kg/h

Case 3. Solvent flow rate = 10,000 kg/h

Docosane mass balance: $0.937\,R + 0.000\,E = 800$

Total mass balance: $R + E = F + S = 1{,}000 + 10{,}000 = 11{,}000$

Solving, $R = 850$ kg/h and $E = 10{,}150$ kg/h

(b) and (c)

The minimum and maximum solvent flow rates for the formation of two liquid phases is obtained from the intersection with the bimodal curve of a straight line between the feed and solvent compositions. The construction is shown on a separate page below. The solvent rates are obtained using the inverse lever-arm rule with that diagram, resulting in the following results:

$S_{min} = 64$ kg/h and $S_{max} = 142{,}000$ kg/h

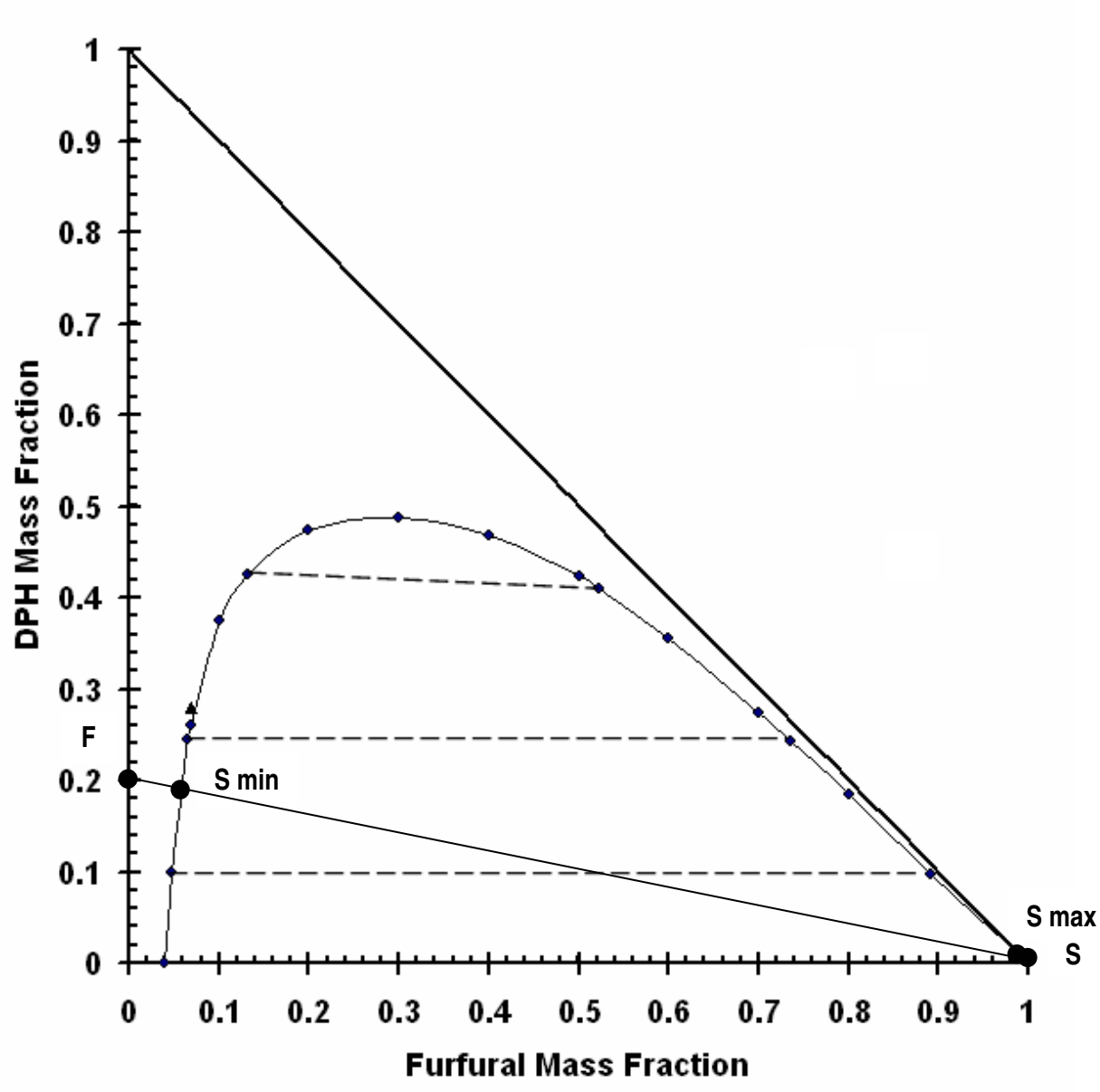
(d) The determination of the raffinate and extract obtained from a two-equilibrium-stage, countercurrent-flow extraction system requires a trial-and-error procedure. One approach is to assume a sequence of equilibrium raffinate compositions and step off the corresponding stages until 2 stages result. A good way to start the start sequence is to solve the single-stage problem in a manner similar to that in Part (a) of this exercise. That construction is shown below and results in a raffinate containing 6.7 wt% DPH. For two stages, the wt% DPH will be less. In this manner, it is found that the raffinate will contain 2.5 wt% DPH for 2 stages. The construction is shown below and the compositions and flow rates of the corresponding raffinate and extract are as follows for the solvent flow rate of 2,000 kg/h:

	Raffinate	Extract
Flow rate, kg/h	855	2,145
DPH, wt %	2.5	8.0
Docosane, wt%	93.3	0.5
Furfural, wt%	4.2	91.5

Exercise 8.23 (continued)

Analysis: (b, c) continued:

The following diagram shows the construction to determine minimum and maximum solvent rates to produce two liquid phases.



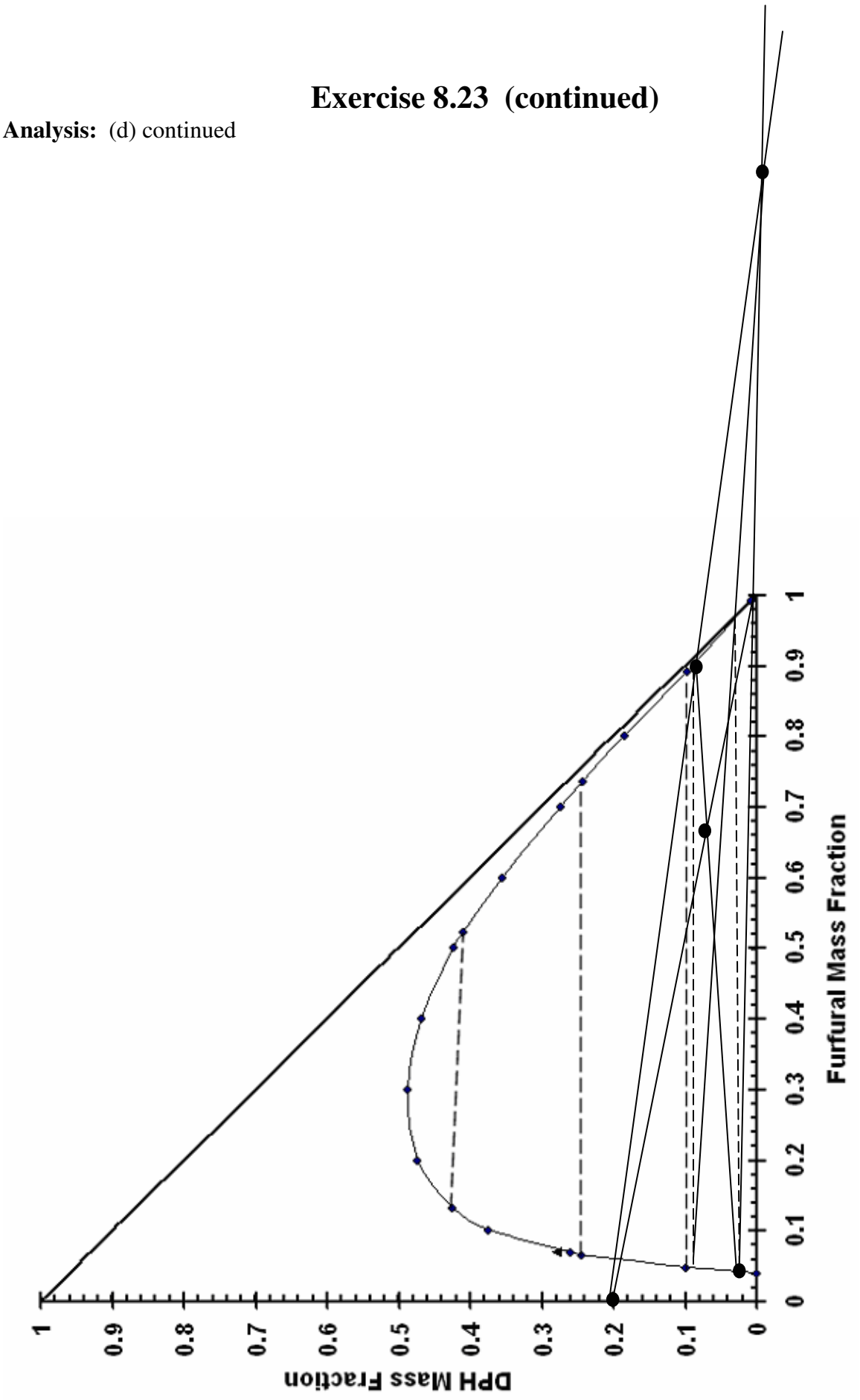
Exercise 8.23 (continued)

Analysis: (d) continued:

The diagram bellows shows construction for an assumed raffinate containing 2.5 wt% DPH and two stages. The mixing point, M, corresponds to 200 kg/h of DPH and 2,000 kg/h of furfural in a total of 3,000 kg/h sent to the extraction unit. This gives 6.7 wt% DPH and 66.7 wt% furfural.

Exercise 8.23 (continued)

Analysis: (d) continued



Exercise 8.24

Subject: Extraction of acetone (A) from water (C) by 1,1,2-trichloroethane (S) at 25°C

Given: Liquid mixture of 27 wt% A and 73 wt% C. Liquid-liquid equilibrium data. Raffinate essentially of acetone

Find:

(a) Minimum solvent-to-feed ratio.
(b) Composition of the extract at the minimum solvent-to-feed ratio.
(c) Composition of the extract stream leaving Stage 2 from the feed end.

Analysis: Using the given equilibrium data in weight fractions, the right-triangle diagram is shown below, where a solid line is used for the equilibrium curve and dashed lines are used for the tie lines, only three of which are given. Additional tie-line locations can be made using either of the two techniques illustrated in Fig. 8.16.

(a) The minimum solvent flow rate corresponds to an infinite number of equilibrium stages. To determine this minimum: (1) Points are plotted on the triangular diagram for the given compositions of the solvent, S (pure S), feed, F (27 wt% A, 73 wt% C), and raffinate, R_N (0 wt% A on the equilibrium curve), followed by drawing an operating line through the points S and R_N and extending it only to the right because the tie lines slope down from left to right; (2) Because the pinch region, where equilibrium stages crowd together, may occur anywhere, additional potential operating lines may be drawn through the tie lines extended to the right until they cross the operating line at the solvent end, drawn in (1) The intersections are not shown in the diagram because they are far off the page. (3) The intersection point farthest from the triangular diagram is the one used to determine the minimum solvent rate. For this exercise, that point is quite sensitive. Assume the controlling line is the one through F, corresponding to a pinch point at the feed end of the cascade; (4) An operating line is drawn from $P_{\min}$ through F to the determine the extract E_1, followed by drawing lines from E_1 to R_N and from S to F, with the intersection of these two lines determining the mixing point, M. The wt% A at the mixing point is approximately 17 wt% From Eq. (8-10),

$$\frac{S_{\min}}{F} = \frac{(x_A)_F - (x_A)_M}{(x_A)_M - (x_A)_S} = \frac{0.27 - 0.17}{0.17 - 0.0} = 0.59$$

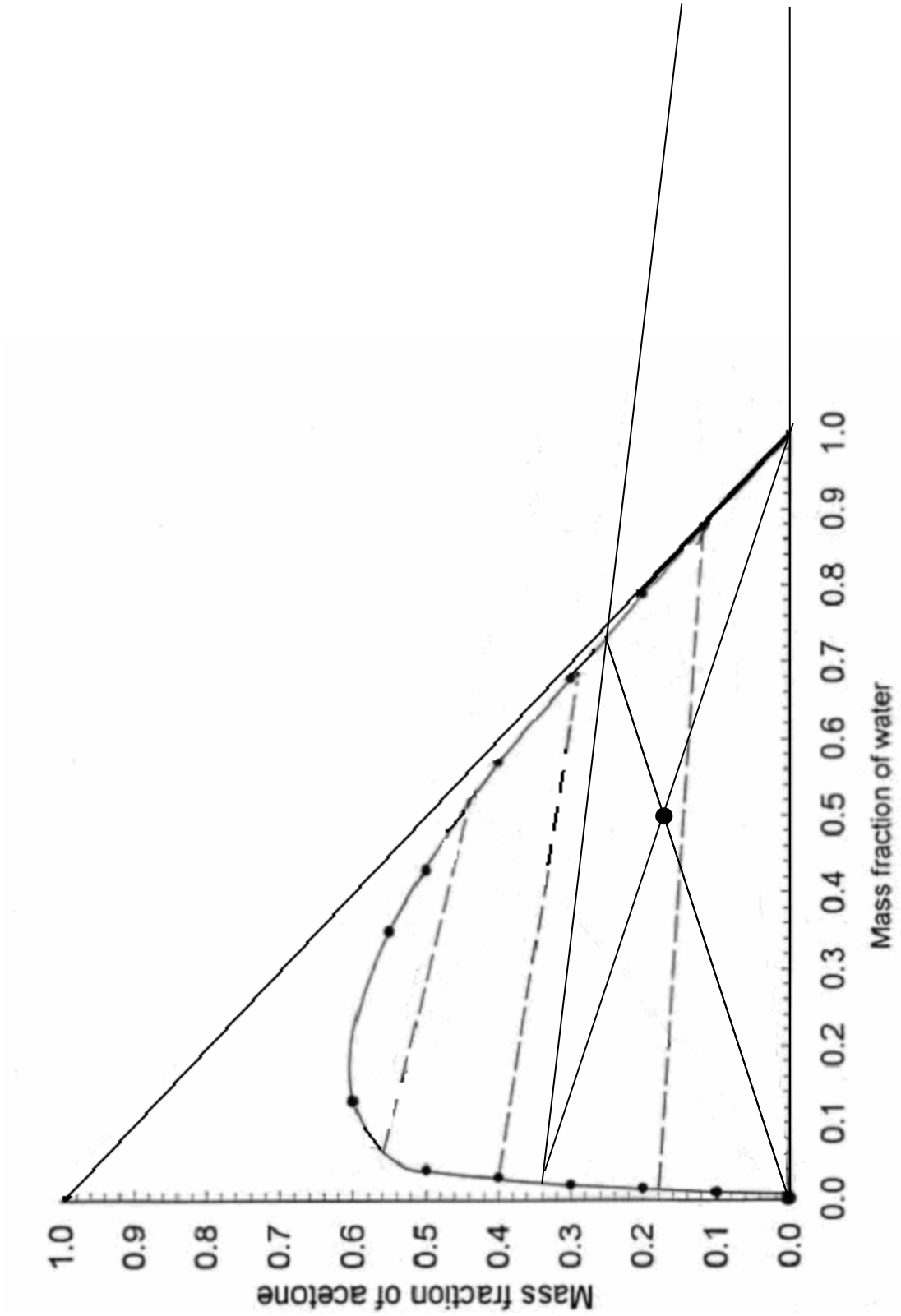
(b) The composition of the extract at the minimum solvent rate is:

34 wt% acetone, 1.5 wt% water, and 64.5 wt% solvent

(c) If the pinch point is at the feed end of the system as assumed above, then the extract leaving Stage 2 is essentially the same composition as the final extract.

Exercise 8.24 (continued)

Analysis: (continued)



Exercise 8.25

Subject: Liquid-liquid extraction of methylcyclohexane (A) from a mixture with n-heptane (C) by aniline (S) as the solvent, using extract reflux.

Given: Feed of 50 wt% C and 50 wt% A. Extract to contain 92.5 wt% A in the extract, and 7.5 wt% A in the raffinate, both on a solvent-free basis. Equilibrium data at 25°C and 1 atm.

Assumptions: Perfect solvent separator.

Find: Using the graphical method of Maloney and Schubert:
(a) Minimum stages.
(b) Minimum extract reflux ratio.
(c) Theoretical stages for an extract reflux ratio = 7.

Analysis: The cascade is like that shown in Fig. 8.26b or 8.32, where extract reflux is used. The Maloney-Schubert method for the use of extract reflux is conducted on a Janecke diagram like that in Figs. 8.31 and 8.33. For the system here, the diagram is shown on the next page, where the composition on the ordinate, Y, is mass of solvent (S) per mass of solvent-free extract (upper curve), and per mass of solvent-free raffinate (lower curve). The abscissa composition, X, is mass of solute (A) per mass of solvent-free extract or raffinate. The dashed lines are the liquid-liquid equilibrium tie lines.

(a) For the minimum number of equilibrium stages, the construction is that is Fig. 8.31a, where all operating lines on the Y - X diagram are vertical lines. As shown on the following page, the number of stages stepped off by alternating between equilibrium tie lines (many of which are added by interpolation) and vertical operating lines starting from the raffinate, L_1, and ending at the extract, V_N , is just less than 10. Call the minimum number of stages 10.

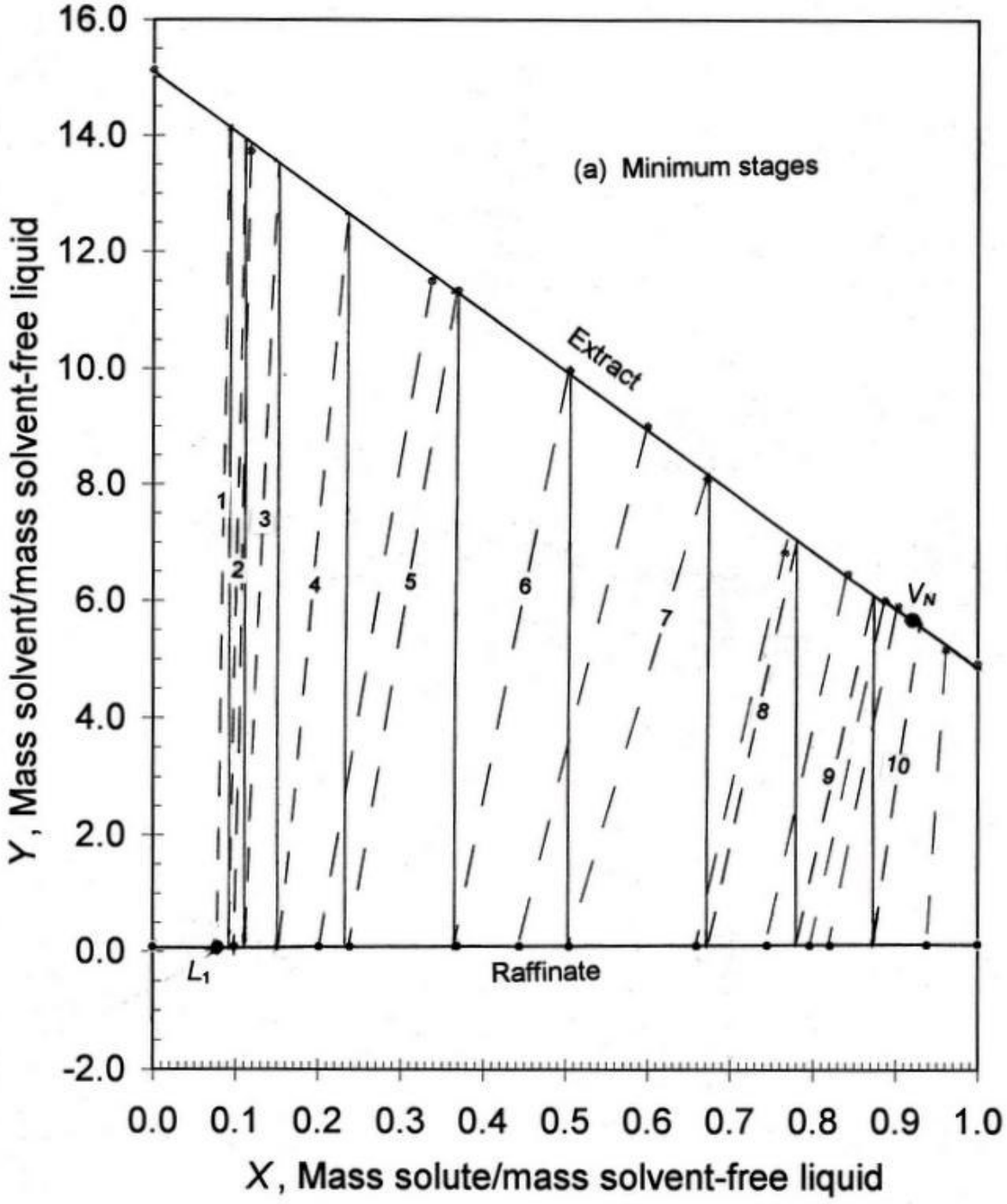
(b) For the minimum extract reflux ratio, the construction is that shown in Figs. 8.31a and b and is given here on the third page of this exercise. A tie line through the feed point, F, establishes the point P' on a vertical line through $X = 0.975$, which is the solvent-free composition of the solute in the extract. No other line drawn through a tie line to the right of the feed tie line or drawn from P'' points (established by tie lines to the right of the feed tie line) through the feed point, intersects the vertical line through $X = 0.975$ at a higher P' point. Therefore, as shown, $P'_{min} = 20.5$. Using Eq. (8-18) with measurements from the diagram,

the minimum reflux ratio = line $P'V_N$ / line V_NL_R = L_R/D = 2.5

(c) With an extract reflux ratio, $L_R/D = 7$ and line $V_NL_R = 5.0$, $P' = 5(7) + 5 = 40$. The construction follows that in Fig. 8.33, as given on the fourth page of this exercise, where 16 stages are stepped off with the feed stage at 11 from the raffinate end.

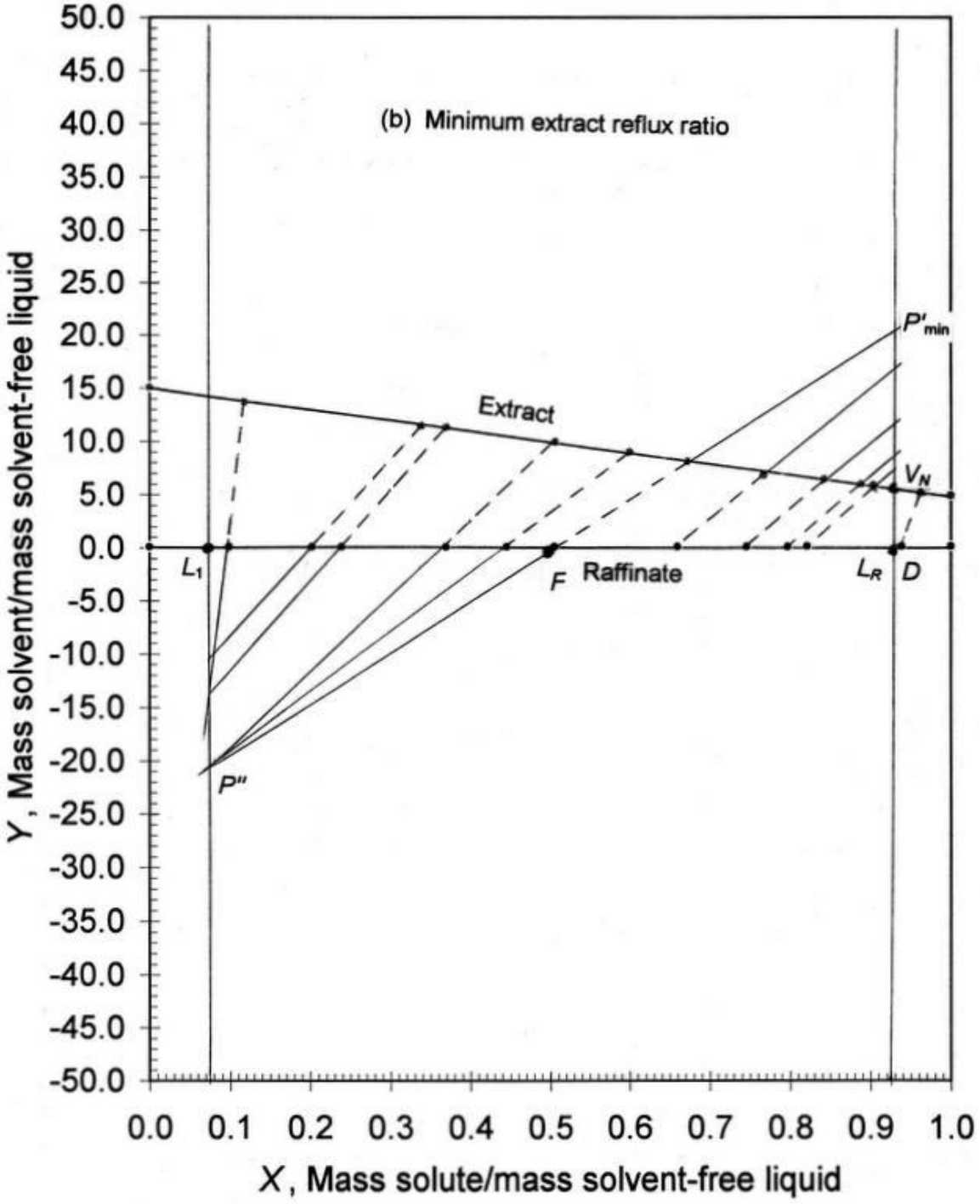
Exercise 8.25 (continued)

Analysis: (a) (continued)



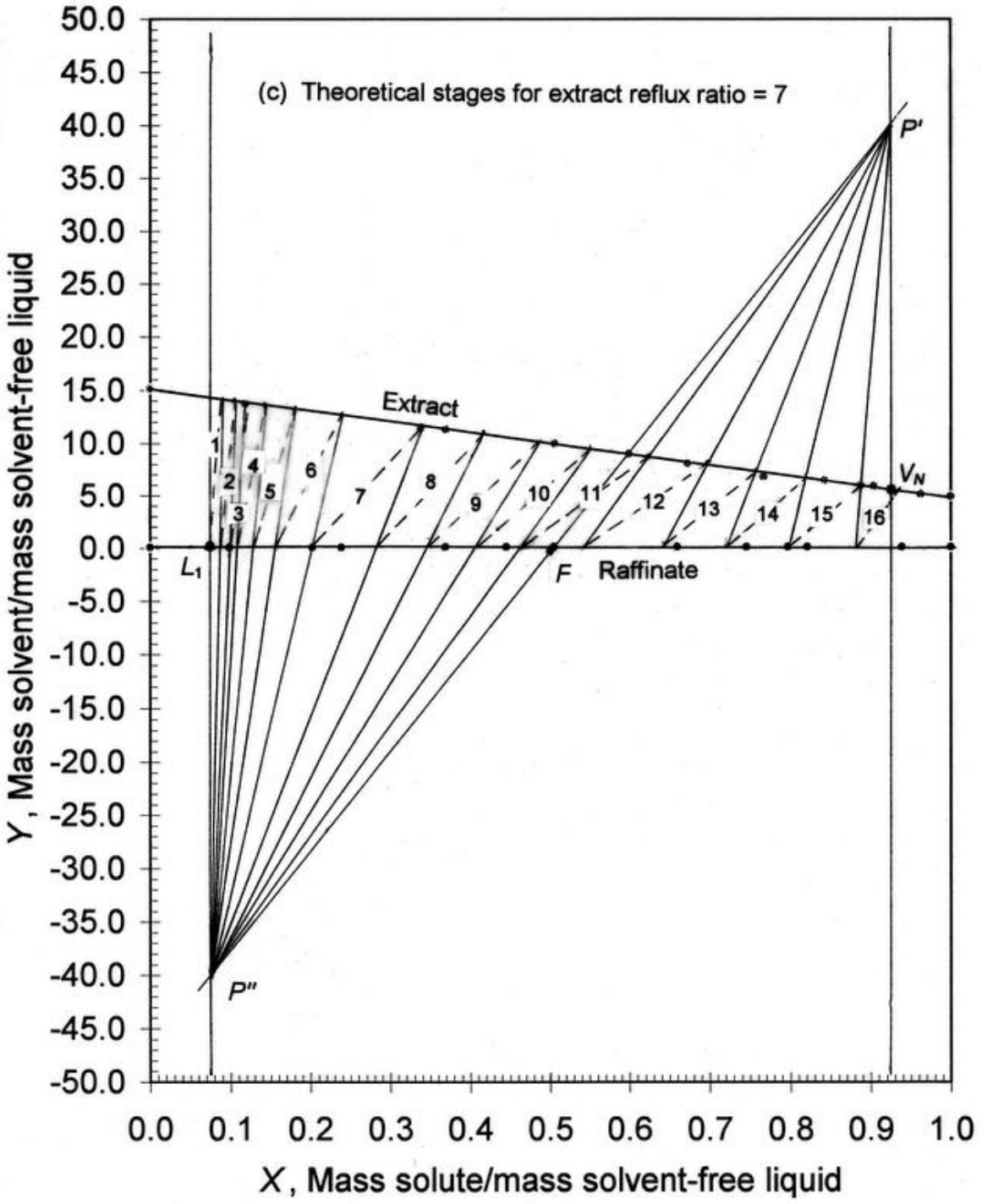
Exercise 8.25 (continued)

Analysis: (b) (continued)



Exercise 8.25 (continued)

Analysis: (c) (continued)



Exercise 8.26

Subject: Liquid-liquid extraction of A from a mixture with B, by solvent C, using extract reflux.

Given: Feed of 1,000 lb/h containing 35 wt% A and 65 wt% B on a solvent-free basis, but as a saturated raffinate. Extract to contain 83 wt% A and 17 wt% B on a solvent-free basis. Raffinate to contain 10 wt% A and 90 wt% B on a solvent-free basis. Liquid-liquid equilibrium data for A,B,C system.

Assumptions: Solvent is completely removed from the extract leaving Stage N in Fig. 8.26b. Thus, the extract reflux, L_R , contains no solvent.

Find: Minimum mass of reflux.
Number of equilibrium stages for twice the minimum reflux ratio.
Masses of streams on a solvent-free basis.

Analysis: Solve the problem using solvent-free coordinates with a Y - X diagram for the solute, A. The same results should be obtained using triangular coordinates. The configuration of the extraction cascade is that in Fig. 8.26b, where the feed is F , the solvent-free extract is D, and the raffinate is B or say B' on a solvent-free basis. The equilibrium data are plotted on the next page as:

$$Y_{\mathrm{A}} = \frac{\text{wt\% A in extract layer}}{(\text{wt\% A} + \text{wt\% B}) \text{ in extract layer}}$$

$$X_{\mathrm{A}} = \frac{\text{wt\% A in raffinate layer}}{(\text{wt\% A} + \text{wt\% B}) \text{ in raffinate layer}}$$

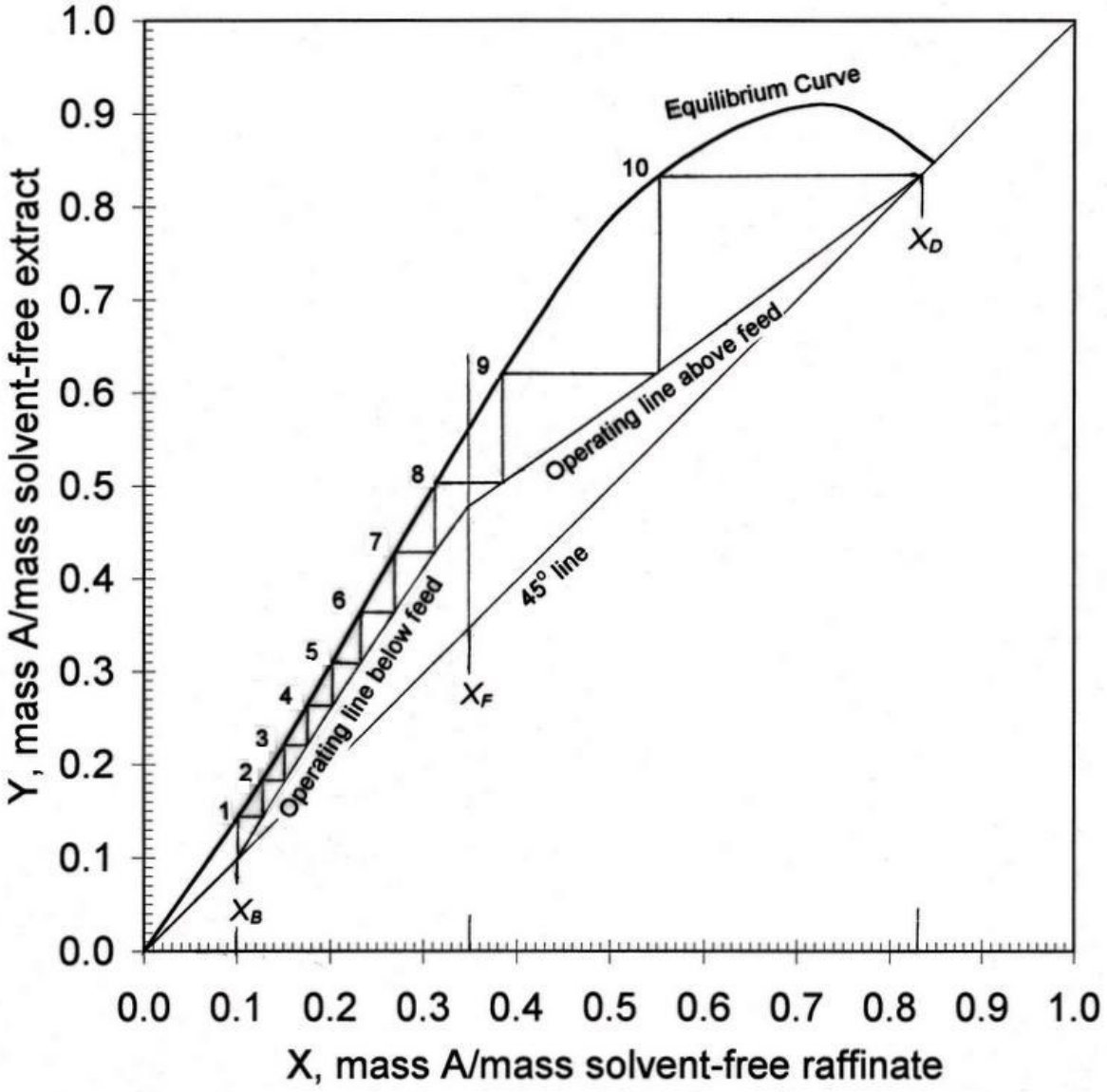
where these values are computed from the given equilibrium data as follows:

Extract:		**Raffinate:**			
wt% A	**wt% B**	**wt% A**	**wt%B**	X_{A}	Y_{A}
0.0	7.0	0.0	92.0	0.000	0.000
1.0	6.1	9.0	81.7	0.099	0.141
1.8	5.5	14.9	75.0	0.166	0.247
3.7	4.4	25.3	63.0	0.287	0.457
6.2	3.3	35.0	51.5	0.405	0.653
9.2	2.4	42.0	41.0	0.506	0.793
13.0	1.8	48.1	29.3	0.621	0.878
18.3	1.8	52.0	20.0	0.722	0.910
24.5	3.0	47.1	12.9	0.785	0.891
31.2	5.6	31.2	5.6	0.848	0.848

Included on the plot are the compositions of the feed, the final extract, and the final raffinate.

Exercise 8.26 (continued)

Analysis: (continued)



Exercise 8.26 (continued)

Analysis: (continued)

An overall component material balance for A, using solvent-free flow rates, gives:

$$1{,}000(0.35) = 350 = Y_D D + X_B B' = 0.83D = 0.10B' \qquad (1)$$

An overall total material balance (on a solvent-free basis) gives:

$$1{,}000 = D + B' \qquad (2)$$

Solving Eqs. (1) and (2), D = 342.5 lb/h and B' = 657.5 lb/h.
To obtain the total flows, including the solvent contributions, the above table of Y-y and X-x compositions can be interpolated, from plots given on the next page. For the feed as a raffinate, saturated with solvent, with $X_A = 0.35$, the wt% C = 12.5%.
Therefore, the total feed rate = 1,000/(1 - 0.125) = 1,140 lb/h, including 140 lb/h of solvent.
The total flow rate of the final raffinate, including the solvent, is found in a similar manner. For $X_A = 0.10$, the wt% C for a saturated raffinate = 9.3.
Therefore, the total final raffinate, $L_1 = B$ = 657.5(1 - 0.093) = 724.9 lb/h.
The solvent in the final total raffinate = 724.9 - 657.5 = 67.4 lb/h.

The total flow rate of the exiting solvent, S_D, can not be found yet because the flow rate, V_N, can not be determined until the extract reflux rate is known. However, for, $Y_A = 0.83$ in the extract leaving Stage N, the wt% C for an extract saturated with solvent = 87.5. Similarly, the entering fresh solvent rate, S_B can not be determined yet.

From the shape of the equilibrium curve on the previous page, at minimum extract reflux, the intersection of the operating lines for the extractor sections above and below the feed would appear to be at the intersection with a vertical line for the wt% A (solvent-free) in the feed, and with the equilibrium curve. Assume this is so. Then at minimum extract reflux, the pinch point will be at the feed stage. Accordingly, the composition of raffinate stream, L_{F+1}, entering the feed stage F (in Fig. 8.26b) is identical to the composition of the feed. From the Y - X plot on the previous page, the solvent-free composition of the extract, V_F, is that in equilibrium with the X = 0.35 of the feed, or $Y = 0.56$. From the figures on the next page, the wt% C in this extract is 91.3. Now, the entering and leaving flow rates can be calculated by material balances for the section of the extractor above the feed stage in Fig. 8.26b.
An overall solvent-free material balance gives the following, where the prime superscript indicates a flow rate on a solvent-free basis:

$$V_F' = L_{F+1}' + D = L_{F+1}' + 342.5 \qquad (3)$$

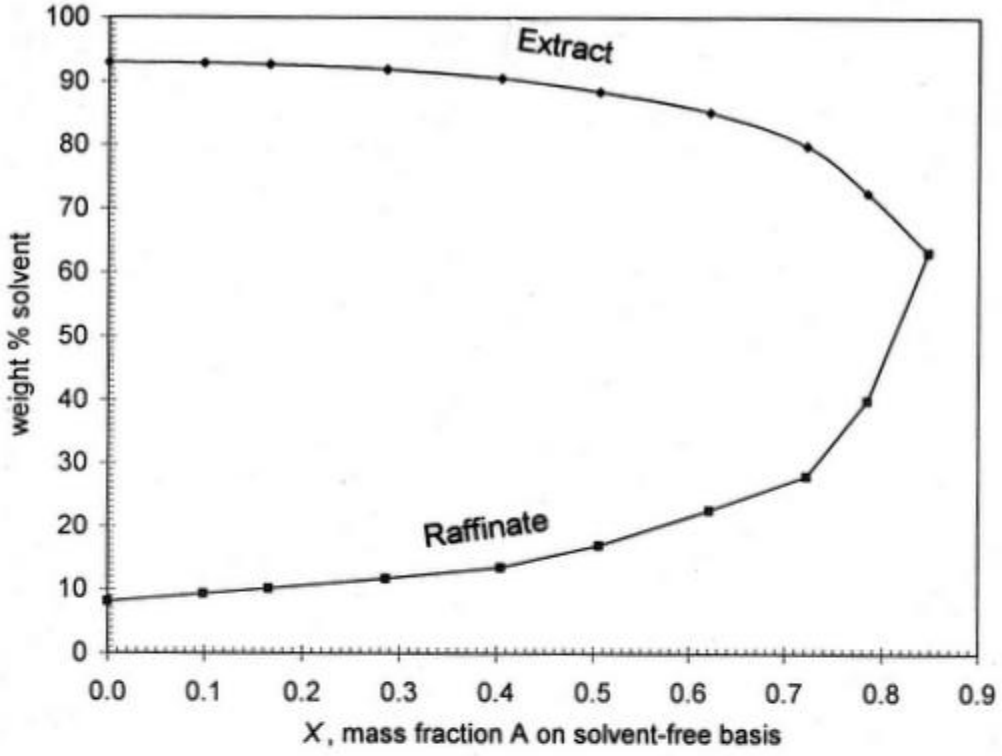
A similar balance on the solute, A, gives:

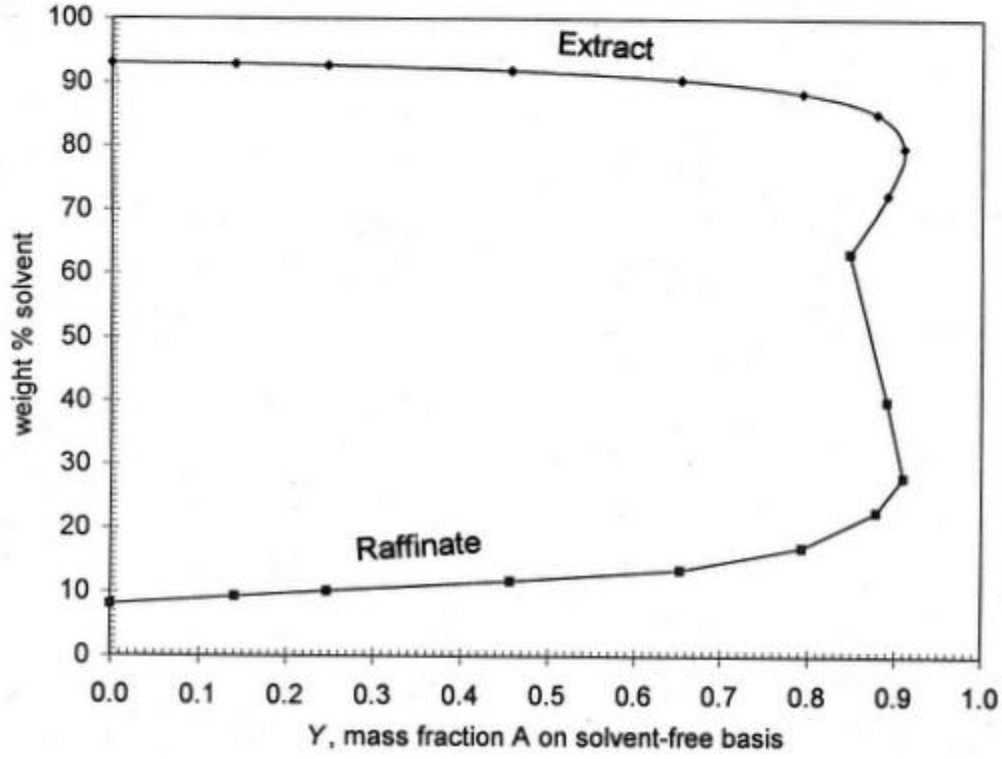
$$Y_{V_F} V_F' = 0.56 V_F' = X_{L_{F+1}} L_{F+1}' + Y_D D = 0.35 L_{F+1}' + 0.83(342.5) = 0.35 L_{F+1}' + 284.3 \qquad (4)$$

Solving Eqs. (3) and (4), gives: $V_F' = 782.9$ lb / h and $L_{F+1}' = 440.4$ lb / h
The corresponding total flow rates (including solvent) are:
V_F = 782.9/(1 - 0.913) = 8,998.9 lb/h of which, 8,998.9 - 782.9 = 8,216.0 is solvent
L_{F+1} = 440.4/(1 - 0.125) = 503.3 lb/h of which 503.3 - 440.4 = 62.9 is solvent
Therefore, the exiting solvent rate, S_D = 8,216.0 - 62.9 = 8,152.1 lb/h

Exercise 8.26 (continued)

Analysis: (continued)





Exercise 8.26 (continued)

Analysis: (continued)

The extract, V_N, contains 83 wt% A on a solvent-free basis. Therefore, From the equilibrium plots on a previous page, the corresponding wt% C in this extract is 87.5 wt%.
Therefore, the total flow rate of V_N = 8,152.1/(0.875) = 9,316.7 lb/h
By total material balance around the solvent removal and stream divider above the top of the cascade (as shown in Fig. 8.26b), $L_D = V_N - S_D - D$ = 9,316.7 - 8,152.1 - 342.5 = 822.1 lb/h.

Therefore, the minimum extract reflux rate = 822.1 lb/h,
and the minimum extract reflux ratio = 822.1/342.5 = 2.40

To compute the number of equilibrium stages, take twice the minimum extract reflux flow rate or 2(822.1) = 1,644.2 lb/h with the same composition of 83 wt% A and 17 wt% B. The solvent-free extract is the same flow rate as before of D = 342.5 lb/h. Therefore, the solvent-free flow rate of V'_N = 1,644.2 + 342.5 = 1,986.7 lb/h.
Since, this flow is 87.5 wt% solvent, total flow rate V_N = 1,986.7/(1 - 0.875) = 15,893.6 lb/h.
The corresponding flow rate of exiting solvent is S_D = 15,893.6 - 1,986.7 = 13,906.9 lb/h

The slope of the solvent-free operating line at the top of the cascade = L_D/V'_N = 1,644.2/1,986.7 = 0.828. However, this slope is not constant because as we move down from the top of the cascade, all three components undergo mass transfer between the two liquid phases in an overall non-equimolar fashion. At the bottom of the cascade, by overall solvent material balance, the entering solvent flow rate = S_B = 13,906.9 + 67.4 - 140 = 13,834.3 lb/h

Next, determine two Y - X points on the operating line above the feed entry by writing the following balances around a section of stages from Stage n above the feed to Stage N at the top, in terms of total stream mass flows, V and L, and mass fractions (including solvent), y and x:

Total mass balance:	$V_{n-1} = L_n + 14{,}249.4$	(5)
Solute mass balance:	$(y_{n-1})_A\, V_{n+1} - (x_n)_A\, L_n = 284.3$	(6)
Solvent mass balance:	$(y_{n-1})_C\, V_{n+1} - (x_n)_C\, L_n = 13{,}906.9$	(7)

Eqs. (5) to (7) are solved by trial and error for a selected value of X_n. To do this, combine Eq. (5) with (6) to eliminate V_{n-1}, and combine Eq. (5) with (7) to eliminate V_{n-1}. We now have two equations for L_n. The selected value of X_n fixes the mass fractions of A and C in the raffinate. Then find a value of Y_{n-1} (which fixes the mass fractions of A and C in the extract) that gives identical values of L_n. The results are as follows, with these two points for Y and X, together with $Y = X = 0.83$ establishing the upper operating line, as shown in the Y - X diagram on the second page of this exercise:

X_n	Y_{n-1}	V_{n-1}, lb/h	L_n, lb/h
0.621	0.670	15,790	1,541
0.405	0.520	15,400	1,151

Exercise 8.26 (continued)

Analysis: (continued)

Next, determine two Y - X points on the operating line below the feed entry by solving the following balances around a section of stages from Stage m below the feed to bottom Stage1:

Total mass balance:	$V_m = L_{m+1}$ - 13,109.4	(8)
Solute mass balance:	$(y_m)_A V_m - (x_{m+1})_A L_{m+1} = -65.7$	(9)
Solvent mass balance:	$(y_m)_C V_m - (x_{m+1})_C L_{m+1} = 13{,}766.9$	(10)

. The results are as follows, with these two points for Y and X, together with $Y = X = 0.10$ establishing the lower operating line, as shown in the Y - X diagram on the second page of this exercise:

X_{m+1}	Y_m	V_m, lb/h	L_{m+1},lb/h
0.287	0.390	15,182	2,073
0.166	0.205	15,064	1,955

From the Y - X plot on the second page of this exercise, 10 equilibrium stages are stepped off, with 2 above the feed stage and 7 below.

The component material balance in lb/h is as follows:

Component	Feed	Solvent in	Extract	Raffinate	Solvent out	Reflux, L_D
A	350.0	0.0	284.3	65.7	0.0	1364.7
B	650.0	0.0	58.2	591.8	0.0	279.5
C	140.0	13834.3	0.0	67.4	13906.9	0.0
Total	1140.0	13834.3	342.5	724.9	13906.9	1644.2

Exercise 8.27

Subject: Extraction of methylcyclohexane (MCH) from n-heptane (C) with aniline (S) at 25°C in a countercurrent-stage extractor.

Given: Feed of 50 wt% MCH in C. On a solvent-free basis, extract contains 95 wt% MCH and raffinate contains 5 wt% MCH. Reflux at both ends as in Fig. 8.26a. Minimum extract reflux ratio = 3.49. Equilibrium data in Exercise 8.22.

Find: With the Maloney-Schubert method on a Y - X Janecke diagram:

(a) Raffinate reflux ratio.

(b) Amount of aniline that must be removed by solvent removal at the top of the extractor, as shown in Fig. 8.26a.

(c) Amount of solvent that must be added to the mixer at the bottom of the extractor, as shown in Fig. 8.26a.

Analysis: The liquid-liquid phase equilibrium data are given, for each phase, as mass % MCH on an aniline-free basis, and mass of aniline per mass of aniline-free mixture. Thus, the data can be plotted directly to obtain the Janecke diagram, which is shown on the next page.

Referring to Fig. 8.26a, the given compositions of the feed, F, the solvent-free extract, D, and the solvent-free raffinate, B, are plotted on the diagram. By construction on the Janecke diagram, on the previous page, the compositions of the solvent-containing extract, V_N , and the solvent-containing raffinate, L_1 , are determined as intersections of vertical lines (drawn up from the solvent-free points to the extract and raffinate equilibrium curves. The wt% compositions of these points are read from the diagram with the aid of the tabulated equilibrium data given in the exercise statementto be:

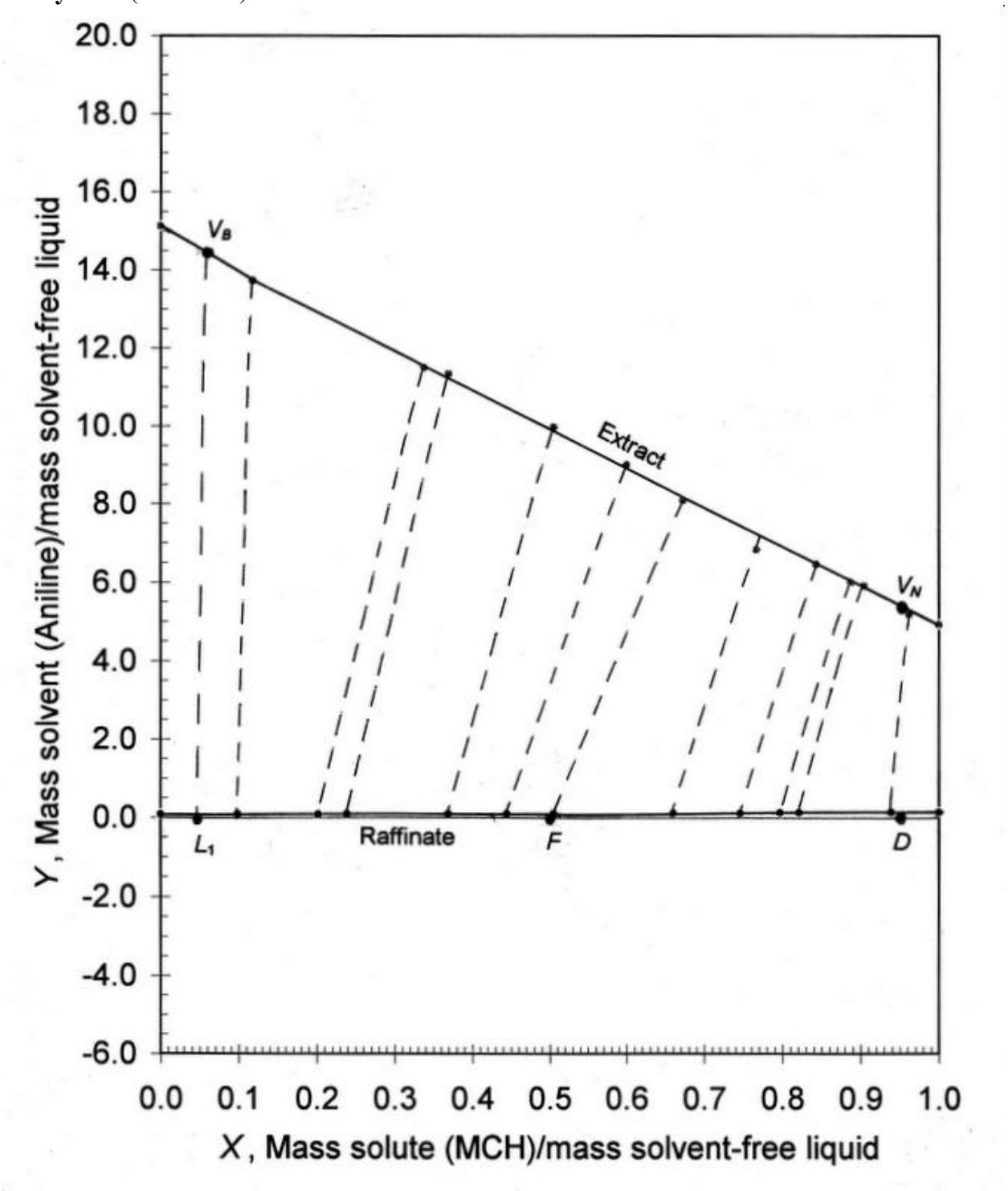
	Wt%:	
Component	**Extract, V_N**	**Raffinate, L_1**
Aniline, S	84.0	7.5
n-Heptane, C	1.0	88.0
Methylcyclohexane, MCH	15.0	4.5
Total:	100.0	100.0

Take a basis of 1,000 kg/h of feed and make material balances for the minimum extract reflux condition. Because the feed is 50 wt% MCH and 50 wt% C, and the two solvent-free product compositions are symmetrical with respect to MCH and C, the solvent-free material balance is quickly determined to be:

	kg/h:		
Component	**Feed, F**	**Extract, D**	**Raffinate, B**
n-Heptane, C	500	25	475
Methylcyclohexane, MCH	500	475	25
Total:	1,000	500	500

Exercise 8.27 (continued)

Analysis: (continued)



Exercise 8.27 (continued)

Analysis: (continued)

(b) Assume the given minimum extract reflux ratio = 3.49 = L_R/D in Fig. 8.36a.
Then, L_R = 3.49(500) = 1,745 kg/h. Therefore, the flow rate of solvent-free extract in stream V_N = 1,745 + 500 = 2,245 kg/h. But, from above, this stream contains 84 wt% aniline solvent.
Therefore, the flow rate of aniline in stream V_N = (84/16)(2,245) = 11,790 kg/h. This is the flow rate of aniline that must be removed by the separator at the top of the cascade.

(c) From above, the raffinate L_1 leaving at the bottom of the cascade is 7.5 wt% aniline.
Therefore, aniline flow rate in B is (7.5/92.5)(500) = 40 kg/h and B = 540 kg/h
The entering solvent rate S_B is, therefore, 40 + 11,790 = 11,830 kg/h.
This is the amount of fresh solvent that must be added to the mixer at the bottom of the column.

(a) Referring to Fig. 8.36a, define the raffinate reflux ratio as (L_1 - B)/B. Because the cascade is operating at minimum reflux, assume infinite stages so that V_B is in equilibrium with L_1. From the Janecke diagram on the previous page, the composition of V_B is obtained by the dashed tie line from B, which gives 14.5 kg aniline/ kg solvent-free extract and 5.7 wt% MCH in the extract. This gives 14.5/15.5 x 100% = 93.5 wt% aniline. A total material balance around the bottom Mixer gives: $S_B - B$ = 11,830 - 540 = 11, 290 = $V_B - L_1$.
An aniline balance around the bottom Mixer gives: 11,830 - 40 = 0.935V_B - 0.075L_1.
Solving these two equations gives L_1 = 1,435 kg/h.
Therefore, the raffinate reflux ratio = (1,435 - 540)/540 = 1.66.

Exercise 8.28

Subject: Design of a mixer-settler unit for extraction of acetic acid (A) from water (C) by isopropyl ether (S).

Given: 12,400 lb/h of 3 wt% A in C. 24,000 lb/h of S. 1.5 minutes residence time in mixer. 4 gal/min-ft^2 in settling vessel.

Find: (a) Diameter, D_T, and height, H, of mixing vessel if $H/D_T = 1$.
(b) Agitator Hp for mixing vessel.
(c) Diameter, D_T, and length, L, of settling vessel, if $L/D_T = 4$.
(d) Residence time in settling vessel in minutes.

Analysis: First compute total volumetric flows into mixer vessel. Because feed is dilute in A, assume density of feed is that of water = 62.4 lb/ft^3. From Perry's Handbook, specific gravity of S = 0.725 or a density of 0.725(62.4) = 45.2 lb/ft^3. Therefore, total flow rate of feed plus solvent =
Q = 12,400/62.4 + 24,000/45.2 = 730 ft^3/h or 12.2 ft^3/min.

(a) Vessel volume = $V = Qt_{res}$ = 12.2(1.5) = 18.3 ft^3
For a cylindrical vessel of $H/D_T = 1$, $V = \pi D_T^2 H/4 = \pi D_T^3/4$
Solving, $D_T^3 = 4V/\pi = 4(18.3)/3.14 = 23.3$ ft^3. Therefore, $D_T = H = 2.85$ ft

(b) Assume 4 Hp/1,000 gallons for mixer agitator power.
Gallons in vessel = 7.48V = 7.48(18.3) = 137 gal
Therefore, need 4(137)/1,000 = 0.55 Hp.

(c) Assume volumetric flow into mixer = volumetric flow leaving settler
Therefore, Q = 12.2 ft^3/min or 7.48(12.2) = 91 gpm
The ft^2 disengaging area needed = 91/4 = 22.8 ft^2 = $D_T L = D_T(4D_T) = 4D_T^2$
Solving, D_T = 2.4 ft and $L = 4D_T$ = 4(2.4) = 9.6 ft.

(d) Settler volume = $V = \pi D_T^2 L/4 = 3.14(2.4)^2(9.6)/4 = 43.4$ ft^3
Residence time of phases in settler = $t_{res} = V/Q$ = 43.4/12.2 = 3.6 minutes

Exercise 8.29

Subject: Extraction of acetic acid (A) from water (C) by ethyl acetate (S) in available extractor.

Given: Cascade of 6 mixer-settler units. Each mixer is 10-ft diameter by 10-ft high with 20-Hp agitator. Each settler is 10-ft diameter by 40-ft long. Feed and solvent compositions , and solvent-to-feed mass ratio, are those in Fig. 8.1.

Find: Allowable feed flow rate.

Analysis: From Fig. 8.1, the total entering component flow rates are as follows, with liquid densities from Perry's Handbook. Assume ideal liquid solutions.

Component	lb/h	density, lb/gal	gpm
Acetic acid	6,660	8.74	12.7
Water	26,100	8.33	52.2
Ethyl acetate	68,600	7.51	152.2

Therefore, total flow rate = Q = 12.7 + 52.2 + 152.2 = 217.1 gpm
The volume of one mixer = $V = \pi D_T^2 H/4$ = 3.14(10)^2(10)/4 = 785 ft^3 or 5,872 gal.

First consider the mixer residence time factor.
With the flow rates in Fig. 8.1, residence time in mixer = $t_{res} = V/Q$ = 5,872/217 = 27 minutes. Since the liquid phase viscosities are each less than 5 cP (actually less than 1 cP) and the density difference computes to be 0.106, which is greater than 0.10, the required residence time in the mixer should not exceed 5 minutes, Therefore, should be able to handle a feed rate of the acetic acid-water mixture of (27/5)(6,660 + 23,600) = 163,400 lb/h or 27/5 = 5.4 times that in Fig. 8.1.

Next, consider the mixer agitator Hp factor.
The vessel volume in gallons = 5,872. Therefore, using the criterion of 4 Hp/1,000 gal, need 4(5,872)/1,000) = 23.5 Hp. This is greater than the given 20 Hp. So reduce allowable feed rate of acetic acid in water to 20/23.5(163,400) = 139,000 lb/h. This increases residence time in mixer to 5(23.5)/20 = 5.9 minutes.

Now, check settler disengaging factor.
Assume that the total volumetric flow leaving the settler is equal to that entering the mixer. Therefore, Q = (27/5)(5/5.9)(217.1) = 994 gpm. Using the settling criterion of 5 gpm/ft^2 of D_TL, Need D_TL = 994/5 = 200 ft^2. The available settler has D_TL = 10(40) = 400 ft^2, which is twice that needed.

Therefore, a feed rate of acetic acid + water of 139,000 lb/h is safe. This is 4.6 times that in Fig. 8.1.

Exercise 8.30

Subject: Sizing an agitator for extraction of acetic acid (A) from water (C) by isopropyl ether (S) at 25°C.

Given: For one of the mixers, flow rates and properties of raffinate and extract are given. Raffinate is dispersed phase in mixer, with residence time of 2.5 minutes.

Find: (a) Dimensions of closed, baffled mixing vessel.
(b) Diameter of flat-bladed impeller.
(c) Minimum rate of rotation of impeller in rpm for complete and uniform dispersion.
(d) Power of agitator at minimum rpm.

Analysis: First, compute the volumetric flow rates of the extract and raffinate.
Extract flow rate = 52,000/45.3 = 1,148 ft^3/h or 1,148(7.48)/60 = 143 gpm
Raffinate flow rate = 21,000/63.5 = 331 ft^3/h or 331(7.48)/60 = 41 gpm
Total flow rate = Q = 1,148 + 331 = 1,479 ft^3/h or 143 + 41 = 184 gpm
Assume this total flow also enters and leave the mixer.

(a) For a residence time of 2.5 minutes,
volume of mixing vessel = $V = Qt_{res}$ = (1,479/60)(2.5) = 62 ft^3
Assume $H = D_T$, then $V = \pi D_T^2 H/4 = \pi D_T^3/4$
Solving, D_T^3 = 4(62)/3.14 = 79 ft^3 and $D_T = H = 4.3$ ft.

(b) Impeller diameter = $D_i = (1/3)D_T$ = 4.3/3 = 1.43 ft.

(c) To determine the minimum impeller rpm, assume that the volume fractions of the two phases in the mixer are in the same ratio as for the flow rates of the phases leaving the settler. Therefore, the volume fractions are: ϕ_E = 1,148/1,479 = 0.78 and ϕ_R = 1 - 0.78 = 0.22. Because the raffinate volume fraction is less than 0.26, the raffinate is probably the dispersed phase. Therefore, ϕ_D = 0.22 and ϕ_C = 0.78. We are given the following properties,

Phase	Density, lb/ft^3	Viscosity, cP
Dispersed (raffinate)	63.5	3.0
Continuous (extract)	45.3	1.0

Also, interfacial tension = σ_I = 13.5 dyne/cm = 388,000 lb/h^2
Density difference = $\Delta\rho$ = 63.5 - 45.3 = 18.2 lb/ft^3
Phase mixture density from Eq. (8-23) = ρ_M = 45.3(0.78) + 63.5(0.22) = 49.3 lb/ft^3
From Eq. (8-24), mixture viscosity is,

$$\mu_M = \frac{\mu_C}{\phi_C}\left[1+\frac{1.5\mu_D\phi_D}{\mu_C+\mu_D}\right] = \frac{1.0}{0.78}\left[1+\frac{1.5(3.0)(0.22)}{1.0+3.0}\right] = 1.6\,\text{cP} \text{ or } 3.87 \text{ lb/ft-h}$$

Exercise 8.30 (continued)

Analysis: (c) (continued)
Compute minimum rpm from Eq. (8-25), where, far-right dimensionless group is,

$$\left(\frac{\mu_M^2\sigma}{D_i^5\rho_M g^2(\Delta\rho)^2}\right)=\left[\frac{3.87^2(388{,}000)}{(1.43)^5(49.3)(4.17\times10^8)(18.2)^2}\right]=3.42\times10^{-16}$$

$$\frac{N_{\min}^2\rho_M D_i}{g\Delta\rho}=1.03\left(\frac{D_T}{D_i}\right)^{2.76}\phi_D^{0.106}\left(\frac{\mu_M^2\sigma}{D_i^5\rho_M g^2(\Delta\rho)^2}\right)^{0.084}=1.03\left(\frac{4.3}{1.43}\right)^{2.76}(0.22)^{0.106}(3.42\times10^{-16})^{0.084}=20.88$$

Therefore, $N_{\min}^2=20.88\dfrac{g\Delta\rho}{\rho_M D_i}=20.88\dfrac{(4.17\times10^8)(18.2)}{(49.3)(1.43)}=9.9\times10^7$ (rph^2)

and $N_{\min}$ = 9,950 rph or 166 rpm

(d) Determine the mixing vessel agitator Hp from Fig. 8.36 (b), which requires N_{Re}.
Assume $N = N_{\min}$ = 9,950 rph

From Eq. (8-22), $N_{\text{Re}}=\dfrac{D_i^2 N\rho_M}{\mu_M}=\dfrac{(1.43)^2(9{,}950)(49.3)}{3.87}=2.6\times10^5$

From Fig. 8.36 (b), for a mixing vessel with baffles (thus, no vortex), N_{po} = 5.7
From Eq. (8-21), the power is given by,

$$P=\frac{N_{\text{Po}}N^3D_i^5\rho_M}{g_c}=\frac{(5.7)(9{,}950)^3(1.43)^5(49.3)}{4.17\times10^8}=4.0\times10^6 \text{ ft-lbf/h or 2 Hp}$$

Compare this to the rule of thumb of 4 Hp/1,000 gallons.
Vessel volume = 62 ft^3 or 464 gal.
Therefore, Hp = 4(464)/1,000 = 1.9 Hp, which is in very good agreement.

Exercise 8.31

Subject: Droplet characteristics for extraction of acetic acid (A) from water (C) by isopropyl ether (S) in a mixer unit.

Given: Conditions in Exercise 8.27.

Find: (a) Sauter mean drop size.
(b) Range of drop sizes.
(c) Interfacial area of emulsion.

Analysis:

(a) The Sauter (surface-mean) diameter, d_{vs} , is given by Eq. (8-38) or (8-39), depending on the Weber number. From Eq. (8-37),

$$N_{\text{We}} = \frac{D_i^3 N^2 \rho_C}{\sigma_i} = \frac{(1.43)^3 (9{,}950)^2 (45.3)}{388{,}000} = 33{,}800$$

Since $N_{\text{We}} > 10{,}000$, Eq. (8-39) applies.

$$d_{vs} = 0.39 D_i \left(N_{\text{We}}\right)^{-0.6} = 0.39(1.43)(33{,}900)^{-0.6} = 0.00107 \text{ ft} \quad \text{or} \quad 0.32 \text{ mm}$$

(b) $d_{\min} = d_{vs}/3 = 0.32/3 = 0.107$ mm

$d_{\max} = 3d_{\text{vs}} = 3(0.32) = 0.96$ mm

(c) From Eq. (8-36), the interfacial surface area per unit volume of emulsion is,

$$a = \frac{6\phi_D}{d_{vs}} = \frac{6(0.22)}{0.00107} = 1{,}234 \text{ ft}^2/\text{ft}^3$$

Exercise 8.32

Subject: Mass transfer characteristics for extraction of acetic acid (A) from water (C) by isopropyl ether (S) in a mixer unit.

Given: Conditions in Exercises 8.27 and 8.28. Diffusivity of acetic acid in each phase. Distribution coefficient of acetic acid.

Find: (a) Dispersed-phase mass-transfer coefficient.
(b) Continuous-phase mass-transfer coefficient.
(c) Murphree dispersed-phase efficiency.
(d) Fraction of A extracted.

Analysis:
(a) For the raffinate, which is the dispersed phase, Eq. (8-40 applies.
Diffusivity of A in C = D_D = 1.3 x 10^{-9} m^2/s and from Exercise 8.28, d_{vs} = 0.32 mm = 0.00032 m

From a rearrangement of Eq. (8-40), $k_D = 6.6\dfrac{D_D}{d_{vs}} = 6.6\dfrac{1.3\times10^{-9}}{0.00032} = 26.8\times10^{-6}$ m/s or 0.32 ft/h

(b) For the extract, which is the continuous phase, Eq. (8-50) applies.
Diffusivity of A in S = D_C = 2.0 x 10^{-9} m^2/s or 7.75 x 10^{-5} ft^2/h

In Eq. (8-44), $N_{Sc} = \dfrac{\mu_C}{\rho_C D_C} = \dfrac{(1.0)(2.42)}{(45.3)(7.75\times10^{-5})} = 690$

In Eq. (8-50), $N_{Re} = \dfrac{D_i^2 N \rho_C}{\mu_C} = \dfrac{(1.43)^2(9{,}950)(45.3)}{(2.42)} = 381{,}000$

In Eq. (8-50), $N_{Fr} = \dfrac{D_i N^2}{g} = \dfrac{(1.43)(9{,}950)^2}{4.17\times10^8} = 0.34$

In Eq. (8-50), D_i / d_{vs} = 1.43/(0.00032/0.3048) = 1,360
In Eq. (8-50, d_{vs}/D_T = (0.00032/0.3048)/4.3 = 2.44 x 10^{-4}

In Eq. (8-50, $N_{Eo} = \dfrac{\rho_D d_{vs}^2 g}{\sigma} = \dfrac{(63.5)(0.00032/0.3048)^2(4.17\times10^8)}{388{,}000} = 0.0752$

From Eq. (8-50),

$$(N_{Sh})_C = \frac{k_C d_{vs}}{D_C} = 1.237\times10^{-5}(N_{Sc})^{1/3}(N_{Re})^{2/3}\phi_D^{-1/2}(N_{Fr})^{5/12}\left(\frac{D_i}{d_{vs}}\right)^2\left(\frac{d_{vs}}{D_T}\right)^{1/2}(N_{Eo})^{5/4}$$

$$= 1.237\times10^{-5}(690)^{1/3}(381{,}000)^{2/3}(0.22)^{-1/2}(0.34)^{5/12}(1{,}360)^2(2.44\times10^{-4})^{1/2}(0.0752)^{5/4} = 889$$

Exercise 8.32 (continued)

Analysis: (b) (continued)

$$k_C = \frac{(N_{Sh})_C D_C}{d_{vs}} = \frac{889(7.75\times10^{-5})}{(0.00032/0.3048)} = 65.6 \text{ ft/h}$$

(c) To compute E_{MD} from Eq. (8-33), K_{OD} must be computed from Eq. (8-28). That equation requires the slope of the equilibrium curve for acetic acid, $m = dc_C/dc_D$. From Perry's Handbook, Section 15, the equilibrium constant under dilute conditions in mass-fraction composition units is $K_D = 0.429$. Converting this to concentration units, mass/unit volume, $m = K_D(\rho_S/\rho_C) = 0.429(45.3/63.5) = 0.306$.

From Eq. (8-28), $K_{OD} = \dfrac{1}{\dfrac{1}{k_D} + \dfrac{1}{mk_C}} = \dfrac{1}{\dfrac{1}{0.32} + \dfrac{1}{0.306(65.6)}} = 0.315$ ft/h

Thus, mass transfer is controlled by the dispersed phase.

In Eq. (8-33), need a, V, and Q_D. From Exercise 8.28, $a = 1{,}234$ ft^2/ft^3, $V = 62$ ft^3, and $Q_D = 331$ ft^3/h. From Eq. (8-33),

$$E_{MD} = \frac{K_{OD}aV/Q_D}{1+K_{OD}aV/Q_D} = \frac{0.315(1{,}234)(62)/331}{1+0.315(1{,}234)(62)/331} = 0.986 \text{ or } 98.6\%$$

(d) To compute the fraction of solute extracted, the relation in Example 8.7 can not be used because in that example, the extract is the dispersed phase. Here, the raffinate is the dispersed phase. Therefore, derive a new equation. By material balance on the solute,

$$Q_D\left(c_{D,\text{in}} - c_{D,\text{out}}\right) = Q_C\left(c_{C,\text{out}}\right)$$

$$\text{or } Q_D\left(1 - \frac{c_{D,\text{out}}}{c_{D,\text{in}}}\right) = Q_C\left(\frac{c_{C,\text{out}}}{c_{D,\text{in}}}\right)$$

$$\text{Therefore, } f_{\text{extracted}} = 1 - \frac{c_{D,\text{out}}}{c_{D,\text{in}}} = \frac{Q_C}{Q_D}\left(\frac{c_{C,\text{out}}}{c_{D,\text{in}}}\right) \qquad (1)$$

$$E_{MD} = \frac{c_{D,\text{in}} - c_{D,\text{out}}}{c_{D,\text{in}} - c^*_{D,\text{out}}} = \frac{c_{D,\text{in}} - c_{D,\text{out}}}{c_{D,\text{in}} - \dfrac{c_{C,\text{out}}}{m}} = \frac{1 - \dfrac{c_{D,\text{out}}}{c_{D,\text{in}}}}{1 - \dfrac{1}{m}\left(\dfrac{c_{C,\text{out}}}{c_{D,\text{in}}}\right)} \qquad (2)$$

Combining Eqs. (1) and (2) and solving for $f_{\text{extracted}}$,

$$f_{\text{extracted}} = \frac{E_{MD}}{1 + \dfrac{E_{MD}}{m}\left(\dfrac{Q_D}{Q_C}\right)} = \frac{0.986}{1 + \dfrac{0.986}{0.306}\left(\dfrac{331}{1{,}148}\right)} = 0.511 \text{ or } 51.1\% \text{ extracted}$$

Exercise 8.33

Subject: Design of mixer unit for extraction of benzoic acid (A) from water (C) by toluene (S).

Given: Conditions in Example 8.4. Properties of raffinate and extract phases. 6-flat-blade impeller in a closed mixer unit with baffles. Extract phase is dispersed.

Find: (a) Minimum rpm of impeller for complete and uniform dispersion.
(b) Power requirement of agitator.
(c) Sauter mean diameter.
(d) Interfacial area.
(e) K_{OD}.
(f) N_{OD}.
(g) E_{MD}.
(h) Fractional extraction of A.

Analysis: From Example 8.4, $D_T = 7.9$ ft. Use $D_i = D_T/3 = 7.9/3 = 2.63$ ft.
Assume $Q_R = Q_F = 500$ gpm, and $Q_E = Q_S = 750$ gpm. Therefore, total $Q = 500 + 750 = 1{,}250$ gpm. Assume phase volume holdups in the mixing vessel are in proportion to the volumetric flow rates. Therefore, with the extract phase dispersed, $\phi_\Delta = 750/1{,}250 = 0.60$ and $\phi_C = 0.40$.

(a) We are given the following properties,

Phase	Density, lb/ft^3	Viscosity, cP	Diffusivity of A, cm/s
Dispersed (extract)	53.7	0.59	1.5 x 10^{-5}
Continuous (raffinate)	62.1	0.95	2.2 x 10^{-5}

Also, interfacial tension = $\sigma_I = 22.0$ dyne/cm = 633,000 lb/h^2
Density difference = $\Delta\rho$ =62.1 - 53.7 = 8.4 lb/ft^3
Phase mixture density from Eq. (8-23) = $\rho_M = 53.7(0.60) + 62.1(0.40) = 57.0$ lb/ft^3
From Eq. (8-24), mixture viscosity is,

$$\mu_M = \frac{\mu_C}{\phi_C}\left[1+\frac{1.5\mu_D\phi_D}{\mu_C+\mu_D}\right] = \frac{0.95}{0.40}\left[1+\frac{1.5(0.59)(0.60)}{0.95+0.59}\right] = 2.65 \text{ cP or } 6.41 \text{ lb/ft-h}$$

Compute minimum rpm from Eq. (8-25), where, far-right dimensionless group is,

$$\left(\frac{\mu_M^2\sigma}{D_i^5\rho_M g^2(\Delta\rho)^2}\right) = \left[\frac{6.41^2(633{,}000)}{(2.63)^5(57.0)(4.17\times10^8)(8.4)^2}\right] = 2.96\times10^{-19}$$

$$\frac{N_{\min}^2\rho_M D_i}{g\Delta\rho} = 1.03\left(\frac{D_T}{D_i}\right)^{2.76}\phi_D^{0.106}\left(\frac{\mu_M^2\sigma}{D_i^5\rho_M g^2(\Delta\rho)^2}\right)^{0.084} = 1.03\left(\frac{7.9}{2.63}\right)^{2.76}(0.60)^{0.106}(2.96\times10^{-19})^{0.084} = 1.004$$

Exercise 8.33 (continued)

Analysis: (a) (continued)

Therefore, $N_{\min}^2 = 1.004\dfrac{g\Delta\rho}{\rho_M D_i} = 1.004\dfrac{(4.17\times10^8)(8.4)}{(57.0)(2.63)} = 23.5\times10^6$ (rph^2)

and $N_{\min}$ =4,840 rph or 81 rpm

(b) Determine the mixing vessel agitator Hp from Fig. 8.36 (b), which requires N_{Re}.
Assume $N = N_{\min}$ =4,840 rph

From Eq. (8-22), $N_{Re} = \dfrac{D_i^2 N\rho_M}{\mu_M} = \dfrac{(2.63)^2(4{,}840)(57.0)}{6.41} = 2.98\times10^5$

From Fig. 8.36 (b), for a mixing vessel with baffles (thus, no vortex), N_{po} = 5.7
From Eq. (8-21), the power is given by,

$$P = \frac{N_{Po}N^3D_i^5\rho_M}{g_c} = \frac{(5.7)(4{,}840)^3(2.63)^5(57.0)}{4.17\times10^8} = 11.10\times10^6 \text{ ft-lbf/h or } 5.6 \text{ Hp}$$

Compare this to the rule of thumb of 4 Hp/1,000 gallons.
Vessel volume = 334 ft^3 or 2,500 gal.
Therefore, Hp = 4(2,500)/1,000 = 10 Hp, which is 80% higher.

(c) The Sauter (surface-mean) diameter, d_{vs}, is given by Eq. (8-38) or (8-39), depending on the Weber number. From Eq. (8-37),

$$N_{We} = \frac{D_i^3N^2\rho_C}{\sigma_i} = \frac{(2.63)^3(4{,}840)^2(57.0)}{633{,}000} = 41{,}800$$

Since N_{We} > 10,000, Eq. (8-39) applies.

$$d_{vs} = 0.39D_i(N_{We})^{-0.6} = 0.39(2.63)(41{,}800)^{-0.6} = 0.00173 \text{ ft} \quad \text{or} \quad 0.53 \text{ mm}$$

(d) From Eq. (8-36), the interfacial surface area per unit volume of emulsion is,

$$a = \frac{6\phi_D}{d_{vs}} = \frac{6(0.60)}{0.00173} = 2{,}080 \text{ ft}^2/\text{ft}^3$$

Exercise 8.33 (continued)

Analysis: (continued)

(e) Eq. (8-28) applies, where, $K_{OD} = \dfrac{1}{\dfrac{1}{k_D} + \dfrac{1}{mk_C}}$

For the extract, which is the dispersed phase, Eq. (8-40 applies.

From a rearrangement of Eq. (8-40), $k_D = 6.6\dfrac{D_D}{d_{vs}} = 6.6\dfrac{1.5\times10^{-5}}{0.0527} = 1.88\times10^{-3}$ cm/s or 0.22 ft/h

For the raffinate, which is the continuous phase, Eq. (8-50) applies, with D_C = 2.2 x 10^{-5} cm^2/s or 8.53 x 10^{-5} ft^2/h.

In Eq. (8-44), $N_{Sc} = \dfrac{\mu_C}{\rho_C D_C} = \dfrac{(0.95)(2.42)}{(62.1)(8.53\times10^{-5})} = 434$

In Eq. (8-50), $N_{Re} = \dfrac{D_i^2 N \rho_C}{\mu_C} = \dfrac{(2.63)^2(4{,}840)(62.1)}{(0.95)(2.42)} = 904{,}000$

In Eq. (8-50), $N_{Fr} = \dfrac{D_i N^2}{g} = \dfrac{(2.63)(4{,}840)^2}{4.17\times10^8} = 0.148$

In Eq. (8-50), D_i / d_{vs} = 2.63/(0.00173 = 1,520
In Eq. (8-50, d_{vs}/D_T = 0.00173/7.9 = 2.19 x 10^{-4}

In Eq. (8-50, $N_{Eo} = \dfrac{\rho_D d_{vs}^2 g}{\sigma} = \dfrac{(53.7)(0.00173)^2(4.17\times10^8)}{633{,}000} = 0.1058$

From Eq. (8-50),

$$(N_{Sh})_C = \frac{k_C d_{vs}}{D_C} = 1.237\times10^{-5}(N_{Sc})^{1/3}(N_{Re})^{2/3}\phi_D^{-1/2}(N_{Fr})^{5/12}\left(\frac{D_i}{d_{vs}}\right)^2\left(\frac{d_{vs}}{D_T}\right)^{1/2}(N_{Eo})^{5/4}$$

$$= 1.237\times10^{-5}(434)^{1/3}(904{,}000)^{2/3}(0.60)^{-1/2}(0.148)^{5/12}(1{,}520)^2(2.19\times10^{-4})^{1/2}(0.1058)^{5/4} = 1{,}052$$

$$k_C = \frac{(N_{Sh})_C D_C}{d_{vs}} = \frac{1{,}052(8.53\times10^{-5})}{0.00173} = 51.8 \text{ ft/h}$$

The slope of the equilibrium curve for dilute conditions is given by Eq. (8-29) as $m = dc_C/dc_D = c_C/c_D$ = 1/21 = 0.0476

From Eq. (8-28), $K_{OD} = \dfrac{1}{\dfrac{1}{k_D} + \dfrac{1}{mk_C}} = \dfrac{1}{\dfrac{1}{0.22} + \dfrac{1}{0.0476(51.8)}} = \dfrac{1}{4.55 + 0.405} = 0.202$ ft/h

where, it is seen that the dispersed phase controls the rate of mass transfer.

Exercise 8.33 (continued)

Analysis: (continued)

(f) From Eq. (8-32, $N_{OD} = \dfrac{K_{OD}aV}{Q_D} = \dfrac{(0.202)(2,080)(334)}{(750)(60)/7.48} = 26.3$

(g) From Eq. (8-33), $E_{MD} = \dfrac{N_{OD}}{1+N_{OD}} = \dfrac{26.3}{1+26.3} = 0.963$ or 96.3%

(h) Because the extract is the dispersed phase, Eq. (3) in Example 8.7 applies,

$$f_{\text{extracted}} = \frac{\dfrac{Q_D E_{MD}}{Q_C m}}{1+\dfrac{Q_D E_{MD}}{Q_C m}} = \frac{\dfrac{750(0.963)}{500\left(\dfrac{1}{21}\right)}}{1+\dfrac{750(0.963)}{500\left(\dfrac{1}{21}\right)}} = 0.968 \text{ or } 96.8\% \text{ extracted}$$

Exercise 8.34

Subject: Diameter of an RDC column for extraction of acetic acid (A) from water (C) by isopropyl ether (S).

Given: Conditions in Exercises 8.28 and 8.30.

Find: Column diameter.

Analysis:

Conditions of Exercise 8.28:

Flow rate of feed/raffinate = 12,400 lb/h. Flow rate of solvent/extract = 24,000 lb/h

Assume raffinate is dispersed.

The following properties are given in Exercise 8.30.

$\rho_R = \rho_D = 63.5$ lb/ft^3 and $\rho_E = \rho_C = 45.3$ lb/ft^3

$\mu_C = 1.0$ cP or 0.000021 lbf-s/ft^2

Interfacial tension = $\sigma_I = 13.5$ dyne/cm or 0.000924 lbf/ft

Assume $\dfrac{u_o \mu_C \rho_C}{\sigma_i \Delta\rho} = 0.01$

Therefore, $u_o = 0.01\dfrac{\sigma_i \Delta\rho}{\mu_C \rho_C} = 0.01\dfrac{(0.000924)(63.5-45.3)}{(0.000021)(45.3)} = 0.177$ ft/s

$\dfrac{U_D}{U_C} = \dfrac{\dot{m}_D/\rho_D}{\dot{m}_C/\rho_C} = \dfrac{12{,}400/63.5}{24{,}000/45.3} = 0.369$ The flooding correlation of Fig. 8.39 is too difficult to read for low values of U_D/U_C. Instead, use Eqs. (8-62) and (8-59).

From Eq. (8-62), with $U_C/U_D = 1/0.369 = 2.71$, (1)

$$\phi_{D_f} = \frac{\left[1+8(U_C/U_D)\right]^{1/2}-3}{4\left[(U_C/U_D)-1\right]} = \frac{\left[1+8(2.71)\right]^{1/2}-3}{4\left[2.71-1\right]} = 0.257$$

From Eq. (8-59), using $\phi_D = (\phi_D)_f = 0.257$,

$$\frac{U_D}{\phi_D} + \frac{U_C}{1-\phi_D} = \frac{U_D}{0.257} + \frac{U_C}{1-0.257} = u_o(1-\phi_D) = 0.177(1-0.257)$$

which simplifies to, $3.891U_D + 1.346U_C = 0.1315$ (2)

Solving Eqs. (1) and (2) simultaneously, $U_C = 0.0473$ ft/s and $U_D = 0.0175$ ft/s

Therefore, at flooding, $(U_D + U_C) = 0.0175 + 0.0473 = 0.0648$ ft/s

Size the column for 50% of flooding. Therefore, $(U_D + U_C) = 0.0648/2 = 0.0324$ ft/s

Total volumetric flow rate = $Q = 12{,}400/63.5 + 24{,}000/45.3 = 725$ ft^3/h $= 0.201$ ft^3/s

Column cross-sectional area = $A_C = Q/(U_D + U_C) = 0.201/0.0324 = 6.2$ ft^2

Column diameter = $D_C = (4A_C/\pi)^{1/2} = [4(6.2)/3.14]^{1/2} =$ 2.8 ft

Exercise 8.34 (continued)

Analysis: (continued)

Conditions of Exercise 8.30:
Flow rate of feed/raffinate = 21,000 lb/h. Flow rate of solvent/extract = 52,000 lb/h
Raffinate is dispersed.
The following properties are given in Exercise 8.30.
$\rho_R = \rho_D = 63.5$ lb/ft^3 and $\rho_E = \rho_C = 45.3$ lb/ft^3
$\mu_C = 1.0$ cP or 0.000021 lbf-s/ft^2
Interfacial tension = $\sigma_I = 13.5$ dyne/cm or 0.000924 lbf/ft

Assume $\dfrac{u_o \mu_C \rho_C}{\sigma_i \Delta\rho} = 0.01$

Therefore, $u_o = 0.01\dfrac{\sigma_i \Delta\rho}{\mu_C \rho_C} = 0.01\dfrac{(0.000924)(63.5-45.3)}{(0.000021)(45.3)} = 0.177$ ft/s

$\dfrac{U_D}{U_C} = \dfrac{\dot{m}_D/\rho_D}{\dot{m}_C/\rho_C} = \dfrac{21{,}000/63.5}{52{,}000/45.3} = 0.288$ The flooding correlation of Fig. 8.39 is too difficult to read for low values of U_D/U_C. Instead, use Eqs. (8-62) and (8-59).
From Eq. (8-62), with $U_C/U_D = 1/0.289 = 3.46$, (1)

$$\phi_{D_f} = \frac{\left[1+8(U_C/U_D)\right]^{1/2}-3}{4\left[(U_C/U_D)-1\right]} = \frac{\left[1+8(3.46)\right]^{1/2}-3}{4\left[3.46-1\right]} = 0.239$$

From Eq. (8-59), using $\phi_D = (\phi_D)_f = 0.239$,

$$\frac{U_D}{\phi_D} + \frac{U_C}{1-\phi_D} = \frac{U_D}{0.239} + \frac{U_C}{1-0.239} = u_o(1-\phi_D) = 0.177(1-0.239)$$

which simplifies to, $4.184U_D + 1.314U_C = 0.1347$ (2)
Solving Eqs. (1) and (2) simultaneously, $U_C = 0.0534$ ft/s and $U_D = 0.0154$ ft/s
Therefore, at flooding, $(U_D + U_C) = 0.0154 + 0.0534 = 0.0688$ ft/s
Size the column for 50% of flooding. Therefore, $(U_D + U_C) = 0.0688/2 = 0.0344$ ft/s
Total volumetric flow rate = $Q = 21{,}000/63.5 + 52{,}000/45.3 = 1{,}480$ ft^3/h = 0.411 ft^3/s
Column cross-sectional area = $A_C = Q/(U_D + U_C) = 0.411/0.0344 = 11.9$ ft^2
Column diameter = $D_C = (4A_C/\pi)^{1/2} = [4(11.9)/3.14]^{1/2} = 3.9$ ft

Exercise 8.35

Subject: Diameter of a Karr column for extraction of benzoic acid (A) from water (C) by toluene (S).

Given: Conditions in Exercise 8.33.

Find: Column diameter.

Analysis:

Volumetric flow rate of feed/raffinate = 500 gal/min
Volumetric flow rate of solvent/extract = 750 gal/min
Extract is dispersed.
The following properties are given in Exercise 8.30.
$\rho_R = \rho_D = 0.860(62.4) = 53.7$ lb/ft^3 and $\rho_E = \rho_C = 0.995(62.4) = 62.1$ lb/ft^3
$\mu_C = 0.95$ cP or 0.000020 lbf-s/ft^2
Interfacial tension = $\sigma_I = 22$ dyne/cm or 0.0015 lbf/ft

Assume $\dfrac{u_o \mu_C \rho_C}{\sigma_i \Delta\rho} = 0.01$

Therefore, $u_o = 0.01\dfrac{\sigma_i \Delta\rho}{\mu_C \rho_C} = 0.01\dfrac{(0.0015)(62.1-53.7)}{(0.000020)(62.1)} = 0.101$ ft/s

$\dfrac{U_D}{U_C} = \dfrac{Q_D}{Q_C} = \dfrac{750}{500} = 1.50$ From Fig. 8.39, $\dfrac{(U_D + U_C)_f}{u_o} = 0.27$

Therefore, $(U_D + U_C)_f = 0.27\ u_o = 0.27(0.101) = 0.0273$ ft/s

Size the column for 50% of flooding. Therefore, $(U_D + U_C) = 0.0273/2 = 0.0137$ ft/s
Total volumetric flow rate = Q =(500 + 750)(60)/7.48 = 10,030 ft^3/h = 2.79 ft^3/s
Column cross-sectional area = $A_C = Q/(U_D + U_C) = 2.79/0.0137 = 204$ ft^2
Column diameter = $D_C = (4A_C/\pi)^{1/2} = [4(204)/3.14]^{1/2} = 16.1$ ft

From Table 8.2, maximum Karr diameter is 1.5 m or 4.9 ft. Therefore, need multiple Karr columns in parallel of maximum cross-sectional area = $(A_c)_{\max} = \dfrac{\pi D^2}{4} = \dfrac{3.14(4.9)^2}{4} = 18.8$ ft^2

Therefore, need 204/18.8 = 11 units in parallel of 1.5 m diameter each.

Would probably be better to specify one RDC column of 16.1 ft diameter or 5 m , which is less than the maximum diameter of 8 m.

Exercise 8.36

Subject: HETS of an RDC column for extraction of acetic acid (A) from water (C) by isopropyl ether (S).

Given: Conditions in Exercises 8.28, 8.30, and 8.34.

Find: HETS.

Analysis: From Fig. 8.40, for an interfacial tension of 13.5 dyne/c from Exercise 8.30,

$$\frac{\text{HETS}}{D_T^{1/3}} = 4 \quad \text{with HETS and } D_T \text{ in inches.}$$

From Exercise 8.34, for the conditions of Exercise 8.28, D_T = 2.8 ft or 33.6 inches.
Therefore, HETS = $4(33.6)^{1/3}$ = 12.9 inches.

From Exercise 8.34, for the conditions of Exercise 8.30, D_T = 3.9 ft or 46.8 inches.
Therefore, HETS = $4(46.8)^{1/3}$ = 14.4 inches.

Exercise 8.37

Subject: HETS of a Karr column for extraction of benzoic acid (A) from water (C) by toluene (S).

Given: Conditions in Exercises 8.32 and 8.35.

Find: HETS.

Analysis: From Fig. 8.40, for an interfacial tension of 22 dyne/c from Exercise 8.33,

$$\frac{\text{HETS}}{D_T^{1/3}} = 5 \quad \text{with HETS and } D_T \text{ in inches.}$$

From Exercise 8.35, D_T = 4.9 ft or 58.8 inches.
Therefore, HETS = $5(58.8)^{1/3}$ = 19.4 inches.

Exercise 9.1

Subject: Selection of type condenser and operating pressure for distillation of propionic and n-butyric acids.

Given: Distillate of 95 mol% propionic acid. Bottoms of 98 mol% n-butyric acid.

Assumptions: Ideal solutions so that Raoult's *K*-values apply.

Find: type condenser and operating pressure

Analysis: From Perry's Handbook or other source, the normal boiling points are:

Propionic acid	141.1°C
n-Butyric acid	163.5°C

Using Fig. 7.16, an operating pressure of 30 psia or less, with a total condenser, might be used. Could also consider using subcooled reflux with a top pressure of just above atmospheric pressure.

Exercise 9.2

Subject: Selection of type condenser and operating pressure for distillation of a mixture of light paraffin hydrocarbons in two columns

Given: Feed and product compositions as follows:

	kmol/h:			
Component	**Feed**	**Product 1**	**Product 2**	**Product 3**
C_1	160	160	0	0
C_2	370	365	5	0
C_3	240	5	230	5
nC_4	25	0	1	24
nC_5	5	0	0	5
Total:	800	530	236	34

Find: Type condensers and operating pressures for:
(a) Direct sequence.
(b) Indirect sequence.

Analysis: Use Chemcad or other simulator to make the bubble-point and dew-point calculations, using the SRK equation of state. The results should be close to hand calculations using *K*-values from Figs. 2.8 and 2.9. Use Fig. 7.16 to determine pressure and type condenser.

Column 1 of direct sequence:

Distillate is Product 1. Can not condense at 120°F because this temperature is above the critical temperatures of methane and ethane. At 415 psia, the dew point temperature is 16°F. Therefore, use a partial condenser with a refrigerant boiling at a temperature of about 6°F. One choice of refrigerant is propane. Bottoms temperature would not be in the decomposition range.

Column 2 of direct sequence:

Distillate is Product 2, which is mainly propane. Bubble-point pressure at 120°F is 256 psia, which is greater than 215 psia. Dew-point pressure at 120°F is 248 psia. Use partial condenser with about 250 psia pressure at the top. Use cooling water in the condenser. Bottoms conditions present no problems.

Column 1 of indirect sequence:

Distillate is a mixture of Products 1 and 2. At 120°F, pressure is very high, even for a partial condenser. Dew-point temperature at 415 psia is 83°F. Raise pressure a little and use cooling water in the condenser. Bottoms conditions present no problems.

Column 2 of indirect sequence:

Conditions at the top are the same as Column 1 of the direct sequence. Therefore, use a partial condenser with a refrigerant for removing heat at 16°F.

Exercise 9.3

Subject: Selection of type condenser and operating pressure for the distillation of a mixture of methane, ethane, benzene, and toluene by the direct sequence in two columns.

Given: Feed and product conditions as follows from Fig. 9.20:

kmol/h:

Component	Feed	Product 1	Product 2	Product 3
Methane	20	20.000	0.000	0.0
Ethane	5	4.995	0.005	0.0
Benzene	500	5.000	485.000	10.0
Toluene	100	0.000	0.500	99.5
Total:	625	29.995	485.505	109.5

Find: Type condenser and operating pressure in each column.

Analysis: Use Chemcad or other simulator to make the bubble-point and dew-point calculations, with the SRK equation of state. Use Fig. 7.16 to determine pressure and type condenser.

Column 1:

Distillate is Product 1. Bubble point on Product 1 at 120°F gives an impossible very high pressure because the critical temperatures of methane and ethane are less than 120°F. A dew point on Product 1 at 120°F gives 31.4 psia because of the presence of benzene. Therefore, can use a partial condenser with cooling water. No problems occur at the bottom.

Column 2:

Distillate is Product 2. Bubble point on Product at 120°F gives 5.1 psia. No need to operate at a vacuum. Raise condenser pressure to 30 psia or just above atmospheric pressure and use a total condenser, possibly with subcooled reflux. No problems at the column bottom.

Exercise 9.4

Subject: Number of equilibrium stages for a deethanizer.

Given: Deethanizer with feed and average relative volatilities as follows from Fig. 9.21:

Component	Feed, kmol/h	Avg. Relative volatility
C_1	160	8.22
C_2	370	2.42
C_3	240	1.00
nC_4	25	0.378
nC_5	5	0.150

Distillate is to contain 2 kmol/h of C_3. Bottoms is to contain 2 kmol/h of C_2. Therefore, LK is C_2 and HK is C_3.

Assumptions: Relative volatilities are relative to C_3.

Find: Number of equilibrium stages for 2.5 times minimum number of stages.

Analysis: To compute the minimum number of stages, use component flow rate form of the Fenske equation given by (9-12):

$$N_{\min} = \frac{\log\left[\left(\frac{d_{C_2}}{d_{C_3}}\right)\left(\frac{b_{C_3}}{b_{C_2}}\right)\right]}{\log \alpha_{C_2,C_3}} = \frac{\log\left[\left(\frac{370-2}{2}\right)\left(\frac{240-2}{2}\right)\right]}{\log 2.42} = 11.3$$

$$N = 2.5N_{\min} = 2.5(11.3) = 28.3$$

Exercise 9.5

Subject: Determination of the minimum number of stages by the Fenske equation for each of three sections in a distillation column with a vapor sidestream

Given: The following feed and product compositions for a distillation column:

kmol/h:

Component	Feed	Distillate	Vapor sidestream	Bottoms
Benzene, B	260	257.0	3.0	0.0
Toluene, T	80	0.1	79.4	0.5
Biphenyl, BP	5	0.0	0.2	4.8
Pressure, kPa	165	130	180	200

Assumptions: Raoult's law for *K*-values.

Find: Using the Fenske equation, the minimum number of stages for sections between:

(a) Distillate and feed.

(b) Feed and vapor sidestream.

(c) Sidestream and bottoms.

Analysis: (a) For this section, take the LK as benzene and the HK as toluene. At the top, have almost pure benzene at 130 kPa = 19 psia. Therefore, from Fig. 2.4, the distillate temperature = boiling point of benzene at 19 psia = 195°F. At the feed point, the pressure = 165 psia = 23.9 psia. Assume a saturated liquid feed. The bubble-point temperature is estimated to be 215° F. Take an average temperature = 205°F, at which the vapor pressures for benzene and toluene, respectively, are 23 psia and 9 psia respectively. From Eq. (2-44), the corresponding *K*-values at the average section pressure of 21.5 psia are 1.07 and 0.42. The relative volatility, from Eq. (2-21) = 1.07/0.42 = 2.55. From the Fenske equation (9-12), applied between the distillate and feed compositions:

$$N_{\min} = \frac{\log\left[\left(\frac{d_B}{d_T}\right)\left(\frac{f_T}{f_B}\right)\right]}{\log \alpha_{B,T}} = \frac{\log\left[\left(\frac{257}{0.1}\right)\left(\frac{80}{260}\right)\right]}{\log 2.55} = 7.1 \text{ stages}$$

(b) For the section between the feed and the vapor sidestream, again take the LK as benzene and the HK as toluene. The pressure at the vapor sidestream = 180 kPa = 26.1 psia. A dew-point on the vapor sidestream gives a temperature of 265°F. Assume an average temperature for the section of 240°F, at which the vapor pressures for benzene and toluene, respectively, are 37 psia and 16 psia respectively. From Eq. (2-44), the corresponding *K*-values at the average section pressure of 25 psia are 1.48 and 0.64. The relative volatility, from Eq. (2-21) = 1.48/0.64 = 2.31.

Exercise 9.5 (continued)

Analysis: (b) (continued)

From the Fenske equation (9-12), applied between the feed and vapor sidestream compositions:

$$N_{min} = \frac{\log\left[\left(\frac{f_B}{f_T}\right)\left(\frac{vs_T}{vs_B}\right)\right]}{\log \alpha_{B,T}} = \frac{\log\left[\left(\frac{260}{80}\right)\left(\frac{79.4}{3}\right)\right]}{\log 2.31} = 5.3 \text{ stages}$$

(c) In the section between the vapor sidestream and bottoms, take toluene as the LK and biphenyl as the HK. At the bottom of the column, the pressure = 200 kPa = 29 psia. Biphenyl boils at 255°C = 491°F at 14.7 psia, which is much higher than toluene. From Perry's Handbook, the following vapor pressure data are obtained for biphenyl:

T, °F	243	274	307	165.2	329	400	445
Vapor pressure, psia	0.19	0.39	0.77	1.16	1.93	3.87	7.74

A bubble point on the bottoms pressure gives 465°F. At this temperature, the relative volatility, $\alpha_{T,BP}$ = vapor pressure of T/vapor pressure of BP = 220/10.6 = 20.8.
At the temperature of the vapor sidestream, 265°F, $\alpha_{T,BP}$ = vapor pressure of T/vapor pressure of BP = 27.9/0.37 = 75.4. Use a geometric mean for this wide range. Thus, $\alpha_{T,BP} = [20.8(75.4)]^{1/2} = 40$.
From the Fenske equation (9-12), applied between the vapor sidestream and bottoms compositions:

$$N_{min} = \frac{\log\left[\left(\frac{vs_T}{vs_{BP}}\right)\left(\frac{b_{BP}}{b_T}\right)\right]}{\log \alpha_{B,T}} = \frac{\log\left[\left(\frac{79.4}{0.2}\right)\left(\frac{4.8}{0.5}\right)\right]}{\log 40} = 2.3 \text{ stages}$$

Exercise 9.6

Subject: Comparison of minimum number of stages by Fenske equation and McCabe-Thiele method for a non-ideal system of acetone (A) and water (W).

Given: A feed of 25 mol% A and 75 mol% W. Distillation at 130 kPa (975 torr) to obtain a distillate of 95 mol% A and a bottoms of 2 mol% A. Infinite-dilution liquid-phase activity coefficients of 8.12 for acetone and 4.13 for water.

Find: Minimum stages by the Fenske equation and by the McCabe-Thiele method.

Analysis: Because the pressure is close to 1 atm, estimate vapor-liquid equilibria from the modified Raoult's law, Eq. (4) in Table 2.3. Obtain vapor pressures from Antoine equations and liquid-phase activity coefficients over the entire composition range from fitting the infinite-dilution coefficients to the van Laar equation, Eq. (3) in Table 2.9, using Eqs. (2-75). Thus,

$$K_A = \frac{y_A}{x_A} = \frac{\gamma_A P_A^s}{P} \quad (1) \quad \text{and} \quad K_W = \frac{y_W}{x_W} = \frac{\gamma_W P_W^s}{P} \quad (2)$$

$$\gamma_A = \exp \frac{A_{AW}}{\left[1 + \frac{x_A A_{WA}}{x_W A_{AW}}\right]^2} \quad (3) \quad \text{and} \quad \gamma_W = \exp \frac{A_{WA}}{\left[1 + \frac{x_W A_{AW}}{x_A A_{WA}}\right]^2} \quad (4)$$

$$A_{AW} = \ln \gamma_A^\infty = \ln(8.12) = 2.094$$

$$A_{WA} = \ln \gamma_W^\infty = \ln(4.13) = 1.418$$

Substituting these van Laar coefficients into Eqs. (3) and (4),

$$\gamma_A = \exp \frac{2.094}{\left[1 + 1.477 \frac{x_A}{(1 - x_A)}\right]^2} \quad (5) \quad \text{and} \quad \gamma_W = \exp \frac{1.418}{\left[1 + 0.6772 \frac{(1 - x_A)}{x_A}\right]^2} \quad (6)$$

From the 7th edition of Perry's Chemical Engineers' Handbook, page 13-21,

$$\log P_A^s = 7.11714 - \frac{1210.595}{T + 229.664} \quad (7) \quad \text{and} \quad \log P_W^s = 8.07131 - \frac{1730.630}{T + 233.426} \quad (8)$$

where P_i^s = vapor pressure of component i in torr and $T = {}^\circ\text{C}$

<u>Minimum stages by the Fenske equation:</u>

First determine the relative volatilities at the top and bottom and take the geometric average for use in the Fenske equation.

Exercise 9.6 (continued)

Analysis: Fenske equation (continued)

Bubble point for the distillate composition.

From Eqs. (4-12), (1), and (2): $$\sum_i x_{D_i} K_i = \sum_i x_{D_i} \frac{\gamma_i P_i^s}{P} = 1 \qquad (9)$$

In the distillate, $x_A = 0.95$ and $x_W = 0.05$. From Eqs. (3) and (4),

$$\gamma_A = \exp\frac{2.094}{\left[1+\frac{(0.95)2.094}{(0.05)1.418}\right]^2} = 1.003 \quad \text{and} \quad \gamma_W = \exp\frac{1.418}{\left[1+\frac{(0.05)1.418}{(0.95)2.094}\right]^2} = 3.75$$

Eq. (9) becomes: $0.95\left(\frac{1.003P_A^s}{975}\right)+0.05\left(\frac{3.75P_A^s}{975}\right)=1$ where vapor pressure is in torr.

Using Eqs. (7) and (8) with a spreadsheet, a trial and error calculation gives a distillate temperature of 64°C. Then from Eqs. (1) and (2), $\alpha_{A,W} = K_A/K_W = 1.48$

Bubble point for the bottoms composition.

In the bottoms, $x_A = 0.02$ and $x_W = 0.98$. From Eqs. (3) and (4),

$$\gamma_A = \exp\frac{2.094}{\left[1+\frac{(0.02)2.094}{(0.98)1.418}\right]^2} = 7.19 \quad \text{and} \quad \gamma_W = \exp\frac{1.418}{\left[1+\frac{(0.98)1.418}{(0.02)2.094}\right]^2} = 1.001$$

Eq. (9) becomes: $0.02\left(\frac{7.19P_A^s}{975}\right)+0.98\left(\frac{1.001P_A^s}{975}\right)=1$ where vapor pressure is in torr.

Using Eqs. (7) and (8) with a spreadsheet, a trial and error calculation gives a distillate temperature of 95°C. Then from Eqs. (1) and (2), $\alpha_{A,W} = K_A/K_W = 27.7$

The geometric mean relative volatility = $[(1.48)(27.7)]^{1/2} = 6.40$

From the Fenske equation (9-11), $$N_{min} = \frac{\log\left[\left(\frac{x_{D_A}}{x_{B_A}}\right)\left(\frac{x_{B_W}}{x_{D_W}}\right)\right]}{\log \alpha_{A,W}} = \frac{\log\left[\left(\frac{0.95}{0.02}\right)\left(\frac{0.98}{0.05}\right)\right]}{\log 6.40} = 3.7$$

Minimum stages by the McCabe-Thiele method:

To obtain a *y-x* equilibrium curve at 975 torr in terms of acetone mole fractions, we can run bubble-point temperature calculations, as above, for a set of points in the range of liquid compositions between the distillate and bottoms compositions. For each point, the *K*-value and vapor mole fraction for acetone are computed from Eq. (1). The results from a spreadsheet are as follows:

Exercise 9.6 (continued)

Analysis: McCabe-Thiele method (continued)

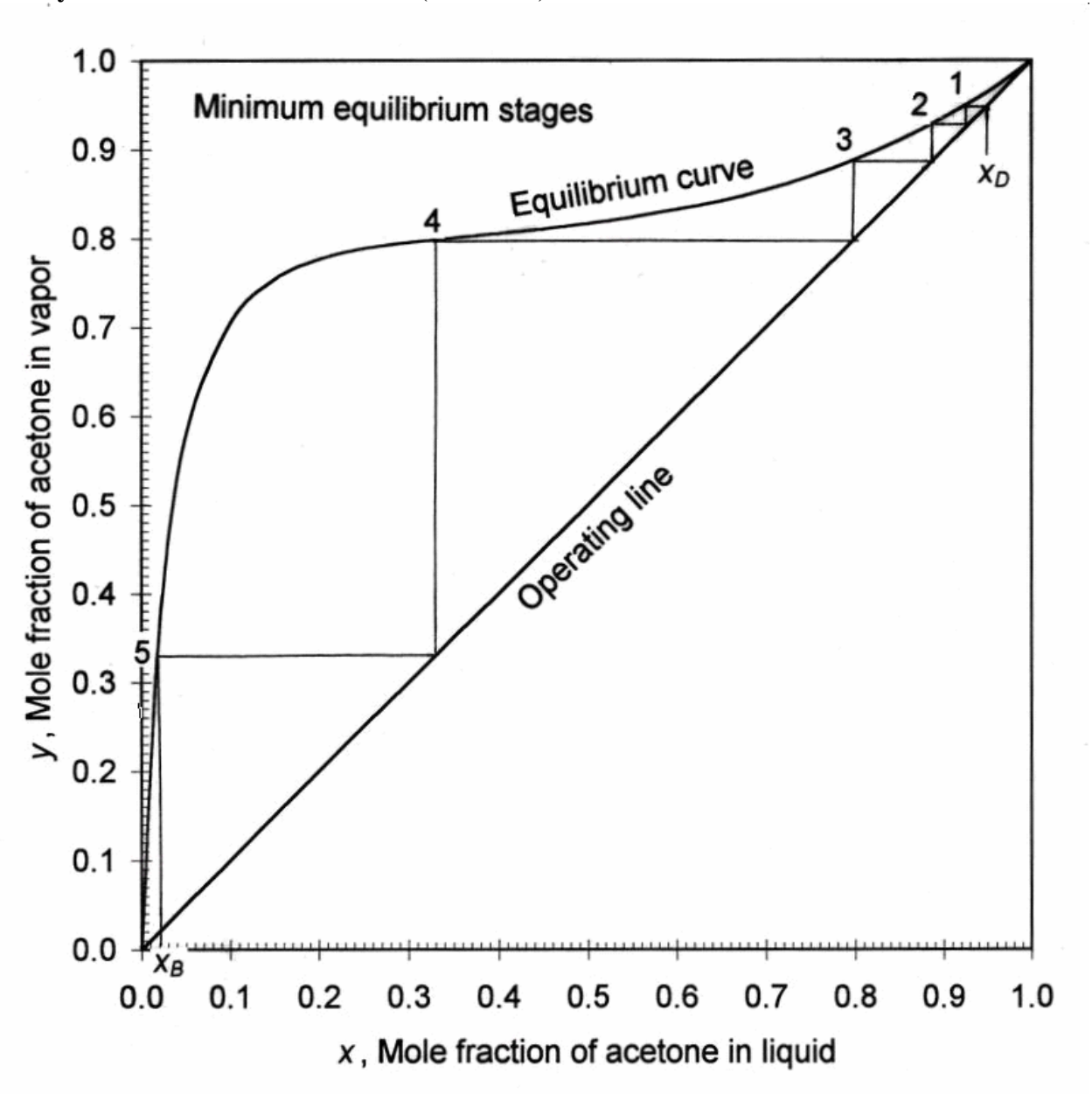
T, °C	y_A	x_A
63.6	1.000	1.000
64.0	0.965	0.950
64.5	0.936	0.900
65.0	0.911	0.850
65.5	0.889	0.800
66.0	0.870	0.750
66.5	0.855	0.700
67.0	0.842	0.650
67.5	0.833	0.600
67.9	0.824	0.550
68.3	0.817	0.500
68.6	0.811	0.450
68.9	0.806	0.400
69.2	0.801	0.350
69.6	0.796	0.300
70.2	0.789	0.250
71.2	0.777	0.200
73.1	0.754	0.150
76.8	0.705	0.100
84.9	0.578	0.050
95.1	0.361	0.020
107.1	0.000	0.000

The McCabe-Thiele plot for these data are shown on the next page. The equilibrium stages for total reflux are stepped off between the equilibrium curve and the 45°line, which represents the operating line, from the acetone $x_D = 0.95$ down to the acetone $x_B = 0.02$.

From the plot, there are 5 minimum stages, which is 35% higher than the 3.7 minimum stages computed from the Fenske equation. The Fenske equation is not reliable for highly nonideal binary systems.

Exercise 9.6 (continued)

Analysis: McCabe-Thiele method (continued)



Exercise 9.7

Subject: Minimum equilibrium stages and distribution of nonkey components using the Fenske equation for distillation of a paraffin hydrocarbon mixture.

Given: Column pressure of 700 kPa. Feed composition and split for two key components in Fig. 9.23. *K*-values from Figs. 2.8 and 2.9.

Find: Minimum number of equilibrium stages.
Distribution of nonkey components at total reflux.

Analysis: To apply the Fenske equation, the geometric mean relative volatility between the distillate and bottoms is needed. From the following crude estimate of the split of all nonkey components, compute the bubble-point temperatures of the distillate and bottoms and use the *K*-values at those temperatures to get the relative volatilities. Use the bubble-point equation, Eq. (4-12). The following results are obtained for a distillate bubble point of 68°F (20°C) and a bottoms bubble point of 257°F (125°C):

Component	Feed, kmol/h	Distillate, kmol/h	*K*-value, distillate	Kx_D	Bottoms, kmol/h	*K*-value, bottoms	Kx_B
Propane	2500	2500	1.250	0.8895	0	5.70	
Isobutane	400	399	0.490	0.0557	1	3.25	0.0078
n-Butane	600	594	0.340	0.0575	6	2.65	0.0382
Isopentane	100	15	0.138	0.0006	85	1.45	0.2955
n-Pentane	200	5	0.108	0.0002	195	1.23	0.5751
n-Hexane	40	0	0.038		40	0.65	0.0623
n-Heptane	50	0	0.013		50	0.33	0.0222
n-Octane	40	0	0.005		40	0.19	0.0177
Total	3930	3513		1.0035	417		1.0188

For the two key components, nC_4 and iC_5, the relative volatilities at the top and bottom are, respectively (0.34/0.138) = 2.46 and (2.65/1.45) = 1.83. The geometric mean $\alpha_{nC4,iC5} = [(2.46)(1.83)]^{1/2} = 2.12$. From the Fenske equation, (9-12),

$$N_{min} = \frac{\log\left[\left(\frac{d_{nC_4}}{d_{iC_5}}\right)\left(\frac{b_{iC_5}}{b_{nC_4}}\right)\right]}{\log \alpha_{nC_4,iC_5}} = \frac{\log\left[\left(\frac{594}{6}\right)\left(\frac{85}{15}\right)\right]}{\log 2.12} = 8.4$$

To compute the distribution of nonkey components at total reflux, use for the lighter than light key components, LLK, Eq. (9-15), and use Eq. (9-16) for the heavier than heavy key, HHK, with iC_5 as the reference component, *r*, and the above value of N_{min}.

Exercise 9.7 (continued)

Analysis: (continued)

Thus, for the LLK, i, $$b_i = \frac{f_i}{1+\left(\frac{d_{iC_5}}{b_{iC_5}}\right)\alpha_{i,iC_5}^{N_{min}}} = \frac{f_i}{1+\left(\frac{15}{85}\right)\alpha_{i,iC_5}^{8.4}} \qquad (1)$$

For the HHK, i, $$d_i = \frac{f_i\left(\frac{d_{iC_5}}{b_{iC_5}}\right)\alpha_{i,iC_5}^{N_{min}}}{1+\left(\frac{d_{iC_5}}{b_{iC_5}}\right)\alpha_{i,iC_5}^{N_{min}}} = \frac{f_i\left(\frac{15}{85}\right)\alpha_{i,iC_5}^{8.4}}{1+\left(\frac{15}{85}\right)\alpha_{i,iC_5}^{8.5}} \qquad (2)$$

Using the above K-values to compute geometric mean values of $\alpha_{i,\,iC5}$, followed by use of Eqs. (1) and (2) with the material balance, $f_i = d_i + b_i$, the following results are obtained:

Component	$\alpha_{i,\,iC5}$ at top	$\alpha_{i,\,iC5}$ at bottom	$\alpha_{i,\,iC5}$ average	d_i, kmol/h	b_i, kmol/h
Propane	9.06	3.93	5.97	2499.996	4.2×10^{-3}
Isobutane	3.55	2.24	2.82	399.63	0.37
n-Butane				594	6
Isopentane	1.00	1.00		15	85
n-Pentane	0.783	0.848	0.815	6.12	193.88
n-Hexane	0.272	0.448	0.349	0.001	39.999
n-Heptane	0.094	0.228	0.146	8.2×10^{-7}	50
n-Octane	0.038	0.128	0.070	1.92×10^{-10}	40

Exercise 9.8

Subject: Type condenser and operating pressure. Minimum equilibrium stages and distribution of nonkey components using the Fenske equation for distillation of a light hydrocarbon mixture.

Given: Feed composition and split of two key components in Fig. 9.24. *K*-values from Figs. 2.8 and 2.9.

Find: Type condenser.
Operating pressure.
Minimum equilibrium stages.
Distribution of nonkey components at total reflux.

Analysis: To determine the type condenser and operating pressure, follow the algorithm in Fig. 7.16. The estimated distillate and bottoms compositions from the given data are:

Component	Feed, lbmol/h	Distillate, lbmol/h	Bottoms, lbmol/h
Methane	1000	1000	0
Ethylene	2500	2500	0
Ethane	2000	1999	1
Propylene	200	5	195
Propane	100	0	100
n-Butane	50	0	50

Using Fig. 2.8, it is quickly shown that at 120°F, both the bubble-point and the dew-point pressures for the estimated distillate composition are greater than 1000 psia because the *K*-value for ethane is greater than 1.0 at 120°F and 1000 psia. Therefore, select the operating pressure as 415 psia and use a partial condenser.
Run a dew point on the distillate at 415 psia. Use Eq. (4-13) in the following form:

$$\sum_i \frac{d_i}{K_i} = D = \frac{1000}{K_{C_1}} + \frac{2500}{K_{C_2^=}} + \frac{1999}{K_{C_2}} + \frac{5}{K_{C_3^=}} = 5504 \qquad (1)$$

By trial and error, using Fig. 2.9 for *K*-values, the temperature that satisfies Eq. (1) is 0°F, which gives:

$$\sum_i \frac{d_i}{K_i} = D = \frac{1000}{5.0} + \frac{2500}{1.05} + \frac{1999}{0.69} + \frac{5}{0.18} = 5505$$

The relative volatility of the two key components is $\alpha_{C2,\,C3=} = 0.69/0.18 = 3.83$

Exercise 9.8 (continued)

Analysis: (continued)

Now run a bubble-point on the estimated bottoms composition at 415 psia. Use Eq. (4-12) in the following form: $\sum_i b_i K_i = B = K_{C_2} + 195K_{C_3^=} + 100K_{C_3} + 50K_{nC_4} = 346$ (2)

By trial and error, using Fig. 2.8 for *K*-values, the temperature that satisfies Eq. (1) is 155°F, which gives: $\sum_i b_i K_i = B = 2.7 + 195(1.15) + 100(1.01) + 50(0.39) = 347$

The relative volatility of the two key components is $\alpha_{C2,\,C3=} = 2.7/1.15 = 2.35$

The geometric mean relative volatility = $[(3.83)(2.35)]^{1/2} = 3.0$

From the Fenske equation, (9-12),

$$N_{min} = \frac{\log\left[\left(\frac{d_{C_2}}{d_{C_3^=}}\right)\left(\frac{b_{C_3^=}}{b_{C_2}}\right)\right]}{\log \alpha_{C_2,C_3^=}} = \frac{\log\left[\left(\frac{1999}{5}\right)\left(\frac{195}{1}\right)\right]}{\log 3.0} = 10.3$$

To compute the distribution of nonkey components at total reflux, use for the lighter than light key components, LLK, Eq. (9-15), and use Eq. (9-16) for the heavier than heavy key, HHK, with $C_3^=$ as the reference component, *r*, and the above value of N_{min}.

Thus, for the LLK, *i*, $b_i = \frac{f_i}{1+\left(\frac{d_{C_3^=}}{b_{C_3^=}}\right)\alpha_{i,C_3^=}^{N_{min}}} = \frac{f_i}{1+\left(\frac{5}{195}\right)\alpha_{i,C_3^=}^{10.3}}$ (3)

For the HHK, *i*, $d_i = \frac{f_i\left(\frac{d_{C_3^=}}{b_{C_3^=}}\right)\alpha_{i,C_3^=}^{N_{min}}}{1+\left(\frac{d_{C_3^=}}{b_{C_3^=}}\right)\alpha_{i,C_3^=}^{N_{min}}} = \frac{f_i\left(\frac{5}{195}\right)\alpha_{i,C_3^=}^{10.3}}{1+\left(\frac{5}{195}\right)\alpha_{i,C_3^=}^{10.3}}$ (4)

Using the above *K*-values to compute geometric mean values of $\alpha_{i,\,C3=}$, followed by use of Eqs. (3) and (4) with the material balance, $f_i = d_i + b_i$, the following results are obtained:

Component	$\alpha_{i,\,C3=}$ at top	$\alpha_{i,\,C3=}$ at bottom	$\alpha_{i,\,C3=}$ average	d_i, lbmol/h	b_i, lbmol/h
Methane	27.8	8.70	15.55	1000	2.1×10^{-8}
Ethylene	5.83	3.22	4.33	2499.973	0.027
Ethane	3.83	2.35	3.00	1999	1
Propylene	1.00	1.00	1.00	5	195
Propane	0.78	0.88	0.83	0.375	99.625
n-Butane	0.18	0.34	0.25	8.1×10^{-7}	50

Exercise 9.9

Subject: Recovery of a key component as a function of distillate flow rate for the distillation of a paraffin hydrocarbon mixture when the minimum number of equilibrium stages is fixed.

Given: Feed composition and flow rate of 1000 lbmol/h. Column pressure of 250 psia. Minimum equilibrium stages = 15. *K*-values from Figs. 2.8 and 2.9.

Find: Percent recovery of propane in the distillate as a function of distillate flow rate.

Analysis: Assume that the average relative volatility between propane and n-butane is not sensitive to the separation. If a perfect separation were made between propane and n-butane at 250 psia, the distillate temperature would be approximately 110°F and the bottoms temperature would be approximately 270°F. Assume an average temperature of 190°F. From Fig. 2.8, the *K*-values and relative volatilities at 250 psia and 190°F, with the light key as propane and the heavy key as n-butane are:

Component	Feed rate, lbmol/h	K-value	α referred to nC_4
Ethane	30	4.3	5.97
Propane	200	1.74	2.42
n-Butane	370	0.72	1.00
n-Pentane	350	0.30	0.417
n-Hexane	50	0.133	0.185
Total:	1000		

Based on these relative volatility values, assume that little of the nonkey components will distribute. Therefore, $D = d_{C_2} + d_{C_3} + d_{nC_4} + d_{nC_5} + d_{nC_6} = 30 + d_{C_3} + d_{nC_4}$ (1)

The Fenske equation, (9-12) becomes:

$$N_{min} = 15 = \frac{\log\left[\frac{d_{C_3}}{d_{nC_4}}\frac{b_{nC_4}}{b_{C_3}}\right]}{\log\left(\alpha_{C_3,nC_4}\right)_{avg}} = \frac{\log\left[\frac{d_{C_3}}{d_{nC_4}}\left(\frac{370-d_{nC_4}}{200-d_{C_3}}\right)\right]}{\log 2.42}$$

Rearranging, $\frac{370-d_{nC_4}}{d_{nC_4}} = \left(\frac{200-d_{C_3}}{d_{C_3}}\right)2.42^{15} = 571800\left(\frac{200-d_{C_3}}{d_{C_3}}\right)$ (2)

Assume a value of *d* for C_3. Calculate *d* for nC_4 from Eq. (2). Then compute *D* from Eq. (1).

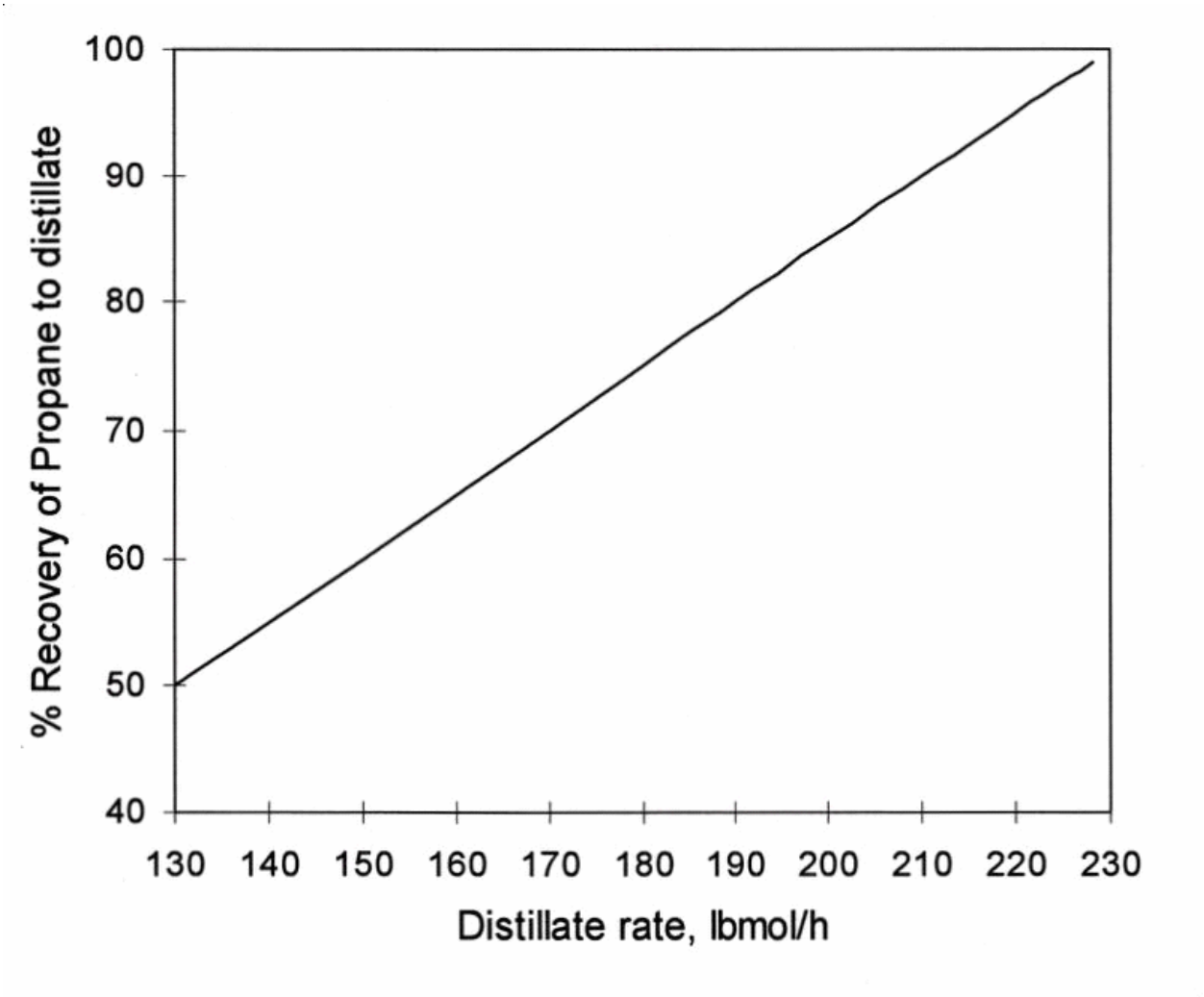
Then compute recovery of $C_3 = d$ for $C_3/200$ and make plot.

Exercise 9.9 (continued)

Analysis: (continued)

d of C_3, lbmol/h	% recovery of C_3	*d* of nC_4, lbmol/h	*D*, lbmol/h
198	99	0.064	228.1
190	95	0.012	220.0
180	90	0.006	210.0
150	75	0.002	180.0
100	50	0.00065	130.0

We see that with 15 minimum stages, the distribution of nC_4 to the distillate is almost negligible.



Exercise 9.10

Subject: Minimum reflux ratio by the Underwood equation for the separation of a binary mixture as a function of feed vaporization.

Given: Binary feed of 30 mol% propane and 70 mol% propylene. Distillate to contain 99 mol% propylene, and bottoms to contain 98 mol% propane. Column pressure of 300 psia. *K*-values in Figs. 2.8 and 2.9.

Find: Minimum reflux ratio by the Underwood equation for:

(a) Bubble-point liquid feed.
(b) Feed of 50 mol% vapor.
(c) Dew-point vapor feed.

Analysis:

Because we have a binary mixture, this is a Class I separation, where all components distribute. Therefore, the Underwood equation that applies is (9-20):

$$\frac{L_{\min}}{D} = \frac{\left[\left(\frac{x_{C_3^=,D}}{x_{C_3^=,\infty}}\right) - \alpha_{C_3^=,C_3}\left(\frac{x_{C_3,D}}{x_{C_3,\infty}}\right)\right]}{\alpha_{C_3^=,C_3} - 1} = \frac{\left[\left(\frac{0.99}{x_{C_3^=,\infty}}\right) - \alpha_{C_3^=,C_3}\left(\frac{0.01}{x_{C_3,\infty}}\right)\right]}{\alpha_{C_3^=,C_3} - 1} \qquad (1)$$

(a) For a bubble-point liquid feed, the liquid-phase mole fractions in the pinch zone are those of the total feed. Thus, $x_{C_3^=,\infty} = 0.70$ and $x_{C_3,\infty} = 0.30$. The relative volatility is that at the pinch. A bubble-point temperature on the feed composition at 300 psia gives 126°F, with $\alpha = 1.035/0.92 = 1.125$. Substitution in Eq. (1) gives $L_{\min}/D = 11.0$

(b) For 50 mol% vaporization, a flash gives about the same temperature of 126°F, and therefore the same α, with liquid-phase mole fractions of 0.688 for propylene and 0.312 for propane. Substitution into Eq. (1) gives $L_{\min}/D = 11.2$.

(c) For a dew-point feed, the temperature still is 126°F, with liquid-phase mole fractions of 0.68 for propylene and 0.32 for propane. Substitution into Eq. (1) gives $L_{\min}/D = 11.4$

Because the relative volatility is close to 1, the % vaporization of the feed has only a small effect on the minimum reflux ratio.

Exercise 9.11

Subject: Minimum reflux rate and distribution of nonkey components for the distillation of a paraffin hydrocarbon mixture.

Given: Column pressure of 700 kPa. Feed composition and split for two key components in Fig. 9.23. Feed is a bubble-point liquid. *K*-values from Figs. 2.8 and 2.9.

Find: Minimum external reflux rate.
Distribution of nonkey components at minimum reflux ratio.

Analysis: Because of the wide range of volatility of the components in the feed, and the relative sharpness of the separation between the LK, n-butane, and the HK, isopentane, assume a Class 2 separation for estimating the minimum reflux ratio by the method of Underwood. Compute the minimum reflux using relative volatilities at the feed temperature. Because the feed is at the bubble point, use Eq. (4-12). For the pressure of 700 kPa (102 psia), a trial-and-error calculation for the bubble-point temperature gives the following results for 80^{o}F, where nC_8 is by extrapolation:

Component	z, feed mole fraction	K at 102 psia and 80^{0}F	Kz	α referred to iso-pentane
Propane	0.6361	1.37	0.8715	8.56
iso-Butane	0.1018	0.56	0.0570	3.50
n-Butane	0.1527	0.39	0.0596	2.44
iso-Pentane	0.0254	0.16	0.0041	1.00
n-Pentane	0.0509	0.12	0.0061	0.75
n-Hexane	0.0102	0.038	0.0004	0.24
n-Heptane	0.0127	0.013	0.0002	0.081
n-Octane	0.0102	0.004	0.0000	0.025
Total:	1.0000		0.9989	

The Underwood equations that apply are Eqs. (9-28) and (9-29). For a bubble-point feed, $1 - q = 0$ and Eq. (9-28) becomes:

$$\sum_i \frac{\alpha_{i,r} z_{i,F}}{\alpha_{i,r} - \theta} = 1 - q = 0 = \frac{8.56(0.6361)}{8.56-\theta} + \frac{3.5(0.1018)}{3.5-\theta} + \frac{2.44(0.1527)}{2.44-\theta} + \frac{1.0(0.0254)}{1.0-\theta} + \frac{0.75(0.0509)}{0.75-\theta} + \frac{0.24(0.0102)}{0.24-\theta} + \frac{0.081(0.0127)}{0.081-\theta} + \frac{0.025(0.0102)}{0.025-\theta} \quad (1)$$

Eq. (1) has 8 roots for θ. However, only 3 roots are probably necessary. These are those between values of α for: (1) iso-butane and n-butane, (2) n-butane and iso-pentane, and (3) iso-

Exercise 9.11 (continued)

Analysis: (continued)

pentane and n-pentane, because iso-butane and n-pentane boil closely to n-butane and iso-pentane, respectively. Using a spreadsheet, the 3 roots of θ are: (1) 2.7159 between 3.50 and 2.44, (2) 1.02575 between 2.44 and 1.00, and (3) 0.78274 between 1.00 and 0.75.
Eq. (9-29) is applied in the following form for each of the three values of θ, in terms of the three unknowns, d_{iC4} , d_{nC5} , and L_{min}. The form used is obtained by multiplying Eq. (9-29) by the total distillate rate, D, which converts distillate mole fractions to component distillate rates, and the reflux ratio, R to L.

$$D + L_{min} = \frac{8.56\ (2500)}{8.56 - 2.7159} + \frac{3.50\ (d_{iC_4})}{3.50 - 2.7159} + \frac{2.44\ (594)}{2.44 - 2.7159} + \frac{1.00\ (15)}{1.00 - 2.7159} + \frac{0.75\ (d_{nC_5})}{0.75 - 2.7159}$$

$$= 3661.8 + 4.4637(d_{iC_4}) - 5253.2 - 8.7418 - 0.3815(d_{nC_5}) = 4.4637(d_{iC_4}) - 1600.14 - 0.3815(d_{nC_5})$$

$$D + L_{min} = \frac{8.56\ (2500)}{8.56 - 1.02575} + \frac{3.50\ (d_{iC_4})}{3.50 - 1.02575} + \frac{2.44\ (594)}{2.44 - 1.02575} + \frac{1.00\ (15)}{1.00 - 1.02575} + \frac{0.75\ (d_{nC_5})}{0.75 - 1.02575}$$

$$= 2840.36 + 1.41457(d_{iC_4}) + 1024.83 - 582.52 - 2.71986(d_{nC_5}) = 1.41457(d_{iC_4}) + 3282.67 - 2.71986(d_{nC_5})$$

$$D + L_{min} = \frac{8.56\ (2500)}{8.56 - 0.78274} + \frac{3.50\ (d_{iC_4})}{3.50 - 0.78274} + \frac{2.44\ (594)}{2.44 - 0.78274} + \frac{1.00\ (15)}{1.00 - 0.78274} + \frac{0.75\ (d_{nC_5})}{0.75 - 0.78274}$$

$$= 2751.61 + 1.28806(d_{iC_4}) + 874.55 + 69.04 - 22.9078(d_{nC_5}) = 1.28806(d_{iC_4}) + 3695.20 - 22.9078(d_{nC_5})$$

Because the total distillate rate, D, is also an unknown, the following equation is also needed:
$D = d_{C3} + d_{iC4} + d_{nC4} + d_{iC5} + d_{nC5} = 2500 + d_{iC4} + 594 + 15 + d_{nC5} = 3109 + d_{iC4} + d_{nC5}$
Solving these 4 linear equations, the following results are obtained:
D = 4712.8 kmol/h, L_{min} = 795.4 kmol/h, d_{iC4} = 1593.4 kmol/h, d_{nC5} = 10.45 kmol/h
Because the flow rate of iC_4 in the distillate is greater than its feed rate, iC_4 does not distribute.
Recalculate omitting the first of the four equations that uses θ = 2.7159. Replace $d_{iC4} = f_{iC4} = 400$ kmol/h. The equations to be solved now are:

$$D + L_{min} + 2.71986\left(d_{nC_5}\right) = 3848.5$$

$$D + L_{min} + 22.9078\left(d_{nC_5}\right) = 4210.4$$

$$D - \left(d_{nC_5}\right) = 3509.0$$

Exercise 9.11 (continued)

Analysis: (continued)

Solving, D = 3526.9 kmol/h, L_{min} = 272.8 kmol/h, and d_{nC5} = 17.9 kmol/h

Because the distillate rate of nC_5 is positive and less than its feed rate, it does distribute.
If we had assumed that only the two key components distributed, then it is only necessary to solve the following two equations using only θ = 1.02575, the one between the two key components, with d_{nC5} = 0.0 :

$$D + L_{min} = 3848.5$$

$$D = 3509.0$$

Then, L_{min} = 3848.5 - 3509.0 = 339.5 kmol/h = internal reflux rate, which is high and incorrect.
Assume that the minimum external reflux rate = minimum internal reflux rate = 272.8 kmol/h

The product compositions at minimum reflux rate are:

Component	Feed, kmol/h	Distillate, kmol/h	Bottoms, kmol/h
Propane	2500	2500	0
iso-Butane	400	400	0
n-Butane	600	594	6
iso-Pentane	100	15	85
n-Pentane	200	17.9	182.1
n-Hexane	40	0	40
n-Heptane	50	0	50
n-Octane	40	0	40
Total:	3930	3526.9	403.1

:

Exercise 9.12

Subject: Minimum reflux ratio and minimum number of equilibrium stages as a function of product purity for the distillation of a binary mixture.

Given: Equimolar bubble-point feed of isobutane and n-butane at column pressure of 100 psia. Purity of iC_4 in the distillate equal to purity of nC_4 in the bottoms. Purity range from 90 mol% to 99.99 mol%

Find: Minimum reflux ratio.
Minimum number of equilibrium stages.
Discuss significance of results.

Analysis: From the vapor pressure plot of Fig. 2.4, for 100 psia, the boiling points are 120°F for iC_4 and 146°F for nC_4. Take an average temperature of 133°F and assume a relative volatility equal to the vapor pressure ratio. Thus, again using Fig. 2.4, $\alpha_{iC4,\,nC4} = 115/85 = 1.35$.
For N_{min} , use the Fenske equation, (9-11), which simplifies to:

$$N_{\min} = \frac{\log\left[\dfrac{\left(x_{iC_4}\right)_D^2}{\left(x_{iC_4}\right)_B^2}\right]}{\log 1.35} = \frac{\log\left[\dfrac{\left(x_{iC_4}\right)_D^2}{\left(1-x_{iC_4}\right)_D^2}\right]}{0.1303} \qquad (1)$$

For R_{min} , use the Class 1 form of the Underwood equation, (9-20), which simplifies to:

$$R_{\min} = \frac{\left\{\left(x_{iC_4,D}/0.5\right) - 1.35\left[\left(1-x_{iC_4,D}\right)/0.5\right]\right\}}{0.35} \qquad (2)$$

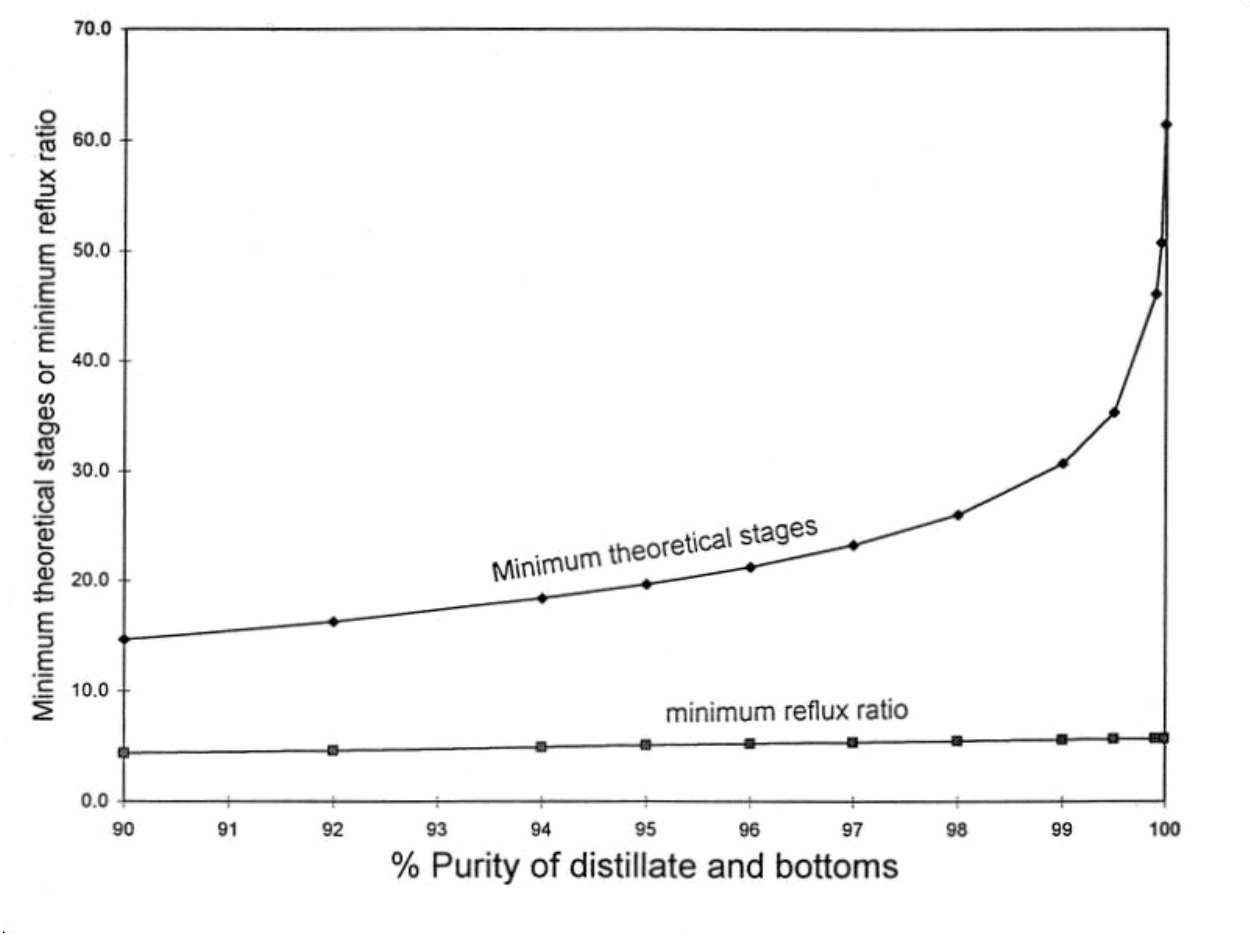
Using a spreadsheet, the following values are computed:

% Purity	N_{min}	R_{min}
90	14.6	4.37
92	16.3	4.64
94	18.3	4.91
95	19.6	5.04
96	21.2	5.18
98	25.9	5.45
99	30.6	5.58
99.5	35.3	5.65
99.9	46.0	5.70
99.95	50.7	5.71
99.99	61.4	5.71

Exercise 9.12 (continued)

Analysis: (continued)

A plot of the results is shown below. It is clearly evident from the table above or the plot below that the minimum reflux increases little and less and less as the purity approaches 100%, while the minimum number of equilibrium stages increases greatly and more and more as the purity approaches 100%,



Exercise 9.13

Subject: Reflux ratio by the FUG method for the distillation of a propylene-propane mixture.

Given: Binary feed of 360 kmol/h of propylene and 240 kmol/h of propane at the bubble point at column pressure. Distillate to contain 347.5 kmol/h of propylene and 3.5 kmol/h of propane. Average relative volatility = 1.11. $N/N_{min} = 2$. Total condenser and partial reboiler.

Assumptions: External reflux ratio = internal reflux ratio at the upper pinch.

Find: Operating reflux ratio by the FUG method.

Analysis: By material balance, the bottoms product contains 12.5 kmol/h of propylene and 236.5 kmol/h of propane. Using the Fenske equation (9-12):

$$N_{min} = \frac{\log\left[\dfrac{d_{C_3^=}}{d_{C_3}}\dfrac{b_{C_3}}{b_{C_3^=}}\right]}{\log\left(\alpha_{C_3^=,C_3}\right)_{avg}} = \frac{\log\left[\dfrac{(347.5)}{(3.5)}\dfrac{(236.5)}{(12.5)}\right]}{\log 1.11} = 72.2$$

$$N = 2\,N_{min} = 2(72.2) = 144.4$$

For minimum reflux, use the Class 1 Underwood equation (9-20), which applies for a binary mixture, where the pinch composition is that of the liquid feed. The distillate mole fractions are 347.5/351 = 0.99 for propylene and 0.01 for propane. In the feed, the mole fractions are 360/600 = 0.60 for propylene and 0.40 for propane. Thus,

$$R_{min} = \frac{L_{min}}{D} = \frac{\left[\left(\dfrac{x_{C_3^=,D}}{x_{C_3^=,F}}\right) - \alpha_{C_3^=,C_3}\left(\dfrac{x_{C_3,D}}{x_{C_3,F}}\right)\right]}{\alpha_{C_3^=,C_3} - 1} = \frac{\left[\left(\dfrac{0.99}{0.60}\right) - 1.11\left(\dfrac{0.01}{0.40}\right)\right]}{1.11 - 1} = 14.75$$

Use either the Gilliland graphs of Figs. 9.10 or 9.11, or the Gilliland correlation equation, (9-34). The latter is more accurate, but requires iteration when solving for X. Apply the equation.

$$Y = \frac{N - N_{min}}{N + 1} = \frac{144.4 - 72.2}{144.4 + 1} = 0.497$$

Using a spreadsheet to solve Eq. (9-34), which is nonlinear in X, we obtain $X = 0.159$

$$X = \frac{R - R_{min}}{R + 1} = 0.159$$ Solving, $R = 17.73$ and $R/R_{min} = 17.73/14.75 = 1.202$

Exercise 9.14

Subject: Number of equilibrium stages by the FUG method for the distillation of a binary mixture of dichlorobenzene (DCB) isomers.

Given: Feed of 62 mol% p-DCB and 38 mol% o-DCB at approximately 1 atm. Distillate to contain 98 mol% p-DCB, and bottoms to contain 96 mol% o-DCB. Total condenser and partial reboiler. Average relative volatility = 1.154 with the para isomer as the LK. Feed condition is q = 0.9 (10 mol% vaporized). Want $R/R_{min} = 1.15$.

Assumptions: External reflux ratio = internal reflux ratio at the upper pinch.

Find: Number of equilibrium stages by the FUG method.

Analysis: Using the Fenske equation (9-11):

$$N_{min} = \frac{\log\left[\frac{(x_{p\text{-DCB}})_D}{(x_{p\text{-DCB}})_B}\left[\frac{(x_{o\text{-DCB}})_B}{(x_{o\text{-DCB}})_D}\right]\right]}{\log \alpha_{p\text{-DCB,o-DCB}}} = \frac{\log\left[\frac{(0.98)}{(0.04)}\frac{(0.96)}{(0.02)}\right]}{\log(1.154)} = 49.3$$

For minimum reflux, use the Class 1 Underwood equation (9-20), which applies for a binary mixture, where the pinch composition is that of the liquid portion of the feed. From the feed composition, determine the equilibrium liquid composition by a flash calculation for 10 mol% vaporization. Do this by combining Eqs. (7-26) for the q-line with (4-8) for equilibrium at a constant relative volatility. Thus, applying these equations to the LK, p-DCB,

$$\frac{\alpha x}{1+x(\alpha-1)} = \frac{1.154x}{1+0.154x} = \left(\frac{q}{q-1}\right)x - \left(\frac{z_F}{q-1}\right) = -9x + \frac{0.62}{0.1} = 6.2 - 9x$$

Solving this nonlinear equation for a positive root of x between 0 and 1 gives $x = x_{p\text{-DCB}} = 0.617$
Then,

$$R_{min} = \frac{L_{min}}{D} = \frac{\left[\left(\frac{x_{p\text{-DCB},D}}{x_{p\text{-DCB},F}}\right) - \alpha_{p-DCB,o-DCB}\left(\frac{x_{o\text{-DCB},D}}{x_{o-DCB,F}}\right)\right]}{\alpha_{p-DCB,o-DCB} - 1} = \frac{\left[\left(\frac{0.98}{0.617}\right) - 1.154\left(\frac{0.02}{0.387}\right)\right]}{1.154 - 1} = 9.93$$

$R = 1.15\ R_{min} = 1.15(9.93) = 11.42$ In the Gilliland equation, (9-34), $X = (R - R_{min})/(R + 1) = (11.42\text{-}9.93)/(11.42+1) = 0.120$. Using Eq. (9.34), $Y = 0.534 = (N - N_{min})/(N + 1)$.
Solving, $N = 107$ stages.

Exercise 9.15

Subject: Shortcomings of the Gilliland correlation

Given: Column with a small ratio of rectifying to stripping stages.

Find: Explanation for possible inapplicability of the Gilliland correlation.

Analysis: When a column has a small ratio of rectifying to stripping stages, stripping of a light key in the stripping section may dominate over absorption of the heavy key in the rectifying section, in determining stage requirements. The Gilliland correlation is based on reflux considerations in the rectifying section. Alternatively, a correlation could have been developed based on boilup considerations in the stripping section, using a modified Underwood equation for minimum boilup ratio. Such a correlation, since it would be empirical, would seem to be favored over the Gilliland correlation, which emphasizes rectification, rather than stripping.

Exercise 9.16

Subject: Use of the FUG method for the distillation of a normal paraffin hydrocarbon mixture.

Given: Bubble-point liquid feed at 300 psia, with composition in mole fractions:

Component	C_2	C_3	nC_4	nC_5	nC_6	nC_7
Mole fraction	0.08	0.15	0.20	0.27	0.20	0.10

Find: (a) For a sharp separation between nC_4 and nC_5, determine column pressure and type condenser for condenser outlet temperature of 120°F.

(b) At total reflux, determine the separation for 8 equilibrium stages, with 0.01 mole fraction of nC_4 in the bottoms.

(c) Minimum reflux ratio for separation in Part (b).

(d) Number of equilibrium stages for $R/R_{min} = 1.5$ using Gilliland correlation.

Analysis: (a) For a sharp split, the distillate composition is as follows:

Component	x_d	K **at 120°F, 250 psia**	Kx_d
C_2	0.186	2.8	0.520
C_3	0.349	1.13	0.394
nC_4	0.465	0.34	0.158
Total:	1.000		1.072

In this table, a distillate bubble-point pressure of 250 psia is assumed and the bubble-point equation (4-12) is applied, using K-values in Fig. 2.8. The summation is 1.072. In order for the sum to be 1.0, an even higher pressure is needed, since the K-value is almost inversely proportional to pressure. But, in Fig. 7.16, we are already > 215 psia, therefore use a partial condenser. To determine the pressure, run a dew point using Eq. (4-13).

Component	y_D	K **at 120°F, 140 psia**	y_D/K	K **at 120°F, 120 psia**	y_D/K
C_2	0.186	4.7	0.040	5.4	0.030
C_3	0.349	1.58	0.221	1.80	0.194
nC_4	0.465	0.53	0.877	0.60	0.775
Total:	1.000		1.138		0.999

On the second trial in the above table, the dew-point pressure is found to be 120 psia. Set the column pressure at this value with a partial condenser.

Exercise 9.16 (continued)

Analysis: (continued)

(b) Run a bubble point on an assumed bottoms composition, using Eq. (4-12):

Component	x_B	K at 320°F, 120 psia	$x_B K$	K at 290°F, 120 psia	$x_B K$
nC_4	0.010	3.3	0.033	2.75	0.028
nC_5	0.469	1.7	0.797	1.38	0.647
nC_6	0.347	0.92	0.319	0.72	0.250
nC_7	0.174	0.48	0.084	0.36	0.063
Total:	1.000		1.233		0.988

A third trial gives a bottoms temperature of 295°F

The K-values and relative volatilities referred to the nC_5, the heavy key, at distillate and bottoms conditions are as follows for a pressure of 120 psia:

Component	K at 120°F, 120 psia	$\alpha_{I,\,nC5}$ at 120°F, 120 psia	K at 295°F, 120 psia	$\alpha_{I,\,nC5}$ at 295°F, 120 psia	Geometric average α
C_2	5.40	25.7	12.0	8.28	14.6
C_3	1.80	8.6	5.8	4.0	5.9
nC_4	0.60	2.86	2.8	1.93	2.35
nC_5	0.21	1.00	1.45	1.00	1.00
nC_6	0.074	0.352	0.74	0.51	0.424
nC_7	0.028	0.133	0.38	0.262	0.187

From the Fenske Eq. (9-12), $N_{min} = 8 = \dfrac{\log\left[\dfrac{d_{nC_4}}{d_{nC_5}}\dfrac{b_{nC_5}}{b_{nC_4}}\right]}{\log\left(\alpha_{nC_4,nC_5}\right)_{avg}} = \dfrac{\log\left[\dfrac{d_{nC_4}}{d_{nC_5}}\dfrac{b_{nC_5}}{b_{nC_4}}\right]}{\log 2.35}$ (1)

Take as a basis, 1 mol of feed. Assume that the distribution of the nonkeys is negligible. That is, only the LK and the HK are found in both the distillate and bottoms. Assume the total bottoms, B, is 0.57 mol. Then $b_{nC4} = 0.01(0.57) = 0.0057$. Therefore, $d_{nC4} = 0.20 - 0.0057 = 0.1943$ mol. Solving Eq. (1), $b_{nC5}/d_{nC5} = 27.3$. Since $b_{nC5} + d_{nC5} = f_{nC5} = 0.27$, $b_{nC5} = 0.2605$ mol and $d_{nC5} = 0.0095$. Therefore, $B = 0.0057 + 0.2605 + 0.20 + 0.10 = 0.5662$. Repeating the calculations with this value of B, the result is $b_{nC4} = 0.00566$, $d_{nC4} = 0.19434$, $b_{nC5} = 0.2604$, and $d_{nC5} = 0.0096$. Using Eq. (1) for each of the nonkey components shows that they do not distribute to any extent. Therefore the distillate and bottoms compositions at total reflux are:

Component	f, mol	d, mol	x_D	b, mol	x_B
C_2	0.08	0.0800	0.184	0.0000	0.000
C_3	0.15	0.1500	0.346	0.0000	0.000
nC_4	0.20	0.1943	0.448	0.0057	0.010
nC_5	0.27	0.0096	0.022	0.2604	0.460
nC_6	0.20	0.0000	0.000	0.2000	0.353
nC_7	0.10	0.0000	0.000	0.1000	0.177
Total	1.00	0.4339	1.000	0.5661	1.000

Exercise 9.16 (continued)

Analysis: (c)

Because the split of the two key components is quite sharp, assume a Class 2 separation for the purpose of minimum reflux. Thus, only components methane to n-pentane will distribute to the distillate. To determine the phase condition of the feed, perform an adiabatic flash with bubble-point conditions at 300 psia upstream of the feed valve to the column, and 120 psia downstream of the valve, using Chemcad. The result is a *V/F* ratio for the feed of 0.334. From Eq. (7-19), $q = 1 - (V/F) = 1 - 0.334 = 0.666$ or $1 - q = 0.334$. From Underwood Eq. (9-28),

$$\sum_i \frac{\alpha_{i,nC_5} z_{i,F}}{\alpha_{i,nC_5} - \theta} = 1 - q = 0.334 = \frac{14.6(0.08)}{14.6 - \theta} + \frac{5.9(0.15)}{0.15 - \theta} + \frac{2.35(0.20)}{2.35 - \theta} + \frac{1.00(0.27)}{1.00 - \theta} + \frac{0.424(0.20)}{0.424 - \theta} + \frac{0.187(0.10)}{0.187 - \theta}$$

Solving this equation for the root between 2.35 and 1.00 gives $\theta = 1.5962$
From Underwood Eq. ((9-29),

$$\sum_i \frac{\alpha_{i,nC_5} x_{i,D}}{\alpha_{i,nC_5} - \theta} = \frac{14.6(0.184)}{14.6 - 1.5962} + \frac{5.9(0.346)}{5.9 - 1.5962} + \frac{2.35(0.448)}{2.35 - 1.5962} + \frac{1.00(0.022)}{1.00 - 1.5962} = 2.04 = 1 + R_{min}$$

Therefore, the internal minimum reflux ratio = 2.04 - 1.00 = 1.04
Assume the external minimum reflux ratio = 1.04

(d) For the number of theoretical stages, use the Gilliland equation, (9-34), where for this exercise, $R = 1.5R = 1.5(1.04) = 1.56$. $X = (R - R_{min})/(R + 1) = (1.56 - 1.04)/(1.56 + 1) = 0.203$. Using Eq. (9.34), $Y = 0.458 = (N - N_{min})/(N + 1)$.

Solving, $N = 15.6$ equilibrium stages.

Exercise 9.17

Subject: Use of the FUG method for the distillation of a light paraffin hydrocarbon mixture.

Given: Feed mixture of:

Component	C_3	iC_4	nC_4	iC_5	nC_5
lbmol/h	5	15	25	20	35

Column pressure = 120 psia. Liquid distillate contains 92.5% of the nC_4 in the feed. Bottoms contains 82 mol% of iC_5 in the feed. Use Chemcad with SRK instead of Figs. 2.8 and 2.9 for *K*-values.

Find: (a) Minimum number of equilibrium stages.
(b) Distribution of nonkey components.
(c) Minimum reflux ratio for a bubble-point liquid feed.
(d) Number of equilibrium stages for $R = 1.2\ R_{min}$.
(e) Feed-stage location.

Analysis: (a) To obtain the average relative volatilities, run bubble points on the following assumed distillate and bottoms compositions, using the given key-component recoveries:

	lbmol/h:		
Component	**Feed**	**Distillate**	**Bottoms**
C_3	5	5.000	0.000
iC_4	15	15.000	0.000
nC_4	25	23.125	1.875
iC_5	20	3.600	16.400
nC_5	35	0.000	35.000
Total:	100	46.725	53.275

The results with K-values and relative volatilities are as follows, using the SRK equation of state for *K*-values and the bubble-point equation, (4-12):

Component	***K*, distillate, 140°F**	**$\alpha_{i,iC5}$, 140°F**	***K*, bottoms, 230°F**	**$\alpha_{i,iC5}$, 230°F**	**$\alpha_{i,iC5}$, geometric mean**
C_3	2.100	5.24	3.880	3.63	4.36
iC_4	1.056	2.63	2.260	2.12	2.36
nC_4	0.818	2.04	1.863	1.74	1.88
iC_5	0.401	1.00	1.068	1.00	1.00
nC_5	0.329	0.82	0.922	0.86	0.84

Exercise 9.17 (continued)

Analysis: (continued)

(a) Using the Fenske equation (9-12), with nC_4 as the LK and iC_5 as the HK,

$$N_{min} = \frac{\log\left[\frac{d_{nC4}}{d_{iC5}}\frac{b_{iC5}}{b_{nC4}}\right]}{\log\left(\alpha_{nC4,iC5}\right)_{avg}} = \frac{\log\left[\frac{(23.125)}{(3.6)}\frac{(16.4)}{(1.875)}\right]}{\log 1.88} = 6.38$$

(b) To compute the distribution of nonkey components at total reflux, use for the lighter than light key components, LLK, Eq. (9-15), and use Eq. (9-16) for the heavier than heavy key, HHK, with iC_5 as the reference component, r, and the above value of N_{min}.

Thus, for the LLK, i, $$b_i = \frac{f_i}{1+\left(\frac{d_{iC_5}}{b_{iC_5}}\right)\alpha_{i,iC_5}^{N_{min}}} = \frac{f_i}{1+\left(\frac{3.6}{16.4}\right)\alpha_{i,iC_5}^{6.38}} \qquad (1)$$

For the HHK, i, $$d_i = \frac{f_i\left(\frac{d_{iC_5}}{b_{iC_5}}\right)\alpha_{i,iC_5}^{N_{min}}}{1+\left(\frac{d_{iC_5}}{b_{iC_5}}\right)\alpha_{i,iC_5}^{N_{min}}} = \frac{f_i\left(\frac{3.6}{16.4}\right)\alpha_{i,iC_5}^{6.38}}{1+\left(\frac{3.6}{16.4}\right)\alpha_{i,iC_5}^{6.38}} \qquad (2)$$

Using the above geometric mean values of $\alpha_{i,iC5}$, followed by use of Eqs. (1) and (2) with the material balance, $f_i = d_i + b_i$, the following results are obtained:

lbmol/h:

Component	Feed	Distillate	Bottoms
C_3	5	4.998	0.002
iC_4	15	14.720	0.280
nC_4	25	23.125	1.875
iC_5	20	3.600	16.400
nC_5	35	2.356	32.644
Total:	100	48.799	51.201

(c) Because the split of the LK and HK components is not sharp and because iC_4 boils close to nC_4, and iC_5 boils close to nC_5, it is possible that both iC_4 and nC_5 will distribute at minimum reflux. It is questionable that C_3 will distribute. Nevertheless, first assume a Class 1 Underwood minimum reflux and use the following rearrangement of Eq. (9-21) for a feed at the bubble point:

$$L_{min} = \frac{F\left[\left(\frac{d_{nC_4}}{f_{nC_4}}\right) - \alpha_{nC_4,iC_5}\left(\frac{d_{iC_5}}{f_{iC_5}}\right)\right]}{\alpha_{nC_4,iC_5} - 1} = \frac{100\left[\left(\frac{23.125}{25}\right) - 1.88\left(\frac{3.6}{20}\right)\right]}{1.88 - 1} = 66.7\,1$$

Exercise 9.17 (continued)

Analyze: (c) (continued)

Now, use the Class 2 Underwood equation, Eq. (9-28),which for a bubble-point feed is:

$$\sum_i \frac{\alpha_{i,\mathrm{iC_5}} z_{i,F}}{\alpha_{i,\mathrm{iC_5}} - \theta} = 1 - q = 0 = \frac{4.36(0.05)}{4.36-\theta} + \frac{2.36(0.15)}{2.36-\theta} + \frac{1.88(0.25)}{1.88-\theta} + \frac{1.00(0.20)}{1.00-\theta} + \frac{0.84(0.35)}{0.84-\theta} \qquad (3)$$

There are four roots to Eq. (3), which from a spreadsheet calculation are:

$\theta = 0.9248,\ \ 1.317,\ 2.173,\ 3.996$

Assume that the C_3 does not distribute. Then, the 3.996 root is not needed and $d_{C3} = 5$ lbmol/h. Eq. (9-29) is applied in the following form for each of the three remaining values of θ, in terms of the three unknowns, d_{iC4} , d_{nC5} , and L_{min}. The form used is obtained by multiplying Eq. (9-29) by the total distillate rate, D, which converts distillate mole fractions to component distillate rates, and the reflux ratio, R to L.

$$D + L_{\min} = \frac{4.36\ (5)}{4.36-0.9248} + \frac{2.36\ (d_{\mathrm{iC_4}})}{2.36-0.9248} + \frac{1.88\ (23.125)}{1.88-0.9248} + \frac{1.00\ (3.6)}{1.00-0.9248} + \frac{0.84\ (d_{\mathrm{nC_5}})}{0.84-0.9248}$$

$$= 6.346 + 1.644(d_{\mathrm{iC_4}}) + 45.514 + 47.872 - 9.9057(d_{\mathrm{nC_5}}) = 1.644(d_{\mathrm{iC_4}}) + 93.386 - 9.9057(d_{\mathrm{nC_5}})$$

$$D + L_{\min} = \frac{4.36\ (5)}{4.36-1.317} + \frac{2.36\ (d_{\mathrm{iC_4}})}{2.36-1.317} + \frac{1.88\ (23.125)}{1.88-1.317} + \frac{1.00\ (3.6)}{1.00-1.317} + \frac{0.84\ (d_{\mathrm{nC_5}})}{0.84-1.317}$$

$$= 7.164 + 2.263(d_{\mathrm{iC_4}}) + 77.22 - 11.36 - 1.761(d_{\mathrm{nC_5}}) = 2.263(d_{\mathrm{iC_4}}) + 73.02 - 1.761(d_{\mathrm{nC_5}})$$

$$D + L_{\min} = \frac{4.36\ (5)}{4.36-2.173} + \frac{2.36\ (d_{\mathrm{iC_4}})}{2.36-2.173} + \frac{1.88\ (23.125)}{1.88-2.173} + \frac{1.00\ (3.6)}{1.00-2.173} + \frac{0.84\ (d_{\mathrm{nC_5}})}{0.84-2.173}$$

$$= 9.968 + 12.62(d_{\mathrm{iC_4}}) - 148.38 - 3.07 - 0.63(d_{\mathrm{nC_5}}) = 12.62(d_{\mathrm{iC_4}}) - 141.48 - 0.63(d_{\mathrm{nC_5}})$$

Because the total distillate rate, D, is also an unknown, the following equation is also needed:

$D = d_{C3} + d_{iC4} + d_{nC4} + d_{iC5} + d_{nC5} = 5 + d_{iC4} + 23.125 + 3.6 + d_{nC5} = 31.725 + d_{iC4} + d_{nC5}$

Solving these 4 linear equations, the following results are obtained:

D = 53.27 lbmol/h, L_{min} = 64.74 lbmol/h, d_{iC4} = 20.61 lbmol/h, d_{nC5} = 0.93 lbmol/h

Note that the distillate rate for iC_4 is impossible because it exceeds the feed rate of 15 lbmol/h. Therefore, iC_4 does not distribute, and the calculations must be repeated, eliminating d_{iC4} as an unknown by replacing it with a value of 15 lbmol/h. Also, the θ root of 2.173 is not used. The following three equations result:

Exercise 9.17 (continued)

Analyze: (c) (continued)

$$D + L_{\min} = 106.96 - 1.761 d_{nC_5}$$
$$D + L_{\min} = 118.05 - 9.9057 d_{nC_5}$$
$$D = 46.725 + d_{nC_5}$$

Solving these three equations: D = 48.085 lbmol/h, $L_{\min}$ = 56.49 lbmol/h, and d_{nC5} = 1.36 lbmol/h
This is the correct value of internal minimum reflux rate. Assume the external minimum reflux ratio = internal minimum reflux ratio = 56.49/48.085 = 1.175. Note that this value is about 15% less than that obtained by assuming a Class 1 separation.

(d) The operating reflux ratio = 1.2(1.175) = 1.41. In the Gilliland equation, (9-34), $X = (R - R_{\min})/(R + 1)$ = (1.41 - 1.175)/1.41+1) = 0.0975. Using Eq. (9.34), Y = 0.556 = $(N - N_{\min})/(N + 1)$.

Solving, N = 15.6 stages.

(e) Apply the Kirkbride equation (9-36):
From above, using the Fenske distribution, D = 48.799 lbmol/h and B = 51.201 lbmol/h

$$\frac{N_R}{N_S} = \left[\left(\frac{z_{iC_5,F}}{z_{nC_4,F}}\right)\left(\frac{x_{nC_4,B}}{x_{iC_5,D}}\right)^2\left(\frac{B}{D}\right)\right]^{0.206} = \left[\left(\frac{0.20}{0.25}\right)\left(\frac{0.0366}{0.0738}\right)^2\left(\frac{51.201}{48.799}\right)\right]^{0.206} = 0.723$$

Therefore, of 15.6 equilibrium stages, (0.723/1.723)(15.6) = 6.5 stages are in the rectifying section. Thus, the feed stage is equilibrium stage 6 or 7 from the top.

Exercise 9.18

Subject: Use of the FUG method for the distillation of a chlorination effluent.

Given: Bubble-point liquid feed with the following composition and average *K*-values:

Component	Mole fraction	Aver. K-value
C_2H_4 , A	0.05	5.10
HCl , B	0.05	3.80
C_2H_6 , C	0.10	3.40
C_2H_5Cl , D	0.80	0.15

Partial condenser and partial reboiler. Column pressure = 240 psia. $(x_D/x_B) = 0.01$ for C_2H_5Cl and 75 for C_2H_6.

Find: Minimum equilibrium stages
Component distribution
Minimum reflux ratio
Number of equilibrium stages for $R = 1.5\ R_{min}$
Feed stage location

Analysis: For minimum equilibrium stages, use the Fenske equation (9-11):

$$N_{min} = \frac{\log\left[\dfrac{(x_D/x_B)_{C_2H_6}}{(x_D/x_B)_{C_2H_5Cl}}\right]}{\log \alpha_{C,D}} = \frac{\log\left[\dfrac{75}{0.01}\right]}{\log(3.4/0.15)} = 2.86$$

For component distribution, use the following rearrangements of the Fenske equation:

$$\left(\frac{x_D}{x_B}\right)_{C_2H_4} = \left(\frac{x_D}{x_B}\right)_{C_2H_5Cl} \alpha_{C_2H_4,C_2H_5Cl}^{N_{min}} = 0.01\left(\frac{5.1}{0.15}\right)^{2.86} = 240$$

$$\left(\frac{x_D}{x_B}\right)_{HCl} = \left(\frac{x_D}{x_B}\right)_{C_2H_5Cl} \alpha_{HCl,C_2H_5Cl}^{N_{min}} = 0.01\left(\frac{3.8}{0.15}\right)^{2.86} = 103$$

Because the separation between the two key components is quite sharp, assume that the two nonkeys do not distribute at minimum reflux. The relative volatilities with respect to the heavy key are: 34 for A, 25.3 for B, and 22.7 for C. Now, use the Class 2 Underwood equation, Eq. (9-28),which for a bubble-point feed is:

Exercise 9.18 (continued)

Analysis: (continued)

$$\sum_i \frac{\alpha_{i,D} z_{i,F}}{\alpha_{i,D} - \theta} = 1 - q = 0 = \frac{34(0.05)}{34-\theta} + \frac{25.3(0.05)}{25.3-\theta} + \frac{22.7(0.10)}{22.7-\theta} + \frac{1.00(0.80)}{1.00-\theta} \quad (1)$$

There are three roots to Eq. (1). The one of interest is the one between 22.7 and 1.0, which from a spreadsheet calculation is θ = 4.318. The composition of the distillate by material balances is:

Component	**distillate, mole fraction**
C_2H_4 , A	0.25405
HCl , B	0.25405
C_2H_6 , C	0.48195
C_2H_5Cl , D	0.00995

Apply Underwood Eq. (9-29):

$$\sum_i \frac{\alpha_{i,D} x_{i,D}}{\alpha_{i,D} - \theta} = \frac{34(0.25405)}{34-4.318} + \frac{25.3(0.25405)}{25.3-4.318} + \frac{22.7(0.48195)}{22.7-4.318} + \frac{1.00(0.00995)}{1.00-4.318} = 1 + R_{\min}$$

$$= 0.291 + 0.306 + 0.595 - 0.003 = 1.189 = 1 + R_{\min}$$

Therefore, $R_{\min} = 0.189$. Assume this is equal to the external minimum reflux ratio.

Operating reflux ratio = 1.5(0.189) = 0.284. In the Gilliland equation, (9-34), $X = (R - R_{\min})/(R + 1) = (0.284 - 0.189)/0.284 + 1) = 0.074$. Using Eq. (9.34), $Y = 0.581 = (N - N_{\min})/(N + 1)$.
Solving, $N = 8.2$ stages.

For feed stage location, apply the Kirkbride equation (9-36):

From above, using the Fenske distribution with a material balance, $D/B = 0.245$.
Also, mole fractions in the bottoms product are: $x_C = 0.0064$ and $x_D = 0.9936$

$$\frac{N_R}{N_S} = \left[\left(\frac{z_{D,F}}{z_{C,F}} \right) \left(\frac{x_{C,B}}{x_{D,D}} \right)^2 \left(\frac{B}{D} \right) \right]^{0.206} = \left[\left(\frac{0.80}{0.10} \right) \left(\frac{0.0064}{0.00995} \right)^2 \left(\frac{1}{0.245} \right) \right]^{0.206} = 1.71$$

Therefore, of 8.2 equilibrium stages, (1.71/2.71)(8.2) = 5.2 stages are in the rectifying section. With a partial condenser acting an equilibrium stage, the feed is about stage 4 from the top stage in the column.

Exercise 9.19

Subject: Use of the FUG method for the distillation of a ficticious ternary mixture.

Given: 100 kmol/h of a bubble-point feed of:

Component	Feed rate, kmol/h	$\alpha_{i,C}$
A	40	5
B	20	3
C	40	1

Find: (a) Product distribution for a distillate rate of 60 kmol/h and 5 minimum theoretical stages.

(b) Minimum reflux and boilup ratios for separation of part (a).

(c) Number of equilibrium stages and feed-stage location for $R = 1.2R_{min}$.

Analysis: (a) With a distillate rate of 60 kmol/h, the LK is B and the HK is C. From the rearranged form of the Fenske equation, given by Eq. (9-14), using component C as the reference,

$$\frac{d_A}{b_A} = \left(\frac{d_C}{b_C}\right)5^5 = 3125\left(\frac{d_C}{b_C}\right)$$

$$\frac{d_B}{b_B} = \left(\frac{d_C}{b_C}\right)3^5 = 243\left(\frac{d_C}{b_C}\right)$$

The following 4 material balances also apply:

$$d_A + b_A = 40$$
$$d_B + b_B = 20$$
$$d_C + b_C = 40$$
$$d_A + d_B + d_C = 60$$

Solving these 6 equations, two of which are nonlinear, in 6 unknowns gives the following results:

Component	z_F	x_D	x_B
A	0.4	0.662	0.007
B	0.2	0.307	0.039
C	0.4	0.031	0.954

(b) Assuming that component A does not distribute, the Underwood Eq. (9-28) for Class 2 applies:

$$\sum_i \frac{\alpha_{i,D} z_{i,F}}{\alpha_{i,D} - \theta} = 1 - q = 0 = \frac{5(0.40)}{5-\theta} + \frac{3(0.20)}{3-\theta} + \frac{1(0.40)}{1-\theta} \qquad (1)$$

Exercise 9.19 (continued)

Analysis: (continued)

There are two roots to Eq. (1). The one of interest is the one between 3 and 1.0, which from a spreadsheet calculation is θ = 1.425. If component A does not distribute, the composition of the distillate by material balances is as follows, if the total distillate rate of 60 kmol/h is maintained:

kmol/h:

Component	Feed	Distillate	Bottoms	x_D	x_B
A	40	40	0.0	0.6667	0.0000
B	20	18.3	1.7	0.3050	0.0425
C	40	1.7	38.3	0.0283	0.9575
Total:	100	60	40	1.0000	1.0000

Apply Underwood Eq. (9-29):

$$\sum_i \frac{\alpha_{i,D} x_{i,D}}{\alpha_{i,D} - \theta} = \frac{5(0.6667)}{5-1.425} + \frac{3(0.3050)}{3-1.425} + \frac{1(0.0283)}{1-1.425} = 1 + R_{\min}$$

$$= 0.9324 + 0.5810 - 0.0666 = 1.447 = 1 + R_{\min}$$

Therefore, $R_{\min}$ = 1.447 - 1.000 = 0.447. Assume this is also the external reflux ratio. Assume constant molar overflow. Then, the reflux rate in the rectifying section = 0.447(60) = 26.8 kmol/h. The reflux rate in the stripping section = 100 + 26.8 = 126.8 kmol/h. The boilup rate in the stripping section = 126.8 - 40 = 86.8 kmol/h. The boilup ratio = 86.8/40 = 2.17.

(c) Operating reflux ratio = 1.2(0.0.447) = 0.536. In the Gilliland equation, (9-34), $X = (R - R_{\min})/(R + 1) = (0.536 - 0.447)/0.536 + 1) = 0.058$. Using Eq. (9.34), $Y = 0.60 = (N - N_{\min})/(N + 1)$.
Solving, N = 14 stages.

For feed stage location, apply the Kirkbride equation (9-36):

From above, using the Fenske distribution with a material balance, D/B = 1.5.

$$\frac{N_R}{N_S} = \left[\left(\frac{z_{C,F}}{z_{B,F}}\right)\left(\frac{x_{B,B}}{x_{C,D}}\right)^2\left(\frac{B}{D}\right)\right]^{0.206} = \left[\left(\frac{0.40}{0.20}\right)\left(\frac{0.039}{0.031}\right)^2\left(\frac{1}{1.5}\right)\right]^{0.206} = 1.166$$

Therefore, of 14 equilibrium stages, (1.166/2.166)(14) = 7.5 stages are in the rectifying section. Assuming a total condenser, the feed stage is stage 7 or 8 from the top.

Exercise 9.20

Subject: Comparison of the Kirkbride, Fenske, and McCabe-Thiele methods for determining feed-stage location.

Given: A feed mixture of 25 mol% acetone (A) and 75 mol% water (W). Distillate to contain 95 mol% A, and bottoms to contain 2 mol% A. Infinite dilution activity coefficients from Exercise 9.6.

Find: Ratio of rectifying to stripping stages by:
(a) Fenske equation.
(b) Kirkbride equation.
(c) McCabe-Thiele method.

Analysis: (a) Fenske equation:
From Exercise 9.6:

Component	z_F	x_D	x_B	$\alpha_{i,W}$, D	$\alpha_{i,W}$, B
Acetone	0.25	0.95	0.02	1.48	27.7
Water	0.75	0.05	0.98	1.00	1.0

The relative volatility at feed conditions is also needed. Assume a bubble-point liquid feed. Also from vapor-liquid, y-x table of Exercise 9.6, $\alpha_{l,W} = [(0.789/0.250)]/[(0.211/0.750)] = 11.2$
From Eq. (9-35),

$$\frac{N_R}{N_S} = \frac{\log\left[(0.95/0.25)(0.75/0.05)\right]}{\log\left[(0.25/0.02)(0.98/0.75)\right]} \frac{\log[(27.7)(11.2)]^{1/2}}{\log[(1.48)(11.2)]^{1/2}} = \frac{1.756(1.246)}{1.213(0.6097)} = 2.96$$

(b) Kirkbride equation:
By material balances on A and W, $B/D = 0.753/0.247 = 3.05$

$$\frac{N_R}{N_S} = \left[\left(\frac{z_{W,F}}{z_{A,F}}\right)\left(\frac{x_{A,B}}{x_{W,D}}\right)^2\left(\frac{B}{D}\right)\right]^{0.206} = \left[\left(\frac{0.75}{0.25}\right)\left(\frac{0.02}{0.05}\right)^2 3.05\right]^{0.206} = 1.08$$

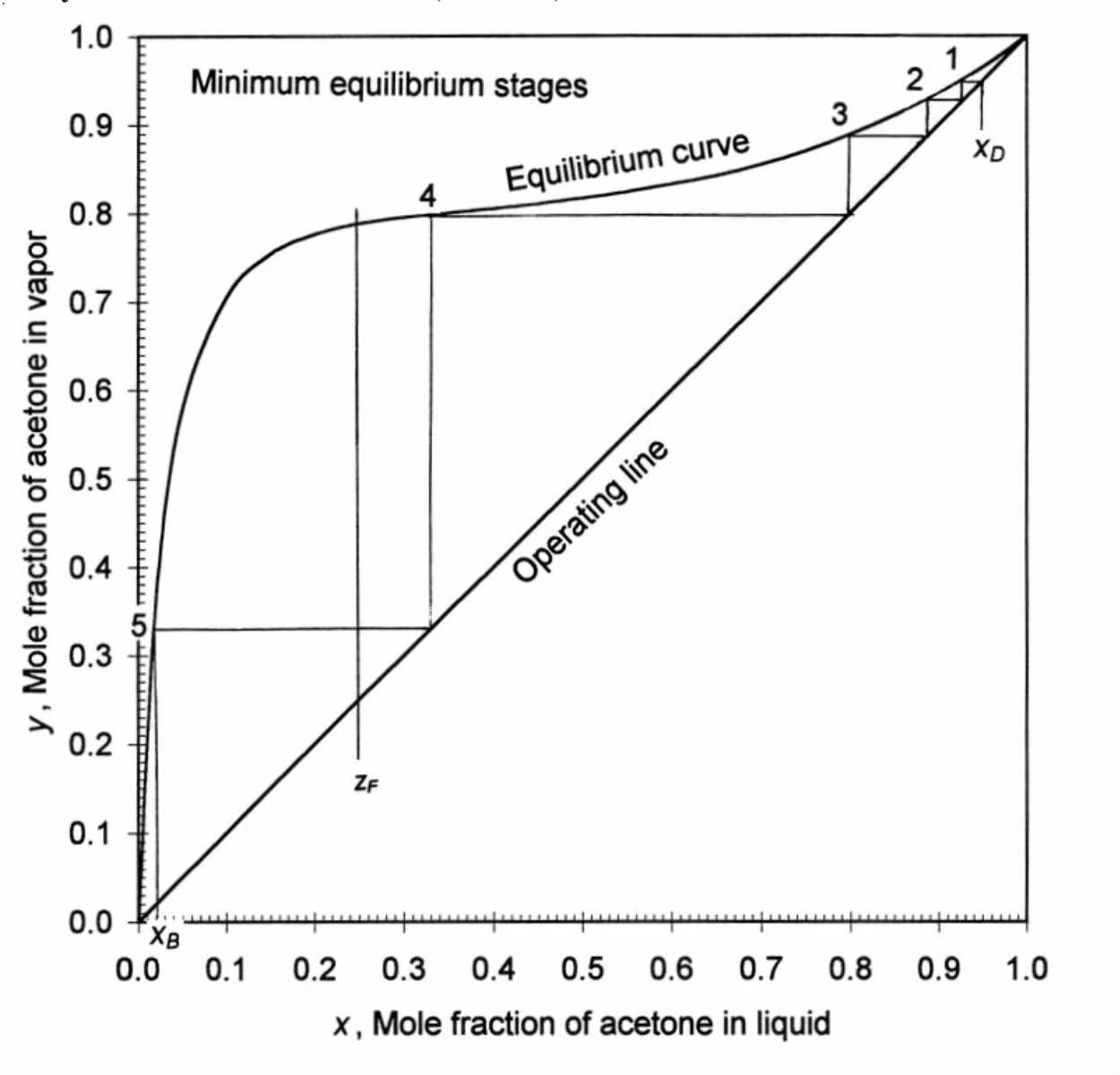
(c) McCabe-Thiele method:
From the McCabe-Thiele graph of Exercise 9.6, shown on the next page, where the total number of minimum stages = 5.

$$\frac{N_R}{N_S} = \frac{4.2}{0.8} = 5.25$$

The McCabe-Thiele method is the most accurate. The Fenske equation is better than the Kirkbride equation because the Kirkbride equation does not take into account the drastic change in relative volatility from the distillate to the bottoms.

Exercise 9.20 (continued)

Analysis: McCabe-Thiele method (continued)



Exercise 9.21

Subject: Derivation of Eq. (9-37) for the effective stripping factor

Given: Equations (5-46) and (5-47)

Analysis: By analogy to Eqs. (5-46) and (5-47), the fraction of species in the entering feed liquid that is not stripped is given for just 2 stages by:

$$\phi_S = \frac{1}{S_N S_1 + S_N + 1} = \frac{1}{S_e^2 + S_e + 1}$$

Therefore,

$$S_e^2 + S_e + 1 = S_N S_1 + S_N + 1$$

Solving for S_e,

$$S_e^2 + S_e - S_N(S_1 + 1) = 0$$

$$S_e = \frac{-1 + \sqrt{1 + 4S_N(S_1 + 1)}}{2} = \sqrt{0.25 + S_N(S_1 + 1)} - 0.5$$

Which is Eq. (9-37).

Exercise 9.22

Subject: Effect of number of stages and pressure on multicomponent absorption

Given: Feed gas of 2,000 lbmol/h of light paraffin hydrocarbons at 60°F, and 500 lbmol/h of nC_{10} absorbent at 90°F. *K*-values in Fig. 2.8.

Find: Separation at following conditions:
(a) 6 stages and 75 psia.
(b) 3 stages and 150 psia.
(c) 6 stages and 150 psia

Analysis: Apply Kremser's method, with absorption factors, $A = L/KV$, computed for L = entering absorbent rate = 500 lbmol/h, V = entering gas rate = 2,000 lbmol/h, and *K*-values from Fig. 2.8 at the average of the two entering temperatures, (90 + 60)/2 = 75°F and each of the two pressures. The feed gas composition and the resulting *K*-values and values of *A* are as follows:

Component	Feed, lbmol/h	*K* at 75 psia	*A* at 75 psia	*K* at 150 psia	*A* at 150 psia
C_1	1660	29	0.00862	15	0.0167
C_2	168	5.8	0.0431	3.1	0.0806
C_3	96	1.68	0.149	0.93	0.269
nC_4	52	0.48	0.521	0.27	0.926
nC_5	24	0.145	1.724	0.08	3.13
Total:	2000				

The fraction of a gas component not absorbed, ϕ_A, is given by the Kremser Eq. (5-48) and by material balance the amount absorbed follows:

$$\phi_A = \frac{A-1}{A^{N+1}-1} \quad \text{and} \quad l_N = (1-\phi_A) f$$

The results for all three cases are as follows:

	Case (a):		Case (b):		Case (c):	
Component	ϕ_A	l_N, lbmol/h	ϕ_A	l_N, lbmol/h	ϕ_A	l_N, lbmol/h
C_1	0.991	14.9	0.983	28.2	0.983	28.2
C_2	0.957	7.2	0.919	13.6	0.919	13.6
C_3	0.851	14.3	0.731	25.8	0.731	25.8
nC_4	0.484	26.8	0.280	37.4	0.178	42.7
nC_5	0.0164	23.6	0.0224	23.5	0.00072	23.98
Total:		86.8		128.5		134.28

The results show that doubling the pressure is much more effective than doubling the number of equilibrium stages. Even Case (c) results in little additional absorption over Case (b) when the stages are doubled for the same pressure.

Exercise 9.23

Subject: Effect of the number of stages on the absorption of a light normal paraffin hydrocarbon gas by the Kremser method.

Given: 1000 kmol/h of gas at 70°F of composition below, and 500 kmol/h of nC_{10} absorbent at 90°F. Absorber operating at 4 atm. *K*-values in Fig.2.8.

Find: Percent absorption for each component for (a) 4 stages, (b) 10 stages, and (c) 30 stages.

Analysis: : Apply Kremser's method, with absorption factors, $A = L/KV$, computed for L = entering absorbent rate = 500 kmol/h, V = entering gas rate = 1,000 kmol/h, and K-values from Fig. 2.8 at the average of the two entering temperatures, (90 + 70)/2 = 80°F and a pressure of 4 atm = 59 psia. The feed gas composition and the resulting K-values and values of A are as follows:

Component	*f*, kmol/h	*K*-value	*A* = *L*/*KV*
C_1	250	35	0.0142
C_2	150	7.7	0.065
C_3	250	2.2	0.227
nC_4	200	0.65	0.769
nC_5	150	0.20	2.50
Total:	1000		

The fraction of a gas component not absorbed, ϕ_A, is given by the Kremser Eq. (5-48), and by material balance the amount absorbed follows:

$$\phi_A = \frac{A-1}{A^{N+1}-1} \quad \text{and} \quad \text{Percent absorbed} = 100(1-\phi_A)$$

The results for all three cases are as follows:

	N = 4 stages:		*N* = 10 stages:		*N* = 30 stages:	
Component	ϕ_A	**% absorbed**	ϕ_A	**% absorbed**	ϕ_A	**% absorbed**
C_1	0.986	1.4	0.986	1.4	0.986	1.4
C_2	0.935	6.5	0.935	6.5	0.935	6.5
C_3	0.773	22.7	0.773	22.7	0.773	22.7
nC_4	0.316	68.4	0.245	75.5	0.231	76.9
nC_5	0.0155	98.4	0.0001	99.99	0.0000	100.0

The above results show that as N increases, the percent absorption of the heavier components increases, but the absorption of the lighter components does not increase. However, beyond 10 stages, little change occurs.

Exercise 9.24

Subject: Flow rate of stripping steam by the Kremser method

Given: Feed of composition below enters a flash drum operating at 150°F and 2 atm. Equilibrium liquid is sent to a 5-equilibrium-stage stripper operating at 2 atm to give 0.5 kmol/h of nC_5 in stripper bottoms.

Find: Flow of steam needed in the stripper.

Analysis: Use Chemcad with the SRK equation of state to flash the feed to determine the liquid feed to the stripper. The result is:

Component	Feed, kmol/h	Distillate, kmol/h	Bottoms, kmol/h
C_1	13.7	13.6	0.1
C_2	101.3	98.2	3.1
C_3	146.9	134.9	12.0
nC_4	23.9	19.1	4.8
nC_5	5.7	3.4	2.3
nC_{12}	196.7	0.4	196.3
Total:	488.2	269.6	218.6

The stripping steam enters the stripper at 2 atm and 300°F. For the stripper, the average temperature of the two feeds = (150 + 300) = 225°F. From Fig. 2.8, the *K*-value of nC_5 at 2 atm and 225°F = 3.0. The average stripping factor for n-pentane can be taken as:

$$S = KV/L = 3V/218.6 = 0.0137\ V$$

The fraction of nC_5 not stripped = $\phi_S = 0.5/2.3 = 0.217$
Use Kremser Eq. (5-50) to compute the value of *S* needed for *N* = 5 theoretical stages.
By trial and error, the result from:

$$\phi_S = \frac{S-1}{S^{N+1}-1} = 0.217$$

is *S* = 0.89. Therefore,

Flow rate of stripping steam = *V* = *S*/0.0137 = 0.89/0.0137 = 65 kmol/h

Exercise 9.25

Subject: Stripping of a hydrocarbon liquid with superheated steam.

Given: 1000 kmol/h of feed liquid at 250°F with composition below. 100 kmol/h of superheated steam at 300°F and 50 psia. Stripper operates at 50 psia and has 3 equilibrium stages.

Assumptions: Negligible stripping of nC_{10} and negligible condensation of steam

Find: Flow rates and compositions of the exiting streams by the group (Kremser) method.

Analysis: Apply Kremser's method, with stripping factors, $S = KV/L$, computed for L = entering feed = 1000 kmol/h, V = entering steam rate = 100 kmol/h, and K-values from Fig. 2.8 at the average of the two entering temperatures, (250 + 300)/2 = 275°F and a pressure of 50 psia. The feed gas composition and the resulting K-values and values of S are as follows:

Component	f, kmol/h	K-value	$S = KV/L$
C_1	0.3	67	6.7
C_2	2.2	26	2.6
C_3	18.2	12.2	1.22
nC_4	44.7	6.0	0.60
nC_5	85.9	2.85	0.285
nC_{10}	848.7		
Total:	1000.0		

The fraction of a gas component not stripped, ϕ_S, is given by the Kremser Eq. (5-50), and by material balance the amounts stripped and not stripped follow:

$$\phi_S = \frac{S-1}{S^{N+1}-1} \quad \text{and} \quad l_1 = \phi_S f \quad \text{and} \quad v_3 = f - l_1$$

The results are as follows:

Component	ϕ_S	l_1, kmol/h	v_3, kmol/h
C_1	0.0028	0.0	0.3
C_2	0.036	0.1	2.1
C_3	0.181	3.3	14.9
nC_4	0.46	20.6	24.1
nC_5	0.72	61.8	24.1
Total:		85.8	65.5

The exiting gas is 65.5 + 100 = 165.5 kmol/h.
The exiting liquid is 85.8 + 848.7 = 934.5 kmol/h.

Exercise 9.26

Subject: Liquid-liquid extraction of a hydrocarbon mixture by diethylene glycol (DEG) by the group (Kremser) method.

Given: 100 kmol/h of an equimolar mixture of benzene (B), toluene (T), n-hexane (C6), and n-heptane (C7). Extraction at 150°C with 300 kmol/h of DEG. Extractor has 5 equilibrium stages. Distribution coefficients given below.

Find: Flow rates and compositions of extract and raffinate.

Analysis: Treat the problem like a stripper. Apply Kremser's method, with extraction factors, Eq. (9-39), $E = K_D V/L$, computed for L = entering feed = 100 kmol/h, V = entering DEG solvent rate = 300 kmol/h, and given values of K_D = mole fraction in extract/mole fraction in raffinate. The extract is like the vapor in stripping and the raffinate is like the liquid in stripping. The feed composition and the K-values and values of S are as follows:

Component	f, kmol/h	K_D	$E = K_D V/L$
Benzene	25	0.33	0.99
Toluene	25	0.29	0.87
n-Hexane	25	0.050	0.15
n-Heptane	25	0.043	0.129
Total:	100		

The fraction of a feed component not extracted, ϕ_E , is given by the Kremser Eq. (9-44), and by material balance the amounts stripped and not stripped follow:

$$\phi_E = \frac{E-1}{E^{N+1}-1} \quad \text{and} \quad l_1 = \phi_E f \quad \text{and} \quad v_3 = f - l_1$$

The results are as follows:

Component	ϕ_E	l_1, kmol/h	v_3, kmol/h
Benzene	0.177	4.3	20.7
Toluene	0.230	5.8	19.2
n-Hexane	0.850	21.2	3.8
n-Heptane	0.871	21.8	3.2
Total:		53.1	46.9

Now compute the transfer of DEG to the raffinate using Eqs. (9-40) and (9-43), using K_D = 30 $U = L/K_D V$ = 100/[30(300)] = 0.0111. ϕ_U = 0.9889. Therefore 0.9889(300) = 296.7 kmol/h of DEG leaves in the extract and 300 - 296.7 = 3.3 kmol/h in the raffinate.

The exiting extract flow rate = 46.9 + 296.7 = 343.6 kmol/h

The exiting raffinate flow rate = 53.1 + 3.3 = 56.4 kmol/h.

Exercise 9.27

Subject: Reboiled stripping of a normal paraffin hydrocarbon feed liquid by the group method.

Given: Feed liquid at 39°F and 300 psia and of composition given below is adiabatically flashed to 150 psia before entering a stripper containing 7 equilibrium stages and a partial reboiler. The bottoms flow rate from the stripper = B = 99.3 lbmol/h.

Find: Compositions of the vapor and liquid products from stripper.

Analysis: First, adiabatically flash the feed given below, using Chemcad with the SRK equation of state. The results of the flash are as follows, where the calculated flash temperature = 26.3°F:

	Lbmol/h:		
Component	**Feed**	**Vapor**	**Liquid**
C_1	59.5	37.67	21.83
C_2	73.6	14.83	58.77
C_3	153.2	8.90	144.30
nC_4	173.5	2.58	170.92
nC_5	58.2	0.23	57.97
nC_6	33.6	0.04	33.56
Total:	551.6	64.25	487.35

The liquid from the adiabatic flash is sent to the reboiled stripper where it is separated into an overhead vapor and a liquid bottoms. The overhead vapor is mixed with the vapor from the adiabatic flash to give the final vapor product.

To solve the reboiled stripper by the group method, apply Edmister's method, rather than Kremser's method, because we do not know the composition and flow rate of the vapor leaving the reboiler and entering the column. For a reboiled stripper, Eq. (5-64) applies:

$$\frac{l_F}{b} = \frac{S_B \phi_{AX} + 1}{\phi_{SX}} \quad (1) \qquad \text{where} \quad S_B = \frac{K_B V_B}{B} \quad (2)$$

For ϕ_{AX} and $\phi_{E\Xi}$, use average absorption and stripping factors computed for L = entering flash liquid = 487.35 kmol/h, V = vapor leaving the reboiler, which can be taken as L - B = 487.35 - 99.30 = 388.05 kmol/h, and K-values from Fig. 2.8 at an average temperature of say 200°F and a pressure of 150 psia. The feed gas composition and the resulting K-values, values of $S = KV/L$ and $A = 1/S$, and corresponding values of ϕ_{AX} and ϕ_{EX}, computed from Eqs. (5-48) and (5-50),

$$\phi_{AX} = \frac{A-1}{A^{N+1}-1} \quad \text{and} \quad \phi_{SX} = \frac{S-1}{S^{N+1}-1}$$

are as follows:

Exercise 9.27 (continued)

Analysis: (continued)

Component	l_F , lbmol/h	K-value	$S = KV/L$	$A = 1/S$	ϕ_{SX}	ϕ_{AX}
C_1	21.83	22	17.5	0.0571	0.000	0.943
C_2	58.77	7.1	5.65	0.177	0.000	0.823
C_3	144.30	2.9	2.31	0.433	0.004	0.569
nC_4	170.92	1.23	0.979	1.021	0.152	0.134
nC_5	57.97	0.52	0.414	2.415	0.587	0.003
nC_5	33.56	0.23	0.183	5.46	0.817	0.000
Total:	487.35					

To compute values of S_B from Eq. (2), the assumed value of V_B is critical. We seek the value of V_B that will give values of S_B , which when substituted into Eq. (1) will give values of b_i that will sum to the specified value of B = 99.3 lbmol/h. Assume the temperature at the bottom is 250°F and obtain from Fig. 2.8 values of K at 250°F and 150 psia. To begin, assume a value of V_B = 500 lbmol/h, calculate $B = \sum b_i$, and then adjust the values of b_i so they sum to the specified B. The results are as follows:

			lbmol/h:		
Component	K_B	S_B	l_F/b	b	Adj. b
C_1	23	116	--	0.00	0.00
C_2	8.8	44.3	---	0.00	0.00
C_3	4.0	20.1	3100	0.05	0.07
nC_4	1.85	9.31	14.8	11.55	25.92
nC_5	0.88	4.43	1.73	33.51	45.87
nC_5	0.45	2.27	1.22	27.44	27.44
Total:				72.55	99.30

The final product distribution is as follows, where it is compared to the result obtained by using Chemcad with the Tower model to also calculate the reboiled stripper:

		Edmister method:		**Rigorous Chemcad:**	
Component	**Feed, lbmol/h**	**Vapor product, lbmol/h**	**Stripped liquid, lbmol/h**	**Vapor product, lbmol/h**	**Stripped liquid, lbmol/h**
C_1	59.5	59.5	0.0	59.5	0.0
C_2	73.6	73.6	0.0	73.6	0.0
C_3	153.2	153.1	0.1	153.1	0.1
nC_4	173.5	147.6	25.9	150.8	22.7
nC_5	58.2	12.3	45.9	12.7	45.5
nC_5	33.6	6.2	27.4	2.6	31.0
Total:	551.6	452.3	99.3	452.3	99.3

The Edmister method is uncertain because average temperature and vapor rate are difficult to estimate.

Exercise 9.28

Subject: Comparison of FUG method with Edmister group method for distillation.

Given: Bubble-point liquid feed in kmol/h of 100 ethylbenzene, 100 paraxylene, 200 metaxylene, and 100 orthoxylene. Column pressures of 25 psia at the top and 35 psia at the bottom. Distillate to contain 1 kmol/h of orthoxylene and bottoms to contain 2 kmol/h metaxylene. Column to be equipped with a total condenser and partial reboiler.

Assumption: Applicability of Raoult's law for estimating *K*-values.

Find: (a) Number of stages and reflux ratio by the FUG method for $R/R_{min} = 1.1$
Feed-stage location by the Kirkbride equation.
(b) Distribution of components between distillate and bottoms by Edmister method.

Analysis: Need *K*-values at distillate, feed, and bottoms conditions. Because metaxylene and paraxylene have very close boiling points, assume the *d*/*b* ratio of paraxylene is the same as that for metaxylene. Therefore, have 1 kmol/h of paraxylene in the bottoms. Use Chemcad to obtain *K*-values by running bubble points on the feed, and estimated distillate and bottoms compositions. The results are:

			***K*-values:**		
Component	***d*, kmol/h**	***b*, kmol/h**	**25 psia, 159.3°C**	**30 psia, 168.4°C**	**35 psia, 180.5°C**
Ethylbenzene, EB	100	0	1.051	1.080	1.206
Paraxylene, PX	99	1	0.986	1.012	1.131
Metaxylene, MX	198	2	0.982	1.012	1.136
Orthoxylene, OX	1	99	0.855	0.884	0.996
Total:	398	101	distillate	feed	bottoms

(a) Using the Fenske equation (9-12), with MX as the LK and OX as the HK, with a geometric mean relative volatility = $[(0.982/0.855)(1.136/0.996)]^{1/2} = 1.144$

$$N_{min} = \frac{\log\left[\frac{d_{MX}}{d_{OX}}\frac{b_{OX}}{b_{MX}}\right]}{\log\left(\alpha_{MX,OX}\right)_{avg}} = \frac{\log\left[\frac{(198)}{(1)}\frac{(99)}{(2)}\right]}{\log 1.144} = 68.3$$

To compute the distribution of nonkey components at total reflux, use for the lighter than light key components, LLK, Eq. (9-15), with OX as the reference component, *r*, and the above value of N_{min}.

Exercise 9.28 (continued)

Analysis: (a) (continued)

Thus, for the LLK, i, $b_i = \dfrac{f_i}{1+\left(\dfrac{d_{OX}}{b_{OX}}\right)\alpha_{i,OX}^{N_{min}}} = \dfrac{f_i}{1+\left(\dfrac{1}{99}\right)\alpha_{i,OX}^{68.3}}$ (1)

Using geometric mean values of $\alpha_{i,OX}$, with Eq. (1) and the material balance, $f_i = d_i + b_i$, the following results are obtained:

kmol/h:

Component	Feed	Distillate	Bottoms
EB	100	99.99	0.01
PX	100	99.00	1.00
MX	200	198.00	2.00
OX	100	1.00	99.00
Total:	500	397.99	102.01

Because it is highly likely that PX, and possibly EB, will distribute, use the Class 2 Underwood equation, Eq. (9-28),which for a bubble-point feed, using relative volatilities at the feed conditions is:

$$\sum_i \frac{\alpha_{i,OX} z_{i,F}}{\alpha_{i,OX} - \theta} = 1 - q = 0 = \frac{1.2217(0.20)}{1.2217-\theta} + \frac{1.1448(0.20)}{1.1448-\theta} + \frac{1.1448(0.40)}{1.1448-\theta} + \frac{1.00(0.20)}{1.00-\theta} \quad (2)$$

There are two roots to Eq. (2), which from a spreadsheet calculation are:

θ = 1.0280 and 1.2027

Eq. (9-29) is applied in the following form for each of the two values of θ, in terms of the two unknowns, d_{EB} and L_{min}. The form used is obtained by multiplying Eq. (9-29) by the total distillate rate, D, which converts distillate mole fractions to component distillate rates, and the reflux ratio, R to L. The distillate rate of PX is not an unknown because it has the same relative volatility as MX. Thus, it must have the same d/b ratio as MX, making its distillate rate as 99 kmol/h.

$$D + L_{\min} = \frac{1.2217\ (d_{EB})}{1.2217 - 1.0280} + \frac{1.1448\ (297)}{1.1448 - 1.0280} + \frac{1.00\ (1)}{1.00 - 1.0280}$$

$$= 6.307(d_{EB}) + 2875.3$$

$$D + L_{\min} = \frac{1.2217(d_{EB})}{1.2217 - 1.2027} + \frac{1.1448(297)}{1.1448 - 1.2027} + \frac{1.00\ (1)}{1.00 - 1.2027}$$

$$= 64.30(d_{EB}) - 5877.2$$

Exercise 9.28 (continued)

Analysis: (a) (continued)

Because the total distillate rate, D, is also an unknown, the following equation is also needed:
$D = d_{EB} + 99 + 198 + 1 = d_{EB} + 298$
Solving these 3 linear equations, the following results are obtained:
D =448.9 kmol/h, $L_{\min}$ = 3378 kmol/h, and d_{EB} = 150.9 kmol/h. Thus, the assumption that EB distributes is incorrect because only 100 kmol/h of EB is in the feed. Therefore discard the root of θ = 1.2027. Also, D now equals 100 + 99 + 198 + 1 = 398 kmol/h. From above for the θ root of 1.0280, $D + L_{\min} = 6.307\ d_{EB} + 2875.3$.
Therefore, $L_{\min}$ = 6.307(100) + 2875.3 - 398 = 3108 kmol/h or $R_{\min} = L_{\min}/D$ = 3108/398 = 7.81

The operating reflux ratio = 1.1(7.81) = 8.59. In the Gilliland equation, (9-34),
$X = (R - R_{\min})/(R + 1)$ = (8.59 - 7.81)/(8.59 + 1) = 0.0813. Using Eq. (9.34), Y = 0.573 = $(N - N_{\min})/(N + 1)$. Solving, for $N_{\min}$ = 68.3, N = 161.3 equilibrium stages.

The Kirkbride Eq. (9-36) is used to determine the feed-stage location.

$$\frac{N_R}{N_S} = \left[\left(\frac{z_{OX,F}}{z_{MX,F}}\right)\left(\frac{x_{MX,B}}{x_{OX,D}}\right)^2\left(\frac{B}{D}\right)\right]^{0.206} = \left[\left(\frac{0.20}{0.40}\right)\left(\frac{0.0196}{0.00251}\right)^2\left(\frac{102.01}{397.99}\right)\right]^{0.206} = 1.53$$

Therefore, the feed stage is located at (1.53/2.53) 161.3 = stage 97.5 from the top.

(b) The Edmister group method is applied by using Eq. (5-66) to estimate the *b/d* ratio for each component:

$$\frac{b}{d} = A_F \frac{\left[\dfrac{\left(A_C \phi_{SE} + 1\right)}{\phi_{AE}}\right]}{\left[\dfrac{\left(S_B \phi_{AX} + 1\right)}{\phi_{SX}}\right]} \qquad (3)$$

For a total condenser, A_C = the reflux ratio = 8.59 for all components. To compute values of ϕ for each component, assume the following values of flow rates and stages for the enriching (rectifying) section and exhausting (stripping) section, based on constant molar overflow and noting that the feed and reboiler stages are not included in these two sections.

Variable	**Enriching Section**	**Exhausting Section**
Number of stages	97	63
Vapor rate, kmol/h	3817	3817
Liquid rate, kmol/h	3419	3919

Exercise 9.28 (continued)

Analysis: (b) (continued)

Because in the above table the *K*-values do not vary much, use arithmetic mean values for each section. These values and those for the feed stage and partial reboiler are as follows along with the corresponding values of the absorption and stripping factors, as defined by equations (5-38), (5-51), below (5-64), and (5-65), where $V_B/B = 3817/102 = 37.4$

Variable	EB	PX	MX	OX
K_E	1.066	0.999	0.997	0.870
A_E	0.840	0.897	0.898	1.030
$S_E = 1/A_E$	1.190	1.115	1.114	0.971
K_F	1.080	1.012	1.012	0.884
A_F	0.951	1.015	1.015	1.161
K_X	1.143	1.072	1.074	0.940
A_X	0.898	0.958	0.956	1.092
$S_X = 1/A_X$	1.114	1.044	1.046	0.918
K_B	1.206	1.131	1.136	0.996
S_B	45.1	42.3	42.5	37.3

Values of ϕ_A and ϕ_S are obtained from Eqs. (5-48) and (5-50), respectively:

Variable	EB	PX	MX	OX
ϕ_{AE}	0.160	0.103	0.102	0.00175
ϕ_{SE}	0.0000	0.0000	0.0000	0.0307
ϕ_{AX}	0.102	0.0449	0.0466	0.0003
ϕ_{SX}	0.0001	0.0030	0.00274	0.0823

Now apply Eq. (3) above to obtain the component distribution:

Variable	EB	PX	MX	OX
f, kmol/h	100	100	200	100
b/d	0.0001	0.0102	0.0091	68.2
d, kmol/h	99.99	98.99	198.20	0.68
b, kmol/h	0.01	1.01	1.80	99.32

Comparing these Edmister method results with the FUG method, we see that the Edmister method predicts a somewhat better split of the two key components than does the FUG method for this problem.

Exercise 10.1

Subject: Independency of MESH equations

Given: Equations (10-1), (10-3), (10-4), and (10-6).

Prove: Equation (10-6) is not independent of the other 3 equations

Analysis: Eq. (10-6) can be derived from the other 3 equations as follows, as outlined in the text between Eqs. (10-5) and (10-6)..

Summing Eq. (10-1) over all C components:

$$L_{j-1}\sum_{i=1}^{C} x_{i,j-1} + V_{j+1}\sum_{i=1}^{C} y_{i,j+1} + F_j \sum_{i=1}^{C} z_{i,F_j} - \left(L_j + U_j\right)\sum_{i=1}^{C} x_{i,j} - \left(V_j + W_j\right)\sum_{i=1}^{C} y_{i,j} = 0 \qquad (1)$$

From Eqs. (10-3) and (10-4), all 5 sums in Eq. (1) are equal to 1. Therefore, Eq. (1) becomes:

$$L_{j-1} + V_{j+1} + F_j - \left(L_j + U_j\right) - \left(V_j + W_j\right) = 0 \qquad (2)$$

Writing Eq. (2) for each stage from Stage 1 to Stage j:

$$\begin{aligned}
&L_0 + V_2 + F_1 - L_1 - U_1 - V_1 - W_1 = 0 \\
&L_1 + V_3 + F_2 - L_2 - U_2 - V_2 - W_2 = 0 \\
&L_2 + V_4 + F_3 - L_3 - U_3 - V_3 - W_3 = 0 \\
&\ldots\ldots \\
&L_{j-2} + V_j + F_{j-1} - L_{j-1} - U_{j-1} - V_{j-1} - W_{j-1} = 0 \\
&L_{j-1} + V_{j+1} + F_j - L_j - U_j - V_j - W_j = 0
\end{aligned} \qquad (3)$$

Summing Eqs. (2), noting that $L_0 = 0$ and that many variables cancel, we obtain:

$$V_{j+1} + \sum_{m=1}^{j}\left(F_m - U_m - W_m\right) - L_j - V_1 = 0$$

or $$L_j = V_{j+1} + \sum_{m=1}^{j}\left(F_m - U_m - W_m\right) - V_1$$

But this is Eq. (10-6). Therefore, it is not independent of Eqs. (10-1), (10-3), and (10-4).

Exercise 10.2

Subject: Revision of MESH equations to account for entrainment, occlusion, and chemical reaction (in the liquid phase).

Given: MESH Eqs. (10-1) to (10-5).

Find: Revised set of MESH equations.

Analysis:

Entrainment:

Let ϕ_j = ratio of entrained liquid (in the exiting vapor) that leaves Stage j to the liquid ($L_j + U_j$) leaving Stage j. Then, the entrained component liquid flow rate leaving Stage $j = \phi_j x_{i,j} (L_j + U_j)$. Correspondingly, the entrained component liquid flow rate entering Stage $j = \phi_{j+1} x_{i,j+1} (L_{j+1} + U_{j+1})$.

Occlusion:

Let θ_j = ratio of occluded vapor (in the exiting liquid) that leaves Stage j to the vapor ($V_j + W_j$) leaving Stage j. Then the occluded component liquid flow rate leaving Stage $j = \theta_j y_{i,j} (V_j + W_j)$. Correspondingly, the occluded component liquid flow rate entering Stage $j = \theta_{j-1} y_{i,j-1} (V_{j-1} + W_{j-1})$.

Chemical Reaction:

Let: M_j = molar liquid volume holdup on Stage j

M = number of independent chemical reactions

$\nu_{i,m}$ = stoichiometric coefficient of component i in chemical reaction m

$r_{k,m,j}$ = chemical reaction rate, $dc_{k,m,j}/dt$, of the mth chemical reaction for the reference reactant component, k, on Stage j

Then, the formation or disappearance of component i by chemical reaction on Stage j is:

$$M_j \sum_{m=1}^{M} \nu_{i,m} r_{k,m,j}$$

The component material balance equations, (10-1), now become:

$$L_{j-1}\sum_{i=1}^{C} x_{i,j-1} + V_{j+1}\sum_{i=1}^{C} y_{i,j+1} + F_j \sum_{i=1}^{C} z_{i,F_j} - \left(L_j + U_j\right)\sum_{i=1}^{C} x_{i,j} - \left(V_j + W_j\right)\sum_{i=1}^{C} y_{i,j} +$$

$$\theta_{j-1}\left(V_{j-1} + W_{j-1}\right) y_{i,j-1} - \theta_j \left(V_j + W_j\right) y_{i,j} + \phi_{j+1}\left(L_{j+1} + U_{j+1}\right) x_{i,j+1} - \phi_j \left(L_j + U_j\right) x_{i,j} - M_j \sum_{m=1}^{M} \nu_{i,m} r_{k,m,j} = 0$$

The equilibrium equations, (1-2) and the summation equations (10-3) and (10-4) do not change.

The energy balance is as follows, where the heat of reaction does not appear because it is assumed that enthalpies are referred to the elements:

$$L_{j-1}h_{L_{j-1}} + V_{j+1}h_{V_{j+1}} + F_j h_{F_j} + \theta_{j+1}\left(V_{j-1} + W_{j-1}\right)h_{V_{j-1}} + \phi_{j+1}\left(L_{j+1} + U_{j+1}\right)h_{L_{j+1}}$$
$$-\left(1+\theta_j\right)\left(V_j + W_j\right)h_{V_j} - \left(1+\phi_j\right)\left(L_j + U_j\right)h_{L_j} = 0$$

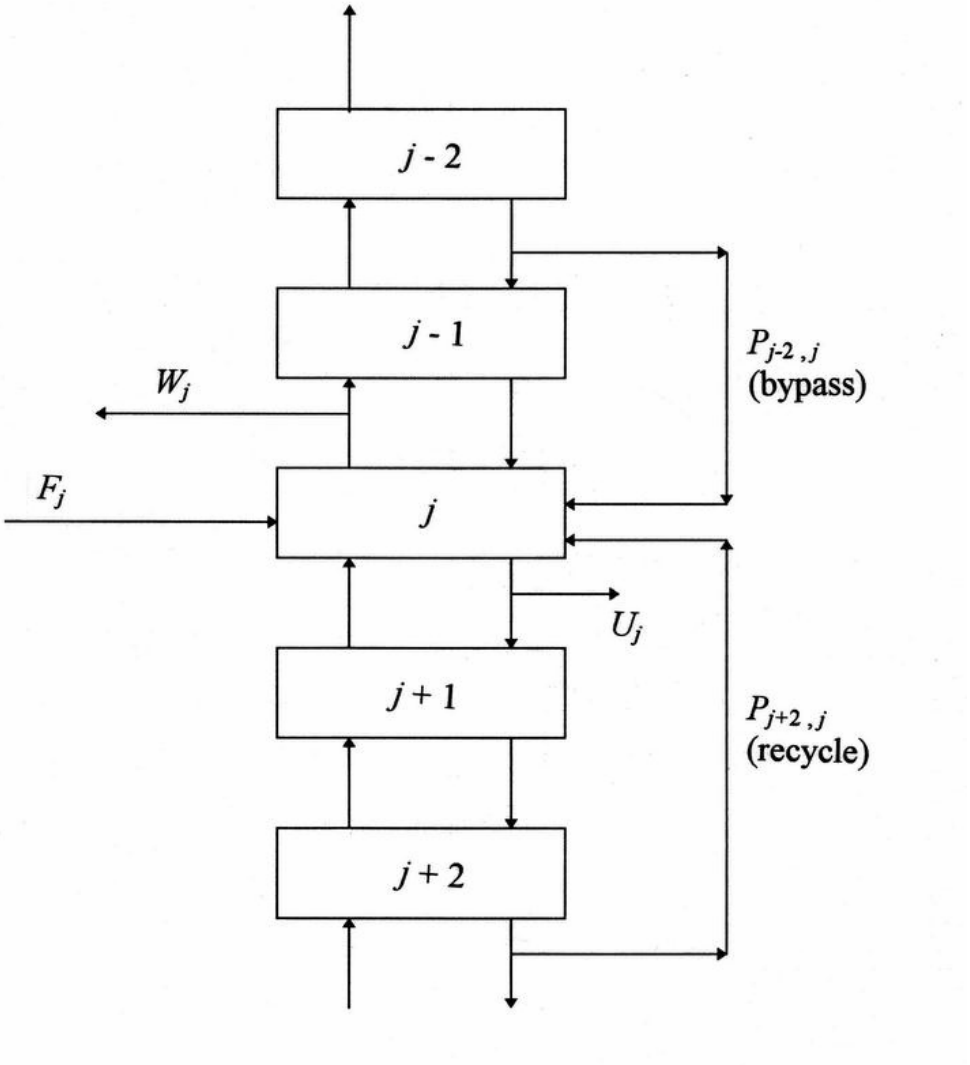
Exercise 10.3

Subject: Revised set of MESH equations.

Given: MESH Eqs. (10-1) to (10-5).

Find: Revised set of MESH equations to account for liquid pumparounds as shown in Fig. 10.2. Revised *M* equations like Eq. (10-7). Possible partitioning to tridiagonal sets.

Analysis: As an example, consider the section of equilibrium stages below, which includes a bypass pumparound and a recycle pumparound. Let $P_{u,v}$ designate a total molar liquid pumparound flow rate from Stage *u* to Stage *v*.



Exercise 10.3 (continued)

Analysis: (continued)

The revised MESH equations for Stage *j* are:

$$M_{i,j} = L_{j-1}x_{i,j-1} + V_{j+1}y_{i,j+1} + P_{j+2,j}x_{i,j+2} + P_{j-2,j}x_{i,j-2} + F_j z_{i,j} - \left(L_j + U_j\right)x_{i,j} - \left(V_j + W_j\right)y_{i,j} = 0 \qquad (1)$$

$$E_{i,j} = y_{i,j} - K_{i,j}x_{i,j} = 0 \qquad (2)$$

$$H_j = L_{j-1}h_{L_{j-1}} + V_{j+1}h_{V_{j+1}} + F_j h_{F_j} + P_{j-2,j}h_{L_{j-2}} + P_{j+2,j}h_{L_{j+2}} - \left(L_j + U_j\right)h_{L_j} - \left(V_j + W_j\right)h_{V_j} - Q_j = 0 \qquad (5)$$

$$L_j = V_{j+1} + \sum_{m=1}^{j}\left(F_m - U_m - W_m\right) - V_1 + P_{j+2,j} = 0 \qquad (6)$$

Equations (1), (2), and (6) are combined to give the following modified $M_{i,j}$ equations in terms of component mole fractions, assuming that all other variables are specified or guessed:

$$M_{i,j} = x_{i,j-1}\left[V_j + \sum_{m=1}^{j-1}\left(F_m - U_m - W_m\right) - V_1 - P_{j-2,j}\right] + x_{i,j+1}K_{i,j+1}V_{j+1} + P_{j+2,j}x_{i,j+2} + P_{j-2,j}x_{i,j-2} + F_j z_{i,j} - x_{i,j}\left[V_{j+1} + \sum_{m=1}^{j}\left(F_m - U_m - W_m\right) - V_1 + P_{j+2,j} + U_j + \left(V_j + W_j\right)K_{i,j}\right] = 0$$

Compared to Eqs. (10-7) to (10-11), we see that the modified $M_{i,j}$ equations contain 5, rather than 3, unknown liquid-phase mole fractions. The additional mole fractions are $x_{i,j+2}$ and $x_{i,j-2}$. Therefore, the set is no longer tridiagonal. We have a banded matrix with 5 bands, one additional band due to the recycle and one due to the bypass.

Exercise 10.4

Subject: Application of tridiagonal matrix algorithm.

Given: Thomas algorithm equations (10-13) to (10-18) and a 3x3 matrix equation below.

Find: Solution to the matrix equation.

Analysis: The matrix equation is:

$$\begin{bmatrix} B_1 & C_1 & 0 \\ A_2 & B_2 & C_2 \\ 0 & A_3 & B_3 \end{bmatrix} \bullet \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} D_1 \\ D_2 \\ D_3 \end{bmatrix} = \begin{bmatrix} -160 & 200 & 0 \\ 50 & -350 & 180 \\ 0 & 150 & -230 \end{bmatrix} \bullet \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 0 \\ -50 \\ 0 \end{bmatrix}$$

Applying the algorithm Eqs. (10-13) to (10-15):

$$p_1 = \frac{C_1}{B_1} = \frac{200}{-160} = -1.25 \qquad q_1 = \frac{D_1}{B_1} = \frac{0}{-160} = 0$$

$$p_2 = \frac{C_2}{B_2 - A_2 p_1} = \frac{180}{-350 - 50(-1.25)} = -0.626$$

$$q_2 = \frac{D_2 - A_2 q_1}{B_2 - A_2 p_1} = \frac{-50 - 50(0)}{-350 - 50(-1.25)} = 0.1739$$

$$p_3 = 0$$

$$q_3 = \frac{D_3 - A_3 q_2}{B_3 - A_3 p_2} = \frac{0 - 150(0.1739)}{-230 - 150(-0.626)} = 0.1917$$

Using Eqs. (10-17) and (10-18):

$x_3 = q_3 = 0.1917$

$x_2 = q_2 - p_2 x_3 = 0.1739 - (-0.626)(0.1917) = 0.2939$

$x_1 = q_1 - p_1 x_2 = 0 - (-1.25)(0.2939) = 0.3674$

Exercise 10.5

Subject: Application of tridiagonal matrix algorithm.

Given: Thomas algorithm equations (10-13) to (10-18) and a 3x3 matrix equation below.

Find: Solution to the matrix equation.

Analysis: The matrix equation is:

$$\begin{bmatrix} B_1 & C_1 & 0 & 0 & 0 \\ A_2 & B_2 & C_2 & 0 & 0 \\ 0 & A_3 & B_3 & C_3 & 0 \\ 0 & 0 & A_4 & B_4 & C_4 \\ 0 & 0 & 0 & A_5 & B_5 \end{bmatrix} \bullet \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \end{bmatrix} = \begin{bmatrix} D_1 \\ D_2 \\ D_3 \\ D_4 \\ D_5 \end{bmatrix} = \begin{bmatrix} -6 & 3 & 0 & 0 & 0 \\ 3 & -4.5 & 3 & 0 & 0 \\ 0 & 1.5 & -7.5 & 3 & 0 \\ 0 & 0 & 4.5 & -7.5 & 3 \\ 0 & 0 & 0 & 4.5 & -4.5 \end{bmatrix} \bullet \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 100 \\ 0 \\ 0 \end{bmatrix}$$

Applying the algorithm Eqs. (10-13) to (10-15):

$$p_1 = \frac{C_1}{B_1} = \frac{3}{-6} = -0.5 \qquad q_1 = \frac{D_1}{B_1} = \frac{0}{-6} = 0$$

$$p_2 = \frac{C_2}{B_2 - A_2 p_1} = \frac{3}{-4.5 - 3(-0.5)} = -1.0 \qquad q_2 = 0$$

$$p_3 = \frac{C_3}{B_3 - A_3 p_2} = \frac{3}{-7.5 - 1.5(-1.0)} = -0.5$$

$$q_3 = \frac{D_3 - A_3 q_2}{B_3 - A_3 p_2} = \frac{100 - 1.5(0)}{-7.5 - 15(-1.0)} = -16.67$$

$$p_4 = \frac{C_4}{B_4 - A_4 p_3} = \frac{3}{-7.5 - 4.5(-0.5)} = -0.57143$$

$$q_4 = \frac{D_4 - A_4 q_3}{B_4 - A_4 p_3} = \frac{0 - 4.5(-16.67)}{-7.5 - 4.5(-0.5)} = -14.28571$$

$$q_5 = \frac{D_5 - A_5 q_4}{B_5 - A_5 p_4} = \frac{0 - 4.5(-14.28571)}{-4.5 - 4.5(-0.57143)} = -33.333$$

Using Eqs. (10-17) and (10-18):

$x_5 = q_5 =$ -33.333

$x_4 = q_4 - p_4 x_5 =$ -14.28571 - (-0.57143)(-33.333) = -33.333

$x_3 = q_3 - p_3 x_4 =$ -16.6667 - (-0.5)(-33.333) = -33.333

$x_2 = q_2 - p_2 x_3 =$ 0.0 - (-1.0)(-33.333) = -33.333

$x_1 = q_1 - p_1 x_2 =$ 0.0 - (-0.5)(-33.333) = -16.667

Exercise 10.6

Subject: Solution of tridiagonal matrix equation for liquid-phase mole fractions to avoid subtraction of nearly equal quantities as claimed by Wang and Henke.

Given: Equations (10-1) to (10-18)

Prove: Claim of Wang and Henke.

Analysis: First investigate the values of p_j. From Eq. (10-14), a subtraction occurs in the denominator:

$$p_j = \frac{C_j}{B_j - A_j p_{j-1}}$$

Starting at the top of the column, $p_1 = C_1/B_1$, therefore, the denominator of Eq. (10-14) becomes:

$B_2 - A_2 p_1 = B_2 - A_2\left(\frac{C_1}{B_1}\right)$ Clearing the fraction, we obtain $B_1 B_2 - A_2 C_1$

Examine this difference by substituting for each of the four quantities. From Eq. (10-8),

$A_2 = V_2 + F_1 - W_1 - U_1 - V_1$

However, by material balance around Stage 1 in Fig. 10.3,

$V_2 + F_1 - W_1 - U_1 - V_1 = L_1$

Therefore, $A_2 = L_1$

From Eq. (10-9),

$B_1 = -[V_2 + F_1 - W_1 - U_1 - V_1 + U_1 + (V_1 + W_1)K_{i,1}]$

However, by material balance around Stage 1 in Fig. 10.3,

$V_2 + F_1 - W_1 - U_1 - V_1 = L_1$

Therefore, $B_1 = -\left[(V_1 + W_1)K_{i,1} + (L_1 + U_1)\right]$

Similarly, $B_2 = -\left[(V_2 + W_2)K_{i,2} + (L_2 + U_2)\right]$

Thus, it is clear that $B_1 B_2$ = a summation of all positive quantities, that is no subtractions.

From Eq. (10-10), $C_1 = V_2 K_{i,2}$ and $A_2 C_1 = L_1 V_2 K_{i,2}$

When $B_1 B_2$ is expanded, it contains a term $-L_1 V_2 K_{i,2}$.

Thus, this potential subtraction in $B_1 B_2 - A_2 C_1$ is cancelled.

There are no subtractions in p_2. The same is found for all p_j.

Now investigate values of q_j. From Eq. (10-15), subtractions occur in the numerator and denominator:

Exercise 10.6 (continued)

Analysis: (continued)

$$q_j = \frac{D_j - A_j q_{j-1}}{B_j - A_j p_{j-1}}$$

The denominator is identical to that already examined in p_j. So we only have to investigate the numerator.

Using Eqs. (10-9), as above, and (10-11),

$$q_1 = \frac{D_1}{B_1} = \frac{-F_1 z_{i,1}}{-\left[\left(V_1 + W_1\right)K_{i,1} + \left(L_1 + U_1\right)\right]}$$ which contains no subtraction problems

Therefore, the numerator in Eq. (10-15) becomes:

$$D_2 - A_2 q_1 = -F_2 z_{i,2} - L_1 \left\{ \frac{-F_1 z_{i,2}}{-\left[\left(V_1 + W_1\right)K_{i,1} + \left(L_1 + U_1\right)\right]} \right\} = \frac{F_2 z_{i,2}\left[\left(V_1 + W_1\right)K_{i,1} + \left(L_1 + U_1\right)\right] + L_1 F_1 z_{i,1}}{-\left[\left(V_1 + W_1\right)K_{i,1} + \left(L_1 + U_1\right)\right]}$$

Thus, no subtractions appear in this numerator. The result is obtained for all q_j.

Therefore, the claim of Wang and Henke is verified.

Exercise 10.7

Subject: Derivation of stagewise component material balance equations in terms of component vapor flow rates rather than liquid-phase mole fractions.

Given: Eq. (10-7).

Find: Component flow rates form of Eq. (10-7). Whether equations can still be partitioned into *C* tridiagonal matrix equations.

Analysis: Start with Eqs. (10-1), (10-2), and (10-6) for L_j and L_{j-1}:

$$M_{i,j} = L_{j-1}x_{i,j-1} + V_{j+1}y_{i,j+1} + F_j z_{i,j} - \left(L_j + U_j\right)x_{i,j} - \left(V_j + W_j\right)y_{i,j} = 0 \qquad (1)$$

$$E_{i,j} = y_{i,j} - K_{i,j}x_{i,j} = 0 \qquad (2)$$

$$L_j = V_{j+1} + \sum_{m=1}^{j}\left(F_m - U_m - W_m\right) - V_1 \qquad (3)$$

$$L_{j-1} = V_j + \sum_{m=1}^{j-1}\left(F_m - U_m - W_m\right) - V_1 \qquad (4)$$

Substituting Eqs. (2) to (4) into (1), to eliminate variables in *L* and *x*,

$$M_{i,j} = \left[V_j + \sum_{m}^{j-1}\left(F_m - U_m - W_m\right) - V_1\right]\frac{v_{i,j-1}}{V_{i,j-1}K_{i,j-1}} + v_{i,j+1} + F_j z_{i,j}$$
$$-\left[V_{j+1} + \sum_{m}^{j}\left(F_m - U_m - W_m\right) - V_1 + U_j\right]\frac{v_{i,j}}{V_j K_{i,j}} - v_{i,j} - W_j\frac{v_{i,j}}{V_j} = 0$$

Collecting terms in the component vapor flow rates,

$$M_{i,j} = \left[V_j + \sum_{m}^{j-1}\left(F_m - U_m - W_m\right) - V_1\right]\frac{v_{i,j-1}}{V_{i,j-1}K_{i,j-1}} +$$
$$-\left\{\left[V_{j+1} + \sum_{m}^{j}\left(F_m - U_m - W_m\right) - V_1 + U_j\right]\frac{1}{V_j K_{i,j}} - 1 - \frac{W_j}{V_j}\right\}v_{i,j} + v_{i,j+1} + F_j z_{i,j} = 0$$

Thus, we will have a set of equations that can be partitioned into *C* tridiagonal sets.

Exercise 10.8

Subject: Computer storage locations for tridiagonal matrix equations

Given: Eqs. (10-7) to (10-11)

Find: Minimum storage locations needed.

Analysis: For a 100-stage column, only need:

99 storage locations for p_j

100 storage locations for q_j

4 storage locations for current values of A_j, B_j, C_j, and D_j

This is total of 203 storage locations.

If A_j, B_j, C_j, and D_j expressions are substituted into the p_j and q_j equations, then only need 199 storage locations.

Exercise 10.9

Subject: Solving a set of two nonlinear equations by the Newton-Raphson method.

Given: Two nonlinear equations in x_1 and x_2:

$$x_1^2 + x_2^2 = 17$$
$$(8x_1)^{1/3} + x_2^{1/2} = 4$$

Find: Solutions for four different starting guesses

Analysis:

(a) Starting guess is $x_1 = 2$, $x_2 = 5$

The Newton-Raphson method converges in 5 iterations:

Iteration	x_1	x_2
Start	2.000	5.000
1	0.5237	4.3911
2	0.8866	4.0569
3	0.9943	4.0032
4	0.9999873	4.0000
5	1.0000	4.0000

(b) Starting guess is $x_1 = 4$, $x_2 = 5$

The Newton-Raphson method fails. After only one iteration, $x_1 = -6.2135$, $x_2 = 10.7719$

(c) Starting guess is $x_1 = 1$, $x_2 = 1$

The Newton-Raphson method fails. After only one iteration, $x_1 = -15.4910$, $x_2 = 24.9880$

(d) Starting guess is $x_1 = 8$, $x_2 = 1$

The Newton-Raphson method fails. After only one iteration, $x_1 = 5.1320$, $x_2 = -0.4449$

Note that by a homotopy continuation method, two roots in the positive domain are obtained:

$x_1 = 1$, $x_2 = 4$

$x_1 = 4.0715$, $x_2 = 0.65027$

If the Newton-Raphson method is damped by using a line search, the method fails less often.

Exercise 10.10

Subject: Solving a set of two nonlinear equations by the Newton-Raphson method.

Given: Two nonlinear equations in x_1 and x_2:

$$\sin(\pi x_1 x_2) - \frac{x_2}{2} - x_1 = 0$$

$$\exp(2x_1)\left[1 - \frac{1}{4\pi}\right] + \exp(1)\left[\frac{1}{4\pi} - 1 - 2x_1 + x_2\right] = 0$$

Find: Solutions for three different starting guesses

Analysis:

(a) Starting guess is $x_1 = 0.4$, $x_2 = 0.9$

The Newton-Raphson method converges in 4 iterations:

Iteration	x_1	x_2
Start	0.4000	0.9000
1	0.1415	0.8394
2	0.2806	0.9073
3	0.2984	0.9026
4	0.2994	0.9030

(b) Starting guess is $x_1 = 0.6$, $x_2 = 0.9$

The Newton-Raphson method converges to a different solution in just 3 iterations.

Iteration	x_1	x_2
Start	0.6000	0.9000
1	0.4901	1.0235
2	0.4999	1.0002
3	0.5000	1.0000

(c) Starting guess is $x_1 = 1$, $x_2 = 1$

The Newton-Raphson method converges with some oscillations in 14 iterations.

Iteration	x_1	x_2	**Iteration**	x_1	x_2
Start	1.0000	1.0000	8	1.0042	0.4451
1	0.9091	0.6914	9	0.7160	1.2837
2	1.0720	0.2987	10	0.6514	0.9886
3	0.9727	0.5500	11	0.5135	1.0452
4	1.1633	-0.0252	12	0.5045	1.0008
5	1.0511	0.3321	13	0.5001	1.0001
6	0.9512	0.6053	14	0.5000	1.0000
7	1.0876	0.2072			

Exercise 10.11

Subject: Calculations for the first iteration of the Bubble-Point method

Given: Feed of 1000 kmol/h of a bubble-point mixture of 60 mol% methanol (M), 20 mol% ethanol (E), and 20 mol% n-propanol (P) is sent to the middle stage of a column with a total condenser, 3 equilibrium stages in the column, and a partial reboiler, and operating at 1 atm. The distillate rate = 600 kmol/h and the reflux rate = 2,000 kmol/h.

Assumptions: Ideal solutions with Raoult's law *K*-values. Constant molar overflow.

Find: Liquid-phase component mole fractions and stage temperatures from the first iteration of the bubble-point method.

Analysis: By material balance, the bottoms flow rate = 1000 - 600 = 400 kmol/h. The liquid rate above the feed = 2000 kmol/h. The liquid rate below the feed = 3000 kmol/h. The boilup rate over the entire column = 3000 - 400 = 2600 kmol/h. Based on the distillate rate, methanol will be mainly in the distillate, with ethanol and n-propanol mainly in the bottoms. The boiling points of these three components are, respectively, 64.7°C, 78.4°C, and 97.8°C. As a first approximation, assume a distillate temperature of 64.7°C and a bottoms temperature of (78.4 + 97.8)/2 = 88.1°C. Therefore, the initial guesses, assuming a linear temperature profile, for the tear variables and the total liquid flow rates are:

Stage j	V_j, kmol/h	T_j, °C	L_j, kmol/h
1 (Total condenser)	0	64.7	2000
2	2600	70.6	2000
3	2600	76.4	3000
4	2600	82.3	3000
5 (Partial reboiler)	2600	88.1	400

Compute *K*-values at 1 atm and the above temperatures for each component by Eq. (2-44), $K = P_i^s/P$. From the 7th edition of Perry's Handbook, on page 2-50 to 2-54, in Table 2-6, vapor pressure data are fitted to an extended Clausius-Clapeyron equation:

$P^s = \exp\left(C1 + \frac{C2}{T} + C3 \ln T + C4 T^{C5} \right)$, P^s is in Pa and T is in K, where the constants are:

Component	$C1$	$C2$	C3	C4	$C5$
M	81.768	-6876	-8.7078	7.1926E-6	2
E	74.475	-7164.3	-7.327	3.1340E-6	2
P	88.134	-8498.6	-9.0766	8.3303E-18	6

Exercise 10.11 (continued)

Analysis: (continued)

Computed *K*-values at the five assumed stage temperatures for P = 101300 Pa are:

Stage	1	2	3	4	5
Temperature, K	337.9	343.7	349.6	355.4	361.3
K-values:					
M	1.0086	1.2639	1.5702	1.9350	2.3665
E	0.5705	0.7309	0.9272	1.1654	1.4521
P	0.2505	0.3294	0.4281	0.5504	0.7002

A plot of the *K*-values as a function of temperature is shown on the next page.

The component material balance equations, combined with the equilibrium equations to eliminate vapor-phase mole fractions, for each of the 5 stages are as follows:

Stage 1: $$-(D+L_1)x_{i,1}+V_2K_{i,2}x_{i,2}=0$$

$$-2600x_{i,1}+2600K_{i,2}x_{i,2}=0 \qquad (1)$$

Stage 2: $$L_1x_{i,1}-(V_2K_{i,2}+L_2)x_{i,2}+V_3K_{i,3}x_{i,3}=0$$

$$2000x_{i,1}-(2600K_{i,2}+2000)x_{i,2}+2600K_{i,3}x_{i,3}=0 \qquad (2)$$

Stage 3: $$L_2x_{i,2}-(V_3K_{i,3}+L_3)x_{i,3}+V_4K_{i,4}x_{i,4}=-F_3z_{i,3}$$

$$2000x_{i,2}-(2600K_{i,3}+2000)x_{i,3}+2600K_{i,4}x_{i,4}=-1000z_{i,3} \qquad (3)$$

Stage 4: $$L_3x_{i,3}-(V_4K_{i,4}+L_4)x_{i,4}+V_5K_{i,5}x_{i,5}=0$$

$$3000x_{i,3}-(2600K_{i,4}+3000)x_{i,4}+2600K_{i,5}x_{i,5}=0 \qquad (4)$$

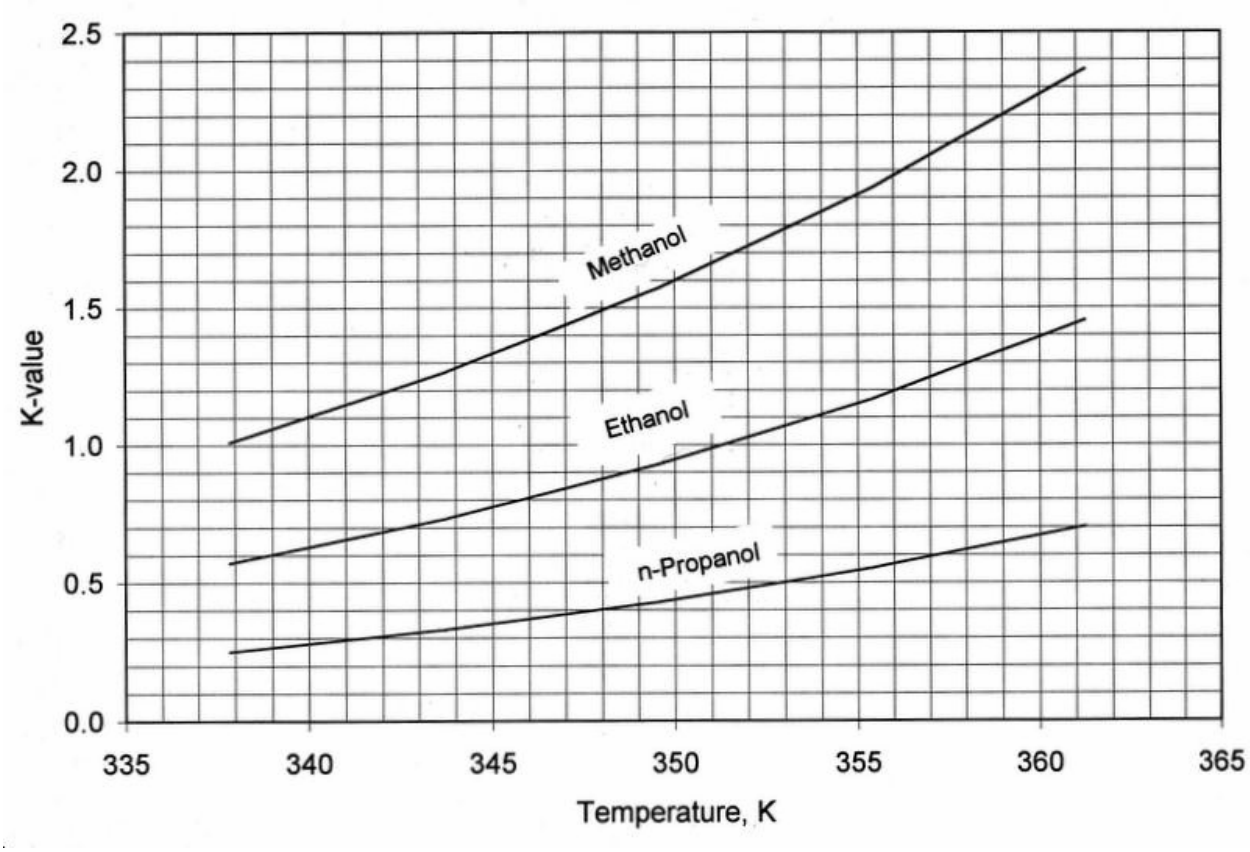
Stage 5: $$L_4x_{i,4}-(V_5K_{i,5}+B)x_{i,5}=0$$

$$3000x_{i,4}-(2600K_{i,5}+400)x_{i,5}=0 \qquad (5)$$

For each component, the *K*-values for each stage are substituted from the table above. The resulting equations form 3 tridiagonal matrix equations, one each for each of the 3 components. These equations are as follows, as produced from a spreadsheet:

Exercise 10.11 (continued)

Analysis: (continued)



Exercise 10.11 (continued)

Analysis: (continued)

Tridiagonal Matrices for combined material balances and phase equilibrium:

MeOH:

Stage 1	-2600.0	3286.1	0.0	0.0	0.0	•	x i,1	=	0
2	2000.0	-5286.1	4082.5	0.0	0.0		x i,2		0
3	0.0	2000.0	-7082.5	5031.1	0.0		x i,3		-600
4	0.0	0.0	3000.0	-8031.1	6153.0		x i,4		0
5	0.0	0.0	0.0	3000.0	-6553.0		x i,5		0

EtOH:

Stage 1	-2600.0	1900.3	0.0	0.0	0.0	•	x i,1	=	0
2	2000.0	-3900.3	2410.7	0.0	0.0		x i,2		0
3	0.0	2000.0	-5410.7	3030.1	0.0		x i,3		-200
4	0.0	0.0	3000.0	-6030.1	3775.5		x i,4		0
5	0.0	0.0	0.0	3000.0	-4175.5		x i,5		0

n-PrOH:

Stage 1	-2600.0	856.5	0.0	0.0	0.0	•	x i,1	=	0
2	2000.0	-2856.5	1113.1	0.0	0.0		x i,2		0
3	0.0	2000.0	-4113.1	1430.9	0.0		x i,3		-200
4	0.0	0.0	3000.0	-4430.9	1820.5		x i,4		0
5	0.0	0.0	0.0	3000.0	-2220.5		x i,5		0

Each of the three matrix equations is solved by the Thomas algorithm, giving the following results:

Mole fraction in liquid phase:

Comp.	Stg 1	2	3	4	5
MeOH	0.9142	0.7233	0.4887	0.2812	0.1288
EtOH	0.2084	0.2851	0.2884	0.2608	0.1874
n-PrOH	0.0362	0.1098	0.2168	0.3299	0.4457
Sum	1.1588	1.1182	0.9939	0.8719	0.7619

Because the mole fractions for each stage do not sum to one, they are normalized using Eq, (10-19), with the following results:

Normalized Mole fraction in liquid phase:

Comp.	Stg 1	2	3	4	5
MeOH	0.7889	0.6468	0.4917	0.3225	0.1691
EtOH	0.1798	0.2550	0.2902	0.2991	0.2460
n-PrOH	0.0312	0.0982	0.2181	0.3784	0.5850
Sum	1.0000	1.0000	1.0000	1.0000	1.0000

Exercise 10.11 (continued)

Analysis: (continued)

A new set of stage temperatures is computed by running bubble-point temperature calculations to find a temperature that satisfies Eq. (10-21), using the normalized mole fractions with the vapor pressure equations and a pressure of 1 atm. The results are as follows compared to the initially assumed values:

Stage j	**T_j, °C initially assumed**	**T_j, °C from 1st iteration**
1 (Total condenser)	64.7	67.2
2	70.6	69.6
3	76.4	73.1
4	82.3	77.8
5 (Partial reboiler)	88.1	84.1

Exercise 10.12

Subject: Solving a block tridiagonal matrix equation.

Given: 9 linear equations in 9 unknowns.

Find: Values of the 9 unknowns using the block form of the Thomas algorithm.

Analysis: To form a block tridiagonal matrix structure, interchange the last 3 equations with the middle group of 3 equations. The result is:

$$\begin{bmatrix} 0 & 1 & 2 & 2 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & 3 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 1 & 1 & 0 & 0 & 0 \\ 1 & 2 & 1 & 1 & 1 & 2 & 3 & 1 & 0 \\ 0 & 1 & 2 & 2 & 1 & 1 & 1 & 1 & 3 \\ 0 & 0 & 1 & 1 & 2 & 1 & 2 & 1 & 1 \\ 0 & 0 & 0 & 1 & 2 & 1 & 2 & 2 & 1 \\ 0 & 0 & 0 & 1 & 1 & 2 & 3 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 2 & 1 \end{bmatrix} \bullet \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \\ x_7 \\ x_8 \\ x_9 \end{bmatrix} = - \begin{bmatrix} -7 \\ -6 \\ -6 \\ -13 \\ -14 \\ -10 \\ -11 \\ -8 \\ -8 \end{bmatrix}$$

The solution proceeds as in Example 10.7, with a matrix of the form:

$$\begin{bmatrix} \overline{B}_1 & \overline{C}_1 & 0 \\ \overline{A}_2 & \overline{B}_2 & \overline{C}_2 \\ 0 & \overline{A}_3 & \overline{B}_3 \end{bmatrix} \bullet \begin{bmatrix} \Delta X_1 \\ \Delta X_2 \\ \Delta X_3 \end{bmatrix} = - \begin{bmatrix} F_1 \\ F_2 \\ F_3 \end{bmatrix}$$

$$\left(\overline{B}_1\right)^{-1} = \begin{bmatrix} -0.5 & 0.5 & 0.5 \\ 0 & -1 & 1 \\ 0.5 & 0.5 & -0.5 \end{bmatrix} \qquad \left(\overline{B}_1\right)^{-1}\left(\overline{C}_1\right) = \begin{bmatrix} -0.5 & 2 & 0 \\ -1 & -2 & 1 \\ 1.5 & 1 & 0 \end{bmatrix} \text{ which replaces } \left(\overline{C}_1\right)$$

$$\left(\overline{B}_1\right)^{-1}\left(\overline{F}_1\right) = \begin{bmatrix} -2.5 \\ 0 \\ -3.5 \end{bmatrix} \text{ which replaces } \left(\overline{F}_1\right) \quad \text{and} \quad I = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \text{ which replaces } \left(\overline{B}_1\right)$$

Exercise 10.12 (continued)

Analysis: (continued)

$$\left(\overline{B}_2 - \overline{A}_2\overline{C}_1\right) = \begin{bmatrix} 2 & 2 & 0 \\ 0 & 1 & 0 \\ -0.5 & 1 & 1 \end{bmatrix} \quad \text{Upon inversion,} \quad \left(\overline{B}_2 - \overline{A}_2\overline{C}_1\right)^{-1} = \begin{bmatrix} 0.5 & -1 & 0 \\ 0 & 1 & 0 \\ 0.25 & -1.5 & 1 \end{bmatrix}$$

$$\left(\overline{B}_2 - \overline{A}_2\overline{C}_1\right)^{-1}\overline{C}_2 = \begin{bmatrix} 0.5 & -0.5 & -3 \\ 1 & 1 & 3 \\ 1.25 & -0.25 & -3.5 \end{bmatrix} \quad \text{which replaces } \overline{C}_2$$

$$\left(\overline{F}_2 - \overline{A}_2\overline{F}_1\right) = \begin{bmatrix} -7 \\ -7 \\ -6.5 \end{bmatrix} \quad \text{which replaces } \overline{F}_2$$

$$\left(\overline{B}_2 - \overline{A}_2\overline{C}_1\right)^{-1}\overline{F}_2 = \begin{bmatrix} 3.5 \\ -7 \\ 2.25 \end{bmatrix} \quad \text{which replaces } \overline{F}_2$$

$\overline{A}_2$ is replaced by $\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$ $\overline{B}_2$ is replaced by $\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$

$$\left(\overline{B}_3 - \overline{A}_3\overline{C}_2\right) = \begin{bmatrix} -1.75 & 0.75 & 1.5 \\ -1 & 0 & 8 \\ -1.25 & 1.25 & 1.5 \end{bmatrix} \quad \text{Upon inversion,} \quad \left(\overline{B}_3 - \overline{A}_3\overline{C}_2\right)^{-1} = \frac{1}{9.25}\begin{bmatrix} -10 & 0.75 & 6 \\ 8.5 & -0.75 & 12.5 \\ -1.25 & 1.25 & 0.75 \end{bmatrix}$$

$$\left(\overline{F}_3 - \overline{A}_3\overline{F}_2\right) = \begin{bmatrix} -2.75 \\ -9 \\ -2.25 \end{bmatrix} \quad \text{which replaces } \overline{F}_3$$

$$\left(\overline{B}_3 - \overline{A}_3\overline{C}_2\right)^{-1}\overline{F}_3 = \begin{bmatrix} 0.13514 \\ -1.13514 \\ -1.10811 \end{bmatrix} \quad \text{which replaces } \overline{F}_3 = -\begin{bmatrix} x_7 \\ x_8 \\ x_9 \end{bmatrix}$$

$$\left(\overline{F}_2 - \overline{C}_2\overline{F}_3\right) = \begin{bmatrix} -0.45947 \\ -2.67567 \\ -2.08110 \end{bmatrix} \quad \text{which replaces } \overline{F}_2 = -\begin{bmatrix} x_4 \\ x_5 \\ x_6 \end{bmatrix}$$

$$\left(\overline{F}_1 - \overline{C}_1\overline{F}_2\right) = \begin{bmatrix} 2.62161 \\ -3.72971 \\ -0.13513 \end{bmatrix} \quad \text{which replaces } \overline{F}_1 = -\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

Exercise 10.12 (continued)

Analysis: (continued)

Therefore, the solution to the 9 equations is:

$x_1 = -2.62161$

$x_2 = 3.72971$

$x_3 = 0.13513$

$x_4 = 0.45947$

$x_5 = 2.67567$

$x_6 = 2.08110$

$x_7 = -0.13514$

$x_8 = 1.13514$

$x_9 = 1.10811$

Exercise 10.13

Subject: Matrix structure when equations are ordered by type.

Given: Mesh equations (10-58) to (10-60).

Find: Whether matrix structure is block tridiagonal.

Analysis: Many matrix structures are possible depending on the order of the equations and the order of the variables. Referring to Eqs. (10-61) to (10-64), try the following orders for a three component system, where *j* refers to the stage number:

$$\mathbf{F} = [\, H_j \,,\, M_{1,j} \,,\, M_{2,j} \,,\, M_{3,j} \,,\, E_{1,j} \,,\, E_{2,j} \,,\, E_{3,j} \,]$$

$$\mathbf{X} = [\, v_{1,j} \,,\, v_{2,j} \,,\, v_{3,j} \,,\, T_j \,,\, l_{1,j} \,,\, l_{2,j} \,,\, l_{3,j} \,]$$

For a three-stage system, the incidence matrix is on the next page, where x denotes that the variable for that column appears in the equation for that row.

It is seen in the incidence diagram that the matrix is not block tridiagonal or banded. If the order of the equations is maintained, it is not possible to permute the variable columns to get a block-banded structure.

Exercise 10.13 (continued)

Analysis: (continued)

Incidence Matrix

	$\nu_{1,1}$	$\nu_{1,2}$	$\nu_{1,3}$	$\nu_{2,1}$	$\nu_{2,2}$	$\nu_{2,3}$	$\nu_{3,1}$	$\nu_{3,2}$	$\nu_{3,3}$	T_1	T_2	T_3	$l_{1,1}$	$l_{1,2}$	$l_{1,3}$	$l_{2,1}$	$l_{2,2}$	$l_{2,3}$	$l_{3,1}$	$l_{3,2}$	$l_{3,3}$
H_1	x	x		x	x		x	x		x	x		x			x			x		
H_2		x	x		x	x		x	x	x	x	x	x	x		x	x		x	x	
H_3			x			x			x		x	x		x	x		x	x		x	x
$M_{1,1}$	x	x											x								
$M_{1,2}$		x	x										x	x							
$M_{1,3}$			x											x	x						
$M_{2,1}$				x	x											x					
$M_{2,2}$					x	x										x	x				
$M_{2,3}$						x											x	x			
$M_{3,1}$							x	x											x		
$M_{3,2}$								x	x										x	x	
$M_{3,3}$									x											x	x
$E_{1,1}$	x			x			x			x			x			x			x		
$E_{1,2}$		x			x			x			x			x			x			x	
$E_{1,3}$			x			x			x			x			x			x			x
$E_{2,1}$	x			x			x			x			x			x			x		
$E_{2,2}$		x			x			x			x			x			x			x	
$E_{2,3}$			x			x			x			x			x			x			x
$E_{3,1}$	x			x			x			x			x			x			x		
$E_{3,2}$		x			x			x			x			x			x			x	
$E_{3,3}$			x			x			x			x			x			x			x

Exercise 10.14

Subject: Obtaining derivatives of *K*-values for use in the Jacobian of the simultaneous-correction method.

Given: Chao-Seader correlation for the *K*-value based on Eq. (2) in Table 2.3.

Find: Analytical derivatives for: $\frac{\partial K_{i,j}}{\partial T_j}$, $\frac{\partial K_{i,j}}{\partial \upsilon_{i,k}}$, and $\frac{\partial K_{i,j}}{\partial l_{i,k}}$.

where, $\upsilon_{l,k} = y_{i,k}V_k$ and $l = x_{i,k}L_k$ and component molar flow rates.

Analysis: From Eq. (2) in Table 2.3, $K_i = \frac{\gamma_{iL}\phi_{iL}}{\phi_{iV}}$ (1)

From Eqs. (2-64) and (2-62),

$$\gamma_{iL} = \exp\left[\frac{v_{iL}}{RT}\left(\delta_i - \sum_{j=1}^{C}\Phi_j\delta_j\right)^2\right] \tag{2}$$

From Eq. (2-61), where for a given component, i, v_{iL} and δ_i are constants,

$$\Phi_i = \frac{x_i v_{iL}}{\sum_{j=1}^{C} x_j v_{iL}} \tag{3}$$

It is important to distinguish between the symbols $\upsilon_{i,k}$ (the molar vapor component flow rate) and v_{iL} (the component molar volume in the liquid phase = a constant).

For the liquid-phase, pure-component, fugacity coefficient, the Chao-Seader equations are:

$$\log\phi_{iL} = \log\phi_{iL}^{(0)} + \omega_i \log\phi_{iL}^{(1)} \tag{4}$$

$$\log\phi_{iL}^{(0)} = A_0 + \frac{A_1}{T_{r_i}} + A_2T_{r_i} + A_3T_{r_i}^2 + A_4T_{r_i}^3 + P_{r_i}\left(A_5 + A_6T_{r_i} + A_7T_{r_i}^2\right) + P_{r_i}^2\left(A_8 + A_9T_{r_i}\right) - \log P_{r_i} \tag{5}$$

$$\log\phi_{iL}^{(1)} = A_{10} + A_{11}T_{r_i} + \frac{A_{12}}{T_{r_i}} + A_{13}T_{r_i}^3 + A_{14}\left(P_{r_i} - 0.6\right) \tag{6}$$

where, $T_r = T/T_c$

Exercise 10.14 (continued)

Analysis (continued)

From Eqs. (2-56), (2-46), (2-47), (2-48), (2-49), and (2-50),

$$\bar{\phi}_{iV} = \exp\left[(Z_V - 1)\frac{B_i}{B} - \ln(Z_V - B) - \frac{A}{B}\left(2\sqrt{\frac{A_i}{A}} - \frac{B_i}{B} \right) \ln\left(1 + \frac{B}{Z_V} \right) \right] \qquad (7)$$

$$Z_V^3 - Z_V^2 + Z_V\left(A - B - B^2 \right) - AB = 0 \qquad (8)$$

$$A = \frac{aP}{R^2T^2} \qquad (9) \qquad B = \frac{bP}{RT} \qquad (10)$$ with a and b given Table 2.5 and Eqs. (2-49) and (2-50)

<u>Derivative</u> $\frac{\partial K_{i,j}}{\partial T_j}$:

Using Eq. (1) with the chain rule, $$\frac{\partial K_{i,j}}{\partial T_j} = \frac{\phi_{iL}}{\bar{\phi}_{iV}} \frac{\partial \gamma_{iL}}{\partial T_j} + \frac{\gamma_{iL}}{\bar{\phi}_{iV}} \frac{\partial \phi_{iL}}{\partial T_j} - \frac{\gamma_{iL}\phi_{iL}}{\bar{\phi}_{iV}^2} \frac{\partial \bar{\phi}_{iV}}{\partial T_j} \qquad (11)$$

From Eq. (2), $$\frac{\partial \gamma_{iL}}{\partial T_j} = -\frac{\gamma_{iL} v_{iL} \left(\delta_i - \sum_{j=1}^{C} \Phi_j \delta_j \right)^2}{RT_j^2}$$

$$\frac{\partial \phi_{iL}}{\partial T_j} = 2.3026\, \phi_{iL} \left[\frac{\partial \log \phi_{iL}^{(0)}}{\partial T_j} + \omega_i \frac{\partial \log \phi_{iL}^{(1)}}{\partial T_j} \right]$$

where from Eqs. (5) and (6),

$$\frac{\partial \log \phi_{iL}^{(0)}}{\partial T_j} = \frac{1}{T_{c_i}} \left[-\frac{A_1}{T_{r_i}^2} + A_2 + 2A_3 T_{r_i} + 3A_4 T_{r_i}^2 + P_{r_i}\left(A_6 + 2A_7 T_{r_i} \right) + P_{r_i}^2 A_9 \right]$$

$$\frac{\partial \log \phi_{iL}^{(1)}}{\partial T_j} = \frac{1}{T_{c_i}} \left[A_{11} - \frac{A_{12}}{T_{r_i}^2} + 3A_{13} T_{r_i}^2 \right]$$

To obtain $\frac{\partial \bar{\phi}_{iV}}{\partial T_j}$, we note that in Eq. (7), Z_V, A, A_i, B, and B_i are functions of T.

Therefore, from Eq. (7),

Exercise 10.14 (continued)

Analysis: (continued)

$$\frac{\partial \bar{\phi}_{iV}}{\partial T_j} = \bar{\phi}_{iV}\left\{ \begin{array}{l} \dfrac{B_i}{B}\dfrac{\partial Z_V}{\partial T} + (Z_V - 1)\left[\dfrac{1}{B}\dfrac{\partial B_i}{\partial T} - \dfrac{B_i}{B^2}\dfrac{\partial B}{\partial T}\right] - \dfrac{1}{(Z_V - B)}\left[\dfrac{\partial Z_V}{\partial T} - \dfrac{\partial B}{\partial T}\right] - \\ \left[\dfrac{1}{B}\left(\sqrt{\dfrac{A_i}{A}} - \dfrac{B_i}{B}\right)\dfrac{\partial A}{\partial T} - \dfrac{A}{B^2}\left(2\sqrt{\dfrac{A_i}{A}} - \dfrac{2B_i}{B}\right)\dfrac{\partial B}{\partial T} + \dfrac{1}{B}\sqrt{\dfrac{A}{A_i}}\dfrac{\partial A_i}{\partial T} - \dfrac{A}{B^2}\dfrac{\partial B_i}{\partial T}\right]\ln\left(1 + \dfrac{B}{Z_V}\right) - \\ \dfrac{A}{BZ_V}\dfrac{\left(\dfrac{\partial B}{\partial T} - \dfrac{B}{Z_V}\dfrac{\partial Z_V}{\partial T}\right)}{\left(1 + \dfrac{B}{Z_V}\right)}\left(2\sqrt{\dfrac{A_i}{A}} - \dfrac{B_i}{B}\right) \end{array} \right\}$$

where, $\dfrac{\partial A}{\partial T} = -2.5\dfrac{A}{T}$, $\dfrac{\partial A_i}{\partial T} = -2.5\dfrac{A_i}{T}$, $\dfrac{\partial B}{\partial T} = -\dfrac{B}{T}$, $\dfrac{\partial B_i}{\partial T} = -\dfrac{B_i}{T}$

$\dfrac{\partial Z_V}{\partial T}$ is obtained as follows by implicit integration from Eq. (8):

$$3Z_V^2\frac{\partial Z_V}{\partial T} - 2Z_V\frac{\partial Z_V}{\partial T} + \left(A - B - B^2\right)\frac{\partial Z_V}{\partial T} + Z_V\left(\frac{\partial A}{\partial T} - \frac{\partial B}{\partial T} - 2B\frac{\partial B}{\partial T}\right) - A\frac{\partial B}{\partial T} - B\frac{\partial A}{\partial T} = 0$$

Solving,

$$\frac{\partial Z_V}{\partial T} = \frac{Z_V\left(\dfrac{\partial A}{\partial T} - \dfrac{\partial B}{\partial T} - 2B\dfrac{\partial B}{\partial T}\right) - A\dfrac{\partial B}{\partial T} - B\dfrac{\partial A}{\partial T}}{2Z_V - 3Z_V^2 - \left(A - B - B^2\right)} = \frac{Z_V\left[-2.5\dfrac{A}{T} + \dfrac{B}{T} + 2\dfrac{B^2}{T}\right] + 3.5\dfrac{AB}{T}}{2Z_V - 3Z_V^2 - \left(A - B - B^2\right)}$$

Substitution of the equations below Eq. (11) into Eq. (11) gives an expression for $\dfrac{\partial K_i}{\partial T}$ for any stage j.

<u>Derivative</u> $\dfrac{\partial K_{i,j}}{\partial \upsilon_{i,k}}$:

Using Eq. (1) with the chain rule, noting that only $\bar{\phi}_{iV}$ is a function of υ_i and letting the subscript $k = j$, but dropping that subscript:

$$\frac{\partial K_i}{\partial \upsilon_i} = -\frac{\gamma_{iL}\phi_{iL}}{\bar{\phi}_{iV}^2}\frac{\partial \bar{\phi}_{iV}}{\partial \upsilon_i} \qquad (12)$$

Exercise 10.14 (continued)

Analysis: (continued)

The mixture vapor fugacity coefficient, $\overline{\phi}_{iV}$, is given by Eq. (7). In this equation only Z_V, A, and B are functions of vapor composition. Also, Z_V, is a function of A and B, which are given by Eqs. (9) and (10), where, from Eqs. (2-49) and (2-50), after substituting $y_i = \dfrac{v_i}{V} = \dfrac{v_i}{\sum_{m=1}^{C} v_m}$:

$$a = \frac{\sum_{r=1}^{C}\left(\sum_{n=1}^{C} v_r v_n \sqrt{a_r a_n}\right)}{\left(\sum_{m=1}^{C} v_m\right)^2} \quad \text{and} \quad b = \frac{\sum_{r=1}^{C} v_r b_n}{\sum_{m=1}^{C} v_m}$$

Therefore,

$$\frac{\partial A}{\partial v_i} = \frac{P}{R^2T^2}\left[\frac{y_i a_i}{V} + \frac{2}{V}\sum_{\substack{n=1\\ n\neq i}}^{C} y_n\sqrt{a_i a_n} - \frac{2}{V}\sum_{r=1}^{C}\left(\sum_{n=1}^{C} y_r y_n \sqrt{a_r a_n}\right)\right] \tag{13}$$

$$\frac{\partial B}{\partial v_i} = \frac{P}{RT}\left[\frac{b_i}{V} - \frac{1}{V}\sum_{r=1}^{C} y_r b_r\right] \tag{14}$$

$\dfrac{\partial Z_V}{\partial v_i}$ is obtained as follows by implicit integration from Eq. (8):

$$3Z_V^2\frac{\partial Z_V}{\partial v_i} - 2Z_V\frac{\partial Z_V}{\partial v_i} + \left(A - B - B^2\right)\frac{\partial Z_V}{\partial v_i} + Z_V\left(\frac{\partial A}{\partial v_i} - \frac{\partial B}{\partial v_i} - 2B\frac{\partial B}{\partial v_i}\right) - A\frac{\partial B}{\partial v_i} - B\frac{\partial A}{\partial v_i} = 0$$

Solving,

$$\frac{\partial Z_V}{\partial v_i} = \frac{Z_V\left(\dfrac{\partial A}{\partial v_i} - \dfrac{\partial B}{\partial v_i} - 2B\dfrac{\partial B}{\partial v_i}\right) - A\dfrac{\partial B}{\partial v_i} - B\dfrac{\partial A}{\partial v_i}}{2Z_V - 3Z_V^2 - \left(A - B - B^2\right)} \tag{15}$$

From Eq. (7),

Exercise 10.14 (continued)

Analysis: (continued)

$$\frac{\partial \bar{\phi}_{iV}}{\partial \upsilon_i} = \bar{\phi}_{iV}\left\{\begin{array}{l} \dfrac{B_i}{B}\dfrac{\partial Z_V}{\partial \upsilon_i} + (Z_V - 1)\left[\dfrac{1}{B}\dfrac{\partial B_i}{\partial \upsilon_i} - \dfrac{B_i}{B^2}\dfrac{\partial B}{\partial \upsilon_i}\right] - \dfrac{1}{(Z_V - B)}\left[\dfrac{\partial Z_V}{\partial \upsilon_i} - \dfrac{\partial B}{\partial \upsilon_i}\right] - \\ \left[\dfrac{1}{B}\left(\sqrt{\dfrac{A_i}{A}} - \dfrac{B_i}{B}\right)\dfrac{\partial A}{\partial \upsilon_i} - \dfrac{A}{B^2}\left(2\sqrt{\dfrac{A_i}{A}} - \dfrac{2B_i}{B}\right)\dfrac{\partial B}{\partial \upsilon_i} + \dfrac{1}{B}\sqrt{\dfrac{A}{A_i}}\dfrac{\partial A_i}{\partial \upsilon_i} - \dfrac{A}{B^2}\dfrac{\partial B_i}{\partial \upsilon_i}\right]\ln\left(1 + \dfrac{B}{Z_V}\right) - \\ \dfrac{A}{BZ_V}\dfrac{\left(\dfrac{\partial B}{\partial \upsilon_i} - \dfrac{B}{Z_V}\dfrac{\partial Z_V}{\partial \upsilon_i}\right)}{\left(1 + \dfrac{B}{Z_V}\right)}\left(2\sqrt{\dfrac{A_i}{A}} - \dfrac{B_i}{B}\right) \end{array}\right\}$$

The final result is obtained by substituting equations below (13), (14), and (15) into this equation, followed by substitution of the result into Equation (12).

Derivative $\dfrac{\partial K_{i,j}}{\partial l_{i,k}}$ **:**

Using Eq. (1) with the chain rule, noting that only γ_{iL} is a function of l_i and letting the subscript $k = j$, but dropping that subscript:

$$\frac{\partial K_i}{\partial l_i} = \frac{\phi_{iL}}{\bar{\phi}_{iV}}\frac{\partial \gamma_{iL}}{\partial l_i} \qquad (16)$$

In Eq. (2), using: $\Phi_m = \dfrac{x_m v_{mL}}{v_L} = \dfrac{l_m v_{mL}}{L v_L} = \dfrac{l_m v_{mL}}{v_L \sum_{n=1}^{C} l_n}$

Eq. (1) becomes: $\gamma_{iL} = \exp\left[\dfrac{v_{iL}}{RT}\left(\delta_i - \dfrac{\sum_{m=1}^{C} l_m v_{mL}\delta_m}{v_L \sum_{n=1}^{C} l_n}\right)^2\right]$

Taking the derivative of this equation with respect to l_i gives:

Exercise 10.14 (continued)

Analysis: (continued)

$$\frac{\partial \gamma_{iL}}{\partial l_i} = \gamma_{iL}\left\{\frac{2v_{iL}}{RT}\left(\delta_i - \frac{\sum_{m=1}^{C} l_m v_{mL}\delta_m}{v_L\sum_{n=1}^{C} l_n}\right)\left[\frac{v_{iL}\delta_i}{v_L\sum_{n=1}^{C} l_n} - \frac{\sum_{m=1}^{C} l_m v_{mL}\delta_m}{v_L\left(\sum_{n=1}^{C} l_n\right)^2}\right]\right\}$$

$$= \gamma_{iL}\left\{\frac{2v_{iL}}{RT}\left(\delta_i - \sum_{m=1}^{C}\Phi_m\delta_m\right)\left[\frac{\Phi_i\delta_i}{x_i L} - \frac{\sum_{m=1}^{C}\Phi_m\delta_m}{L}\right]\right\}$$

Substitution of this equation into Eq. (16) gives the final result

Exercise 10.15

Subject: Development of a partial simultaneous correction method.

Given: MESH equations (10-1) to (10-6).

Find: (a) The two indexed equations for solving for temperatures and vapor flow rates.
(b) Truncated Taylor series expansions for the two indexed equations.
(c) Order of equations and variables to permit an efficient solution procedure.

Analysis: Instead of computing a new set of total vapor flow rates from the energy balance equations as in the bubble-point method and a new set of temperatures from the energy balance equations as in the sum-rates method, a good procedure to simultaneously compute a new set of total vapor flow rates and a new set of temperatures from a combination of the energy balance, sum rates, and equilibrium equations. This procedure is as follows:
(a) Combine the energy balance equation (10-5) with the total mole balance (10-6) to eliminate variables in L_j so as to obtain the following equation in terms of V_j and T_j, assuming that mole fraction compositions have just been calculated:

$$H_j = H_j\{V_j, T_j\} = \left[V_j + \sum_{m=1}^{j-1}(F_m - U_m - W_m) - V_1\right]h_{L_{j-1}} + V_{j+1}h_{V_{j+1}} + F_j h_{F_j} - \left[V_{j+1} + \sum_{m=1}^{j}(F_m - U_m - W_m) - V_1 + U_j\right]h_{L_j} - (V_j + W_j)h_{V_j} - Q_j = 0 \quad (1)$$

Instead of using the sum-rates equation (10-33) in terms of total liquid flow rates, use the following similar equation in terms of the total vapor flow rates:

$$V_j^{(k+1)} = V_j^{(k)} \sum_{i=1}^{C} y_{i,j}$$

Combining this equation with equation (10-2)

$$V_j^{(k+1)} = V_j^{(k)} \sum_{i=1}^{C} K_{i,j} x_{i,j}$$

Writing this equation as a sums function, S_j, gives:

$$S_j = S_j\{V_j, T_j\} = V_j^{(k+1)} - V_j^{(k)} \sum_{i=1}^{C} K_{i,j} x_{i,j} = 0 \quad (2)$$

Equations (1) and (2) are the indexed equations for computing new sets of V_j and T_j, where in Eq. (1), $V_j = V_j^{(k+1)}$ and all T_j implicit in the K-values and enthalpies are $T_j^{(k+1)}$.

Exercise 10.15 (continued)

Analysis: (continued)

(b) The truncated Taylor's series expansions for Eqs. (1) and (2) are:

$$0 = H_j^{(k)} + \left(\frac{\partial H_j}{\partial T_{j-1}}\right)^{(k)} \Delta T_{j-1} + \left(\frac{\partial H_j}{\partial T_j}\right)^{(k)} \Delta T_j + \left(\frac{\partial H_j}{\partial T_{j+1}}\right)^{(k)} \Delta T_{j+1} + \left(\frac{\partial H_j}{\partial V_j}\right)^{(k)} \Delta V_j + \left(\frac{\partial H_j}{\partial V_{j+1}}\right)^{(k)} \Delta V_{j+1} \quad (3)$$

$$0 = S_j^{(k)} + \left(\frac{\partial S_j}{\partial V_j}\right)^{(k)} \Delta V_j + \left(\frac{\partial S_j}{\partial T_j}\right)^{(k)} \Delta T_j \quad (4)$$

The derivatives for Eq. (3) are:

$$\frac{\partial H_j}{\partial T_{j-1}} = \left[V_j + \sum_{m=1}^{j-1}(F_m - U_m - W_m) - V_1\right]\left(\frac{\partial h_{L_{j-1}}}{\partial T_{j-1}}\right)$$

$$\frac{\partial H_j}{\partial T_j} = \left[V_{j+1} + \sum_{m=1}^{j}(F_m - U_m - W_m) - V_1\right]\left(\frac{\partial h_{L_j}}{\partial T_j}\right) - (V_j + W_j)\left(\frac{\partial h_{V_j}}{\partial T_j}\right)$$

$$\frac{\partial H_j}{\partial T_{j+1}} = V_{j+1}\left(\frac{\partial h_{V_{j+1}}}{\partial T_{j+1}}\right)$$

$$\frac{\partial H_j}{\partial V_j} = h_{L_{j-1}} - h_{V_j}$$

$$\frac{\partial H_j}{\partial V_{j+1}} = h_{V_{j+1}} - h_{L_j}$$

The derivatives for Eq. (4) are:

$$\frac{\partial S_j}{\partial V_j} = 1$$

$$\frac{\partial S_j}{\partial T_j} = -V_j^{(k)} \sum_{i=1}^{C}\left(\frac{\partial K_{i,j}}{\partial T_j}\right) x_{i,j}$$

Exercise 10.15 (continued)

Analysis: (continued)

(c) Consider a simple case of 3 equilibrium stages. The set of 3 equations each for Eq. (3) and Eq. (4), will form a block tridiagonal matrix structure if the equations and correction variables are ordered as shown below. More details on this method are given by J. F. Tomich, AIChE Journal, 16, 229 (1970).

The following is the incidence matrix for the Jacobian matrix:

	ΔV_1	ΔT_1	ΔV_2	ΔT_2	ΔV_3	ΔT_3
S_1	x	x				
H_1	x	x	x	x		
S_2			x	x		
H_2		x	x	x	x	x
S_3					x	x
H_3				x	x	x

Exercise 10.16

Subject: Effect of interlinking streams of a thermally coupled distillation system on the Jacobian matrix structure.

Given: Thermally coupled system of Fig. 10.31. Solution of the equations by the Newton-Raphson method.

Find: Whether the matrix equation retains a block tridiagonal structure.

Analysis: Consider the system shown below, where the stages in the first column are numbered from 12 to 15 and the stages in the second column are numbered from 1 to 11 and from 16 to 19. The component material balance equations, similar to Eq. (10-58, around stages 4, 12, 11, and 16, respectively are:

$$M_{i,4} = l_{i,4}\left(1+s_4\right)+\upsilon_{i,4}-l_{i,12}-l_{i,3}-\upsilon_{i,5}=0$$

$$M_{i,12} = l_{i,12}+\upsilon_{i,12}-l_{i,4}s_4-\upsilon_{i,13}=0$$

$$M_{i,11} = l_{i,11}+\upsilon_{i,11}-l_{i,10}-\upsilon_{i,16}=0$$

$$M_{i,16} = l_{i,16}+\upsilon_{i,16}\left(1+S_{16}\right)-l_{i,15}-l_{i,11}-\upsilon_{i,17}=0$$

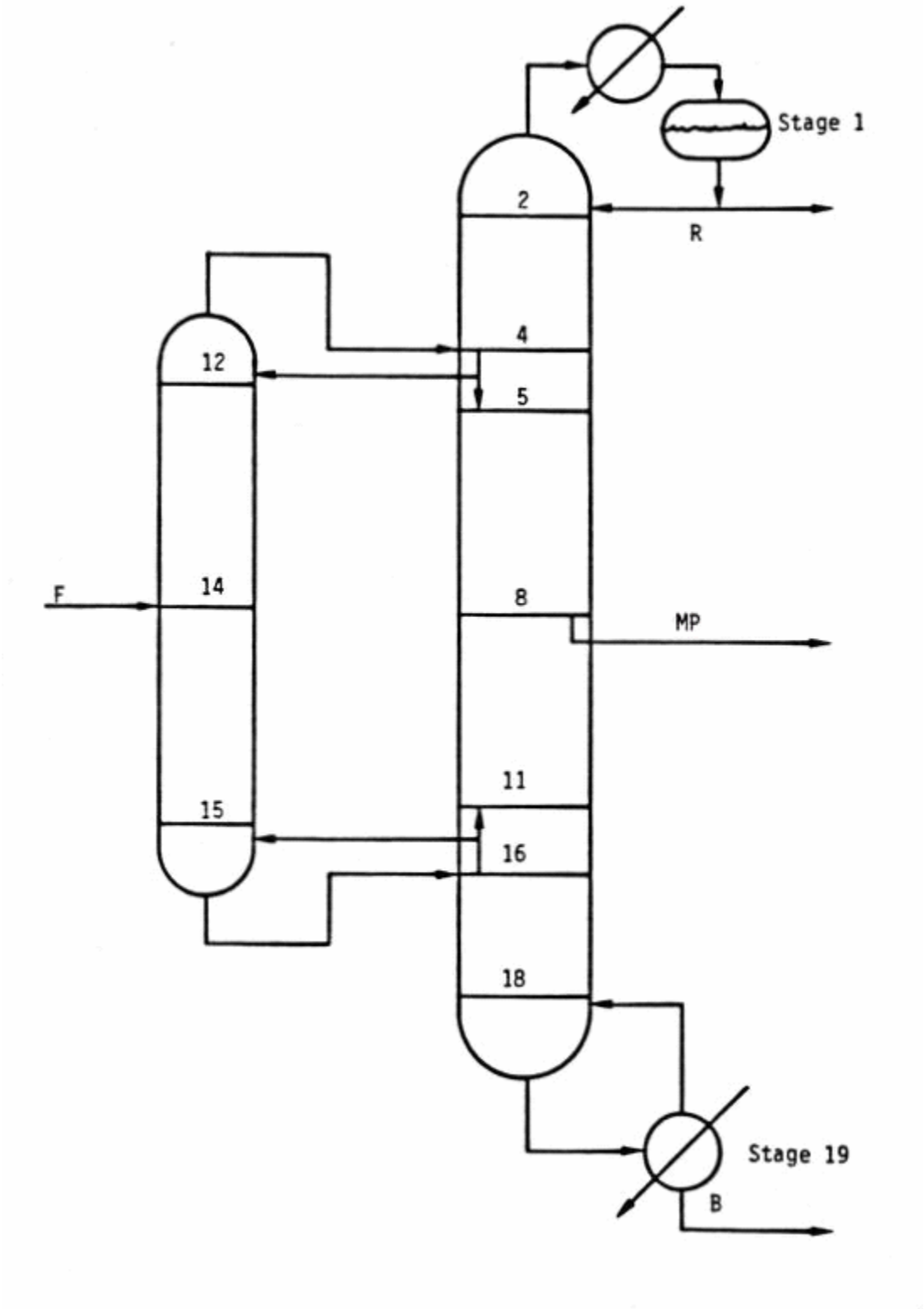
Note that:

Stage 4 includes flow rates for stages 3, 4, 5, and 12.
Stage 12 includes flow rates for stages 4, 12, and 13.
Stage 11 includes flow rates for stages 10, 11, and 16.
Stage 16 includes flow rates for stages 11, 15, 16, and 17.

The same stages appear in the energy balance equations. Therefore, the matrix structure has the diverse A and C blocks as shown in the diagram below. The matrix is not block tridiagonal.

Exercise 10.16 (continued)

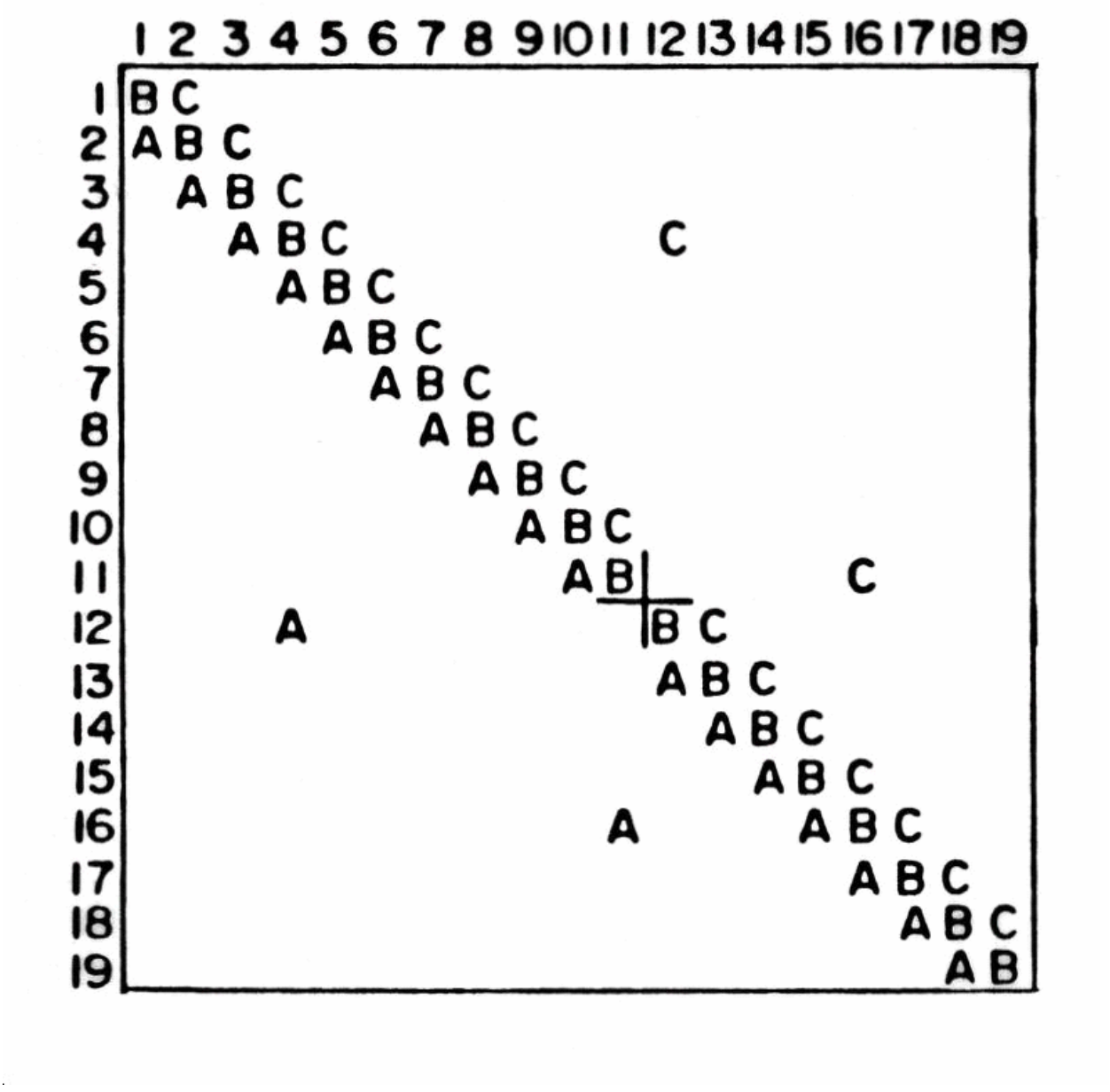
Analysis: (continued)



Exercise 10.16 (continued)

Analysis: (continued)

Matrix Structure



Exercise 10.17

Subject: Effect of changing variable and equation ordering.

Given: Ordering equations (10-63) and (10-64).

Find: Consequences of changing ordering in the above two equations.

Analysis: With the variable ordering *v, T, l,* as seen in Eq. (10-68), the non-zero variables in the $\overline{\mathrm{A}}_j$ submatrix are pushed to the right, close to the $\overline{\mathrm{B}}_j$ submatrix, while the non-zero variables in the $\overline{\mathrm{C}}_j$ submatrix are pushed to the left, close to the $\overline{\mathrm{B}}_j$ submatrix. Thus, the non-zero variables are arranged across the block row of these three submatrices in the most compact manner.

If the ordering is changed to *l, v, T* , the nonzero variables are spread out over the entire width of the row of the three submatrices. That is, the non-zero variables in the $\overline{\mathrm{A}}_j$ submatrix are now pushed to the left, away from the $\overline{\mathrm{B}}_j$ submatrix, while the non-zero variables in the $\overline{\mathrm{C}}_j$ submatrix are pushed to the right, away from the $\overline{\mathrm{B}}_j$ submatrix. This is the least compact arrangement.

If the ordering of the equations is changed from *H, M, E* to *E, M, H*, there is little change.

Thus, the orderings given by Eqs. (10-63) and (10-64) appear to as efficient or more efficient than the other orderings given above.

Exercise 10.18

Subject: Detailed method for determining the scalar multiplier, S_b , in (10-104).

Given: Inside-out method procedure in Section 10.5.

Find: Details of the subject method.

Analysis: From Eq. (10-104), when uncorrected, $S_{i,j} = \alpha_{I,j}\, S_{b,j}$.
This product appears in the component material balance equations (10-83).
Using initial estimates from steps 1-7 of the Initialization Procedure, values of $l_{i,j}$ are computed from step 9.
If the sum of $l_{i,j}$ for the Nth stage, i.e.

$$B = \sum_{i=1}^{C} l_{i,N}$$

is not the specified B, then use,

$$S_{i,j} = S_b \alpha_{i,j} S_{b,j}$$

where S_b is determined by a search, e.g. a Fibonacci search to make B = specified B.
Typically, the search might be over the range of 0.75 to 1.25.

Exercise 10.19

Subject: Error function for the Inside-out method.

Given: Error function for the simultaneous correction method.

Find: Error function

Analysis: Rewrite Eqs. (10-82) and (10-84) in residual form:

$$E_{i,j} = \upsilon_{i,j} - \alpha_{i,j} S_{b,j} l_{i,j} = 0$$

$$M_{i,j} = L_{i,j-1} - \left(R_{Lj} + \alpha_{i,j} \ldots..\right) l_{i,j} + \left(\alpha_{i,j} \ldots.\right) l_{i,j+1} + f_{i,j} = 0$$

$$H_j = h_{L_j} R_{Lj} L_j + \ldots\ldots\ldots - h_{F_j} F_j - Q_j = 0$$

Then, following Eq. (10-75),

$$\tau = \sum_{j=1}^{N} \left\{ \left(\frac{H_j}{\text{scale factor}} \right)^2 + \sum_{i-1}^{C} \left[\left(M_{i,j} \right)^2 + \left(E_{i,j} \right)^2 \right] \right\} \leq \varepsilon$$

where the scale factor is a nominal heat of vaporization, some $h_{V_j} - h_{L_j}$

Exercise 10.20

Subject: Distillation of a light normal paraffin hydrocarbon mixture by a rigorous equilibrium-stage method.

Given: Feed of composition below as a bubble-point liquid at column pressure of 250 psia. Column has a partial condenser, partial reboiler, and 15 equilibrium stages in the column with feed entering the middle stage. Distillate rate = 23.0 lbmol/h and reflux rate = 150.0 lbmol/h. Soave-Redlich-Kwong equation of state for *K*-values and enthalpies.

Find: Product compositions. Stage temperatures, vapor and liquid flow rates, and compositions. Reboiler and condenser duties.

Analysis: The calculations were made with the TOWER model (Inside-out method) of the Chemcad program, with the following specifications:
Partial condenser
Top pressure = 250 psia
No condenser or stage pressure drop. Therefore, bottom pressure also = 250 psia
Number of stages = 17 (includes partial condenser and partial reboiler)
Feed stage = 9 from the top
At the top, reflux rate = 150 lbmol/h
At the bottom, bottoms rate = $B = F - D$ = 100 - 23 = 77 lbmol/h
Estimated distillate rate = 23 lbmol/h (actual rate)
Estimated reflux rate = 150 lbmol/h (actual rate)
Estimated temperature of stage 1 = 120°F
Estimated temperature of bottom stage = 300°F
Estimated temperature of stage 2 = 140°F

Although the feed was given as a bubble-point liquid at 250 psia and 213.9°F, the SRK equation of state gave a bubble-point temperature of 210.7°F, which was the value used. Based on the feed composition below, the distillate rate of 23 lbmol/h corresponded to a desired split between propane and n-butane. The calculations converged rapidly in 3 outer-loop iterations with results given below and on the following pages.

Condenser duty = 862,300 Btu/h
Reboiler duty = 1,119,800 Btu/h

Top temperature = 115.8°F compared to assumed value of 120°F
Bottom temperature = 264.2°F compared to assumed value of 300°F
Stage 2 temperature = 125.4°F compared to assumed value of 140°F

Exercise 10.20 (continued)

Analysis: (continued)

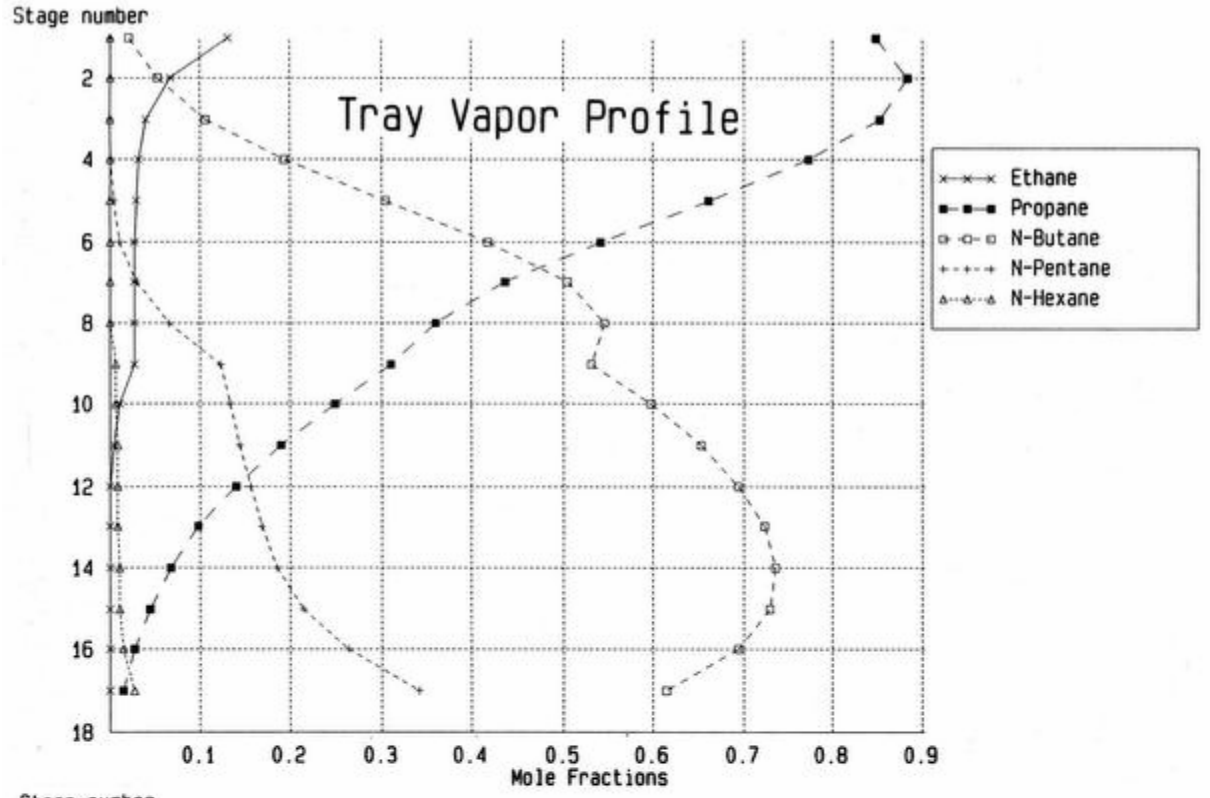
Stream No.	1	2	3
Stream Name	Feed	Distillate	Bottoms
Temp F	210.6565	115.8243	264.1976
Pres psia	250.0000*	250.0000*	250.0000
Enth MMBtu/h	-6.0186	-1.0173	-4.7439
Vapor mole fraction	0.00000*	1.0000*	0.00000
Total lbmol/h	100.0000	22.9993	77.0006
Total lb/h	6078.8164	979.3469	5099.4668
Total std L ft3/hr	165.5281	32.0148	133.5132
Total std V scfh	37947.86	8727.75	29220.09
Flowrates in lbmol/h			
Ethane	3.0000	2.9998	0.0002
Propane	20.0000	19.4835	0.5165
N-Butane	37.0000	0.5158	36.4842
N-Pentane	35.0000	0.0003	34.9997
N-Hexane	5.0000	0.0000	5.0000

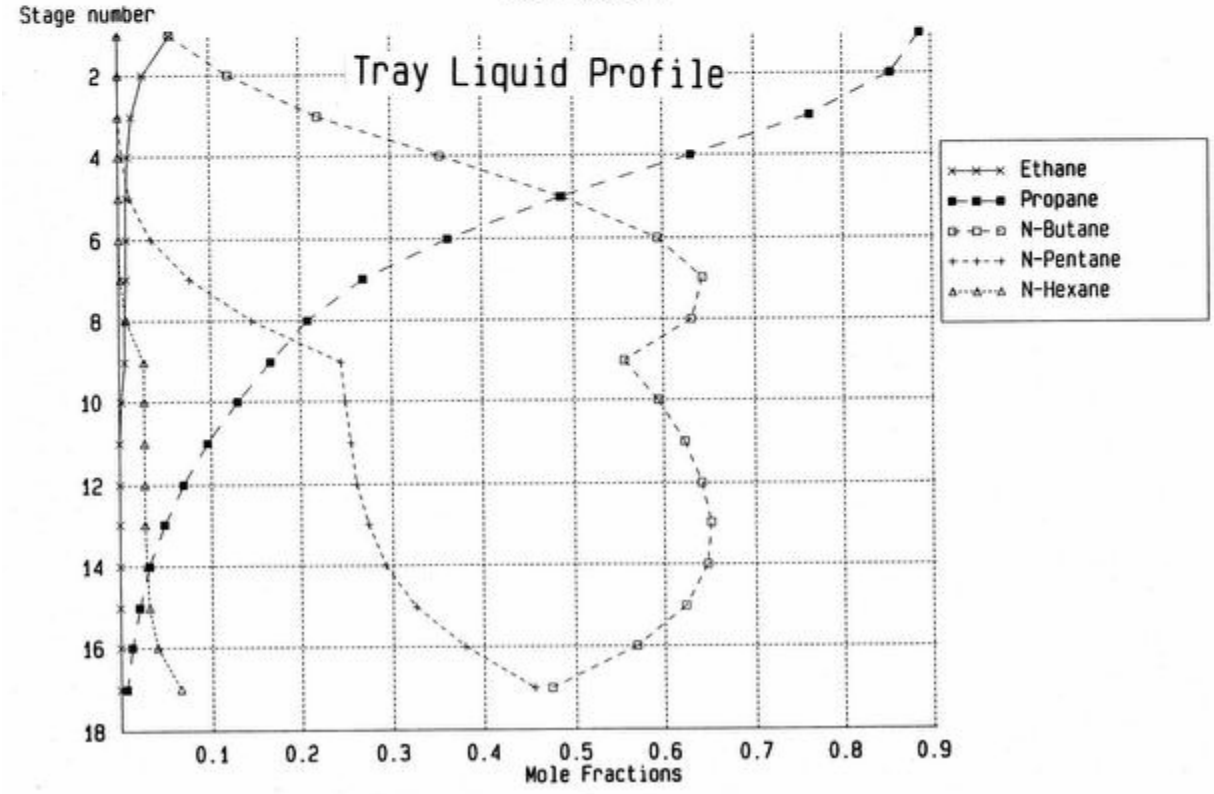
			* Net Flows *			
Stg	Temp F	Pres psia	Liquid lbmol/h	Vapor lbmol/h	Feeds lbmol/h	Product lbmol/h
1	115.8	250.00	149.99			23.00
2	125.4	250.00	146.52	172.99		
3	135.4	250.00	140.68	169.52		
4	147.9	250.00	134.63	163.68		
5	162.3	250.00	130.11	157.63		
6	176.5	250.00	127.01	153.11		
7	189.5	250.00	123.93	150.01		
8	201.9	250.00	119.55	146.93		
9	215.6	250.00	224.90	142.55	100.00	
10	223.1	250.00	229.17	147.90		
11	229.0	250.00	232.51	152.17		
12	233.8	250.00	235.05	155.51		
13	237.9	250.00	236.73	158.05		
14	241.9	250.00	237.35	159.73		
15	246.6	250.00	236.72	160.35		
16	253.4	250.00	234.47	159.71		
17	264.2	250.00		157.47		77.00

Mole Reflux ratio 6.522

Exercise 10.20 (continued)

Analysis: (continued)





Exercise 10.21

Subject: Optimal feed-stage location for separation of Exercise 10.20

Given: Conditions given in Exercise 10.20 except that the optimal feed location is to be determined rather than using the middle stage (stage 9).

Find: Optimal feed stage, assuming that this corresponds to the stage that gives the best separation between propane and n-butane.

Analysis: The calculations were made with the TOWER model (Inside-out method) of the Chemcad program, in exactly the same way as with Exercise 10.20 except that several runs were made with different feed stage locations. The results are as follows for the flow rate of propane (the light key) in the bottoms:

Feed stage location (from top)	lbmol/h C_3 in bottoms
6	0.5258
7	0.4743
8	0.4730
9 (Exercise 10.20)	0.5165
10	0.6138
11	0.7769

The optimal feed stage is seen to be stage 8, with stage 9 giving almost the same result.

Exercise 10.22

Subject: Distillation with a vapor sidestream

Given: Conditions given in Exercise 10.20 except that a vapor side stream is withdrawn from the fourth stage (stage 13 from the top) from the bottom at a rate of 37.0 lbmol/h in an attempt to obtain a nC_4-rich product. Therefore, the remaining specifications are still a feed of composition below as a bubble-point liquid at column pressure of 250 psia. Column has a partial condenser, partial reboiler, and 15 equilibrium stages in the column with feed entering the middle stage. Distillate rate = 23.0 lbmol/h and reflux rate = 150.0 lbmol/h. Soave-Redlich-Kwong equation of state for *K*-values and enthalpies.

Find: Product compositions. Stage temperatures, vapor and liquid flow rates, and compositions. Reboiler and condenser duties.

Analysis: The calculations were made with the TOWER model (Inside-out method) of the Chemcad program, with the following specifications:
Partial condenser
Top pressure = 250 psia
No condenser or stage pressure drop. Therefore, bottom pressure also = 250 psia
Number of stages = 17 (includes partial condenser and partial reboiler)
Feed stage = 9 from the top
Sidestream from stage 13 from the top, as a vapor at a flow rate of 37 lbmol/h
At the top, reflux rate = 150 lbmol/h
At the bottom, bottoms rate = $B = F - D - S$ = 100 - 23 - 37 = 40 lbmol/h
Estimated distillate rate = 23 lbmol/h (actual rate)
Estimated reflux rate = 150 lbmol/h (actual rate)
Estimated temperature of stage 1 = 120°F
Estimated temperature of bottom stage = 300°F
Estimated temperature of stage 2 = 140°F

Although the feed was given as a bubble-point liquid at 250 psia and 213.9°F, the SRK equation of state gave a bubble-point temperature of 210.7°F, which was the value used. Based on the feed composition below, the distillate rate of 23 lbmol/h corresponded to a desired split between propane and n-butane. The calculations converged rapidly in 3 outer-loop iterations with results given below and on the following pages. The vapor side stream contains 69.5 mol% nC_4.

Condenser duty = 914,000 Btu/h
Reboiler duty = 1,440,000 Btu/h

Top temperature = 124.4°F compared to assumed value of 120°F
Bottom temperature = 290.5°F compared to assumed value of 300°F
Stage 2 temperature = 140.9°F compared to assumed value of 140°F

Exercise 10.22 (continued)

Analysis: (continued)

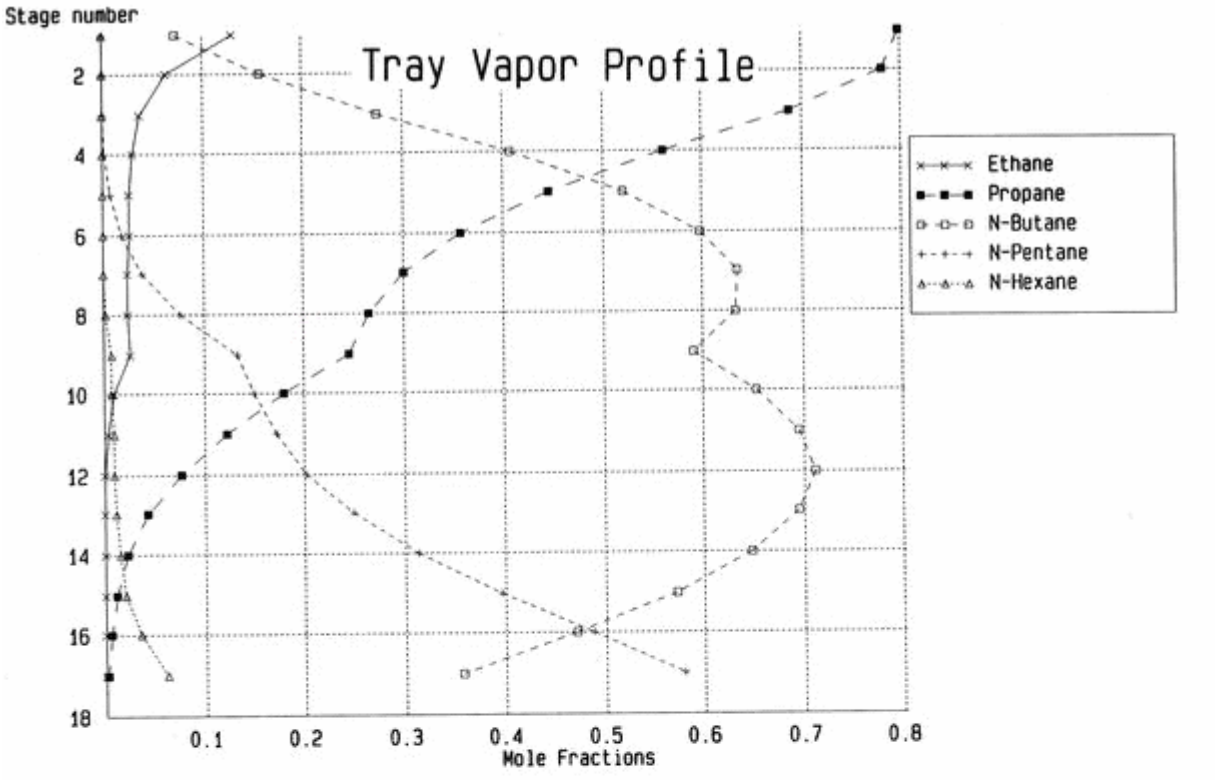
Stream No.	1	2	3	4
Stream Name	Feed	Distillate	Bottoms	Side stream
Temp F	210.6565	124.3623	290.5048	250.1544
Pres psia	250.0000*	250.0000*	250.0000	250.0000
Enth MMBtu/h	-6.0186	-1.0238	-2.5265	-1.9427
Vapor mole fraction	0.00000*	1.0000*	0.00000	1.0000
Total lbmol/h	100.0000	22.9999	40.0003	36.9998
Total lb/h	6078.8164	995.7477	2813.5579	2269.5105
Total std L ft3/hr	165.5281	32.2489	72.1757	61.1034
Total std V scfh	37947.86	8727.95	15179.27	14040.64
Flowrates in lbmol/h				
Ethane	3.0000	2.9840	0.0000	0.0160
Propane	20.0000	18.3489	0.0457	1.6053
N-Butane	37.0000	1.6656	9.6245	25.7100
N-Pentane	35.0000	0.0013	25.7803	9.2184
N-Hexane	5.0000	0.0000	4.5498	0.4502

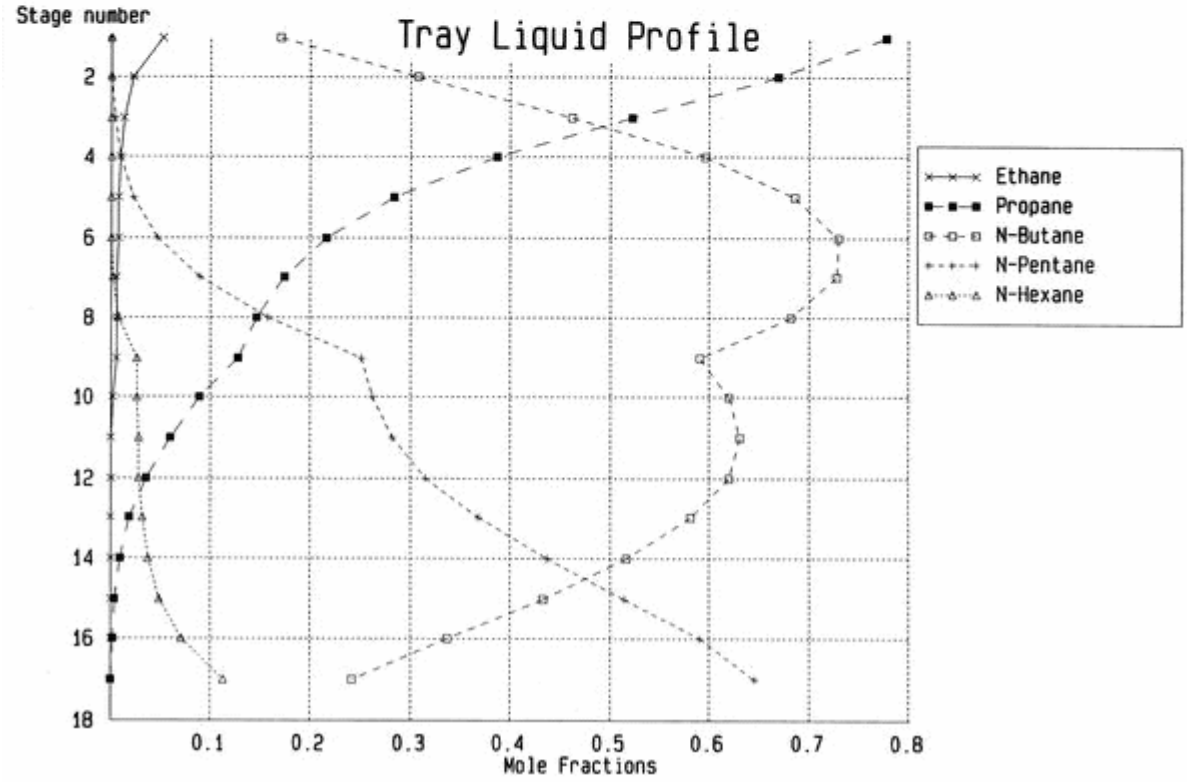
			* Net Flows *			
Stg	Temp F	Pres psia	Liquid lbmol/h	Vapor lbmol/h	Feeds lbmol/h	Product lbmol/h
1	124.4	250.00	150.00			23.00
2	140.9	250.00	144.31	173.00		
3	157.3	250.00	139.86	167.31		
4	172.5	250.00	137.64	162.86		
5	184.9	250.00	136.57	160.64		
6	194.5	250.00	135.40	159.57		
7	202.5	250.00	132.86	158.40		
8	211.0	250.00	128.42	155.86		
9	221.7	250.00	234.93	151.42	100.00	
10	229.8	250.00	239.18	157.93		
11	236.5	250.00	242.01	162.18		
12	242.8	250.00	242.96	165.01		
13	250.2	250.00	242.61	165.96		
						37.00
14	258.1	250.00	241.38	202.61		
15	267.4	250.00	239.91	201.38		
16	278.2	250.00	238.58	199.91		
17	290.5	250.00		198.58		40.00

Mole Reflux ratio 6.522

Exercise 10.22 (continued)

Analysis: (continued)





Exercise 10.23

Subject: Distillation with an intercooler and an interheater

Given: Conditions given in Exercise 10.20 except that an intercooler with a duty of 200,000 Btu/h is placed on the fourth stage from the top (Stage 5 counting the partial condenser), and an interheater with a duty of 300,000 Btu/h is placed on the fourth stage from the bottom (stage 13 from the top counting the partial condenser). Therefore, the remaining specifications are still a feed of composition below as a bubble-point liquid at column pressure of 250 psia. Column has a partial condenser, partial reboiler, and 15 equilibrium stages in the column with feed entering the middle stage. Distillate rate = 23.0 lbmol/h and reflux rate = 150.0 lbmol/h. Soave-Redlich-Kwong equation of state for *K*-values and enthalpies.

Find: Product compositions. Stage temperatures, vapor and liquid flow rates, and compositions. Reboiler and condenser duties.

Analysis: The calculations were made with the TOWER model (Inside-out method) of the Chemcad program, with the following specifications, where TOWER treats intercooler and interheater stages as feed stages with heat transferred out as negative and heat transferred in as positive:
Partial condenser and Top pressure = 250 psia
No condenser or stage pressure drop. Therefore, bottom pressure also = 250 psia
Number of stages = 17 (includes partial condenser and partial reboiler)
Feed stage one = 5 from the top for the intercooler
Feed stage two = 9 from the top for the feed to the column
Feed stage three = 13 from the top for the interheater
At the top, reflux rate = 150 lbmol/h
At the bottom, bottoms rate = $B = F - D$ = 100 - 23 = 77 lbmol/h
Estimated distillate rate = 23 lbmol/h (actual rate)
Estimated reflux rate = 150 lbmol/h (actual rate)
Estimated temperature of stage 1 = 120°F
Estimated temperature of bottom stage = 300°F
Estimated temperature of stage 2 = 140°F

Although the feed is given as a bubble-point liquid at 250 psia and 213.9°F, the SRK equation of state gave a bubble-point temperature of 210.7°F, which was the value used. Based on the feed composition below, the distillate rate of 23 lbmol/h corresponded to a desired split between propane and n-butane. The calculations converged rapidly in 3 outer-loop iterations with results given below and on the following pages:

Condenser duty = 856,200 Btu/h Reboiler duty = 1,014,000 Btu/h

Top temperature = 115°F compared to assumed value of 120°F
Bottom temperature = 264.4°F compared to assumed value of 300°F
Stage 2 temperature = 123.7°F compared to assumed value of 140°F

Exercise 10.23 (continued)

Analysis: (continued)

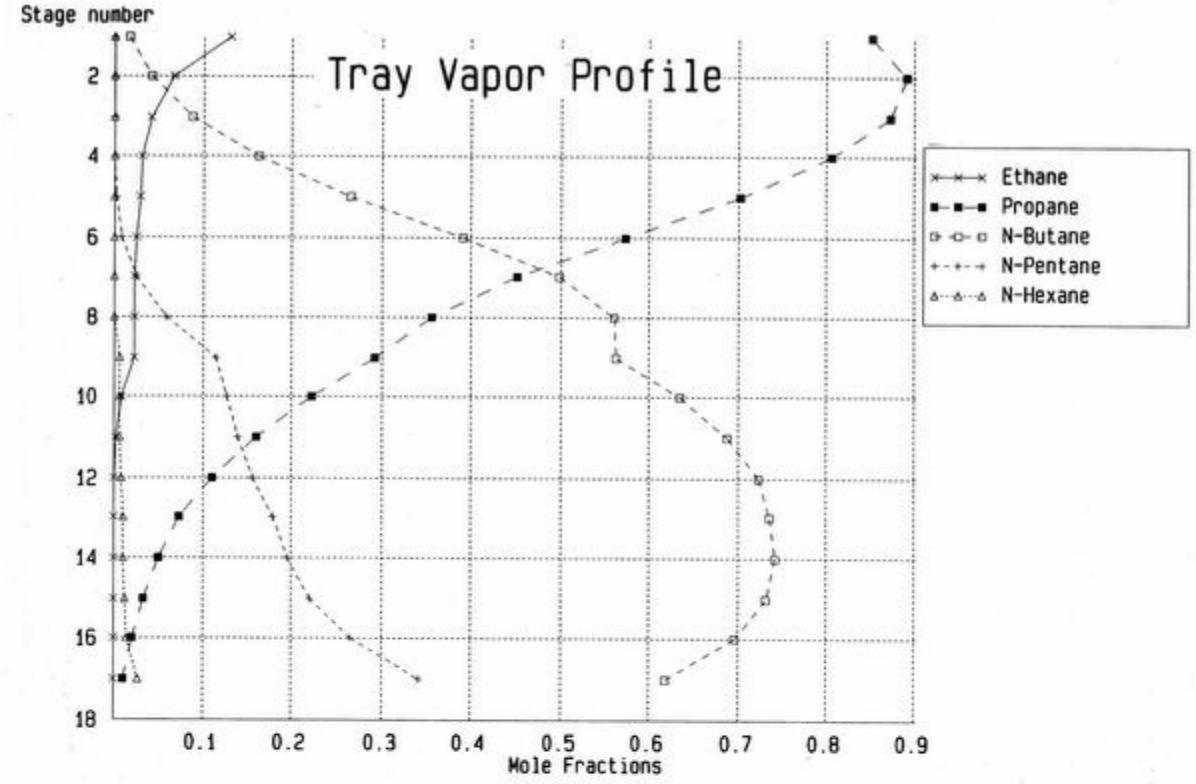
Stream No.	1	2	3	4	5
Stream Name	Intercooler	Feed	Interheater	Distillate	Bottoms
Temp F	0.0000	210.6565	0.0000	114.9880	264.4223
Pres psia	0.0000	250.0000*	0.0000	250.0000	250.0000
Enth MMBtu/h	-0.20000	-6.0186	0.30000	-1.0166	-4.7440
Vapor mole fraction	0.00000	0.00000*	0.00000	1.0000	0.00000
Total lbmol/h	0.0000	100.0000	0.0000	22.9977	77.0023
Total lb/h	0.0000	6078.8164	0.0000	977.7671	5101.0503
Total std L ft3/hr	0.0000	165.5281	0.0000	31.9908	133.5373
Total std V scfh	0.00	37947.86	0.00	8727.13	29220.74
Flowrates in lbmol/h					
Ethane	0.0000	3.0000	0.0000	2.9998	0.0002
Propane	0.0000	20.0000	0.0000	19.5891	0.4110
N-Butane	0.0000	37.0000	0.0000	0.4086	36.5914
N-Pentane	0.0000	35.0000	0.0000	0.0002	34.9998
N-Hexane	0.0000	5.0000	0.0000	0.0000	5.0000

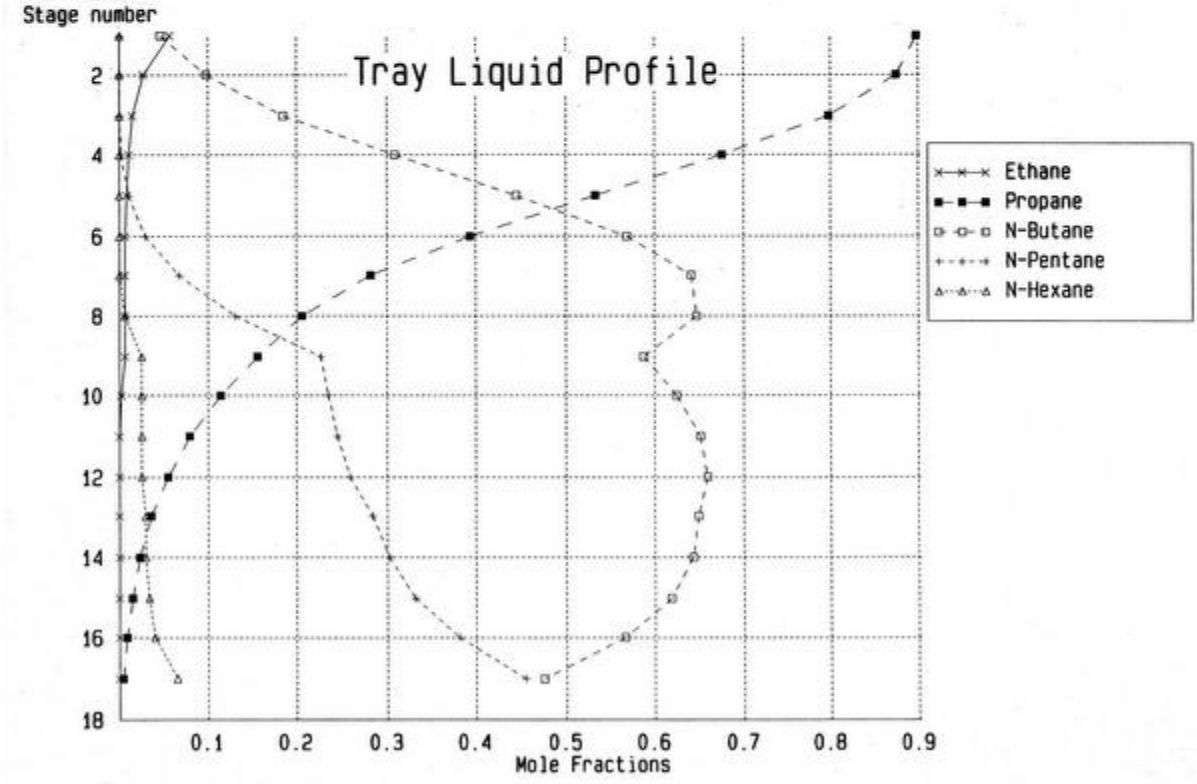
			* Net Flows *				
Stg	Temp F	Pres psia	Liquid lbmol/h	Vapor lbmol/h	Feeds lbmol/h	Product lbmol/h	Duties MMBtu/h
1	115.0	250.00	149.97			23.00	-0.8562
2	123.7	250.00	147.16	172.97			
3	132.4	250.00	141.68	170.16			
4	143.7	250.00	135.45	164.68			
5	157.5	250.00	160.94	158.45			-0.2
6	173.3	250.00	156.57	183.94			
7	188.0	250.00	152.94	179.57			
8	201.6	250.00	148.14	175.94			
9	216.0	250.00	254.30	171.14	100.00		
10	224.1	250.00	259.07	177.29			
11	230.3	250.00	262.45	182.07			
12	235.6	250.00	264.38	185.44			
13	240.8	250.00	222.23	187.38			0.3
14	244.0	250.00	222.59	145.23			
15	248.0	250.00	221.93	145.59			
16	254.1	250.00	219.86	144.93			
17	264.4	250.00		142.85		77.00	1.014

Mole Reflux ratio 6.521

Exercise 10.23 (continued)

Analysis: (continued)





Exercise 10.24

Subject: Determination of optimal feed locations for two feeds of light normal paraffin hydrocarbon mixtures by a rigorous equilibrium-stage method.

Given: Feeds of compositions below as a bubble-point liquids at a constant column pressure of 250 psia. Column has a partial condenser, partial reboiler, and 30 equilibrium stages in the column. Distillate rate = 36.0 lbmol/h and reflux rate = 150.0 lbmol/h. Peng-Robinson equation of state for *K*-values and enthalpies. Suggested feed locations are stage 15 (stage 17 from the top counting the partial condenser), and stage 6 (stage 26 from the top counting the partial condenser) from the bottom for the heaviest feed, F_2. Peng-Robinson equation of state for *K*-values and enthalpies.

Find: Optimal feed-stage locations.

Analysis: The calculations were made with the TOWER model (Inside-out method) of the Chemcad program, with the following specifications:
Partial condenser
Top pressure = 250 psia
No condenser or stage pressure drop. Therefore, bottom pressure also = 250 psia
Number of stages = 32 (includes partial condenser and partial reboiler)
Feed one initially to stage = 17 from the top
Feed two initially to stage = 26 from the top
At the top, reflux rate = 150 lbmol/h
At the bottom, bottoms rate = $B = F - D$ = 100 - 36 = 64 lbmol/h
Estimated distillate rate = 36 lbmol/h (actual rate)
Estimated reflux rate = 150 lbmol/h (actual rate)
Estimated temperature of stage 1 = 120°F
Estimated temperature of bottom stage = 250°F
Estimated temperature of stage 2 = 140°F

Based on the feed compositions below, the distillate rate of 36 lbmol/h corresponds to a desired split between propane and n-butane. The calculations converged rapidly in 3 outer-loop iterations with results given below and on the following pages. The separation with feed stages at 12 and 15 from the top is much better than the separation with feed stages at 17 and 26. For the better stage locations:
Top temperature = 118.3°F compared to assumed value of 120°F
Bottom temperature = 252.8°F compared to assumed value of 300°F

Exercise 10.24 (continued)

Analysis: (continued)

Feed 1 to Stage 17 and Feed 2 to Stage 26

Stream No.	1	2	3	4
Stream Name	Feed 1	Feed 2	Distillate	Bottoms
Temp F	161.9428	214.1007	119.4775	252.1078
Pres psia	250.0000*	250.0000*	250.0000	250.0000
Enth MMBtu/h	-2.8036	-2.9957	-1.6101	-3.8921
Vapor mole fraction	0.00000*	0.00000*	1.0000	0.00000
Total lbmol/h	50.0000	50.0000	35.9998	64.0002
Total lb/h	2646.6519	3039.4070	1563.1553	4122.9053
Total std L ft3/hr	76.5635	82.5318	50.1094	108.9859
Total std V scfh	18973.93	18973.93	13661.16	24286.71
Flowrates in lbmol/h				
Ethane	1.5000	0.5000	1.9999	0.0001
Propane	24.0000	10.0000	33.7322	0.2678
N-Butane	16.5000	22.0000	0.2678	38.2322
N-Pentane	7.5000	14.5000	0.0000	22.0000
N-Hexane	0.5000	3.0000	0.0000	3.5000

Feed 1 to Stage 12 and Feed 2 to Stage 15

Stream No.	1	2	3	4
Stream Name	Feed 1	Feed 2	Distillate	Bottoms
Temp F	161.9428	214.1007	118.3058	252.7568
Pres psia	250.0000*	250.0000*	250.0000	250.0000
Enth MMBtu/h	-2.8036	-2.9957	-1.6088	-3.8927
Vapor mole fraction	0.00000*	0.00000*	1.0000	0.00000
Total lbmol/h	50.0000	50.0000	36.0000	63.9999
Total lb/h	2646.6519	3039.4070	1559.6190	4126.4351
Total std L ft3/hr	76.5635	82.5318	50.0586	109.0366
Total std V scfh	18973.93	18973.93	13661.22	24286.61
Flowrates in lbmol/h				
Ethane	1.5000	0.5000	2.0000	0.0000
Propane	24.0000	10.0000	33.9845	0.0154
N-Butane	16.5000	22.0000	0.0154	38.4845
N-Pentane	7.5000	14.5000	0.0000	22.0000
N-Hexane	0.5000	3.0000	0.0000	3.5000

Exercise 10.25

Subject: Distillation of a hydrocarbon mixture and comparison with solution in Perry's Handbook.

Given: Bubble-point liquid feed of composition given below. Column has partial condenser, partial reboiler, and 9 equilibrium stages in the column, with operation at 120 psia. Reflux rate = 126.1 lbmol/h and vapor distillate rate = 48.9 lbmol/h. Grayson-Streed correlation for *K*-values and Redlich-Kwong equation of state for enthalpies.

Find: Product compositions, stage temperatures, interstage flow rates and compositions, reboiler duty, and condenser duty.

Analysis: The calculations were made with the TOWER model (Inside-out method) of the Chemcad program, with the following specifications:
Partial condenser
Top pressure = 120 psia
No condenser or stage pressure drop. Therefore, bottom pressure also = 120 psia
Number of stages = 11 (includes partial condenser and partial reboiler)
Feed stage = 6 from the top
At the top, reflux rate = 126.1 lbmol/h
At the bottom, bottoms rate = $B = F - D$ = 100 - 48.9 = 51.1 lbmol/h
Estimated distillate rate = 48.9 lbmol/h (actual rate)
Estimated reflux rate = 126.1 lbmol/h (actual rate)
Estimated temperature of stage 1 = 120°F
Estimated temperature of bottom stage = 250°F
Estimated temperature of stage 2 = 140°F

The feed is given as a bubble-point liquid at 120 psia. Using the Grayson-Streed correlation, the temperature is computed to be 180.8°F. Based on the feed composition below, the distillate rate of 48.9 lbmol/h corresponds to a desired split between n-butane and isopentane. The calculations converged rapidly in 3 outer-loop iterations with results given below and on the following pages.

Condenser duty = 1,002,600 Btu/h
Reboiler duty = 1,427,000 Btu/h

Top temperature = 161.4°F compared to assumed value of 120°F
Bottom temperature = 230.0°F compared to assumed value of 250°F
Stage 2 temperature = 173.9°F compared to assumed value of 140°F

Exercise 10.25 (continued)

Analysis: (continued)

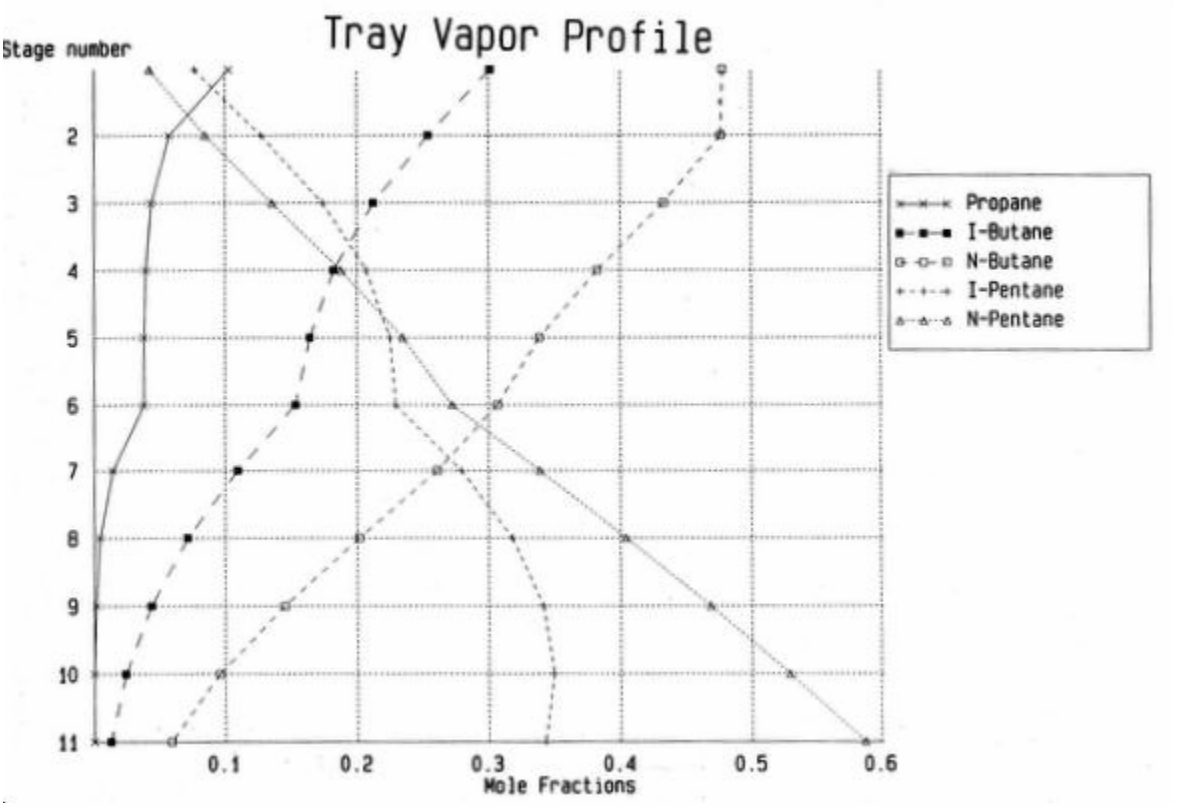
Stream No.	1	2	3
Stream Name	Feed	Distillate	Bottoms
Temp F	180.8180	161.3887	229.9752
Pres psia	120.0000*	120.0000	120.0000
Enth MMBtu/h	-6.5002	-2.6340	-3.4418
Vapor mole fraction	0.00000*	1.0000	0.00000
Total lbmol/h	100.0000	48.8970	51.1030
Total lb/h	6513.6504	2852.9138	3660.7361
Total std L ft3/hr	173.0095	79.3246	93.6849
Total std V scfh	37947.86	18555.35	19392.51
Flowrates in lbmol/h			
Propane	5.0000	4.9976	0.0024
I-Butane	15.0000	14.7104	0.2896
N-Butane	25.0000	23.4160	1.5840
I-Pentane	20.0000	3.7100	16.2900
N-Pentane	35.0000	2.0630	32.9371

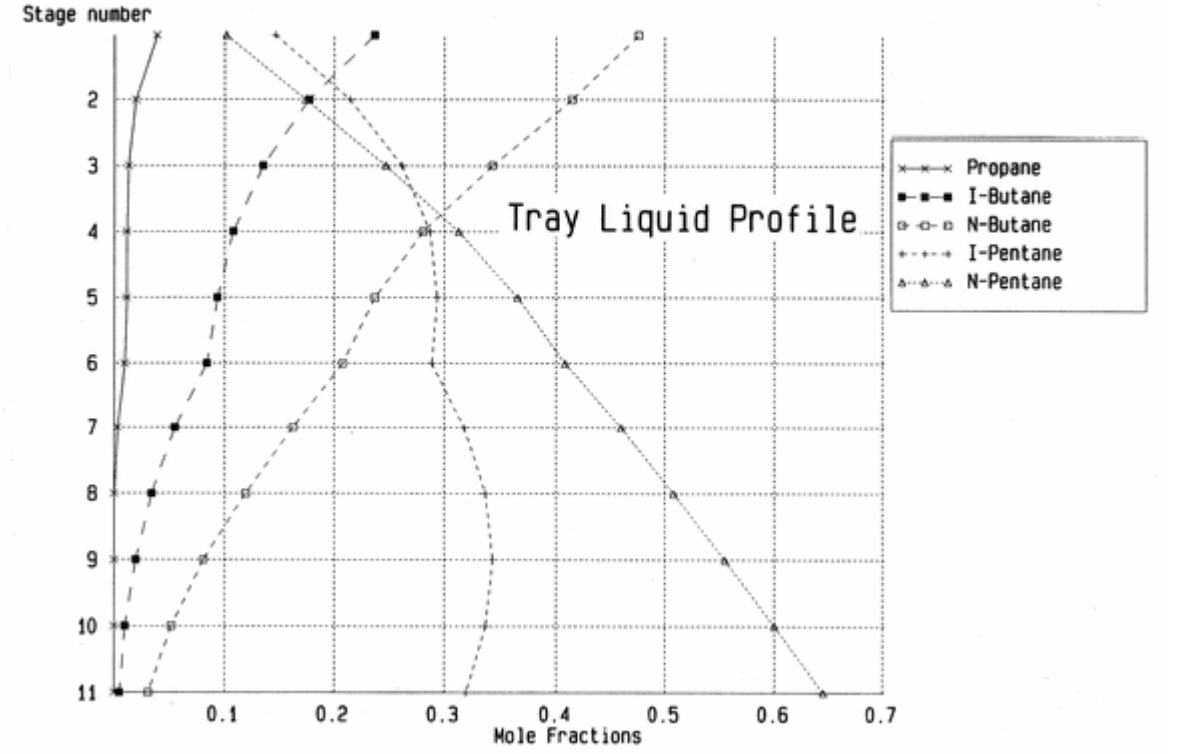
			* Net Flows *			
Stg	Temp F	Pres psia	Liquid lbmol/h	Vapor lbmol/h	Feeds lbmol/h	Product lbmol/h
1	161.4	120.00	126.10			48.90
2	173.9	120.00	123.29	175.00		
3	183.9	120.00	121.47	172.19		
4	191.6	120.00	120.53	170.36		
5	196.9	120.00	120.17	169.43		
6	200.4	120.00	221.81	169.06	100.00	
7	209.4	120.00	223.53	170.71		
8	216.7	120.00	224.74	172.42		
9	222.4	120.00	226.07	173.64		
10	226.7	120.00	227.04	174.96		
11	230.0	120.00		175.94		51.10

Mole Reflux ratio	2.579

Exercise 10.25 (continued)

Analysis: (continued)





Exercise 10.25 (continued)

Analysis: (continued)

The above results for the product compositions are compared to the results in Perry's Handbook as follows:

		Perry's Handbook:		This exercise:	
Component	**Feed, lbmol/h**	**Distillate, lbmol/h**	**Bottoms, lbmol/h**	**Distillate, lbmol/h**	**Bottoms, lbmol/h**
Propane	5.00	5.00	0.00	5.00	0.00
Isobutane	15.00	14.82	0.18	14.71	0.29
n-Butane	25.00	23.60	1.40	23.42	1.58
Isopentane	20.00	3.21	16.79	3.71	16.29
n-Pentane	35.00	2.30	32.70	2.06	32.94
Total:	100.00	48.93	51.07	48.90	51.10

The example in Perry's Handbook is for a column with a total condenser, while this exercise calls for a partial condenser. Thus, this exercise has 11 instead of 10 equilibrium stages. Nevertheless, the solution from Perry's Handbook shows a slightly sharper separation. This is probably due to the differences in *K*-values. For example at a mid-column temperature of 210°F, the Grayson-Streed correlation predicts a relative volatility between n-butane and isopentane of 1.82, while the graphical correlation used in Perry's Handbook predicts a higher value of 1.94.

Exercise 10.26

Subject: Distillation of an light alcohol mixture using UNIFAC equation.

Given: Feed of 1000 kmol/h of a bubble-point mixture of 60 mol% methanol (M), 20 mol% ethanol (E), and 20 mol% n-propanol (P) is sent to the middle stage of a column with a total condenser, 3 equilibrium stages in the column, and a partial reboiler, and operating at 1 atm. The distillate rate = 600 kmol/h and the reflux rate = 2,000 kmol/h.

Find: Product compositions, stage temperatures and vapor and liquid traffic, reboiler and condenser duties, and stage compositions for converged solution.

Analysis: The calculations were made with the TOWER model (Inside-out method) of the Chemcad program, with the following specifications:
Total condenser
Top pressure = 1 atm
No condenser or stage pressure drop. Therefore, bottom pressure also = 1 atm
Number of stages = 5 (includes total condenser and partial reboiler)
Feed stage = 3 from the top
At the top, reflux rate = 2,000 kmol/h
At the bottom, bottoms rate = $B = F - D$ = 1000 - 600 = 400 kmol/h
Estimated distillate rate = 600 kmol/h (actual rate)
Estimated reflux rate = 2000 kmol/h (actual rate)
Estimated temperature of stage 1 = 30°C
Estimated temperature of bottom stage = 100°C
Estimated temperature of stage 2 = 40°C

The feed is given as a bubble-point liquid at 1 atm. The UNIFAC equation gives a bubble-point temperature of 70.1°C. Based on the feed composition, the distillate rate of 600 kmol/h corresponds to a desired split between methanol and ethanol. The enthalpies were computed by the Latent Heat model with a correction for the heat of solution based on liquid-phase activity coefficients from the UNIFAC equation. The calculations converged in 8 outer-loop iterations with results given below and on the following pages.

Condenser duty = 93,592 MJ/h
Reboiler duty = 93,841 MJ/h

Top temperature = 70.1°C compared to assumed value of 30°C
Bottom temperature = 79.2°C compared to assumed value of 100°C
Stage 2 temperature = 67.3°C compared to assumed value of 40°C

Exercise 10.26 (continued)

Analysis: (continued)

Stream No.	1	2	3
Stream Name	Feed	Distillate	Bottoms
Temp C	70.1364	65.9428	79.1889
Pres atm	1.0000*	1.0000	1.0000
Enth J/h	-2.5444E+011	-1.4510E+011	-1.0909E+011
Vapor mole fraction	0.00000*	0.00000	0.00000
Total kmol/h	1000.0000	600.0019	399.9977
Total kg/h	40458.1998	20749.2569	19708.9322
Total std L m3/h	50.6325	26.0453	24.5872
Total std V m3/h	22413.65	13448.23	8965.41
Flowrates in kmol/h			
Methanol	600.0000	503.1963	96.8032
Ethanol	200.0000	84.9639	115.0361
N-Propanol	200.0000	11.8417	188.1584

			* Net Flows *			
Stg	Temp C	Pres atm	Liquid kmol/h	Vapor kmol/h	Feeds kmol/h	Product kmol/h
1	65.9	1.00	2000.01			600.00
2	67.3	1.00	1963.42	2600.01		
3	69.7	1.00	2915.30	2563.42	1000.00	
4	73.0	1.00	2827.77	2515.31		
5	79.2	1.00		2427.77		400.00

Mole Reflux ratio 3.333

Exercise 10.26 (continued)

Analysis: (continued)

Stage # 1	65.94 C	1.00 atm	
	V Mole frac	L Mole frac	K
Methanol	0.00000	0.83866	0.00000
Ethanol	0.00000	0.14161	0.00000
N-Propanol	0.00000	0.01974	0.00000
Total kmol/h	0.0000	2000.0070	
Stage # 2	67.29 C	1.00 atm	
	V Mole frac	L Mole frac	K
Methanol	0.83866	0.73618	1.13920
Ethanol	0.14161	0.20220	0.70031
N-Propanol	0.01974	0.06161	0.32033
Total kmol/h	2600.0094	1963.4186	
Stage # 3	69.70 C	1.00 atm	
	V Mole frac	L Mole frac	K
Methanol	0.76017	0.59527	1.27702
Ethanol	0.18802	0.25292	0.74340
N-Propanol	0.05181	0.15181	0.34128
Total kmol/h	2563.4210	2915.3035	
Stage # 4	73.02 C	1.00 atm	
	V Mole frac	L Mole frac	K
Methanol	0.65144	0.43743	1.48927
Ethanol	0.24741	0.29846	0.82893
N-Propanol	0.10115	0.26411	0.38299
Total kmol/h	2515.3057	2827.7653	
Stage # 5	79.19 C	1.00 atm	
	V Mole frac	L Mole frac	K
Methanol	0.46962	0.24201	1.94051
Ethanol	0.30025	0.28759	1.04403
N-Propanol	0.23012	0.47040	0.48921
Total kmol/h	2427.7677	399.9977	

Exercise 10.27

Subject: Distillation of a 4-component mixture with two sidestreams in an attempt to obtain four nearly pure products.

Given: Feed of composition given below at 150°F and 25 psia. Column pressure of 20 psia at top and 25 psia at the bottom Column has a total condenser giving saturated liquid, a partial reboiler, and 28 equilibrium stages in the column with feed entering stage 14. Distillate rate = 14.08 lbmol/h and reflux ratio = 20. A liquid sidestream of 19.53 lbmol/h is withdrawn at stage 10 from the top, and a vapor sidestream of 24.78 lbmol/h is withdrawn at stage 24 from the top. Peng-Robinson equation of state for *K*-values and enthalpies.

Find: Product compositions. Stage temperatures, vapor and liquid flow rates, and compositions. Reboiler and condenser duties.

Analysis: The calculations were made with the TOWER model (Inside-out method) of the Chemcad program, with the following specifications:
Total condenser
Top pressure = 20 psia
Total stage pressure drop = 5 psia. Therefore, bottom pressure = 25 psia
Number of stages = 30 (includes total condenser and partial reboiler)
Feed stage = 15 from the top
Liquid sidestream from stage 11 from the top, at a flow rate of 19.53 lbmol/h
Vapor sidestream from stage 25 from the top, at a flow rate of 24.78 lbmol/h
At the top, reflux ratio = 20
At the bottom, bottoms rate = $B = F - D - S_1 - S_2$ = 98.33 - 14.08 - 19.53 - 24.78 = 39.94 lbmol/h
Estimated distillate rate = 14.08 lbmol/h (actual rate)
Estimated reflux rate = 280 lbmol/h (close to actual rate of 281.6 lbmol/h)
Estimated temperature of stage 1 = 120°F
Estimated temperature of bottom stage = 200°F
Estimated temperature of stage 2 = 140°F
Estimated 1st draw rate = 19.53 lbmol/h (actual rate)
Estimated 2nd draw rate = 24.78 lbmol/h (actual rate)

The feed condition at the specified temperature and pressure is computed to be just slightly greater than the bubble-point temperature. Based on the feed composition below, the distillate, sidestreams, and bottoms correspond to the flow rates of the four components in the feed. The calculations converged rapidly in 4 outer-loop iterations with results given below and on the following pages.

Condenser duty = 2,834,600 Btu/h
Reboiler duty = 3,493,700 Btu/h

Top temperature = 47.7°F compared to assumed value of 120°F
Bottom temperature = 289.0°F compared to assumed value of 200°F
Stage 2 temperature = 49.9°F compared to assumed value of 140°F

Exercise 10.27 (continued)

Analysis: (continued)

A high reflux ratio is needed to minimize the effect of feed composition when attempting to obtain nearly pure sidestreams.

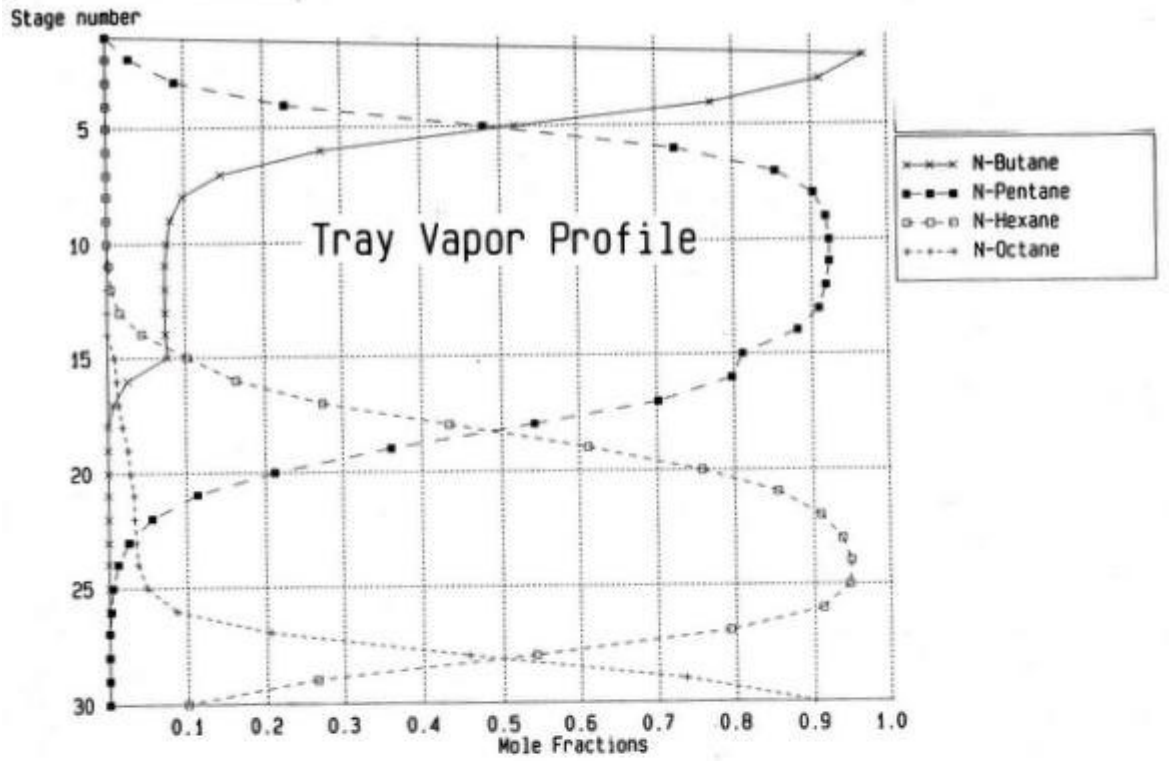
Stream No.	1	2	3	4	5
Stream Name	Feed	Distillate	Bottoms	Liquid SS	Vapor SS
Temp F	150.0000*	47.7093	289.0057	115.4295	198.5749
Pres psia	25.0000*	20.0000	25.0000	21.6071	24.1071
Enth MMBtu/h	-8.3843	-0.91036	-3.7035	-1.4212	-1.6901
Vapor mole fraction	0.000052847	0.00000	0.00000	0.00000	1.0000
Total lbmol/h	98.3300	14.0801	39.9400	19.5301	24.7799
Total lb/h	8925.3135	824.6918	4528.2456	1404.6851	2167.6921
Total std L ft3/hr	213.3971	22.5616	102.8821	35.7475	52.2059
Total std V scfh	37314.13	5343.09	15156.36	7411.24	9403.45
Flowrates in lbmol/h					
N-Butane	14.0800	13.6298	0.0000	0.4502	0.0000
N-Pentane	19.5300	0.4503	0.0001	18.9440	0.1356
N-Hexane	24.7800	0.0000	1.2167	0.1358	23.4275
N-Octane	39.9400	0.0000	38.7232	0.0000	1.2168

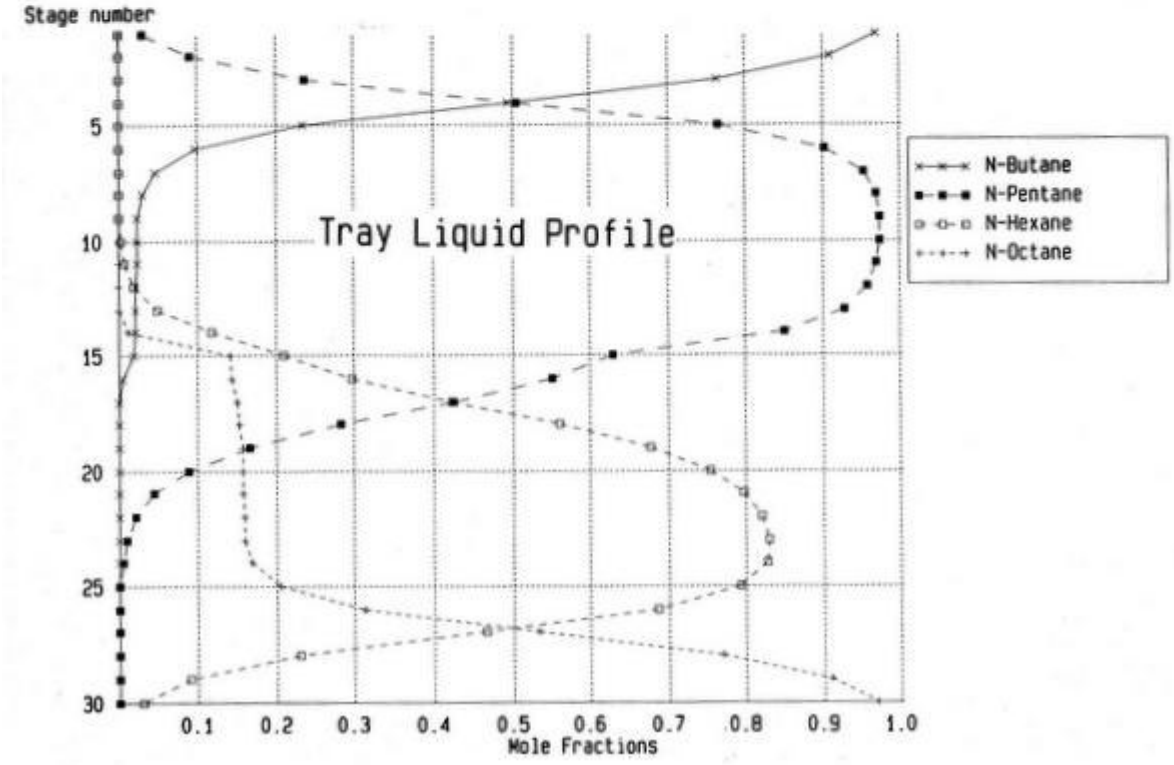
			* Net Flows *			
Stg	Temp F	Pres psia	Liquid lbmol/h	Vapor lbmol/h	Feeds lbmol/h	Product lbmol/h
1	47.7	20.00	281.60			14.08
2	49.9	20.00	276.37	295.68		
3	56.1	20.18	265.29	290.45		
4	69.5	20.36	250.22	279.37		
5	88.6	20.54	243.19	264.30		
6	103.1	20.71	244.16	257.27		
7	110.0	20.89	245.69	258.24		
8	112.7	21.07	246.44	259.77		
9	113.9	21.25	246.76	260.52		
10	114.7	21.43	246.90	260.84		
11	115.4	21.61	227.02	260.98		
						19.53
12	116.4	21.79	226.03	260.63		
13	118.1	21.96	223.37	259.64		
14	122.1	22.14	212.63	256.98		
15	136.5	22.32	305.59	246.24	98.33	
16	144.6	22.50	303.01	240.87		
17	154.5	22.68	300.08	238.29		
18	165.8	22.86	299.41	235.36		
19	176.4	23.04	301.06	234.69		
20	184.1	23.21	303.80	236.34		
21	189.0	23.39	305.81	239.08		
22	191.9	23.57	307.08	241.09		
23	193.8	23.75	307.49	242.36		
24	195.4	23.93	306.12	242.77		
25	198.6	24.11	299.50	241.40		
						24.78
26	207.1	24.29	284.14	259.56		
27	227.1	24.46	267.50	244.20		
28	255.6	24.64	265.60	227.56		
29	277.9	24.82	274.13	225.66		
30	289.0	25.00		234.19		39.94

Mole Reflux ratio 20.000

Exercise 10.27 (continued)

Analysis: (continued)





Exercise 10.28

Subject: Distillation of a hydrocarbon mixture given in Exercise 10.25.

Given: Bubble-point liquid feed of composition given below. Column has a partial condenser and a partial reboiler, with operation at 120 psia. Recovery of light key, n-butane, to distillate = 98%. Recovery of heavy key, isopentane, to bottoms = 98%. Grayson-Streed correlation for *K*-values and Redlich-Kwong equation of state for enthalpies.

Find: Product compositions, reflux ratio, numbers of equilibrium stages above and below the feed, stage temperatures, interstage flow rates and compositions, reboiler duty, and condenser duty.

Analysis: The calculations were made with the TOWER model (Inside-out method). Initially, it was assumed that the same number of stages and feed stage location could be used as in Exercise 10.25. Also, the same reflux rate and distillate rate as specified for Exercise 10.25 were given for initial estimates. It was understood that the Chemcad TOWER model would adjust the reflux rate and distillate rate in an attempt to achieve the desired LK and HK recoveries. Thus, the initial specifications for the TOWER model of the Chemcad program were:

Partial condenser
Top pressure = 120 psia
No condenser or stage pressure drop. Therefore, bottom pressure also = 120 psia
Number of stages = 11 (includes partial condenser and partial reboiler)
Feed stage = 6 from the top
At the top, component recovery of n-butane (component 3) = 0.98
At the bottom, component recovery of isopentane (component 4) = 0.98
Estimated distillate rate = 48.9 lbmol/h (actual rate)
Estimated reflux rate = 126.1 lbmol/h (actual rate)
Estimated temperature of stage 1 = 120^{o}F
Estimated temperature of bottom stage = 250^{o}F
Estimated temperature of stage 2 = 140^{o}F

The feed is given as a bubble-point liquid at 120 psia. Using the Grayson-Streed correlation, the temperature is computed to be 180.8^{o}F. After 50 iterations, the calculations were not converged, even though the reflux rate was increased from 126.1 lbmol/h to 8000.4 lbmol/h. The 98% recoveries of the two key components could not be achieved. This indicated that the number of stages was probably below the minimum number.

Exercise 10.28 (continued)

Analysis: (continued)

To obtain a better estimate of the stage requirements, the Fenske equation can be applied in the following manner, where the separation achieved in Exercise 10.25 for 11 stages is ratioed to the separation desired here. That separation in Exercise 10.25 is 93.66% recovery of nC_4 and 81.4% recovery of iC_5. Thus, applying Eq. (9-12) in this manner:

$$N = \frac{\log\left[\left(\frac{98}{2}\right)\left(\frac{98}{2}\right)\right]}{\log\left[\left(\frac{93.7}{6.3}\right)\left(\frac{81.5}{8.5}\right)\right]}(11) = 17.\ 3 \text{ equilibrium stages}$$

With this result, it was decided to try 19 stages (including the partial condenser and partial reboiler) with the feed to stage 10. Otherwise, the specifications for the TOWER model were unchanged from above. This time convergence was achieved rapidly in just 2 iterations. The reflux rate was increased by TOWER from 126.1 to 161.0 lbmol/h and the distillate rate was reduced from 48.9 lbmol/h to 44.93 lbmol/h. Other results were as follows:

Condenser duty = 1,195,400 Btu/h
Reboiler duty = 1,586,600 Btu/h

Top temperature = 147.9°F compared to assumed value of 120°F
Bottom temperature = 232.3°F compared to assumed value of 250°F
Stage 2 temperature = 152.9°F compared to assumed value of 140°F

Exercise 10.28 (continued)

Analysis: (continued)

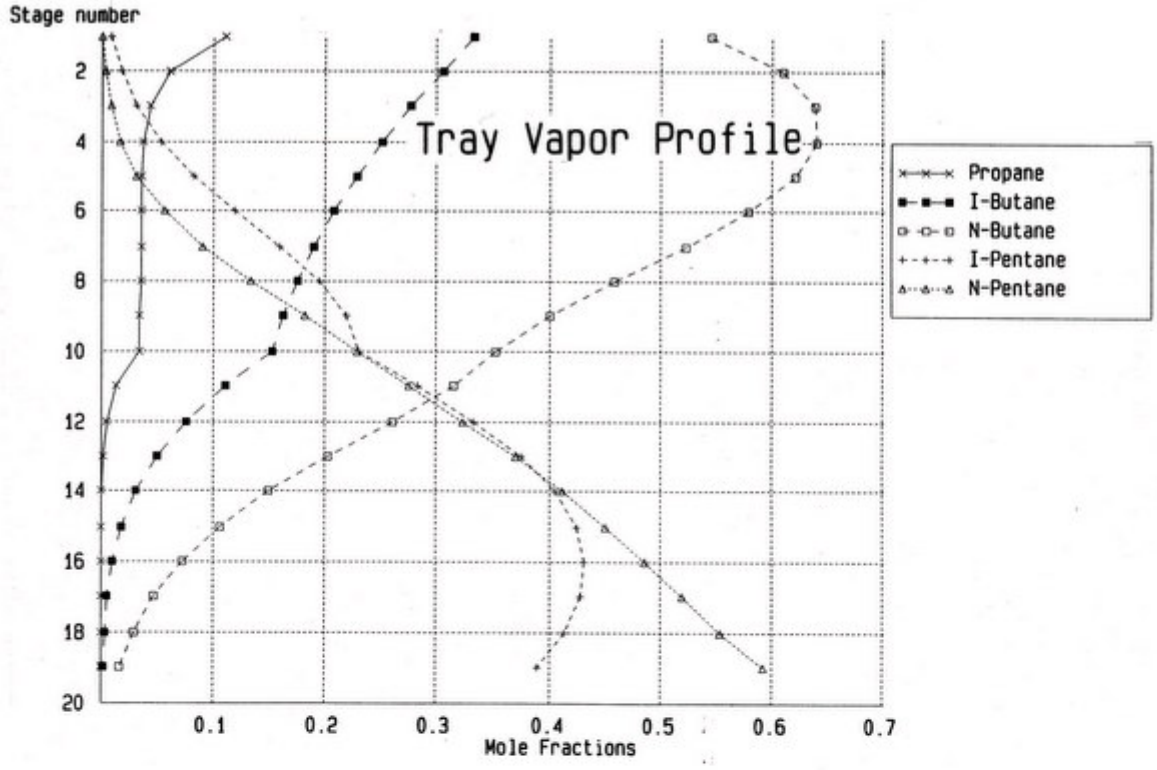
Stream No.	1	2	3
Stream Name	Feed	Distillate	Bottoms
Temp F	180.8180	147.8854	232.3231
Pres psia	120.0000*	120.0000	120.0000
Enth MMBtu/h	-6.5002	-2.3879	-3.7215
Vapor mole fraction	0.00000*	1.0000	0.00000
Total lbmol/h	100.0000	44.9301	55.0699
Total lb/h	6513.6504	2547.9216	3965.7314
Total std L ft3/hr	173.0095	71.6650	101.3446
Total std V scfh	37947.86	17050.03	20897.86
Flowrates in lbmol/h			
Propane	5.0000	5.0000	0.0000
I-Butane	15.0000	14.9608	0.0392
N-Butane	25.0000	24.5001	0.4999
I-Pentane	20.0000	0.4000	19.6000
N-Pentane	35.0000	0.0693	34.9307

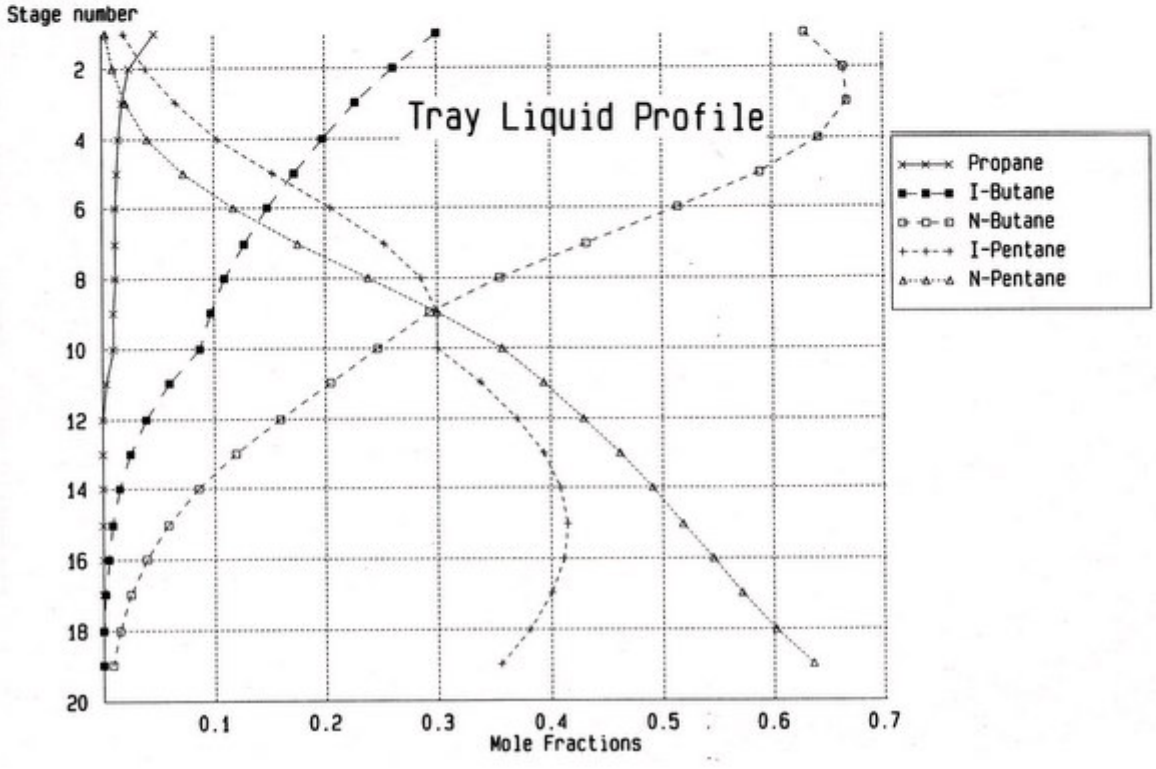
			* Net Flows *			
	Temp	Pres	Liquid	Vapor	Feeds	Product
Stg	F	psia	lbmol/h	lbmol/h	lbmol/h	lbmol/h
1	147.9	120.00	161.05			44.93
2	152.9	120.00	160.21	205.98		
3	156.6	120.00	158.40	205.14		
4	160.6	120.00	155.78	203.33		
5	165.7	120.00	152.56	200.71		
6	172.0	120.00	149.29	197.49		
7	179.1	120.00	146.60	194.22		
8	186.1	120.00	144.79	191.53		
9	192.2	120.00	143.74	189.72		
10	197.0	120.00	245.26	188.67	100.00	
11	205.0	120.00	246.54	190.19		
12	211.8	120.00	247.79	191.47		
13	217.4	120.00	249.03	192.72		
14	221.8	120.00	250.20	193.96		
15	225.2	120.00	251.17	195.13		
16	227.7	120.00	251.90	196.10		
17	229.6	120.00	252.38	196.83		
18	231.1	120.00	252.67	197.31		
19	232.3	120.00		197.60		55.07

Mole Reflux ratio 3.584

Exercise 10.28 (continued)

Analysis: (continued)





Exercise 10.29

Subject: Distillation of a light hydrocarbon mixture with a specified split.

Given: Saturated liquid feed at 125 psia of 200 lbmol/h of 5 mol% iC_4, 20 mol% nC_4, 35 mol% iC_5, and 40 mol% nC_5. Column is equipped with a total condenser and a partial reboiler, operating at 125 psia. Recovery of nC_4 to the distillate = 95%. Recovery of iC_5 to the bottoms = 95%. Number of equilibrium stages = 2 times that of the minimum stages by the Fenske equation. SRK for *K*-values and enthalpies.

Find: A suitable design. Assume this consists of products, profiles, and stage compositions.

Analysis: The Shortcut model of Chemcad computes a minimum number of stages = 10.7 and a minimum reflux ratio of 3.36. Therefore, select 2(10.7) = 21.4 or 22 stages (including the partial reboiler). Estimate the reflux ratio at 1.3(3.36) = 4.4.
For the rigorous TOWER model of chemcad, use the following specifications:

Total condenser
Top pressure = 125 psia
No condenser or stage pressure drop. Therefore, bottom pressure also = 125 psia
Number of stages = 23 (includes total condenser and partial reboiler)
Feed stage = 12 from the top
At the top, component recovery of n-butane (component 2) = 0.95
At the bottom, component recovery of isopentane (component 3) = 0.95
Estimated distillate rate = 50 lbmol/h (actual rate)
Estimated reflux rate = 50(3.36) = 168 lbmol/h (actual rate)
Estimated temperature of stage 1 = 120°F
Estimated temperature of bottom stage = 250°F
Estimated temperature of stage 2 = 140°F

The feed is given as a bubble-point liquid at 125 psia. Using the SRK correlation, the temperature is computed to be 210°F. After 4 iterations, the calculations are converged, while increasing the reflux rate to 267.9 lbmol/h, and the distillate rate to 52.11 lbmol/h, at which the 95% recoveries of the two key components are achieved. The computed results are as follows on this page and the next pages.

Condenser duty = 2,517,800 Btu/h
Reboiler duty = 2,582,500 Btu/h

Top temperature = 160.8°F compared to assumed value of 120°F
Bottom temperature = 233.2°F compared to assumed value of 250°F
Stage 2 temperature = 165.8°F compared to assumed value of 140°F

Exercise 10.29 (continued)

Analysis: (continued)

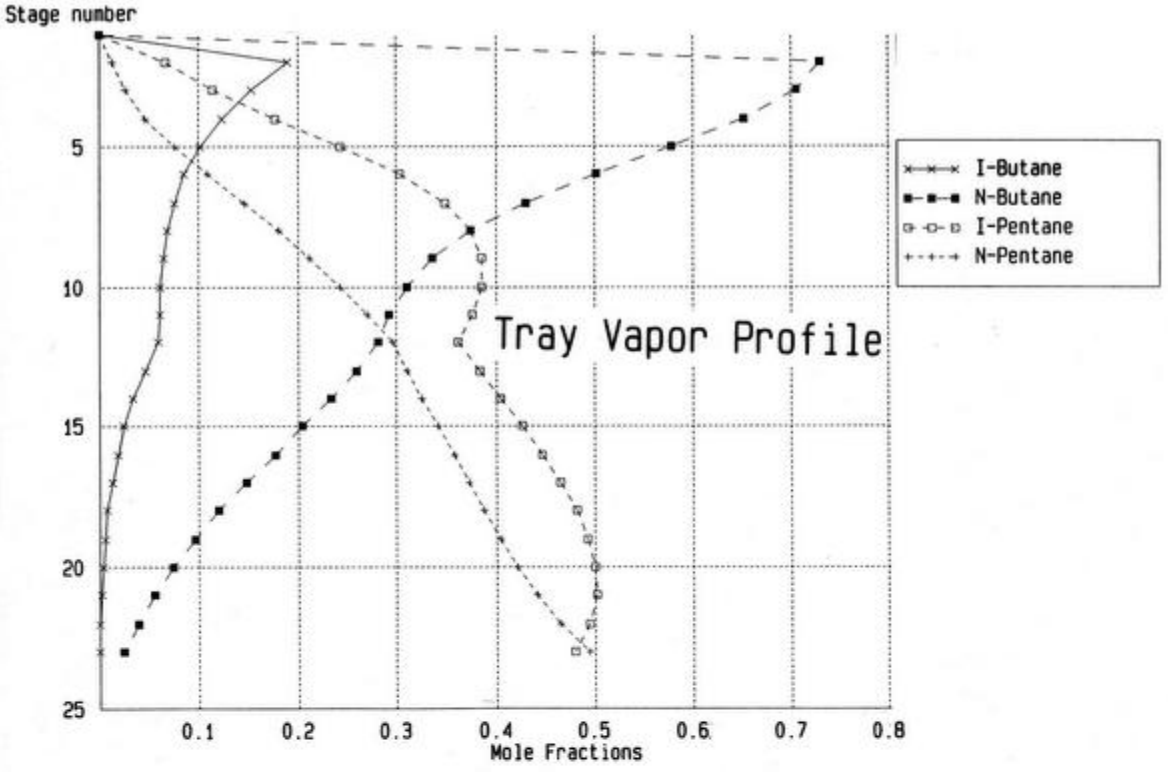
Stream No.	1	2	3
Stream Name	Feed	Distillate	Bottoms
Temp F	210.0201	160.8284	233.2131
Pres psia	125.0000*	125.0000	125.0000
Enth MMBtu/h	-13.410	-3.2228	-10.123
Vapor mole fraction	0.00000*	0.00000	0.00000
Total lbmol/h	200.0000	52.1137	147.8863
Total lb/h	13728.6504	3087.5322	10641.1172
Total std L ft3/hr	357.1210	84.7885	272.3325
Total std V scfh	75895.73	19776.04	56119.68
Flowrates in lbmol/h			
I-Butane	10.0000	9.9412	0.0588
N-Butane	40.0000	38.0000	1.9999
I-Pentane	70.0000	3.4999	66.5001
N-Pentane	80.0000	0.6725	79.3275

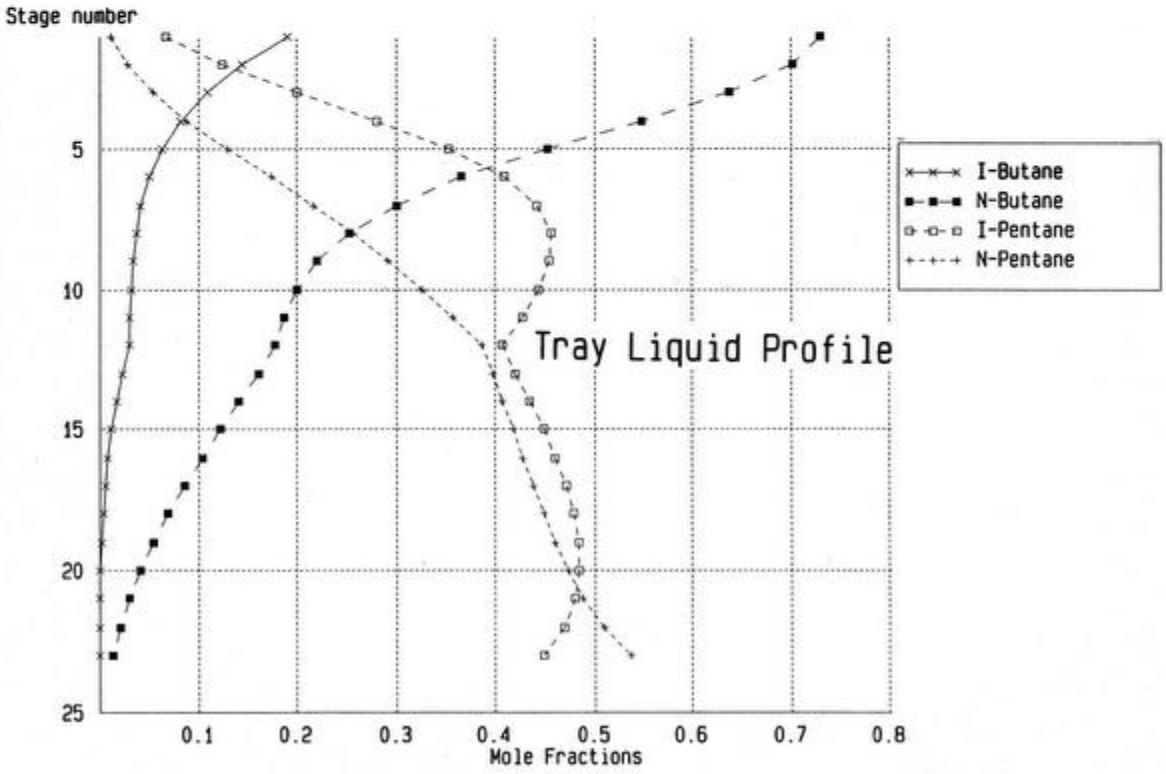
			* Net Flows *			
Stg	Temp F	Pres psia	Liquid lbmol/h	Vapor lbmol/h	Feeds lbmol/h	Product lbmol/h
1	160.8	125.00	267.86			52.11
2	165.8	125.00	262.03	319.97		
3	172.3	125.00	255.78	314.14		
4	179.9	125.00	250.21	307.89		
5	187.9	125.00	246.19	302.33		
6	195.2	125.00	243.79	298.30		
7	201.2	125.00	242.55	295.90		
8	205.7	125.00	241.92	294.66		
9	208.9	125.00	241.54	294.04		
10	211.1	125.00	241.22	293.65		
11	212.6	125.00	240.92	293.34		
12	213.8	125.00	441.50	293.03	200.00	
13	216.2	125.00	442.22	293.61		
14	218.5	125.00	443.04	294.33		
15	220.7	125.00	443.94	295.16		
16	222.9	125.00	444.88	296.06		
17	224.8	125.00	445.82	297.00		
18	226.6	125.00	446.70	297.93		
19	228.2	125.00	447.50	298.82		
20	229.6	125.00	448.18	299.62		
21	230.9	125.00	448.69	300.29		
22	232.1	125.00	449.03	300.81		
23	233.2	125.00		301.14		147.89

Mole Reflux ratio	5.140

Exercise 10.29 (continued)

Analysis: (continued)





Exercise 10.30

Subject: Design of a depropanizer distillation column.

Given: Feed at column average pressure of 315 psia and 66 mol% vaporized. Composition of feed in lbmol/h is as follows: 26 C_1, 9 C_2, 25 C_3, 17 nC_4, 11 nC_5, 12 nC_6. Separation is between C_3 (0.4 lbmol/h in bottoms) and nC_4 (0.3 lbmol/h in distillate). Cooling water available at 65°F and steam available at 315 psia. Total column pressure drop = 2 psi.

Assumptions: Partial reboiler. Grayson-Streed correlation for *K*-values and Redlich-Kwong equation for enthalpies.

Find: (a) Type condenser.
(b) Feed temperature. *K*-values and relative volatilities at feed temperature and pressure.
(c) Reflux ratio for 1.3 times minimum reflux ratio. Number of equilibrium stages in rectifying and stripping sections.
(d) Separation. Separation for reflux ratio = 1.5 times minimum, 15 theoretical stagess, feed stage at stage 9.
(e) Temperature and compositions at each stage for Part (c). Effect on these results if reflux and stages of Part (d) are used.

Analysis: Use the Flash, Shortcut, and TOWER models of Chemcad to make the calculations.
(a) Assume a pressure at the top of 314 psia, with 316 psia at the bottom and 315 psia at the feed location. Using the Flash model, run a bubble-point temperature calculation of the assumed distillate in lbmol/h of 26 C_1, 9 C_2, 24.6 C_3, and 0.3 nC_4 at 314 psia for both 0% (total condenser case) and 100% vaporized (partial condenser case). For a total condenser, the distillate temperature is found to be -100°F, which is infeasible. For a partial condenser, the distillate temperature is 73.1°F, which is possible, but very close to the cooling water temperature of 65°F. A bubble point calculation on the assumed bottoms in lbmol/h of 0.4 C_3, 16.7 nC_4, 11 nC_5, and 12 nC_6, at 316 psia is 301.9°F. The saturation temperature of steam at 315 psia is 421°F. Therefore, the steam is adequate, but may have to be throttled to a lower pressure to avoid film boiling in the reboiler.
(b) When the feed is flashed at 315 psia to 66 mol% vapor, the temperature = 183.3°F. The computed *K*-values and relative volatilities (relative to the HK, nC_4) are:

Component	*K*-value	α referred to nC_4
Methane	9.250	15.29
Ethane	3.081	5.09
Propane, LK	1.405	2.32
n-Butane, HK	0.605	1.00
n-Pentane	0.274	0.453
n-Hexane	0.126	0.208

Exercise 10.30 (continued)

Analysis (continued)

(c) The recovery of the LK, C_3, to the distillate = 24.6/25 = 0.984. The recovery of the HK, nC_4, to the distillate = 0.3/17 = 0.01765. Using the Shortcut (FUG) model of Chemcad, the following results are obtained:

Minimum equilibrium stages = 10.5
Minimum reflux ratio = 0.87
Actual reflux ratio for 1.3 times minimum = 1.131
Number of equilibrium stages = 23.5
Feed stage from top = 11.5
Therefore, use, say, 10 theoretical plates in rectifying section plus a partial condenser, and 12 theoretical plates in the stripping section plus a partial reboiler.

(d) For the rigorous TOWER model of chemcad, first use the following specifications for the case of a reflux ratio = 1.3 times minimum:

Partial condenser
Top pressure = 314 psia
No condenser pressure drop. Column pressure drop = 2 psi
Therefore, bottom pressure = 316 psia
Number of stages = 24 (includes partial condenser and partial reboiler)
Feed stage = 12 from the top
At the top, reflux ratio = 1.131
At the bottom, bottoms flow rate = 40.1 lbmol/h
Estimated distillate rate = 59.9 lbmol/h (actual rate)
Estimated reflux rate = 59.9(1.131) = 67.75 lbmol/h (actual rate)
Estimated temperature of stage 1 = 73°F
Estimated temperature of bottom stage = 302°F
Estimated temperature of stage 2 = 83°F

The TOWER model converged in 4 iterations, with the following results, including the temperatures and concentrations at each stage, as requested in Part (e):

Condenser duty = 417,600 Btu/h
Reboiler duty = 482,500 Btu/h
Top temperature = 72.9°F compared to assumed value of 73°F
Bottom temperature = 302°F compared to assumed value of 302°F
Stage 2 temperature = 105.2°F compared to assumed value of 83°F

Note that the desired split of the two key components is achieved with:

0.2747 lbmol/h of nC_4 (HK) in the distillate compared to a specification of 0.3 lbmol/h
0.3747 lbmol/h of C_3 (LK) in the bottoms compared to a specification of 0.4 lbmol/h

Exercise 10.30 (continued)

Analysis: (d) (continued)

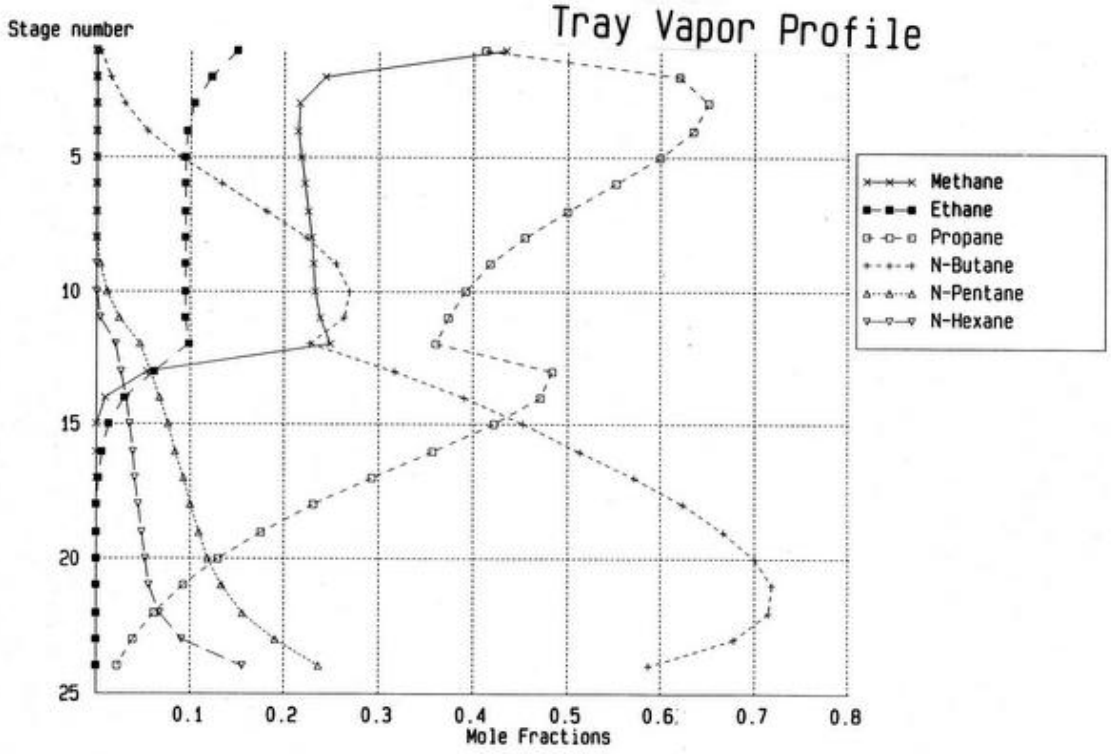
Stream No.	1	2	3
Stream Name	Feed	Distillate	Bottoms
Temp F	183.3298	72.9214	301.9649
Pres psia	315.0000*	314.0000	316.0000
Enth MMBtu/h	-4.8458	-2.3194	-2.4616
Vapor mole fraction	0.66000*	1.0000	0.00000
Total lbmol/h	100.0000	59.9000	40.1000
Total lb/h	4606.0127	1789.5911	2816.4219
Total std L ft3/hr	141.5698	69.2016	72.3682
Total std V scfh	37947.86	22730.76	15217.10
Flowrates in lbmol/h			
Methane	26.0000	26.0000	0.0000
Ethane	9.0000	9.0000	0.0000
Propane	25.0000	24.6253	0.3747
N-Butane	17.0000	0.2747	16.7253
N-Pentane	11.0000	0.0000	11.0000
N-Hexane	12.0000	0.0000	12.0000

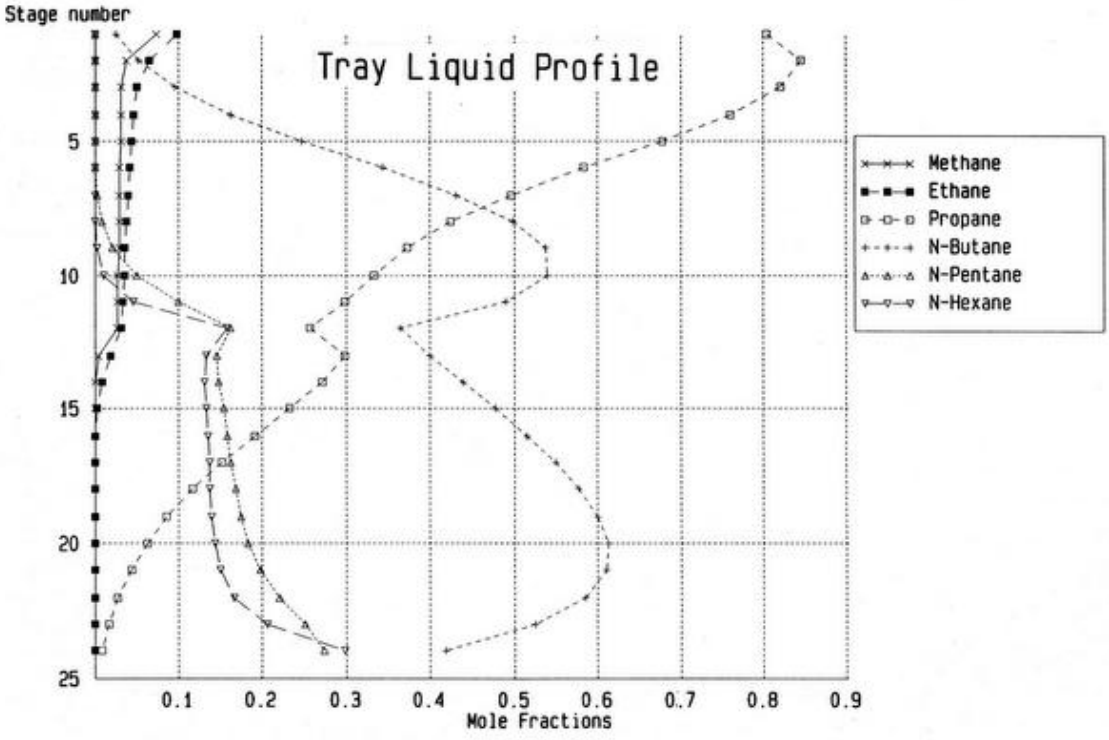
			* Net Flows *			
	Temp	Pres	Liquid	Vapor	Feeds	Product
Stg	F	psia	lbmol/h	lbmol/h	lbmol/h	lbmol/h
1	72.9	314.00	67.75			59.90
2	105.2	314.00	73.68	127.65		
3	113.4	314.09	72.34	133.58		
4	118.8	314.18	69.83	132.24		
5	125.2	314.27	67.01	129.73		
6	132.6	314.36	64.41	126.90		
7	140.2	314.45	62.40	124.31		
8	147.0	314.55	60.81	122.30		
9	152.8	314.64	59.16	120.71		
10	158.6	314.73	56.21	119.06		
11	167.0	314.82	50.22	116.11		
12	183.3	314.91	83.80	110.12	100.00	
13	209.2	315.00	106.58	43.70		
14	223.2	315.09	110.47	66.48		
15	232.3	315.18	111.17	70.37		
16	239.8	315.27	111.36	71.07		
17	246.5	315.36	111.63	71.26		
18	252.3	315.45	112.04	71.53		
19	257.5	315.55	112.56	71.94		
20	262.3	315.64	112.99	72.46		
21	267.3	315.73	113.12	72.89		
22	273.7	315.82	112.65	73.02		
23	284.0	315.91	111.65	72.55		
24	302.0	316.00		71.55		40.10

Mole Reflux ratio 1.131

Exercise 10.30 (continued)

Analysis: (d) (continued)





Exercise 10.30 (continued)

Analysis: (d) (continued)

For the rigorous TOWER model of chemcad, now use the following specifications for the case of a reflux ratio = 1.5 times minimum, with 15 theoretical plates and feed to plate 9 (assume from the top):

Partial condenser
Top pressure = 314 psia
No condenser pressure drop. Column pressure drop = 2 psi
Therefore, bottom pressure = 316 psia
Number of stages = 17 (includes partial condenser and partial reboiler)
Feed stage = 10 from the top
At the top, reflux ratio = 1.5(0.87) = 1.305
At the bottom, bottoms flow rate = 40.1 lbmol/h
Estimated distillate rate = 59.9 lbmol/h (actual rate)
Estimated reflux rate = 59.9(1.305) = 78.17 lbmol/h (actual rate)
Estimated temperature of stage 1 = 73°F
Estimated temperature of bottom stage = 302°F
Estimated temperature of stage 2 = 83°F

The TOWER model converged in 3 iterations, with the following results for the products:
Note that the desired split of the two key components is not achieved:
0.6269 lbmol/h of nC_4 (HK) in the distillate compared to a specification of 0.3 lbmol/h
0.7256 lbmol/h of C_3 (LK) in the bottoms compared to a specification of 0.4 lbmol/h

Stream No.	1	2	3
Stream Name	Feed	Distillate	Bottoms
Temp F	183.3298	74.8766	300.3983
Pres psia	315.0000*	314.0000	316.0000
Enth MMBtu/h	-4.8458	-2.3210	-2.4639
Vapor mole fraction	0.66000*	1.0000	0.00000
Total lbmol/h	100.0000	59.8995	40.1005
Total lb/h	4606.0127	1794.5383	2811.4741
Total std L ft3/hr	141.5698	69.2722	72.2976
Total std V scfh	37947.86	22730.59	15217.27
Flowrates in lbmol/h			
Methane	26.0000	26.0000	0.0000
Ethane	9.0000	8.9982	0.0018
Propane	25.0000	24.2744	0.7256
N-Butane	17.0000	0.6269	16.3731
N-Pentane	11.0000	0.0001	10.9999
N-Hexane	12.0000	0.0000	12.0000

Exercise 10.30 (continued)

Analysis: (e) (continued)

The calculations with the TOWER model of Chemcad are repeated here for the case of a reflux ratio = 1.3 times the minimum, with 24 total stages (including the partial condenser and partial reboiler) and a variable feed stage in an attempt to make the best separation. We compare the results on the basis of the lbmol/h of nC_4 (HK) in the distillate product as follows:

Feed stage from top	lbmol/h of nC_4 in distillate
7	0.509
8	0.364
9	0.276
10	0.244
11	0.246
12	0.275
13	0.343
14	0.439
15	0.559

From these results, it is seen that the optimal feed location is stage 11 (stage 10 in the column), with stage 10 giving almost the same separation.

For the case of a reflux ratio of 1.5 time the minimum, the desired separation could not be achieved for any feed stage location.

Exercise 10.31

Subject: Separation of toluene from biphenyl (diphenyl) by distillation

Given: The following feed at 264°F and 37.1 psia, and the desired products:

lbmol/h:

Component	Feed	Distillate	Bottoms
Benzene	3.4	3.4	0.0
Toluene	84.6	82.5	2.1
Biphenyl	5.1	1.0	4.1
Total	93.1	86.9	6.2

Reflux ratio = 1.3 times minimum with total condenser and partial reboiler. Pressure at top = 36 psia. Pressure at bottom = 38.2 psia.

Assumptions: SRK equation of state for *K*-values and enthalpies.

Find: (a) Actual reflux, number of equilibrium stages, and feed stage location.
(b) Separation for a *D/F* = 86.9/93.1 = 0.9334
(c) Specified separation by adjusting reflux ratio in Part (b)

Analysis: (a) The recovery of the LK, toluene, to the distillate = 82.5/84.6 = 0.9752. The recovery of the HK, biphenyl, to the distillate = 1.0/5.1 = 0.1980. Using the Shortcut (FUG) model of Chemcad, the following results are obtained:

Minimum equilibrium stages = 2.5

Therefore, assume that a rectifying section is not needed. Try a reboiled stripper with 4 stages plus a partial reboiler.

(b) For the rigorous TOWER model of chemcad, use the following specifications:
No condenser
Top pressure = 36 psia
No condenser pressure drop. Column pressure drop = 2.2 psi
Therefore, bottom pressure = 38.2 psia
Number of stages = 5 (includes partial reboiler)
Feed stage = top stage
At the bottom, bottoms flow rate = 6.2 lbmol/h (corresponds to the specified *D/F* ratio.
Estimated distillate rate = 86.9 lbmol/h (desired rate)
Estimated reflux rate = feed rate = 93.1 lbmol/h)
Estimated temperature of stage 1 = 300°F
Estimated temperature of bottom stage = 400°F
Estimated temperature of stage 2 = 320°F

The TOWER model converged in 5 iterations, with the following results:

Exercise 10.31 (continued)

Analysis: (b) (continued)

Reboiler duty = 1,379,300 Btu/h

Stream No.	1	2	3
Stream Name	Feed	Distillate	Bottoms
Temp F	264.0000*	296.1456	438.4632
Pres psia	37.1000*	36.0000	38.2000
Enth MMBtu/h	1.4830	2.4617	0.40058
Vapor mole fraction	0.00000	1.0000	0.00000
Total lbmol/h	93.1000	86.8999	6.2001
Total lb/h	8847.1865	7965.9634	881.2267
Total std L ft3/hr	160.4649	146.3956	14.0694
Total std V scfh	35329.46	32976.66	2352.81
Flowrates in lbmol/h			
Benzene	3.4000	3.3979	0.0021
Toluene	84.6000	83.3960	1.2041
Diphenyl	5.1000	0.1060	4.9940

Note that the desired split of the two key components is better than desired with:
1.204 lbmol/h of toluene (LK) in the bottoms compared to a specification of 2.1 lbmol/h
0.106 lbmol/h of diphenyl (HK) in the distillate compared to a specification of 1.0 lbmol/h

(c) Because the column has no reflux, the flow rate of the toluene in the bottoms was specified on the basis that the reboiler duty would be adjusted to obtained that flow rate. The TOWER model converged in 4 iterations with the following results, which did give the desired toluene rate in the bottoms, but much less than desired diphenyl in the distillate:

Reboiler duty = 1,354,500 Btu/h

Stream No.	1	2	3
Stream Name	Feed	Distillate	Bottoms
Temp F	264.0000*	296.1283	400.2492
Pres psia	37.1000*	36.0000	38.2000
Enth MMBtu/h	1.4830	2.4366	0.40086
Vapor mole fraction	0.00000	1.0000	0.00000
Total lbmol/h	93.1000	86.0014	7.0985
Total lb/h	8847.1865	7883.1265	964.0591
Total std L ft3/hr	160.4649	144.8726	15.5923
Total std V scfh	35329.46	32635.71	2693.74
Flowrates in lbmol/h			
Benzene	3.4000	3.3965	0.0035
Toluene	84.6000	82.5001	2.0999
Diphenyl	5.1000	0.1049	4.9951

Exercise 10.32

Subject: Comparison of two sequences of two distillation columns each for the separation of a mixture into three products.

Given: Feed at 100°F and 480 psia and desired products with the following compositions in component flow rates:

	lbmol/h:			
Component	**Feed**	**Product 1**	**Product 2**	**Product 3**
Hydrogen	1.5	1.5		
Methane	19.3	19.2	0.1	
Benzene	262.8	1.3	258.1	3.4
Toluene	84.7		0.1	84.6
Biphenyl	5.1			5.1
Total:	373.4	22.0	258.3	93.1

In Sequence 1, the keys in Column 1 are methane and benzene, and the keys in Column 2 are benzene and toluene. For Sequence 2, the keys in Column 1 are benzene and toluene, and the keys in Column 2 are methane and benzene. Use partial condensers when the bulk of the methane is taken overhead and set condenser pressures to at least 20 psia, with distillate temperatures of about 130°F.

Assumptions: SRK for *K*-values and enthalpies. Isobaric operation of columns.

Find: Column pressures, type condensers, and reflux and stage requirements for columns in each sequence, using a reflux ratio of 1.3 times minimum reflux ratio.

Analysis: First determine column pressures and type condensers, using Chemcad.

Sequence 1, Column 1: Distillate is Product 1.
The computed dew-point pressure at 130°F = 118 psia. Set top pressure to 118 psia with a partial condenser.
Sequence 1, Column 2: Distillate is Product 2. The computed bubble-point pressure at 130°F = 8.4 psia. This is too low. Therefore, set top pressure to 20 psia with a total condenser.
Distillate temperature at this pressure = 187°F.

Sequence 2, Column 1: Distillate is the sum of Products 1 and 2. The computed dew-point pressure at 130°F = 6.7 psia. This is too low. Therefore, set top pressure to 20 psia with a partial condenser. Distillate temperature at this pressure = 190°F.
Sequence 2, Column 2: Distillate is Product 1. Therefore, again set pressure to 118 psia with a partial condenser.

Exercise 10.32 (continued)

Analysis: (continued)

Now, use the Shortcut model in Chemcad to estimate stage and reflux ratios using $R = 1.3R_{min}$. Results are as follows, where recoveries are of the column feed to the distillate:

	Sequence 1 Column 1	**Sequence 1 Column 2**	**Sequence 2 Column 1**	**Sequence 2 Column 2**
Pressure, psia	118	20	20	118
Light key, LK	Methane	Benzene	Benzene	Methane
Heavy key, HK	Benzene	Toluene	Toluene	Benzene
Recovery of LK	0.9948	0.9870	0.9870	0.9948
Recovery of HK	0.00495	0.00118	0.00118	0.005012
Minimum stages	2.04	14.37	13.28	2.01
Min. reflux ratio	0.0685	1.188	0.930	5.628
Reflux ratio	0.0822	1.425	1.209	7.317
No. of stages	8.97	32.35	29.23	4.55
Feed stage from top	4.60	23.99	21.34	2.26

Now design the two sequences using the rigorous Tower model of Chemcad. For each column, the top specification is the flow rate of the LK in the distillate and the bottom specification is the flow rate of the HK in the bottoms. The stage specifications and estimated reflux and distillate rates are taken from the above shortcut results, with some modest changes. The rigorous Tower model then computes the required reflux ratio and distribution of nonkey components. The results are as follows, where the total stages includes the condenser (total or partial) and the reboiler. The feed stage is counted from the condenser as stage 1.

	Sequence 1 Column 1	**Sequence 1 Column 2**	**Sequence 2 Column 1**	**Sequence 2 Column 2**
Top pressure, psia	118	20	20	118
Pressure drop, psia	2	2	2	2
Total stages	3	30	30	5
Feed stage	2	22	21	2
Reflux ratio	2.2	1.363	1.101	0.0042
Condenser duty, Btu/h	892,100	8,122,800	4,074,800	1,900
Reboiler duty, Btu/h	4,227,300	6,135,800	8,843,100	2,748,100
T of bottoms, ^{o}F	347.4	258.8	258.8	404.6
Lbmol/h of toluene in Product 1	0.063			0.0002

Sequence 2 requires an expensive two-stage compression system to take the vapor distillate from Column 1 at 20 psia and increase its pressure to 119 psia to deliver it to Column 2. Note that Column 2 uses such a small amount of reflux, that it is essentially just a reboiled stripper. Sequence 1 is simpler and preferred over Sequence 2. However, the first column in Sequence 1 would benefit with more reflux and stages to reduce the loss of toluene.

Exercise 10.33

Subject: Separation of propylene from propane by distillation using a rigorous equilibrium-stage model

Given: Feed of 360 lbmol/h of propylene and 240 lbmol/h of propane at 125.7°F and 294 psia. Distillate is to be 99 mol% propylene, and bottoms is to be 95 mol% propane. Column is equipped with a partial condenser and a partial reboiler. Pressure is 280 psia in the reflux drop. Condenser pressure drop is 2 psia, and tray pressure drop is 0.1 psi/tray. Tray efficiency is 100%. Column is to contain 200 trays. Therefore, bottoms pressure = 280 + 2 + 20 = 302 psia. Reflux ratio is approximately 15.9. Feed-stage location is approximately tray 140 from the top tray.

Assumptions: SRK equation of state for *K*-values and enthalpies.

Find: Reflux ratio for the optimal feed tray location.

Analysis: The calculations were made with the SCDS Column model (Simultaneous-correction method) because of the small number of components and the large number of stages. It was understood that the Chemcad SCDS model would adjust the reflux rate and distillate rate to achieve the specified distillate and bottoms purities. Thus, the initial specifications for the SCDS Column model of the Chemcad program were:
Partial condenser
Top pressure = 280 psia
Condenser pressure drop = 2 psia. Column pressure drop = 20 psia.
Number of stages = 202 (includes partial condenser and partial reboiler)
Feed stage =140 from the top as a first estimate of the optimal feed stage
At the top, distillate purity = 99 mol% propylene
At the bottom, bottoms purity = 95 mol% propane
Estimated distillate rate = 350 lbmol/h
Estimated reflux rate = 5582 lbmol/h
Estimated temperature of stage 1 = 120°F
Estimated temperature of bottom stage = 140°F
Estimated temperature of stage 2 = 122°F
Estimated temperature of next to bottom stage = 138°F
When flashed, the feed was computed to be 69.11 mol% vaporized.

Convergence of the calculations was achieved rapidly in 6 iterations, with a converged reflux ratio of 14.0047 compared to the initial estimate of 5582/350 = 15.95.
The effect of feed-stage location on the reflux ratio was then studied with the results shown below.

Exercise 10.33 (continued)

Analysis: (continued)

Feed stage from top	Reflux ratio
145	14.269
140	14.005
135	13.824
130	13.711
125	13.644
120	13.596
119	13.593
118	13.592
117	13.592
116	13.612
115	13.615
110	13.646

As shown above, the optimal feed stage is in the range of stages 117 to 119. For the feed stage at 117 (116 in the column), the product distribution is as follows, accompanied by:

Condenser duty = 25,727,400 Btu/h

Reboiler duty = 25,434,800 Btu/h

The vapor and liquid compositions in the region of the feed stage, shown below, prove that a pinch condition does not exist, but the mole fractions are not changing rapidly.

Stream No.	1	2	3
Stream Name	Feed	Distillate	Bottoms
Temp F	125.7000*	115.5267	136.4598
Pres psia	294.0000*	280.0000	302.0000
Enth MMBtu/h	-8.8195	2.6698	-11.780
Vapor mole fraction	0.69111	1.0000	0.00000
Total lbmol/h	600.0000	351.0667	248.9359
Total lb/h	25732.2012	14780.1973	10952.0039
Total std L ft3/hr	799.5687	454.1352	345.4335
Total std V scfh	227687.17	133222.33	94465.87
Flowrates in lbmol/h			
Propylene	360.0000	347.5533	12.4467
Propane	240.0000	3.5107	236.4893

Stage from top	Mole fraction C_3 in liquid
115	0.41794
116	0.41814
117	0.41931
118	0.42000
119	0.42073

Exercise 10.34

Subject: Use of a stabilizer to remove hydrogen and methane from an aromatic mixture.

Given: A feed mixture of composition given below at 240°F and 275 psia. Column to contain about 10 equilibrium stages, with a partial condenser and a partial reboiler. Condenser outlet temperature = 100°F. Bottoms to contain no more than 0.05 mol% methane plus ethane. Tray efficiency = 70%. Column top pressure = 128 psia. Column bottom pressure = 132 psia. Suggested estimates of 2 for the reflux ratio and 49.4 lbmol/h

Assumptions: SRK for *K*-values and enthalpies

Find: A suitable design with number of trays, feed location, and reflux ratio.

Analysis: A valve is used to drop the feed pressure to column pressure. The calculations were made with the Tower model (Inside-out method) of Chemcad. It was understood that the Chemcad TOWER model would adjust the reflux rate and distillate rate to achieve the specified distillate temperature and bottoms impurities. Thus, the initial specifications for the TOWER model of the Chemcad program were as follows, where it was assumed that the main impurity in the bottoms product would be ethane.
Partial condenser
Top pressure = 128 psia
Condenser pressure drop = 0 psi. Column pressure drop = 4 psi.
Number of stages = 12 (includes partial condenser and partial reboiler)
Feed stage =3 from the top as a first estimate.
At the top, distillate temperature = 100°F.
At the bottom, bottoms purity = 0.0005 mole fraction of ethane
Estimated distillate rate = 50 lbmol/h
Estimated reflux rate = 100 lbmol/h
Estimated temperature of stage 1 = 100°F (actual specification)
Estimated temperature of bottom stage = 400°F
Estimated temperature of stage 2 = 300°F
A flash of the feed at feed conditions upstream of the feed valve showed it to be liquid. Convergence of the calculations was achieved rapidly in 6 iterations, with a converged reflux ratio, however of only 0.186, with a distillate rate of 48.715 lbmol/h. Thus, the reflux rate to the top stage was only 9.06 lbmol/h compared to 1748.4 lbmol/h of feed. This is considered to be unsatisfactory. Therefore, a second run was made with the feed entering the top stage (Stage 2) and reducing the number of stages to 7 (including the partial condenser and partial reboiler). A converged result shown on the next two pages was obtained in 5 iterations. This design is considered more satisfactory and achieves the specifications. The impurity in the bottoms is mainly ethane, as assumed. Other results are: reflux ratio = 0.0.211, condenser duty = 2,515,000 Btu/h, and reboiler duty = 12,976,000 Btu/h. The column will contain 5/0.7 = 8 trays.

Exercise 10.34 (continued)

Analysis: (continued)

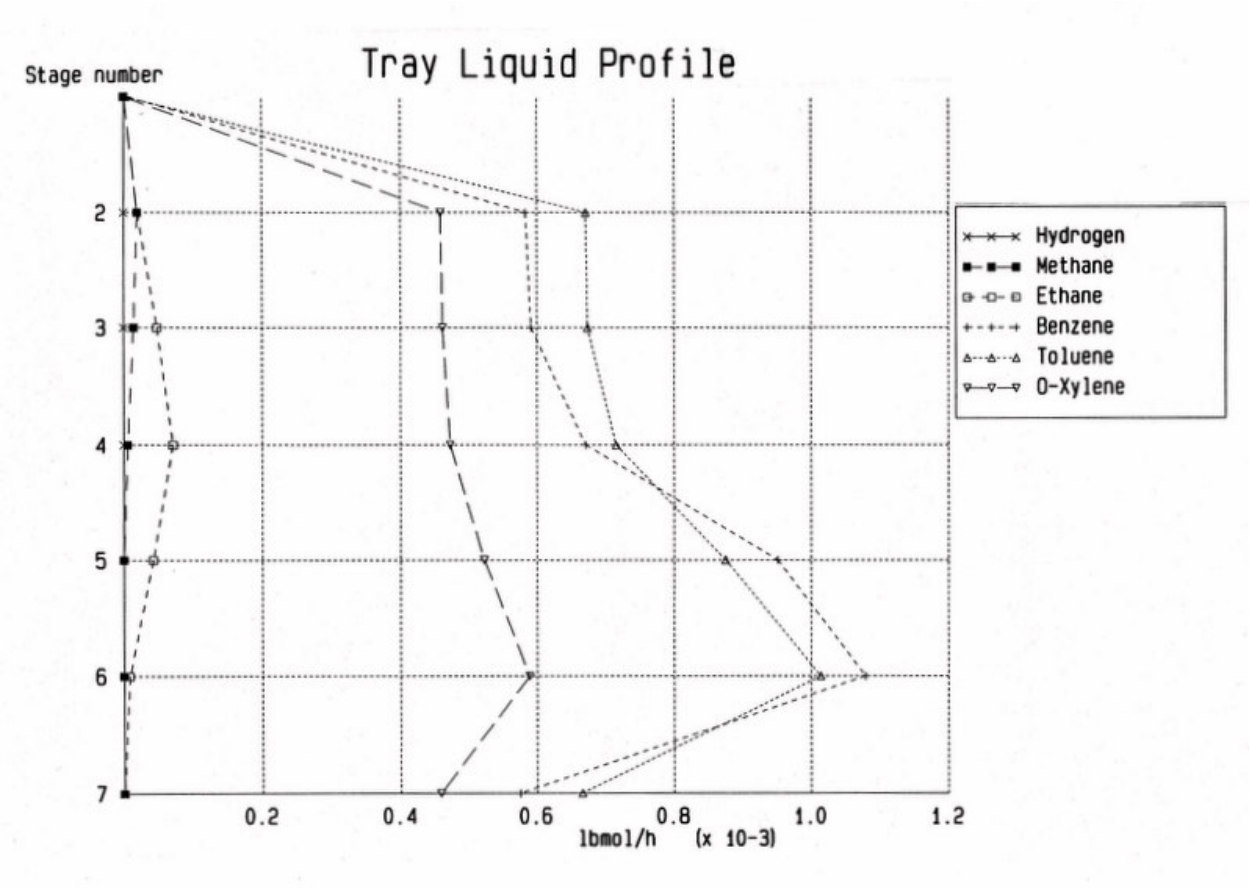
Stream No.	1	2	3
Stream Name	Feed	Distillate	Bottoms
Temp F	240.0000*	99.9997	396.6196
Pres psia	275.0000*	128.0000	132.0000
Enth MMBtu/h	20.617	-1.2567	34.598
Vapor mole fraction	0.00000	1.0000	0.00000
Total lbmol/h	1748.4000	48.5089	1699.8914
Total lb/h	155775.9688	844.1500	154931.8438
Total std L ft3/hr	2868.4204	43.1325	2825.2885
Total std V scfh	663480.44	18408.08	645072.44
Flowrates in lbmol/h			
Hydrogen	8.3000	8.3000	0.0000
Methane	30.7000	30.6917	0.0083
Ethane	9.4000	8.5501	0.8499
Benzene	576.0000	0.8073	575.1928
Toluene	666.0000	0.1489	665.8512
O-Xylene	458.0000	0.0108	457.9893

Stg	Temp F	Pres psia	Liquid lbmol/h	Vapor lbmol/h	Feeds lbmol/h	Product lbmol/h
1	100.0	128.00	10.25			48.51
2	240.5	128.00	1749.47	58.76	1748.40	
3	245.2	128.80	1790.48	49.58		
4	273.0	129.60	1936.03	90.59		
5	344.8	130.40	2389.86	236.14		
6	381.8	131.20	2691.87	689.97		
7	396.6	132.00		991.98		1699.89

Mole Reflux ratio 0.211

Exercise 10.34 (continued)

Analysis: (continued)



Exercise 10.35

Subject: Simulation of a four-stage, nearly isothermal distillation process by flash calculations.

Given: Problem specifications in Figure 10.36, consisting of the feed conditions and temperature and pressure for each of four isothermal flashes.

Assumptions: Grayson-Streed correlation for *K*-values and Redlich-Kwong equation for enthalpies.

Find: Component flow rates for all equilibrium vapor and liquid streams.

Analysis: The Chemcad simulator was used with its FLASH model in the isothermal flash mode. Referring to Figure 10.36, the recycle process was simulated with L1, V3, and V4 as the cut (tear) streams, with the sequence of calculations being Stages 2, 1, 3, and 4. No initial estimates were given for the cut streams. Convergence was achieved in 19 iterations using direct substitution. The resulting stream compositions are given below:

Stream No.	1	2	3	4
Stream Name	V2	V1	L1	Feed
Temp F	120.0000	100.0000	100.0000	120.0000*
Pres psia	284.7000	814.7000	814.7000	284.7000*
Enth MMBtu/h	-1276.8	-1098.2	-203.17	-2445.8
Vapor mole fraction	1.0000	1.0000	0.00000	0.28830
Total lbmol/h	14946.5947	12545.4219	2401.1743	27340.5977
Total lb/h	540674.5000	435558.9062	105115.5469	1887668.8750
Total std L ft3/hr	15735.2624	12779.9441	2955.3204	46946.9339
Total std V scfh	5671913.00	4760719.50	911194.31	10375172.00
Flowrates in lbmol/h				
Nitrogen	397.3700	357.2920	40.0780	358.2000
Carbon Dioxide	5548.3325	4845.4121	702.9205	4965.6001
Hydrogen Sulfide	361.9400	296.0045	65.9355	339.4000
Methane	3185.7625	2992.7168	193.0456	2995.5000
Ethane	2690.0774	2287.4573	402.6201	2395.5000
Propane	1860.0775	1339.7996	520.2780	2291.0000
I-Butane	216.1843	128.3031	87.8812	604.1000
N-Butane	393.7204	211.0347	182.6857	1539.9000
I-Pentane	92.5707	36.6693	55.9014	790.4000
N-Pentane	97.7764	34.2706	63.5058	1129.9000
N-Hexane	55.1167	11.6775	43.4391	1764.7000
N-Heptane	33.2392	4.0115	29.2277	2606.7000
N-Octane	9.5188	0.6192	8.8995	1844.5000
N-Nonane	3.7523	0.1342	3.6181	1669.0000
N-Decane	0.8568	0.0176	0.8392	831.7000
N-Dodecane	0.3007	0.0022	0.2985	1214.5000

Exercise 10.35 (continued)

Analysis (continued)

Stream No.	5	6	7	8	9
Stream Name	V3	L2	V4	L3	L4
Temp F	96.0000	120.0000	85.0000	96.0000	85.0000
Pres psia	63.7000	284.7000	27.7000	63.7000	27.7000
Enth MMBtu/h	-675.99	-2058.4	-119.59	-1502.5	-1383.6
Vapor mole fraction	1.0000	0.00000	1.0000	0.00000	0.00000
Total lbmol/h	8402.7148	23194.3184	1710.7906	16501.9355	14791.1426
Total lb/h	357758.8750	1809711.0000	81103.4141	1533032.1250	1451928.7500
Total std L ft3/hr	10163.7611	44326.0964	2307.5652	36469.2098	34161.6444
Total std V scfh	3188650.75	8801748.00	649208.50	6262132.00	5612922.50
Flowrates in lbmol/h					
Nitrogen	108.3765	109.2545	6.7771	7.6559	0.8787
Carbon Dioxide	2532.9700	2652.5479	323.6844	443.2775	119.5932
Hydrogen Sulfide	269.1588	312.4413	53.8546	97.1283	43.2736
Methane	531.7516	534.4218	25.4473	28.1215	2.6742
Ethane	1508.8750	1616.4463	229.2151	336.7780	107.5629
Propane	2104.3110	3053.8770	581.9407	1531.2031	949.2624
I-Butane	316.3194	791.9449	109.8002	585.3838	475.5836
N-Butane	599.3074	1927.8882	216.5925	1545.1007	1328.5082
I-Pentane	145.4621	899.1387	55.5465	809.2080	753.6614
N-Pentane	150.7828	1246.3589	57.6756	1153.2367	1095.5610
N-Hexane	77.5092	1830.5073	29.2771	1782.2683	1752.9911
N-Heptane	42.2924	2644.9680	15.5321	2618.2041	2602.6719
N-Octane	10.7732	1854.6506	3.8125	1847.6892	1843.8767
N-Nonane	3.8165	1672.6809	1.3053	1670.1697	1668.8643
N-Decane	0.7834	832.4655	0.2590	831.9411	831.6821
N-Dodecane	0.2263	1214.7239	0.0704	1214.5679	1214.4974

Exercise 10.36

Subject: Effect of number of stages, absorbent flow rate, and absorbent temperature on the absorption of a paraffin hydrocarbon gas.

Given: 2,000 lbmol/h of a gas mixture containing in mole fractions, 0.830 C_1, 0.084 C_2, 0.048 C_3, 0.026 nC_4, and 0.012 nC_5, at 75 psia and 60°F. Absorbent oil of MW = 161.

Assumptions: SRK for *K*-values and enthalpies.

Find: For the following four cases, compute product flow rates and compositions, and interstage vapor and liquid flowrates and compositions:

Case	No. of Stages	Absorbent rate, lbmol/h	Absorbent temperature, °F
(a)	6	500	90
(b)	12	500	90
(c)	6	1,000	90
(d)	6	500	60

Analysis: Chose nC_{11} , MW = 156, for the absorbent oil The calculations were made with the Tower model (Inside-out method) of Chemcad. For Case (a), the specs are:
No condenser with top pressure = 75 psia
Column pressure drop = 0 psi.
Number of stages = 6
Feed gas to stage 6
Absorbent to stage 1
At the top, no condenser
At the bottom, no reboiler
Estimated distillate rate = 2,000 lbmol/h
Estimated reflux rate = 500 lbmol/h
Estimated temperature of stage 1 = 100°F
Estimated temperature of bottom stage = 100°F
Estimated temperature of stage 2 = 100°F
Specifications for the other 3 cases differed only in the number of equilibrium stages and the flow and temperature of the absorbent oil, plus changes in the estimates. Convergence of each case was achieved in 3 or 4 iterations.
The results for each case are given on the following
s, where it is observed that
1. Doubling the number of stages, only increases the absorption of nC_5. It is the only feed gas component with an absorption factor, $A = L/KV, > 1$.
2. Doubling the absorbent rate almost doubles the amount absorbed of each feed gas component.
3. Lowering the absorbent temperature increases somewhat the absorption of lighter components

Exercise 10.36 (continued)

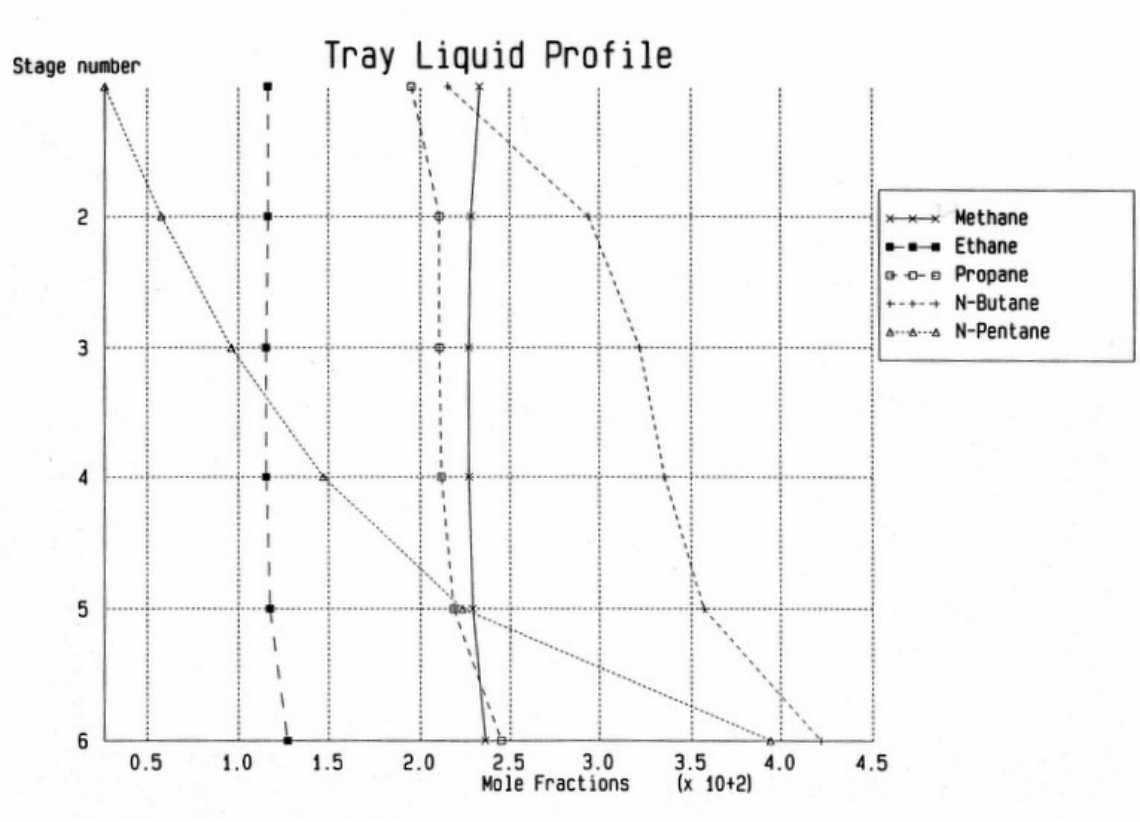
Analysis: (a) (continued)

Stream No.	1	2	3	4
Stream Name	Absorbent	Feed gas	Gas out	Oil out
Temp F	90.0000*	60.0000*	97.2038	87.1761
Pres psia	75.0000*	75.0000*	75.0000	75.0000
Enth MMBtu/h	-69.564	-68.578	-63.772	-74.370
Vapor mole fraction	0.00000	1.0000	1.0000	0.00000
Total lbmol/h	500.0000	2000.0000	1917.5823	582.4178
Total lb/h	78156.0000	40670.3516	36599.9297	82226.4062
Total std L ft3/hr	1684.1408	1911.2911	1790.1733	1805.2587
Total std V scfh	189739.31	758957.25	727681.50	221015.09
Flowrates in lbmol/h				
Methane	0.0000	1660.0000	1646.2473	13.7528
Ethane	0.0000	168.0000	160.5868	7.4132
Propane	0.0000	96.0000	81.7405	14.2594
N-Butane	0.0000	52.0000	27.4041	24.5959
N-Pentane	0.0000	24.0000	1.0402	22.9598
N-Undecane	500.0000	0.0000	0.5633	499.4366

			* Net Flows *			
Stg	Temp F	Pres psia	Liquid lbmol/h	Vapor lbmol/h	Feeds lbmol/h	Product lbmol/h
1	97.2	75.00	542.81		500.00	1917.58
2	99.2	75.00	549.95	1960.39		
3	99.9	75.00	553.86	1967.53		
4	99.4	75.00	557.86	1971.44		
5	96.5	75.00	564.63	1975.44		
6	87.2	75.00		1982.21	2000.00	582.42

Exercise 10.36 (continued)

Analysis: (a) (continued)



Exercise 10.36 (continued)

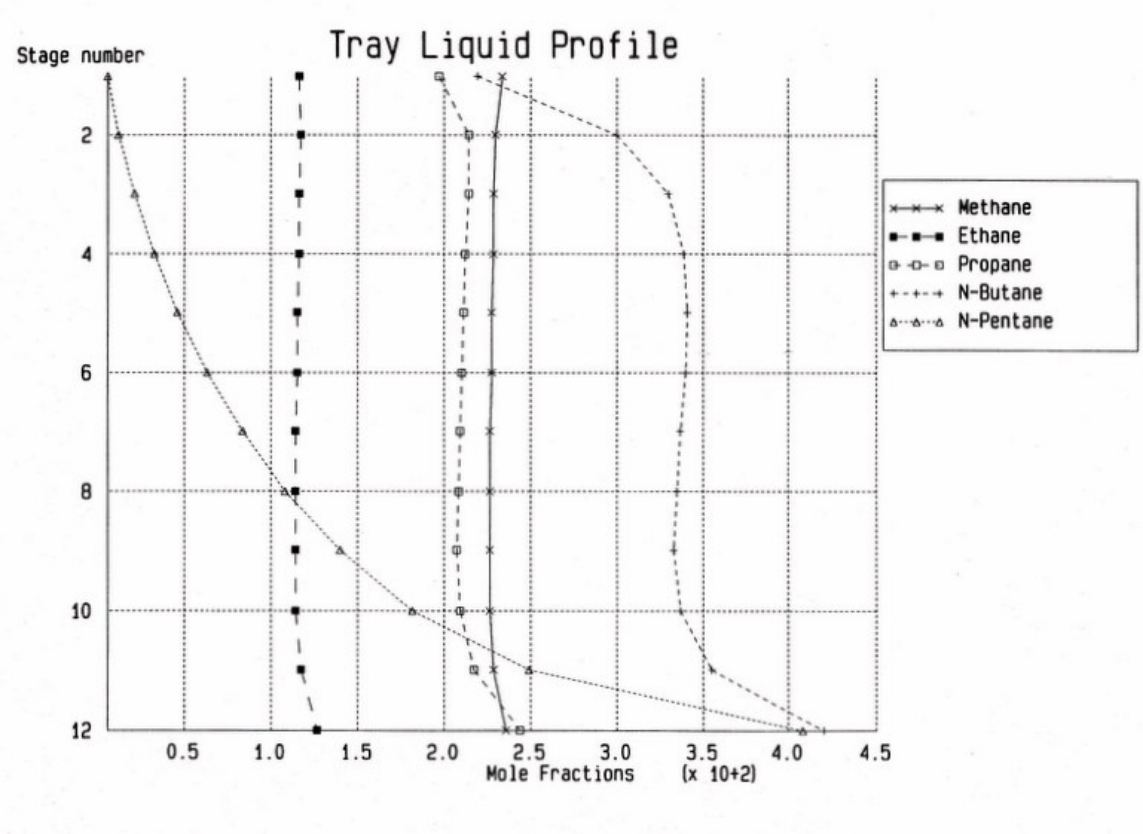
Analysis: (b) (continued)

Stream No.	1	2	3	4
Stream Name	Absorbent	Feed gas	Gas out	Oil out
Temp F	90.0000*	60.0000*	96.7574	87.5725
Pres psia	75.0000*	75.0000*	75.0000	75.0000
Enth MMBtu/h	-69.564	-68.578	-63.740	-74.402
Vapor mole fraction	0.00000	1.0000	1.0000	0.00000
Total lbmol/h	500.0000	2000.0000	1916.9973	583.0032
Total lb/h	78156.0000	40670.3516	36551.1328	82275.2422
Total std L ft3/hr	1684.1408	1911.2911	1788.9948	1806.4377
Total std V scfh	189739.31	758957.25	727459.50	221237.25
Flowrates in lbmol/h				
Methane	0.0000	1660.0000	1646.2675	13.7327
Ethane	0.0000	168.0000	160.6116	7.3885
Propane	0.0000	96.0000	81.8097	14.1903
N-Butane	0.0000	52.0000	27.5283	24.4717
N-Pentane	0.0000	24.0000	0.2257	23.7743
N-Undecane	500.0000	0.0000	0.5546	499.4456

			* Net Flows *			
Stg	Temp F	Pres psia	Liquid lbmol/h	Vapor lbmol/h	Feeds lbmol/h	Product lbmol/h
1	96.8	75.00	541.87		500.00	1917.00
2	98.4	75.00	547.87	1958.87		
3	99.1	75.00	550.07	1964.86		
4	99.6	75.00	551.19	1967.06		
5	100.0	75.00	552.02	1968.19		
6	100.5	75.00	552.85	1969.02		
7	100.9	75.00	553.82	1969.84		
8	101.3	75.00	555.07	1970.82		
9	101.3	75.00	556.85	1972.07		
10	100.5	75.00	559.78	1973.85		
11	97.2	75.00	565.83	1976.77		
12	87.6	75.00		1982.83	2000.00	583.00

Exercise 10.36 (continued)

Analysis: (b) (continued)



Exercise 10.36 (continued)

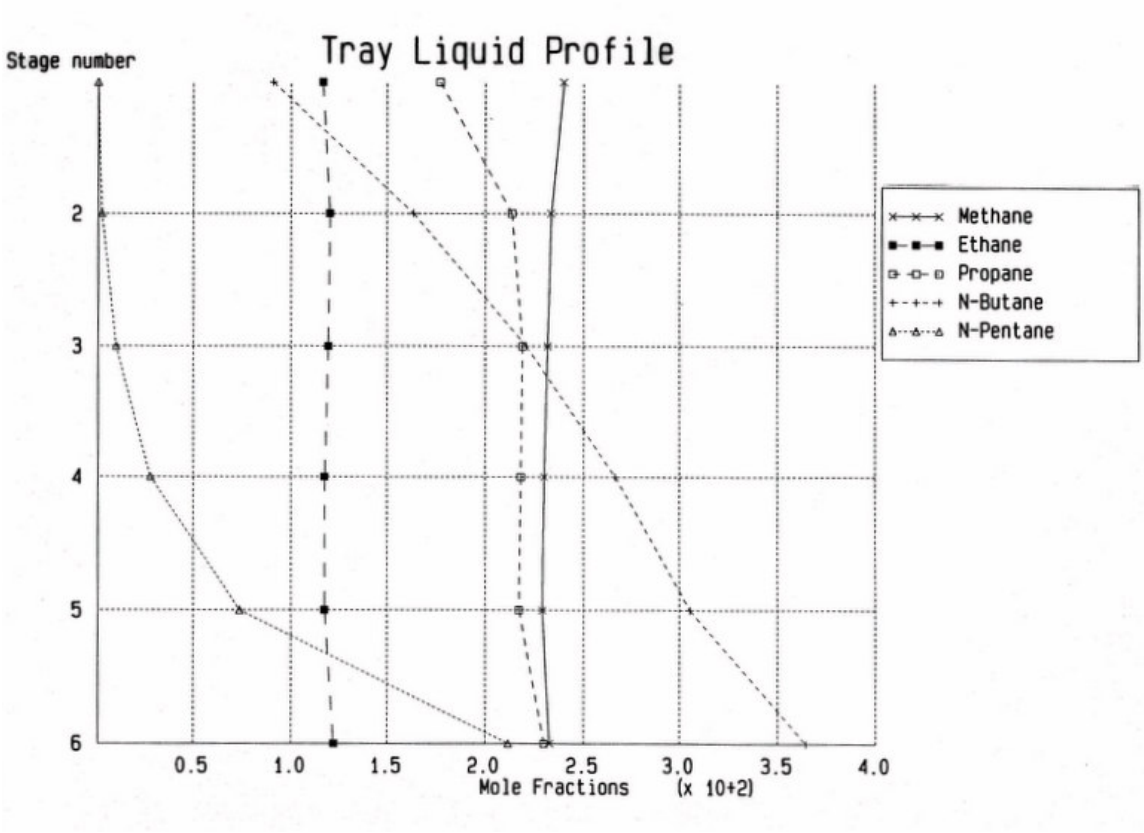
Analysis: (c) (continued)

Stream No.	1	2	3	4
Stream Name	Absorbent	Feed gas	Gas out	Oil out
Temp F	90.0000*	60.0000*	94.4939	92.8343
Pres psia	75.0000*	75.0000*	75.0000	75.0000
Enth MMBtu/h	-139.13	-68.578	-61.697	-146.01
Vapor mole fraction	0.00000	1.0000	1.0000	0.00000
Total lbmol/h	1000.0000	2000.0000	1869.1399	1130.8601
Total lb/h	156312.0000	40670.3516	34638.7734	162343.5938
Total std L ft3/hr	3368.2817	1911.2911	1725.7838	3553.7892
Total std V scfh	379478.62	758957.25	709298.62	429137.25
Flowrates in lbmol/h				
Methane	0.0000	1660.0000	1633.6517	26.3482
Ethane	0.0000	168.0000	154.1892	13.8108
Propane	0.0000	96.0000	69.9722	26.0278
N-Butane	0.0000	52.0000	10.7881	41.2119
N-Pentane	0.0000	24.0000	0.0369	23.9631
N-Undecane	1000.0000	0.0000	0.5018	999.4983

			* Net Flows *			
Stg	Temp F	Pres psia	Liquid lbmol/h	Vapor lbmol/h	Feeds lbmol/h	Product lbmol/h
1	94.5	75.00	1066.91		1000.00	1869.14
2	96.0	75.00	1079.46	1936.05		
3	97.1	75.00	1087.26	1948.60		
4	97.9	75.00	1094.26	1956.40		
5	97.8	75.00	1104.10	1963.40		
6	92.8	75.00		1973.24	2000.00	1130.86

Exercise 10.36 (continued)

Analysis: (c) (continued)

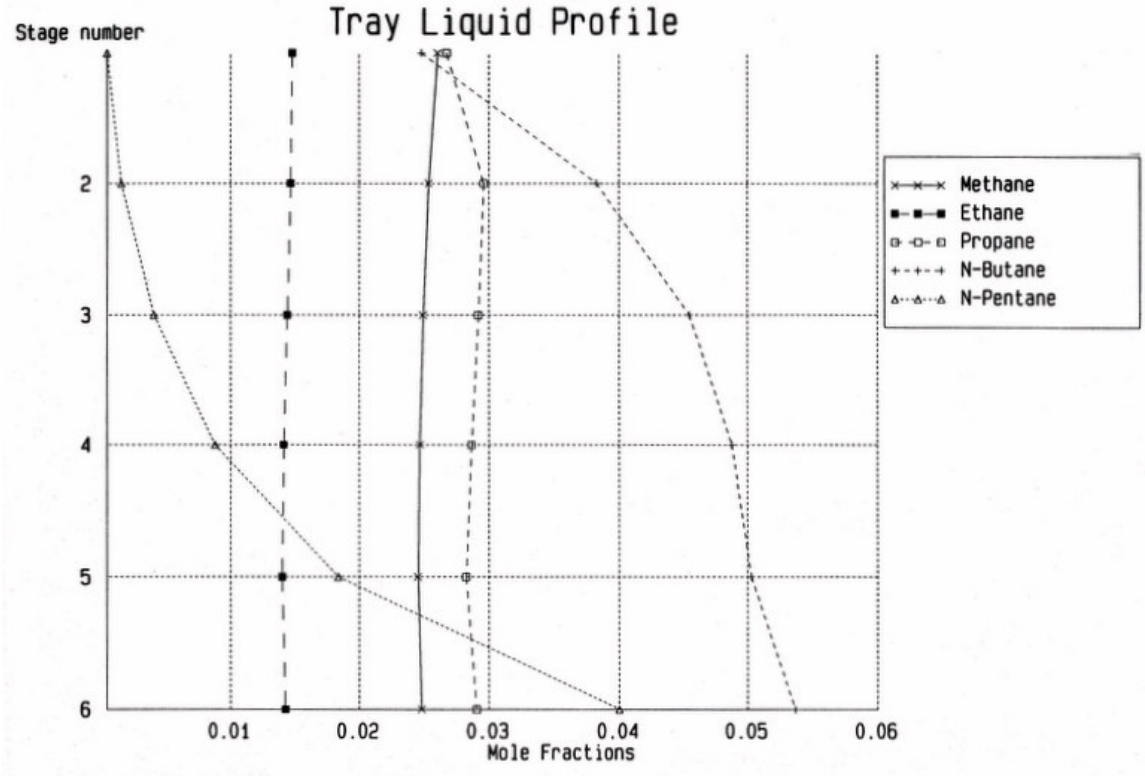


Exercise 10.36 (continued)

Analysis: (d) (continued)

Stream No.	1	2	3	4
Stream Name	Absorbent	Feed gas	Gas out	Oil out
Temp F	60.0000*	60.0000*	69.3833	74.1250
Pres psia	75.0000*	75.0000*	75.0000	75.0000
Enth MMBtu/h	-70.757	-68.578	-63.578	-75.757
Vapor mole fraction	0.00000	1.0000	1.0000	0.00000
Total lbmol/h	500.0000	2000.0000	1903.7129	596.2873
Total lb/h	78156.0000	40670.3516	35860.1055	82966.2422
Total std L ft3/hr	1684.1408	1911.2911	1768.7935	1826.6386
Total std V scfh	189739.31	758957.25	722418.38	226278.28
Flowrates in lbmol/h				
Methane	0.0000	1660.0000	1645.2346	14.7655
Ethane	0.0000	168.0000	159.4820	8.5180
Propane	0.0000	96.0000	78.6892	17.3107
N-Butane	0.0000	52.0000	19.9909	32.0091
N-Pentane	0.0000	24.0000	0.1334	23.8666
N-Undecane	500.0000	0.0000	0.1826	499.8174

			* Net Flows *			
Stg	Temp F	Pres psia	Liquid lbmol/h	Vapor lbmol/h	Feeds lbmol/h	Product lbmol/h
1	69.4	75.00	551.23		500.00	1903.71
2	72.6	75.00	561.56	1954.95		
3	74.6	75.00	566.93	1965.28		
4	76.1	75.00	571.40	1970.65		
5	76.7	75.00	578.37	1975.11		
6	74.1	75.00		1982.08	2000.00	596.29



Exercise 10.37

Subject: Absorption of a hydrocarbon gas with n-decane.

Given: 1000 lbmol/h of a paraffin hydrocarbon gas, of composition below, at 90°F and 75 psia. 1000 lbmol/h of nC_{10} absorbent at the same temperature and pressure. Absorber has 4 equilibrium stages and operates at 75 psia.

Assumptions: SRK for *K*-values and enthalpies.

Find: Product rates and compositions, stage temperatures, and interstage vapor and liquid flow rates and compositions.

Analysis: As shown below, when the gas feed was flashed, it was found to contain 7.2 mol% liquid. The calculations were made with the Tower model (Inside-out method) of Chemcad, with the following specifications:
No condenser
Column pressure drop = 0 psi.
Number of stages = 4
Feed gas to stage 4
Absorbent to stage 1
At the top, no condenser
At the bottom, no reboiler
Estimated distillate rate = 1,000 lbmol/h
Estimated reflux rate = 1,000 lbmol/h
Estimated temperature of stage 1 = 90°F
Estimated temperature of bottom stage = 90°F
Estimated temperature of stage 2 = 90°F

Convergence was achieved only with great difficulty after 29 iterations. The problem was also solved with the SCDS Column model (simultaneous correction method) in only 8 iterations. The percent absorption of each component is as follows:

Component	% Absorbed
Methane	4.8
Ethane	21.0
Propane	60.6
n-Butane	97.3
n-Pentane	99.95

The other results are presented on the next two pages.

Exercise 10.37 (continued)

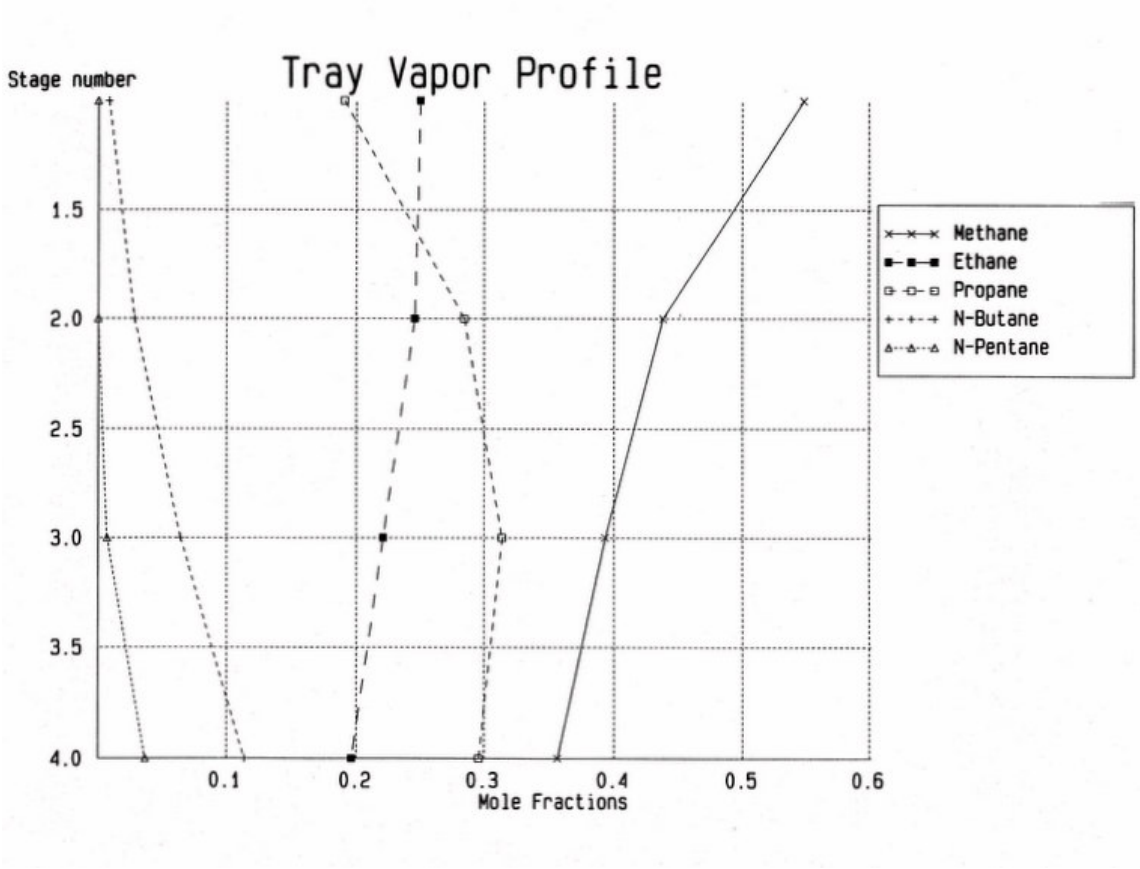
Analysis: (continued)

Stream No.	1	2	3	4
Stream Name	Oil in	Gas in	Gas out	Oil out
Temp F	90.0000*	90.0000*	104.5381	128.2643
Pres psia	75.0000*	75.0000*	75.0000	75.0000
Enth MMBtu/h	-128.25	-44.807	-17.671	-155.39
Vapor mole fraction	0.00000	0.92792	1.0000	0.00000
Total lbmol/h	1000.0000	1000.0000	495.9015	1504.0986
Total lb/h	142285.0000	40393.3164	12608.2266	170070.0938
Total std L ft3/hr	3107.3641	1332.8264	541.8405	3898.3501
Total std V scfh	379478.62	379478.62	188184.02	570773.25
Flowrates in lbmol/h				
Methane	0.0000	286.0000	272.2161	13.7839
Ethane	0.0000	157.0000	124.0583	32.9417
Propane	0.0000	240.0000	94.4751	145.5249
N-Butane	0.0000	169.0000	4.5497	164.4503
N-Pentane	0.0000	148.0000	0.0780	147.9221
N-Decane	1000.0000	0.0000	0.5242	999.4758

			* Net Flows *			
Stg	Temp F	Pres psia	Liquid lbmol/h	Vapor lbmol/h	Feeds lbmol/h	Product lbmol/h
1	104.5	75.00	1163.90		1000.00	495.90
2	113.0	75.00	1233.93	659.80		
3	122.2	75.00	1305.92	729.83		
4	128.3	75.00		801.82	1000.00	1504.10

Exercise 10.37 (continued)

Analysis: (continued)



Exercise 10.38

Subject: Effect of intercooler location on the absorption of a light hydrocarbon mixture.

Given: Feed gas and absorbent oil of Figure 10.17 of Example 10.4. Incooler with a duty of 500,000 Btu/h.

Assumptions: SRK for *K*-values and enthalpies. Absorbent oil is nC_{12}.

Find: Effectiveness of the intercooler and its preferred location. Possible change in duty if intercooler stage temperature is at least 100°F.

Analysis: The calculations of Example 10.4 were first repeated using the TOWER model of Chemcad. The following results differ from those of Example 10.4 because of the different methods used for computing *K*-values and enthalpies:

	lbmol/h:			
Component	**Feed gas**	**Absorbent**	**Gas out**	**Liquid out**
C_1	160.00	0.00	146.25	13.75
C_2	370.00	0.00	268.83	101.17
C_3	240.00	0.00	96.41	143.59
nC_4	25.00	0.05	1.11	23,94
nC_5	5.00	0.78	0.21	5.57
nC_{12}	0.00	164.17	0.15	164.02
Total:	800.00	165.00	512.96	452.04
Temp., °F	105	90	144.9	144.4

Compared to results of Example 10.4, more is absorbed, but the temperature rise is less.
For the effect of the intercooler, the calculations were also made with the Tower model (Inside-out method) of Chemcad. The specifications for an intercooler of -500,000 Btu/h located at Stage 2 from the top were as follows, where it should be noted that the intercooler is treated as a feed between the absorbent and feed gas.
No condenser
Top pressure = 400 psia
Column pressure drop = 0 psi.
Number of stages = 6
Absorbent to stage 1
Intercooler with -0.500 MMBtu/h enthalpy (as a feed) at stage 2
Feed gas to stage 6
At the top, no condenser
At the bottom, no reboiler
Estimated distillate rate = 500 lbmol/h
Estimated reflux rate = 200 lbmol/h

Exercise 10.38 (continued)

Analysis: (continued)
Estimated temperature of stage 1 = 120°F
Estimated temperature of bottom stage = 130°F
Estimated temperature of stage 2 = 120°F

Convergence was achieved in 6 iterations. The calculations were repeated for the intercooler located at stages 3, 4, and 5. The following results show that the outlet gas temperature was reduced and the amount of absorption was considerably increased, but the effect of stage location is not significant, although a location at stage 4 or 5 appeared to be very slightly best.

Case	Liquid out, lbmol/h	Temp., gas out, °F
Base - no intercooler	452.04	144.9
(a) - intercooler stage 2	498.69	133.8
(b) - intercooler stage 3	500.53	137.3
(c) - intercooler stage 4	500.74	138.6
(d) - intercooler stage 5	500.74	138.6

Because the temperature was still significantly higher than the lower limit of 100°F, a higher intercooler heat duty of -2,000,000 Btu/h was tried at stage 5. However, the temperature of that stage dropped to 84°F. For a duty of -1,500,000 Btu/h, the temperature of stage 5 was an acceptable value of 102°F. The liquid out increased to 599.68 lbmol/h and the temperature of the gas out decreased to 127.5°F. The corresponding component absorption rates compared to those of the base case (no intercooler) were as follows:

	lbmol/h:	
Component	**No intercooler**	**-1,500,000 Btu/h, stage 5**
C_1	13.75	21.09
C_2	101.17	171.52
C_3	143.59	212.32
nC_4	23.94	24.98
nC_5	5.57	5.66
Total:	288.02	435.57

Thus, the effect of the intercooler is very significant. The corresponding stage temperatures compared to those of the base case are also of interest:

	°F:					
Stage	**1**	**2**	**3**	**4**	**5**	**6**
No intercooler	144.9	153.1	156.1	157.3	154.6	144.3
-1,500,000 Btu/h - stage 5	127.5	134.1	135.1	128.5	102.1	114.9

Exercise 10.39

Subject: Design of a an absorber with two absorbent oil feeds.

Given: Feed gas at 90°F and 400 psia with the composition given below. Column has 8 equilibrium stages. Lean oil, assumed to be nC_{12}, at 80°F and 400 psia at 250 lbmol/h enters the top stage. Secondary oil at 80°F and 400 psia, of the composition given below, enters stage 7 from the top. 150,000 Btu/h (-0.15 MMBtu/h) is removed by intercooling from stage 7. The feed gas enters stage 8.

Assumptions: SRK for *K*-values and enthalpies.

Find: Product rates and compositions, stage temperatures, and interstage vapor and liquid flow rates and compositions.

Analysis: The calculations were made with the Tower model (Inside-out method) of Chemcad, with the following specifications:
No condenser
Top pressure = 400 psia
Column pressure drop = 0 psi.
Number of stages = 8
Lean oil (1st feed) to stage 1
Secondary oil (2nd feed) to stage 4
Intercooler (3rd feed) at stage 7
Feed gas (4th feed) to stage 8
At the top, no condenser
At the bottom, no reboiler
Estimated distillate rate = 450 lbmol/h
Estimated reflux rate = 350 lbmol/h
Estimated temperature of stage 1 = 110°F
Estimated temperature of bottom stage = 100°F
Estimated temperature of stage 2 = 100°F
Note that the intercooler is treated as the 3rd feed with a specification as a stream of -0.15 MM Btu/h. Convergence was achieved in 4 iterations. The results are shown on the following two pages. Note that the degree of absorption was good with following results:

Component	**% in Feed gas absorbed**
C_1	15.2
C_2	73.4
C_3	99.2
nC_4	99.98
nC_5	100.00

Exercise 10.39 (continued)

Analysis: (continued)

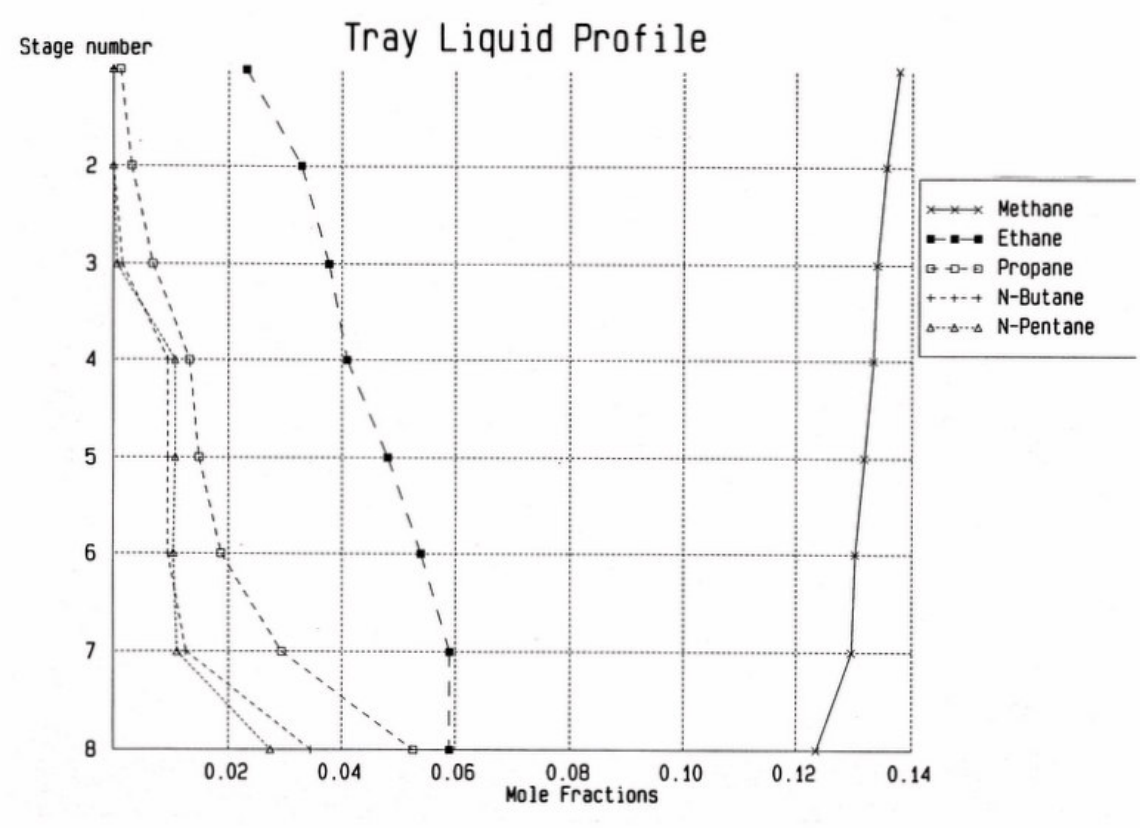
Stream No.	1	2	3	4
Stream Name	Lean oil	Second oil	Intercooler	Feed gas
Temp F	80.0000*	80.0000*	0.0000	90.0000*
Pres psia	400.0000*	400.0000*	0.0000	400.0000*
Enth MMBtu/h	-37.632	-21.724	-0.15000	-15.684
Vapor mole fraction	0.00000	0.00000	0.00000	1.0000
Total lbmol/h	250.0000	164.0000	0.0000	450.0000
Total lb/h	42584.5000	24064.0254	0.0000	9674.0244
Total std L ft3/hr	906.7842	525.9892	0.0000	439.8758
Total std V scfh	94869.66	62234.50	0.00	170765.38
Flowrates in lbmol/h				
Methane	0.0000	13.0000	0.0000	360.0000
Ethane	0.0000	3.0000	0.0000	40.0000
Propane	0.0000	4.0000	0.0000	25.0000
N-Butane	0.0000	4.0000	0.0000	15.0000
N-Pentane	0.0000	5.0000	0.0000	10.0000
N-Dodecane	250.0000	135.0000	0.0000	0.0000

Stream No.	5	6
Stream Name	Lean gas	Rich oil
Temp F	85.2781	93.1521
Pres psia	400.0000	400.0000
Enth MMBtu/h	-10.261	-64.929
Vapor mole fraction	1.0000	0.00000
Total lbmol/h	316.1613	547.8389
Total lb/h	5228.4995	71094.0625
Total std L ft3/hr	276.4982	1596.1514
Total std V scfh	119976.46	207893.14
Flowrates in lbmol/h		
Methane	305.3157	67.6844
Ethane	10.6399	32.3601
Propane	0.1933	28.8067
N-Butane	0.0023	18.9977
N-Pentane	0.0000	15.0000
N-Dodecane	0.0101	384.9900

			* Net Flows *			
Stg	Temp F	Pres psia	Liquid lbmol/h	Vapor lbmol/h	Feeds lbmol/h	Product lbmol/h
1	85.3	400.00	298.53		250.00	316.16
2	86.1	400.00	302.03	364.69		
3	86.8	400.00	305.41	368.19		
4	85.8	400.00	486.03	371.57	164.00	
5	86.4	400.00	490.26	388.20		
6	87.0	400.00	495.38	392.43		
7	85.6	400.00	507.56	397.54	-0.15 MMBtu/h	
8	93.2	400.00		409.72	450.00	547.84

Exercise 10.39 (continued)

Analysis: (continued)



Exercise 10.40

Subject: Reboiled absorber for the separation of a hydrocarbon mixture.

Given: Absorbent oil of nC_9 at 60°F and 230 psia and 40 lbmol/h. Feed at 120°F and 230 psia with the composition given below. Column has 15 equilibrium stages plus a partial reboiler. Absorbent oil enters stage 1 (top stage). Feed enters stage 9. Interreboiler with a heat duty of 1.0 MMBtu/h at stage13. Column operates at 230 psia. Overhead flow rate = 103 lbmol/h.

Assumptions: SRK for *K*-values and enthalpies.

Find: Product rates and compositions, stage temperatures, and interstage vapor and liquid flow rates and compositions. Reboiler duty with and without the interreboiler. Whether an interreboiler is worthwhile and if an intercooler should be considered.

Analysis: The calculations were made with the Tower model (Inside-out method) of Chemcad, with the following specifications:
No condenser
Top pressure = 230 psia
Column pressure drop = 0 psi.
Number of stages = 15 plus a partial reboiler
Absorbent oil (1st feed) to stage 1
Feed (2nd feed) to stage 9
Interreboiler (3rd feed) to stage 13
At the top, no condenser
At the bottom, bottoms flow rate = 459 - 103 = 356 lbmol/h
Estimated distillate rate = 103 lbmol/h (specified rate)
Estimated reflux rate = 40 lbmol/h
Estimated temperature of stage 1 = 80°F
Estimated temperature of bottom stage = 300°F
Estimated temperature of stage 2 = 90°F
Note that the interreboiler is treated as the 3rd feed with a specification as a stream of 1.00 MMBtu/h. Convergence was achieved in 7 iterations. The results are shown on the following two pages. The column feed is 14.2% vaporized. The distillate rate is set to send the methane and ethane overhead, while a portion of the propane and all heavier components to the bottoms. The temperature of the interreboiler stage is 202.6°F compared to a bottoms temperature of 302.4°F. The heat duty of the reboiler is 3.164 MMBtu/h. Thus, almost 25% of the total required heat duty can be supplied by waste heat..

Results without the interreboiler, on a subsequent page, show only a small effect on the separation, with the major effect being 17% more ethane leaving in the overhead vapor and a reboiler duty of 4.177 MMBtu/h. If an intercooler of a heat duty of 100,000 MMBtu/h is added at stage 4, along with the interreboiler at stage 13, as shown below, less ethane leaves in the overhead vapor. Thus, the use of an intercooler is not desirable.

Exercise 10.40 (continued)

Analysis: (continued) **With interreboiler**

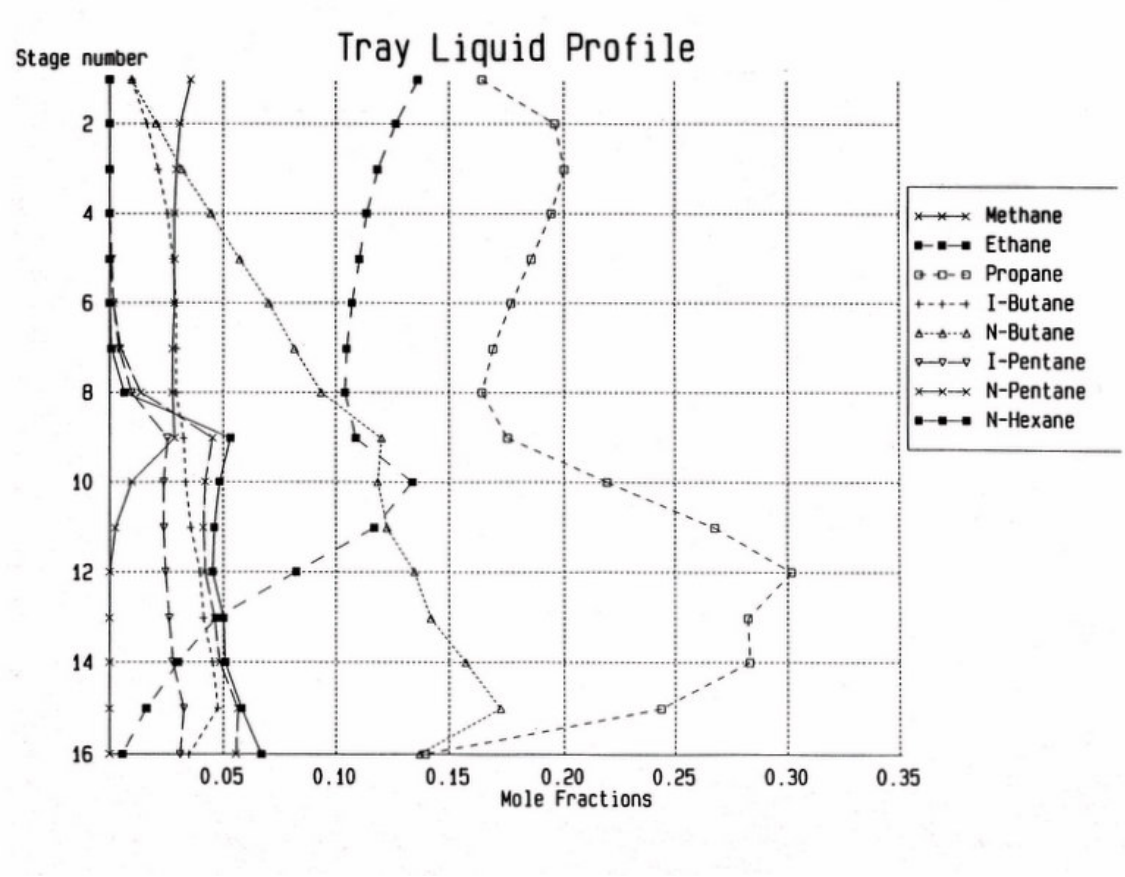
Stream No.	1	2	3	4
Stream Name	Absorbent	Feed	Interboiler	Overhead
Temp F	60.0000*	120.0000*	0.0000	110.6094
Pres psia	230.0000*	230.0000*	0.0000	230.0000
Enth MMBtu/h	-4.7762	-31.622	1.0000	-3.6928
Vapor mole fraction	0.00000	0.14171	0.00000	1.0000
Total lbmol/h	40.0000	419.0000	0.0000	102.9982
Total lb/h	5130.3198	31801.9609	0.0000	2717.2722
Total std L ft3/hr	113.8082	816.0397	0.0000	117.6431
Total std V scfh	15179.14	159001.55	0.00	39085.62
Flowrates in lbmol/h				
Methane	0.0000	46.0000	0.0000	45.9994
Ethane	0.0000	42.0000	0.0000	39.7727
Propane	0.0000	66.0000	0.0000	16.2856
I-Butane	0.0000	13.0000	0.0000	0.4496
N-Butane	0.0000	49.0000	0.0000	0.3403
I-Pentane	0.0000	11.0000	0.0000	0.0002
N-Pentane	0.0000	20.0000	0.0000	0.0001
N-Hexane	0.0000	24.0000	0.0000	0.0000
N-Nonane	40.0000	148.0000	0.0000	0.1503

Stream No.	5
Stream Name	Bottoms
Temp F	302.3542
Pres psia	230.0000
Enth MMBtu/h	-28.541
Vapor mole fraction	0.00000
Total lbmol/h	356.0018
Total lb/h	34215.0156
Total std L ft3/hr	812.2049
Total std V scfh	135095.08
Flowrates in lbmol/h	
Methane	0.0006
Ethane	2.2273
Propane	49.7144
I-Butane	12.5504
N-Butane	48.6597
I-Pentane	10.9998
N-Pentane	19.9999
N-Hexane	24.0000
N-Nonane	187.8497

Stg	Temp F	Pres psia	Liquid lbmol/h	Vapor lbmol/h	Feeds lbmol/h	Product lbmol/h
1	110.6	230.00	62.22		40.00	103.00
2	121.5	230.00	65.82	125.22		
3	126.8	230.00	67.16	128.82		
4	130.8	230.00	67.86	130.16		
5	134.3	230.00	68.39	130.86		
6	137.6	230.00	68.92	131.39		
7	140.6	230.00	69.81	131.92		
8	141.5	230.00	72.84	132.81		
9	132.1	230.00	458.60	135.84	419.00	
10	148.0	230.00	509.97	102.60		
11	161.4	230.00	548.52	153.97		
12	175.5	230.00	576.51	192.52		
13	202.6	230.00	518.42	220.51		
14	211.1	230.00	532.88	162.41		
15	230.9	230.00	533.99	176.88		
16	302.4	230.00		177.99		356.00

Exercise 10.40 (continued)

Analysis: (continued) **With interreboiler**



Exercise 10.40 (continued)

Analysis: (continued) **Without interreboiler**

Stream No.	1	2	3	4
Stream Name	Absorbent	Feed	Interboiler	Overhead
Temp F	60.0000*	120.0000*	0.0000	110.1263
Pres psia	230.0000*	230.0000*	0.0000	230.0000
Enth MMBtu/h	-4.7762	-31.622	0.00000	-3.6921
Vapor mole fraction	0.00000	0.14171	0.00000	1.0000
Total lbmol/h	40.0000	419.0000	0.0000	103.0512
Total lb/h	5130.3198	31801.9609	0.0000	2713.8337
Total std L ft3/hr	113.8082	816.0397	0.0000	117.6941
Total std V scfh	15179.14	159001.55	0.00	39105.73
Flowrates in lbmol/h				
Methane	0.0000	46.0000	0.0000	45.9997
Ethane	0.0000	42.0000	0.0000	40.1513
Propane	0.0000	66.0000	0.0000	15.9835
I-Butane	0.0000	13.0000	0.0000	0.4392
N-Butane	0.0000	49.0000	0.0000	0.3287
I-Pentane	0.0000	11.0000	0.0000	0.0002
N-Pentane	0.0000	20.0000	0.0000	0.0001
N-Hexane	0.0000	24.0000	0.0000	0.0000
N-Nonane	40.0000	148.0000	0.0000	0.1485

Stream No.	5
Stream Name	Bottoms
Temp F	302.9691
Pres psia	230.0000
Enth MMBtu/h	-28.528
Vapor mole fraction	0.00000
Total lbmol/h	355.9489
Total lb/h	34218.4531
Total std L ft3/hr	812.1540
Total std V scfh	135075.00
Flowrates in lbmol/h	
Methane	0.0003
Ethane	1.8487
Propane	50.0165
I-Butane	12.5608
N-Butane	48.6713
I-Pentane	10.9998
N-Pentane	19.9999
N-Hexane	24.0000
N-Nonane	187.8515

Stg	Temp F	Pres psia	Liquid lbmol/h	Vapor lbmol/h	Feeds lbmol/h	Product lbmol/h
1	110.1	230.00	62.12		40.00	103.05
2	120.9	230.00	65.69	125.17		
3	126.3	230.00	67.02	128.74		
4	130.3	230.00	67.70	130.07		
5	133.8	230.00	68.22	130.75		
6	137.1	230.00	68.76	131.27		
7	140.1	230.00	69.63	131.81		
8	141.0	230.00	72.66	132.68		
9	131.6	230.00	457.66	135.72	419.00	
10	146.5	230.00	506.73	101.71		
11	158.3	230.00	543.10	150.78		
12	169.0	230.00	573.76	187.15		
13	179.9	230.00	601.49	217.82		
14	193.4	230.00	621.49	245.54		
15	219.9	230.00	607.06	265.54		
16	303.0	230.00		251.11		355.95

Exercise 10.40 (continued)

Analysis: (continued) **With interreboiler and intercooler**

Stream No.	1	2	3	4
Stream Name	Absorbent	Intercooler	Feed	Interboiler
Temp F	60.0000*	0.0000	120.0000*	0.0000
Pres psia	230.0000*	0.0000	230.0000*	0.0000
Enth MMBtu/h	-4.7762	-0.10000	-31.622	1.0000
Vapor mole fraction	0.00000	0.00000	0.14171	0.00000
Total lbmol/h	40.0000	0.0000	419.0000	0.0000
Total lb/h	5130.3198	0.0000	31801.9609	0.0000
Total std L ft3/hr	113.8082	0.0000	816.0397	0.0000
Total std V scfh	15179.14	0.00	159001.55	0.00
Flowrates in lbmol/h				
Methane	0.0000	0.0000	46.0000	0.0000
Ethane	0.0000	0.0000	42.0000	0.0000
Propane	0.0000	0.0000	66.0000	0.0000
I-Butane	0.0000	0.0000	13.0000	0.0000
N-Butane	0.0000	0.0000	49.0000	0.0000
I-Pentane	0.0000	0.0000	11.0000	0.0000
N-Pentane	0.0000	0.0000	20.0000	0.0000
N-Hexane	0.0000	0.0000	24.0000	0.0000
N-Nonane	40.0000	0.0000	148.0000	0.0000

Stream No.	5	6
Stream Name	Overhead	Bottoms
Temp F	106.7999	304.1045
Pres psia	230.0000	230.0000
Enth MMBtu/h	-3.6834	-28.514
Vapor mole fraction	1.0000	0.00000
Total lbmol/h	102.9977	356.0023
Total lb/h	2696.2712	34236.0156
Total std L ft3/hr	117.4588	812.3892
Total std V scfh	39085.44	135095.25
Flowrates in lbmol/h		
Methane	45.9997	0.0003
Ethane	40.6306	1.3694
Propane	15.9919	50.0081
I-Butane	0.1666	12.8334
N-Butane	0.0732	48.9268
I-Pentane	0.0000	11.0000
N-Pentane	0.0000	20.0000
N-Hexane	0.0000	24.0000
N-Nonane	0.1358	187.8642

Stg	Temp F	Pres psia	Liquid lbmol/h	Vapor lbmol/h	Feeds lbmol/h	Product lbmol/h
1	106.8	230.00	61.85		40.00	103.00
2	114.0	230.00	65.70	124.85		
3	113.2	230.00	68.57	128.70		
4	102.5	230.00	76.76	131.57		
5	109.6	230.00	78.27	139.76		
6	115.5	230.00	78.75	141.27		
7	122.1	230.00	79.07	141.75		
8	129.4	230.00	80.98	142.07		
9	132.4	230.00	473.16	143.98	419.00	
10	151.3	230.00	533.33	117.16		
11	165.7	230.00	576.46	177.33		
12	179.5	230.00	602.79	220.46		
13	204.1	230.00	538.22	246.79		
14	212.3	230.00	550.57	182.22		
15	232.1	230.00	546.24	194.57		
16	304.1	230.00		190.24		356.00

Exercise 10.41

Subject: Design of a reboiled stripper.

Given: Feed of composition below at 39.2°F and 150 psia. Column with 7 equilibrium stages plus a partial reboiler, operating at 150 psia. Bottoms flow rate of 99.33 lbmol/h.

Assumptions: SRK for *K*-values and enthalpies.

Find: Product compositions, stage temperatures, interstage flow rates and compositions, and reboiler duty.

Analysis: : The calculations were made with the Tower model (Inside-out method) of Chemcad, with the following specifications:
No condenser
Top pressure = 230 psia
Column pressure drop = 0 psi.
Number of stages = 7 plus a partial reboiler
Feed to stage 1
At the top, no condenser
At the bottom, bottoms flow rate = 99.33 lbmol/h
Estimated distillate rate = 450 lbmol/h (actual rate = 551.59 - 99.33 = 452.26 lbmol/h)
Estimated reflux rate = 550 lbmol/h
Estimated temperature of stage 1 = 50°F
Estimated temperature of bottom stage = 250°F
Estimated temperature of stage 2 = 80°F

Convergence was achieved in 4 iterations. The results are shown on the following two pages. The column feed is 14.5 mol% vaporized. The heat duty of the reboiler is 4.4674 MMBtu/h.

The % stripping of each component in the feed is as follows:

Component	% Stripped
N_2	100.00
C_1	100.00
C_2	100.00
C_3	99.92
nC_4	86.26
nC_5	23.61
nC_6	8.03

Exercise 10.41 (continued)

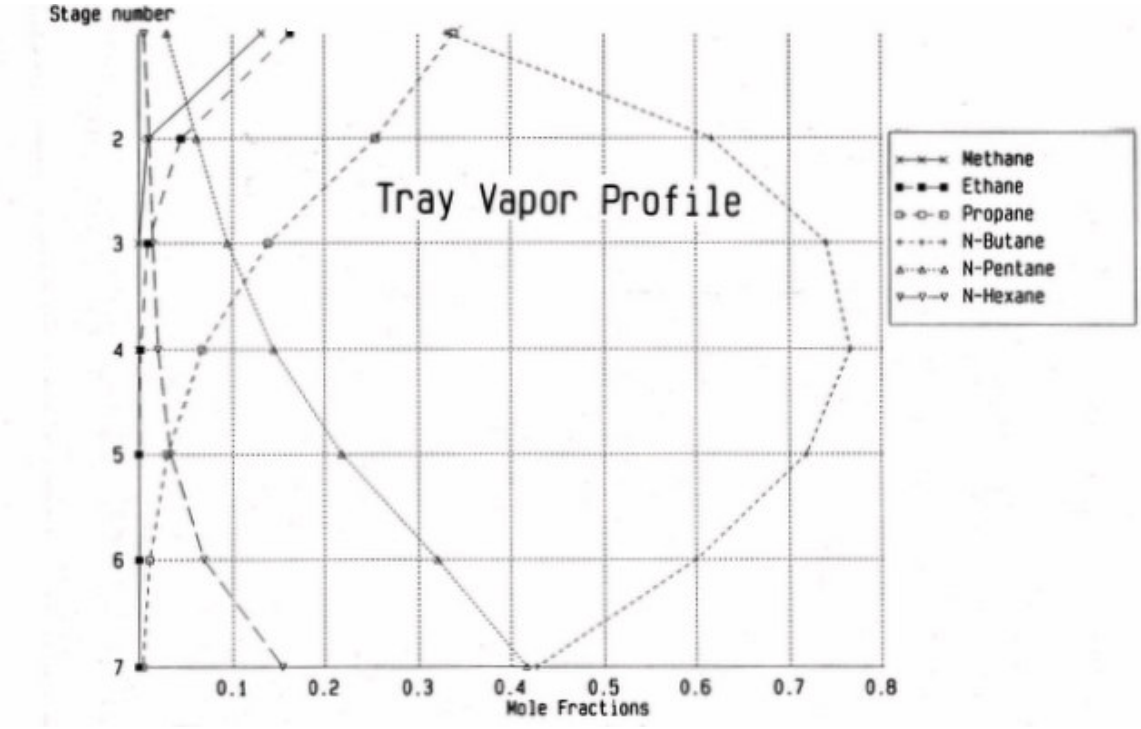
Analysis: (continued)

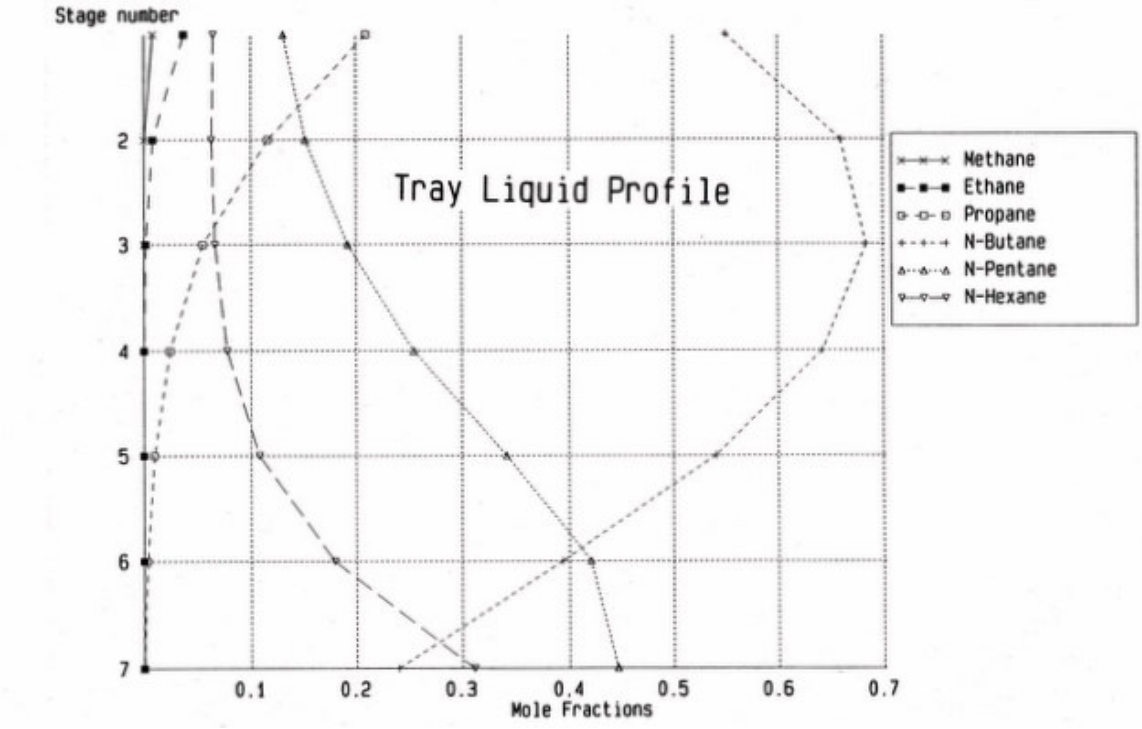
Stream No.	1	2	3
Stream Name	Feed	Overhead	Bottoms
Temp F	39.2000*	129.2775	249.6189
Pres psia	150.0000*	150.0000	150.0000
Enth MMBtu/h	-31.511	-20.355	-6.6891
Vapor mole fraction	0.14483	1.0000	0.00000
Total lbmol/h	551.5900	452.2596	99.3303
Total lb/h	27096.2930	19833.1309	7263.1558
Total std L ft3/hr	817.1388	633.0022	184.1365
Total std V scfh	209316.62	171622.86	37693.71
Flowrates in lbmol/h			
Nitrogen	0.2200	0.2200	0.0000
Methane	59.5100	59.5100	0.0000
Ethane	73.5700	73.5698	0.0002
Propane	153.2200	153.0933	0.1267
N-Butane	173.2200	149.4215	23.7984
N-Pentane	58.2200	13.7454	44.4746
N-Hexane	33.6300	2.6996	30.9304

			* Net Flows *			
	Temp	Pres	Liquid	Vapor	Feeds	Product
Stg	F	psia	lbmol/h	lbmol/h	lbmol/h	lbmol/h
1	129.3	150.00	561.26		551.59	452.26
2	169.4	150.00	615.05	461.93		
3	185.5	150.00	625.75	515.72		
4	196.8	150.00	620.03	526.42		
5	209.4	150.00	604.09	520.70		
6	226.7	150.00	584.08	504.76		
7	249.6	150.00		484.75		99.33

Exercise 10.41 (continued)

Analysis: (continued)





Exercise 10.42

Subject: Liquid-liquid extraction of a mixture of cyclohexane (1) and cyclopentane (2) with methanol (3).

Given: Feed of 700 lbmol/h of cyclohexane and 300 lbmol/h of cyclopentane. Methanol solvent of 1,000 lbmol/h. Extractors with various numbers of equilibrium stages, operating at 25°C.

Assumptions: Phase equilibria predicted by NRTL or UNIQUAC equations.

Find: Product rates and compositions, and interstage flow rates and compositions for 1, 2, 5, and 10 equilibrium stages.

Analysis: Reference 55 in Chap. 2 presents L/L equilibria data for the ternary system at 25°C (77°F). These data are fitted to the NRTL and UNIQUAC equations in "Liquid-Liquid Equilibrium Data Collection - Ternary Systems", Vol. V, Part 2 of the Chemical Data Series, by J. M. Sorenson and W. Arlt, DECHEMA (1980). Their fit to the simpler NRTL equation is almost as good as the UNIQUAC fit. Therefore, the NRTL equation is used here, with the following binary interaction parameters for use in the Chemcad program, where from Eq. (2-94),

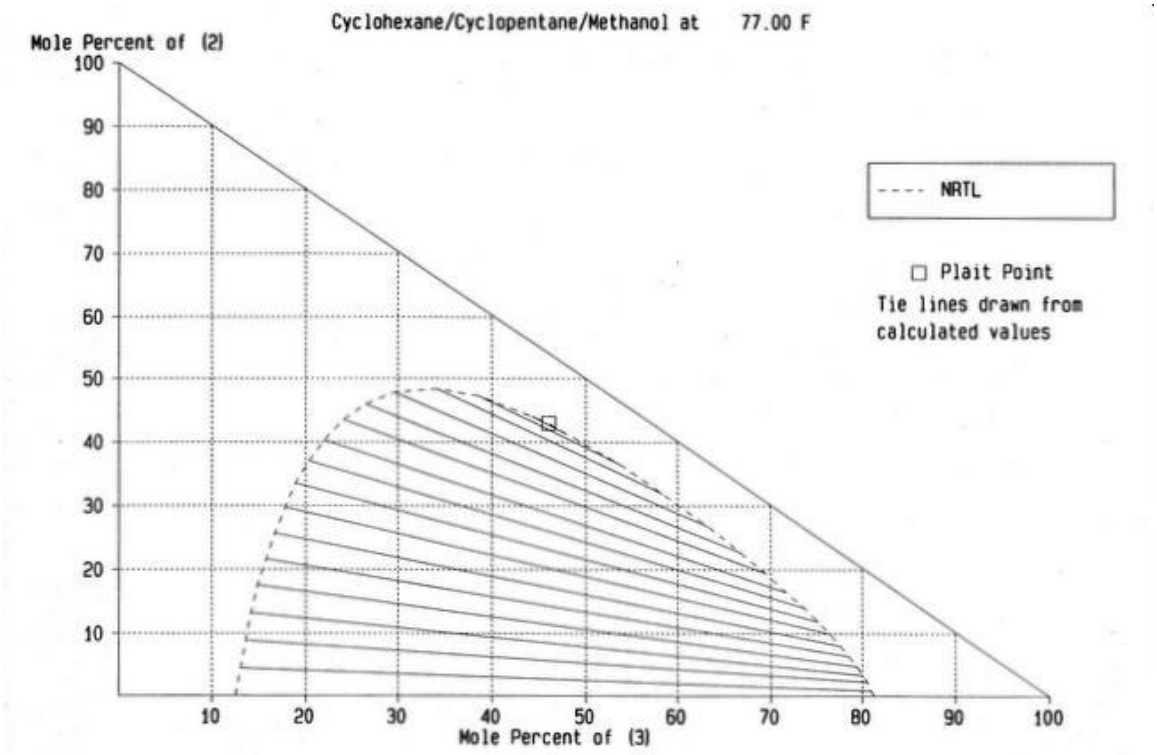
$$\tau_{ij} = \frac{g_{ij} - g_{jj}}{RT} = \frac{B_{ij}}{T}, \text{ where } T \text{ is in Kelvins}$$

I	J	B_{IJ}	B_{JI}	α_{IJ}
1	2	-97.419	-56.868	0.2
1	3	544.82	318.02	0.2
2	3	361.38	234.33	0.2

Using the Binodal Plot feature of the Chemcad program, a predicted ternary liquid-liquid equilibrium diagram is obtained, as shown on the next page, along with a corresponding table of predicted tie lines. It is seen that at 25°C, cyclopentane is completely soluble in methanol, but cyclohexane is only partially soluble in methanol. Is methanol a good solvent for the separation of cyclopentane from cyclohexane? From the slope of the tie lines, the answer is no; Cyclopentane distributes preferably to the cyclohexane-rich phase. For example, for one equilibrium stage, using the LLVF model of Chemcad, the following two liquid phases (raffinate and extract) are calculated when the given feed and solvent are mixed and brought to equilibrium at 25°C and 30 psia, where the pressure exceeds the bubble-point pressures of the feed (2.69 psia) and solvent (2.44 psia) so that a vapor phase does not form. Very little separation of (1) and (2) occurs.

Exercise 10.42 (continued)

Analysis: (continued)



Computed Binodal Curve in Mole Percent:

(1) = Cyclohexane
(2) = Cyclopentane
(3) = Methanol

Left Phase			Right Phase		
(1)	(2)	(3)	(1)	(2)	(3)
87.516	0.000	12.484	18.836	0.000	81.164
82.500	4.476	13.024	18.064	1.069	80.867
77.500	8.880	13.620	17.304	2.228	80.468
72.500	13.220	14.280	16.553	3.490	79.957
67.500	17.485	15.015	15.815	4.864	79.321
62.500	21.663	15.837	15.090	6.362	78.548
57.500	25.738	16.762	14.379	8.002	77.619
52.500	29.690	17.810	13.682	9.804	76.513
47.500	33.491	19.009	13.001	11.796	75.202
42.500	37.102	20.398	12.337	14.016	73.647
37.500	40.468	22.032	11.692	16.516	71.792
32.500	43.502	23.998	11.073	19.374	69.553
27.500	46.064	26.436	10.491	22.716	66.793
22.500	47.895	29.605	9.982	26.758	63.259
17.500	48.414	34.086	9.661	31.949	58.389
14.218	47.285	38.497	9.768	36.500	53.732
11.606	44.238	44.157	10.571	41.500	47.929
11.028	42.937	46.036	11.023	42.937	46.040

Exercise 10.42 (continued)

Analysis: (continued)

Stream Name	Feed	Solvent	Raffinate	Extract
Temp F	77.0000*	77.0000*	77.0000	77.0000
Pres psia	30.0000*	30.0000*	30.0000	30.0000
Enth MMBtu/h	-60.552	-102.73	-61.500	-101.78
Vapor mole fraction	0.00000	0.00000	0.00000	0.00000
Total lbmol/h	1000.0000	1000.0000	908.9450	1091.0549
Total lb/h	79952.9062	32042.0000	65649.7891	46345.1172
Total std L ft3/hr	1655.3704	643.8834	1355.7807	943.4731
Total std V scfh	379478.62	379478.62	344925.19	414032.03
Flowrates in lbmol/h				
Cyclohexane	700.0000	0.0000	540.1685	159.8316
Cyclopentane	300.0000	0.0000	219.7923	80.2077
Methanol	0.0000	1000.0000	148.9843	851.0157

The Extract model of the Chemcad program was used to calculate a 10-stage extraction unit for the given conditions. The model converged in 12 iterations, with the results given below. The product compositions differ little from those computed for 1 stage. Also, the interstage flow rates are almost constant for stages 1 to 7. Thus, a significant separation is not possible for any number of stages. The reason for this is clear if a line on the above ternary diagram is drawn from the feed point [30 mol% (2) at 0 mol% (3)] to the solvent point [100 mol% (3)]. This line is almost collinear with a tie line. Regardless of the number of stages and the number of equilibrium stages, a significant separation of cyclopentane and cyclohexane can not be made.

Stream No.	1	2	3	4
Stream Name	Feed	Solvent	Extract	Raffinate
Temp F	77.0000*	77.0000*	77.0001	76.9996
Pres psia	30.0000*	30.0000*	30.0000	30.0000
Enth MMBtu/h	-60.552	-102.73	-102.13	-61.156
Vapor mole fraction	0.00000	0.00000	0.00000	0.00000
Total lbmol/h	1000.0000	1000.0000	1096.9170	903.0831
Total lb/h	79952.9062	32042.0000	46669.6719	65325.2305
Total std L ft3/hr	1655.3704	643.8834	950.4258	1348.8280
Total std V scfh	379478.62	379478.62	416256.56	342700.72
Flowrates in lbmol/h				
Cyclohexane	700.0000	0.0000	158.6151	541.3849
Cyclopentane	300.0000	0.0000	85.4615	214.5385
Methanol	0.0000	1000.0000	852.8403	147.1597

			* Net Flows *			
	Temp	Pres	Heavy	Light	Feeds	Product
Stg	F	psia	lbmol/h	lbmol/h	lbmol/h	lbmol/h
1	77.0	30.00	1272.35		1000.00	1096.92
2	77.0	30.00	1272.34	1369.26		
3	77.0	30.00	1272.33	1369.26		
4	77.0	30.00	1272.29	1369.25		
5	77.0	30.00	1272.19	1369.21		
6	77.0	30.00	1271.90	1369.11		
7	77.0	30.00	1271.07	1368.82		
8	77.0	30.00	1268.75	1367.99		
9	77.0	30.00	1262.21	1365.66		
10	77.0	30.00		1359.12	1000.00	903.08

Exercise 10.43

Subject: Liquid-liquid extraction of acetic acid from water by ethyl acetate at 100°F

Given: Feed of 6,660 lb/h of acetic acid and 23,600 lb/h of water. Solvent of 68,600 lb/h of ethyl acetate and 2,500 lb/h of water. Ccountercurrent-flow extractor.

Assumptions: NRTL equation for activity coefficients using the following parameters:

I	J	B_{IJ}	B_{JI}	α_{IJ}
Ethyl acetate	Water	166.36	1190.1	0.2
Ethyl acetate	Acetic acid	643.30	-702.57	0.2
Water	Acetic acid	-302.63	-1.683	0.2

Find: Number of equilibrium stages to extract 99.5% of the acetic acid.

Analysis: The Extract model of Chemcad was used starting with 2 equilibrium stages and increasing by one until 99.5% extraction was achieved. For each run, convergence was achieved in 12 to 13 iterations. The results were:

No. of stages	% Extraction of Acetic acid
2	90.59
3	96.68
4	98.80
5	99.56
6	99.86

The results show that 5 stages are needed, but 6 stages is safer.

Detailed results for 6 stages are:

Stream No.	1	2	3	4
Stream Name	Feed	Solvent	Extract	Raffinate
Temp F	100.0000*	100.0000*	100.0007	100.0002
Pres psia	15.0000*	15.0000*	15.0000	15.0000
Enth MMBtu/h	-182.04	-176.98	-223.40	-135.61
Vapor mole fraction	0.00000	0.00000	0.00000	0.00000
Total lbmol/h	1420.9215	917.3808	1242.0226	1096.2797
Total lb/h	30260.0020	71100.0000	80419.7266	20940.2734
Total std L ft3/hr	480.0398	1257.2091	1398.9560	338.2928
Total std V scfh	539209.31	348126.41	471321.03	416014.69
Flowrates in lb/h				
Ethyl Acetate	0.0000	68600.0000	67112.6562	1487.3413
Water	23600.0020	2500.0000	6657.8828	19442.1172
Acetic Acid	6660.0000	0.0000	6649.1841	10.8155

Stg	Temp F	Pres psia	Heavy lb/h	Light lb/h	Feeds lb/h	Product lb/h
1	100.0	15.00	26419.95		30260.00	80419.73
2	100.0	15.00	22731.68	76579.67		
3	100.0	15.00	21510.06	72891.40		
4	100.0	15.00	21075.03	71669.79		
5	100.0	15.00	20916.35	71234.76		
6	100.0	15.00		71076.08	71100.00	20940.28

Exercise 11.1

Subject: Azeotropes and approximate residue curve map for the system n-hexane - methanol - methyl acetate at 1 atm

Given:. Ternary system n-hexane - methanol - methyl acetate at 1 atm.

Find: All binary and ternary azeotropes from suitable references. Approximate residue curve map showing distillation boundaries. Type of node for each azeotrope and pure component.

Analysis: The following azeotrope data were obtained from the "Handbook of Chemistry and Physics" or the 6th edition of "Perry's Chemical Engineers' Handbook":
At 1 atm, the molecular weights and boiling points of the three components are:

Component	Molecular weight	Normal b. pt., ^{o}C
n-Hexane	86.17	69.0
Methanol	32.04	64.7
Methyl acetate	74.08	57.0

Binary azeotropes (all minimum boiling):

Mixture, A/B	Boiling pt., ^{o}C	Wt% A/B	Mol% A/B
n-Hexane/Methanol	50.6		49.0/51.0
n-Hexane/Methyl acetate	51.8	39.3/60.7	35.8/64.2
Methanol/Methyl acetate	53.5	19.0/81.0	35.2/64.8

Ternary azeotrope (minimum boiling):

Mixture, A/B/C	Boiling pt., ^{o}C	Wt% A/B/C	Mol% A/B/C
n-Hexane/Methanol/ Methyl acetate	47.4	48.6/14.6/36.8	37.2/30.1/32.7

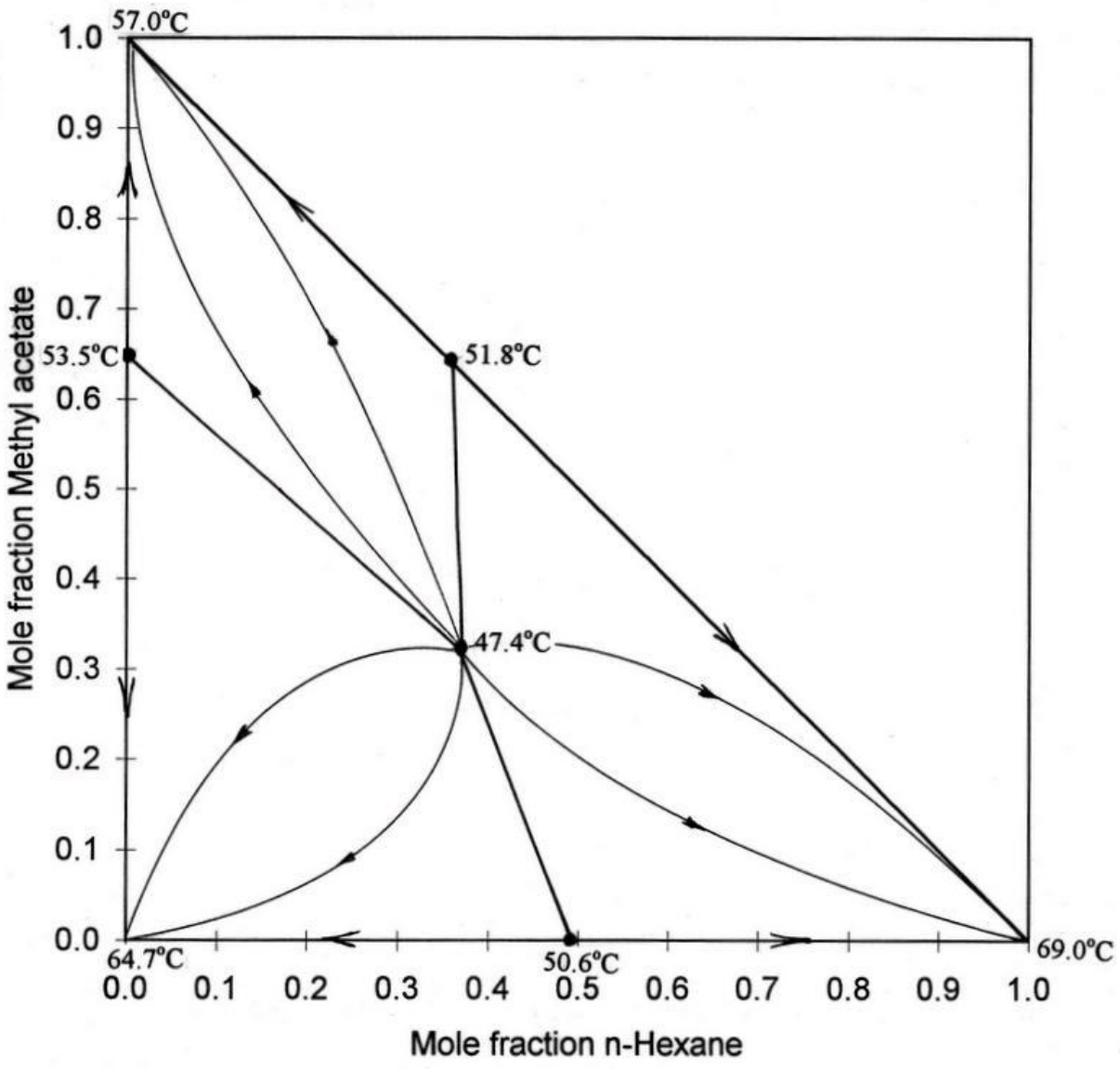
An approximate residue curve map on a right triangular diagram, of the type developed in Fig. 11.7, is shown on the next page. From that diagram, which includes approximate distillation boundaries, the following types of nodes are determined using Fig. 11.6:

Component or Azeotrope	Normal boiling pt., ^{o}C	Type node
n-Hexane	69.0	stable
Methanol	64.7	stable
Methyl acetate	57.0	stable
n-Hexane/Methanol	50.6	saddle
n-Hexane/Methyl acetate	51.8	saddle
Methanol/Methyl acetate	53.5	saddle
n-Hexane/Methanol/Methyl acetate	47.4	unstable

A computed residue curve map is given by van Dongen and Doherty, IEC Fundamentals, Vol. 24, 454 (1985).

Exercise 11.1 (continued)

Analysis: (continued)



Exercise 11.2

Subject: Calculation of a residue curve for the system n-hexane - methanol - methyl acetate.

Given:. Ternary system n-hexane - methanol - methyl acetate at 1 atm.
Assumptions: UNIFAC method for computing *K*-values.

Find: Portion of a residue curve starting from a bubble-point liquid of 20 mol% n-Hexane (1), 60 mol% methanol (2), and 20 mol% methyl acetate (3), at 1 atm.

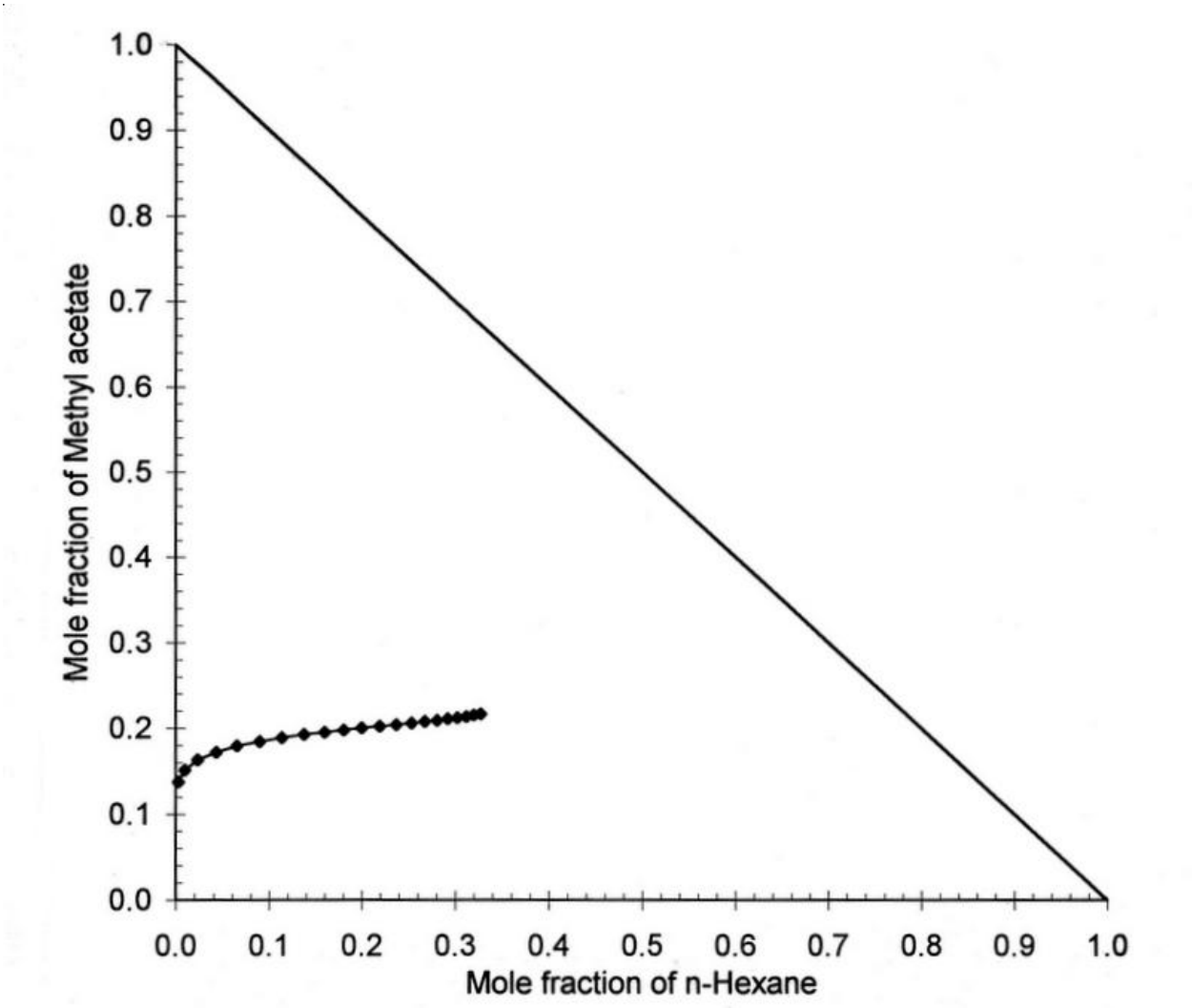
Analysis: The residue curve is computed numerically, in the same manner as in Example 11.1, except that the bubble-point calculations at each step are made with the Chemcad FLASH model. To begin, a bubble point is run with Chemcad on the above initial liquid composition, $x_i^{(0)}$, at 1 atm. The computed vapor composition, $y_i^{(0)}$, is then used with the Euler form of Eqs. (11-5) and (11-6) to compute $x_i^{(1)}$: $x_i^{(1)} = x_i^{(0)} + \left(x_i^{(0)} - y_i^{(0)}\right)\Delta\xi$, i = 1 to C -1

The procedure is repeated in steps of $\Delta\xi = 0.1$ in the forward direction from $\xi = 0$ to $\xi = 1$, and $\Delta\xi = -0.1$in the backward direction from $\xi = 0$ to $\xi = -1$. The results are as follows, with a plot on the following page.

ξ	x (1)	x (2)	x (3)	y (1)	y (2)	y (3)	T, °C
-1.0	0.3277	0.4560	0.2163	0.3933	0.3770	0.2297	47.88
-0.9	0.3203	0.4647	0.2150	0.3942	0.3773	0.2285	47.88
-0.8	0.3120	0.4744	0.2136	0.3950	0.3776	0.2274	47.88
-0.7	0.3027	0.4852	0.2121	0.3959	0.3779	0.2262	47.88
-0.6	0.2923	0.4970	0.2107	0.3966	0.3782	0.2252	47.88
-0.5	0.2806	0.5102	0.2092	0.3973	0.3786	0.2241	47.88
-0.4	0.2676	0.5248	0.2076	0.3978	0.3790	0.2232	47.88
-0.3	0.2531	0.5409	0.2060	0.3979	0.3796	0.2225	47.89
-0.2	0.2371	0.5587	0.2042	0.3975	0.3804	0.2221	47.90
-0.1	0.2194	0.5784	0.2022	0.3964	0.3818	0.2218	47.93
0.0	0.2000	0.6000	0.2000	0.3940	0.3840	0.2220	47.99
0.1	0.1806	0.6216	0.1978	0.3900	0.3871	0.2229	48.08
0.2	0.1597	0.6451	0.1952	0.3835	0.3920	0.2245	48.24
0.3	0.1373	0.6704	0.1923	0.3730	0.3995	0.2275	48.51
0.4	0.1137	0.6974	0.1889	0.3566	0.4114	0.2320	48.96
0.5	0.0894	0.7260	0.1846	0.3311	0.4300	0.2389	49.68
0.6	0.0652	0.7556	0.1792	0.2920	0.4588	0.2492	50.80
0.7	0.0426	0.7853	0.1721	0.2350	0.5019	0.2631	52.44
0.8	0.0233	0.8137	0.1630	0.1591	0.5617	0.2792	54.59
0.9	0.0097	0.8389	0.1514	0.0797	0.6300	0.2903	56.83
1.0	0.0028	0.8598	0.1374	0.0260	0.6866	0.2874	58.46

Exercise 11.2 (continued)

Analysis: (continued)



Exercise 11.3

Subject: : Calculation of a portion of a distillation curve for the system n-hexane - methanol - methyl acetate.

Given:. Ternary system n-hexane - methanol - methyl acetate at 1 atm.

Assumptions: UNIFAC method for computing *K*-values.

Find: Portion of a distillation curve starting from a bubble-point liquid of 20 mol% n-Hexane (1), 60 mol% methanol (2), and 20 mol% methyl acetate (3), at 1 atm, using a simulation program.

Analysis: The distillation curve is computed stagewise using the FLASH model in Chemcad, in the same manner as in Example 11.2, except that here the calculation is made in both directions. To begin, a bubble point is run with Chemcad on the above initial liquid composition, $x_i^{(1)}$, at 1 atm. The computed vapor composition, $y_i^{(1)}$, is set equal to $x_i^{(2)}$, according to Eq. (11-14) so that the compositions of passing vapor and liquid streams are made equal, and the bubble-point calculation is repeated. In this manner, we step in the first direction. The sequence is repeated, starting again from $x_i^{(1)}$, but this time running a sequence of dew points to step in the opposite direction. The results are as follows, with a plot on the following page.

***x* (1)**	***x* (2)**	***x* (3)**	***y* (1)**	***y* (2)**	***y* (3)**	***T*, °C**
0.3753	0.3594	0.2653	0.3731	0.3562	0.2707	47.84
0.3783	0.3635	0.2582	0.3753	0.3594	0.2653	47.84
0.3822	0.3689	0.2489	0.3783	0.3635	0.2582	47.85
0.3873	0.3757	0.2370	0.3822	0.3689	0.2489	47.86
0.3939	0.3840	0.2221	0.3873	0.3757	0.2370	47.89
0.2000	0.6000	0.2000	0.3939	0.3840	0.2221	47.99
0.0272	0.8662	0.1066	0.2000	0.6000	0.2000	55.01
0.0022	0.9586	0.0392	0.0272	0.8662	0.1066	61.89
0.0002	0.9869	0.0129	0.0022	0.9586	0.0392	63.74
0.0000	0.9958	0.0042	0.0002	0.9869	0.0129	64.25
0.0000	0.9987	0.0013	0.0000	0.9958	0.0042	64.41
0.0000	0.9996	0.0004	0.0000	0.9987	0.0013	64.46

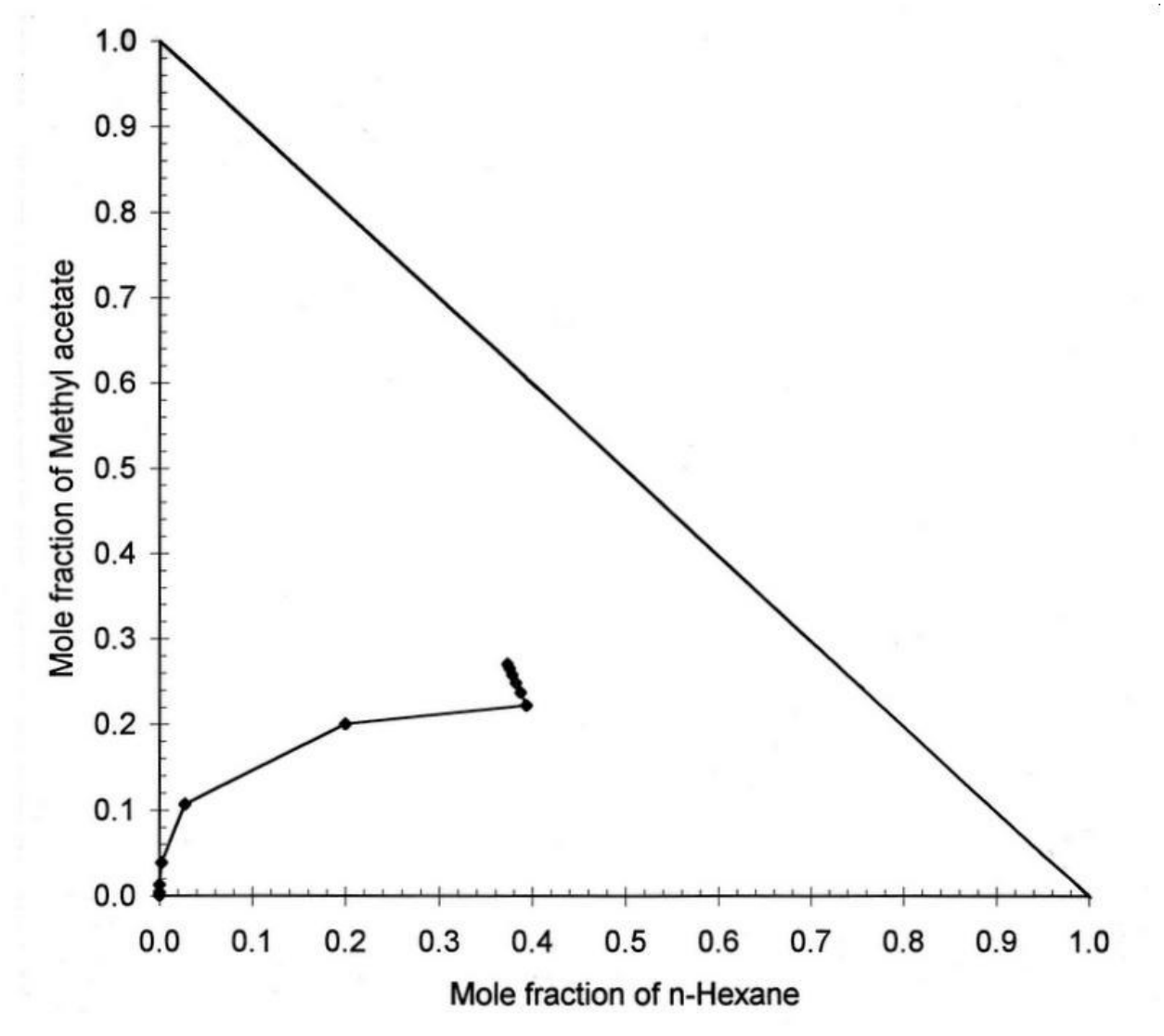
In the plot on the next page, the distillation curve is seen to take a sharp turn at a n-hexane mole fraction of approximately 0.40. This may be due to the drastic changes that occur to the *K*-values along the distillation curve for this very non-ideal system. Starting from almost pure methyl alcohol and moving along the distillation curve to right, the *K*-values change as follows:

Exercise 11.3 (continued)

Analysis: (continued)

Component	***K*-values:**					
nC_6	14.29	12.20	7.37	1.97	0.98	0.99
MeOH	1.00	0.90	0.69	0.64	0.98	0.99
MeAc	3.16	2.73	1.88	1.11	1.07	1.01

Note how the final *K*- values are tending toward the azeotropic condition. This may explain the sharp turn of the distillation curve on the plot below.



Exercise 11.4

Subject: Azeotropes and approximate residue curve map for the system n-hexane - methanol - methyl acetate at 1 atm

Given:. Ternary system acetone - benzene - n-heptane at 1 atm.

Find: All binary and ternary azeotropes from suitable references. Approximate distillation curve map showing distillation boundaries. Type of node for each azeotrope and pure component.

Analysis: The following azeotrope data were obtained from the "Handbook of Chemistry and Physics".
At 1 atm, the molecular weights and boiling points of the three components are:

Component	Molecular weight	Normal b. pt., ^{o}C
n-Heptane	100.2	98.4
Benzene	78.11	80.1
Acetone	58.08	56.5

Binary azeotropes (all minimum boiling):

Mixture, A/B	Boiling pt., ^{o}C	Wt% A/B	Mol% A/B
n-Heptane/Benzene	80.1	0.7/99.3	0.5/99.5
n-Heptane/Acetone	55.9	10.5/89.5	6.5/93.5
Benzene/Acetone	No azeotrope		

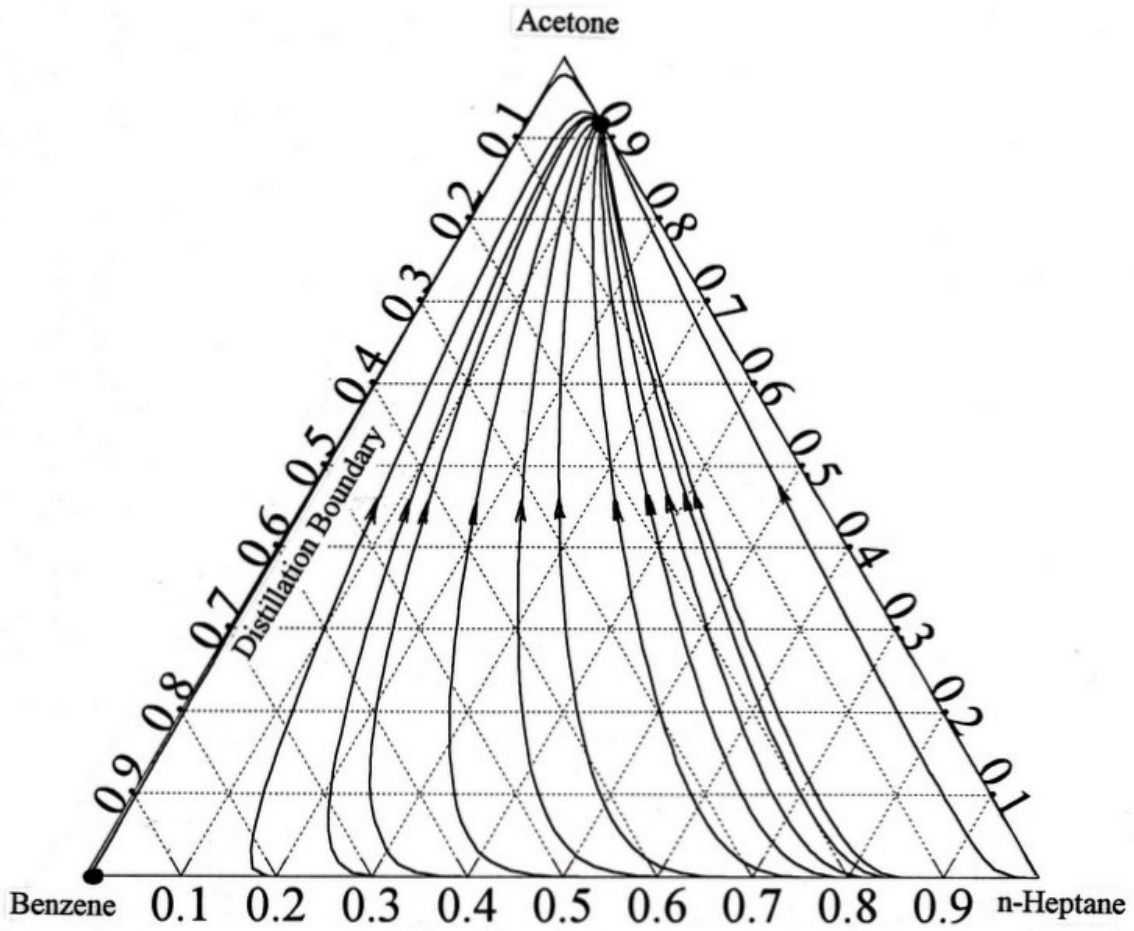
No ternary azeotrope

An approximate distillation curve map on a equilateral triangular diagram, of the type in Fig. 11.3, is shown on the next page. However, it is not a sketch, but is a residue curve map drawn by the Aspen Plus program and modified to represent a distillation curve map. The distillation boundary extends from one binary azeotrope to the other, but is barely discernible. From that diagram, the following types of nodes are determined using Fig. 11.6:

Component or Azeotrope	Normal boiling pt., ^{o}C	Type node
n-Heptane	98.4	stable
Benzene	80.1	stable
Acetone	56.5	saddle
n-Heptane/Benzene	80.1	saddle
n-Heptane/Acetone	55.9	unstable

Exercise 11.4 (continued)

Analysis: (continued)



Exercise 11.5

Subject: Calculation of a residue curve for the system acetone - benzene - n-heptane.

Given:. Ternary system acetone - benzene - n-heptane at 1 atm.

Assumptions: UNIFAC method for computing *K*-values.

Find: Portion of a residue curve starting from a bubble-point liquid of 20 mol% acetone (1), 60 mol% benzene (2), and 20 mol% n-heptane (3), at 1 atm.

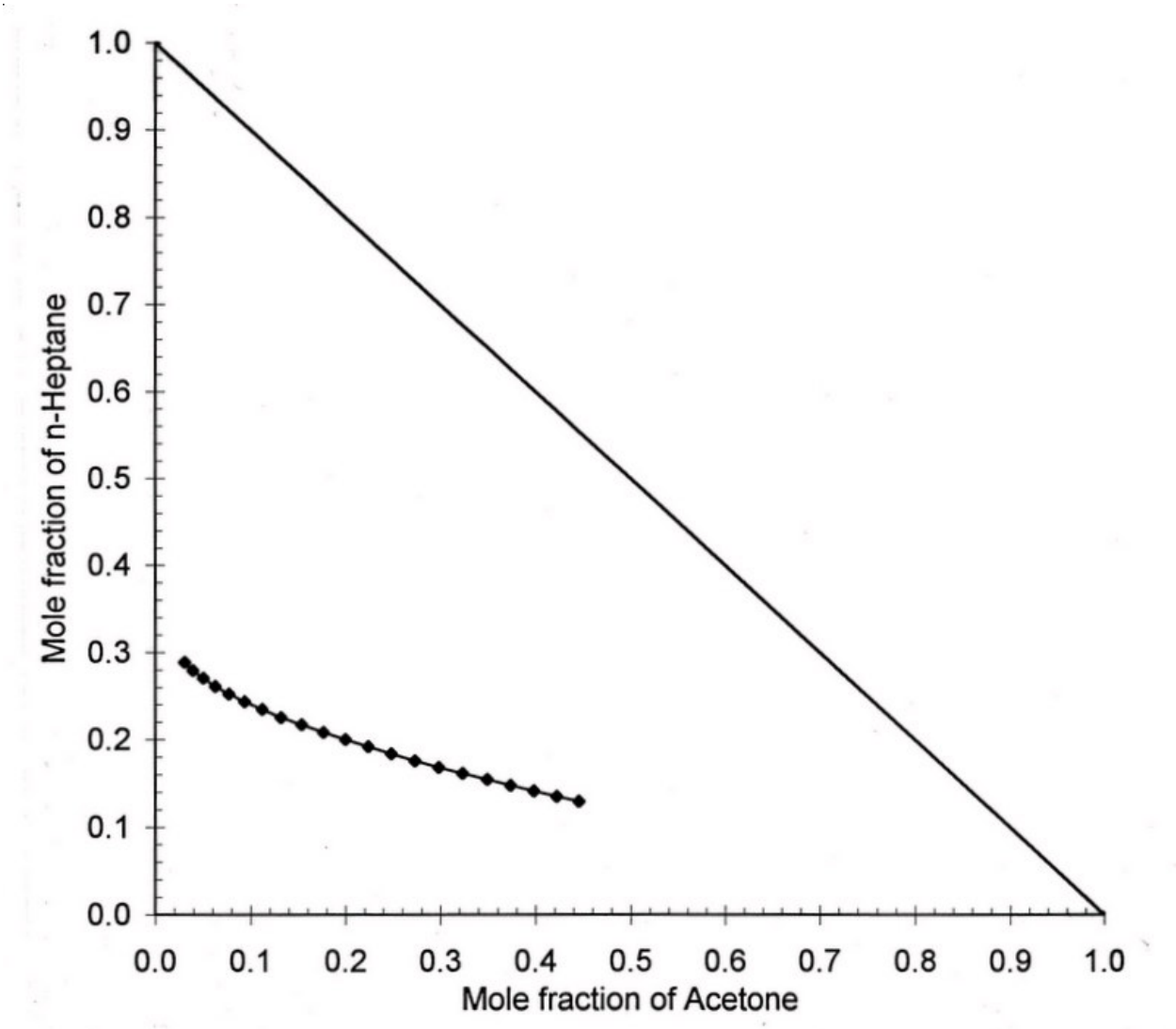
Analysis: The residue curve is computed numerically, in the same manner as in Example 11.1, except that the bubble-point calculations at each step are made with the Chemcad FLASH model. To begin, a bubble point is run with Chemcad on the above initial liquid composition, $x_i^{(0)}$, at 1 atm. The computed vapor composition, $y_i^{(0)}$, is then used with the Euler form of Eqs. (11-5) and (11-6) to compute $x_i^{(1)}$: $x_i^{(1)} = x_i^{(0)} + \left(x_i^{(0)} - y_i^{(0)}\right)\Delta\xi$, i = 1 to C -1

The procedure is repeated in steps of $\Delta\xi = 0.1$ in the forward direction from $\xi = 0$ to $\xi = 1$, and $\Delta\xi = -0.1$in the backward direction from $\xi = 0$ to $\xi = -1$. The results are as follows, with a plot on the following page.

ξ	*x* (1)	*x* (2)	*x* (3)	*y* (1)	*y* (2)	*y* (3)	*T*, °C
-1.0	0.4458	0.4248	0.1294	0.6723	0.2519	0.0758	63.02
-0.9	0.4224	0.4425	0.1351	0.6558	0.2658	0.0784	63.53
-0.8	0.3985	0.4604	0.1411	0.6381	0.2807	0.0812	64.07
-0.7	0.3740	0.4786	0.1474	0.6189	0.2968	0.0843	64.67
-0.6	0.3491	0.4969	0.1540	0.5981	0.3141	0.0878	65.30
-0.5	0.3239	0.5151	0.1610	0.5758	0.3326	0.0916	65.99
-0.4	0.2986	0.5332	0.1682	0.5518	0.3525	0.0957	66.73
-0.3	0.2733	0.5509	0.1758	0.5259	0.3738	0.1003	67.52
-0.2	0.2483	0.5681	0.1836	0.4983	0.3964	0.1053	68.35
-0.1	0.2238	0.5845	0.1917	0.4690	0.4202	0.1108	69.23
0.0	0.2000	0.6000	0.2000	0.4381	0.4452	0.1167	70.14
0.1	0.1762	0.6155	0.2083	0.4043	0.4726	0.1231	71.13
0.2	0.1534	0.6298	0.2169	0.3689	0.5010	0.1301	72.14
0.3	0.1318	0.6426	0.2255	0.3322	0.5303	0.1375	73.18
0.4	0.1118	0.6539	0.2343	0.2951	0.5596	0.1453	74.21
0.5	0.0935	0.6633	0.2432	0.2581	0.5884	0.1535	75.23
0.6	0.0770	0.6708	0.2522	0.2218	0.6162	0.1620	76.21
0.7	0.0625	0.6763	0.2612	0.1874	0.6420	0.1706	77.13
0.8	0.0500	0.6797	0.2703	0.1556	0.6651	0.1793	77.98
0.9	0.0395	0.6811	0.2794	0.1272	0.6851	0.1877	78.74
1.0	0.0307	0.6807	0.2886	0.1019	0.7020	0.1961	79.42

Exercise 11.5 (continued)

Analysis: (continued)



Exercise 11.6

Subject: : Calculation of a portion of a distillation curve for the system acetone - benzene - n-heptane.

Given:. Ternary system acetone - benzene - n-heptane at 1 atm.

Assumptions: UNIFAC method for computing *K*-values.

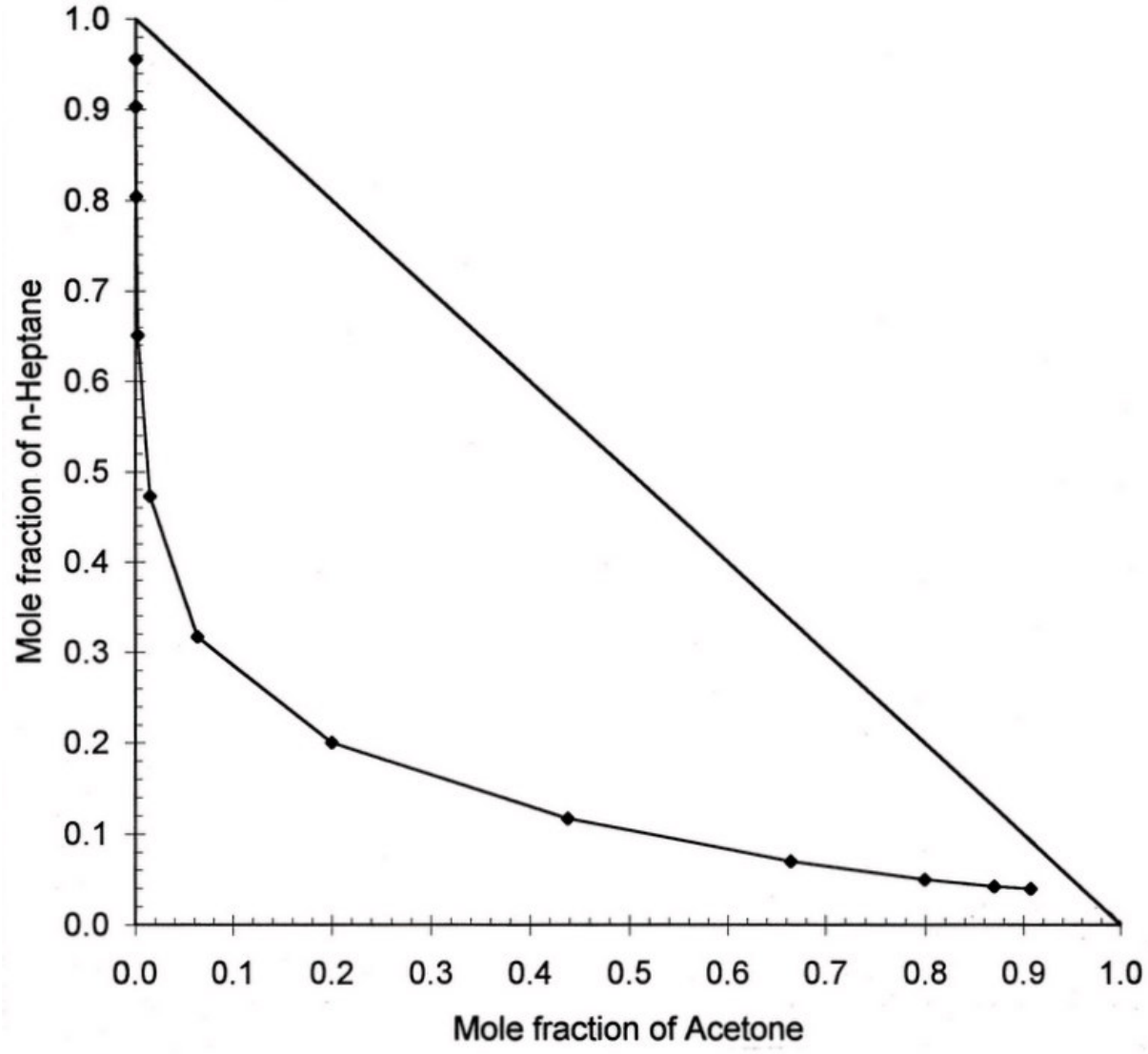
Find: Portion of a distillation curve starting from a bubble-point liquid of 20 mol% Acetone (1), 60 mol% Benzene (2), and 20 mol% n-Heptane (3), at 1 atm, using a simulation program.

Analysis: The distillation curve is computed stagewise using the FLASH model in Chemcad, in the same manner as in Example 11.2, except that here the calculation is made in both directions. To begin, a bubble point is run with Chemcad on the above initial liquid composition, $x_i^{(1)}$, at 1 atm. The computed vapor composition, $y_i^{(1)}$, is set equal to $x_i^{(2)}$, according to Eq. (11-14) so that the compositions of passing vapor and liquid streams are made equal, and the bubble-point calculation is repeated. In this manner, we step in the first direction. The sequence is repeated, starting again from $x_i^{(1)}$, but this time running a sequence of dew points to step in the opposite direction. The results are as follows, with a plot on the following page.

x (1)	x (2)	x (3)	y (1)	y (2)	y (3)	T, °C
0.0000	0.0445	0.9555	0.0000	0.0967	0.9033	96.65
0.0000	0.0967	0.9033	0.0003	0.1953	0.8044	94.59
0.0003	0.1953	0.8044	0.0024	0.3464	0.6512	91.23
0.0024	0.3464	0.6512	0.0146	0.5125	0.4729	86.98
0.0146	0.5125	0.4729	0.0633	0.6196	0.3171	82.59
0.0633	0.6196	0.3171	0.2000	0.6000	0.2000	77.39
0.2000	0.6000	0.2000	0.4384	0.4447	0.1169	70.19
0.4384	0.4447	0.1169	0.6643	0.2695	0.0698	70.20
0.6643	0.2695	0.0698	0.7996	0.1510	0.0494	63.31
0.7996	0.1510	0.0494	0.8702	0.0879	0.0419	59.44
0.8702	0.0879	0.0419	0.9076	0.0526	0.0397	57.73
0.9076	0.0526	0.0397	0.0000	0.9996	0.0004	56.94

Exercise 11.6 (continued)

Analysis: (continued)



Exercise 11.7

Subject: Regions of feasible product composition on a ternary diagram

Given: Residue curve map of Fig. 11.13, which shows a highly curved distillation boundary

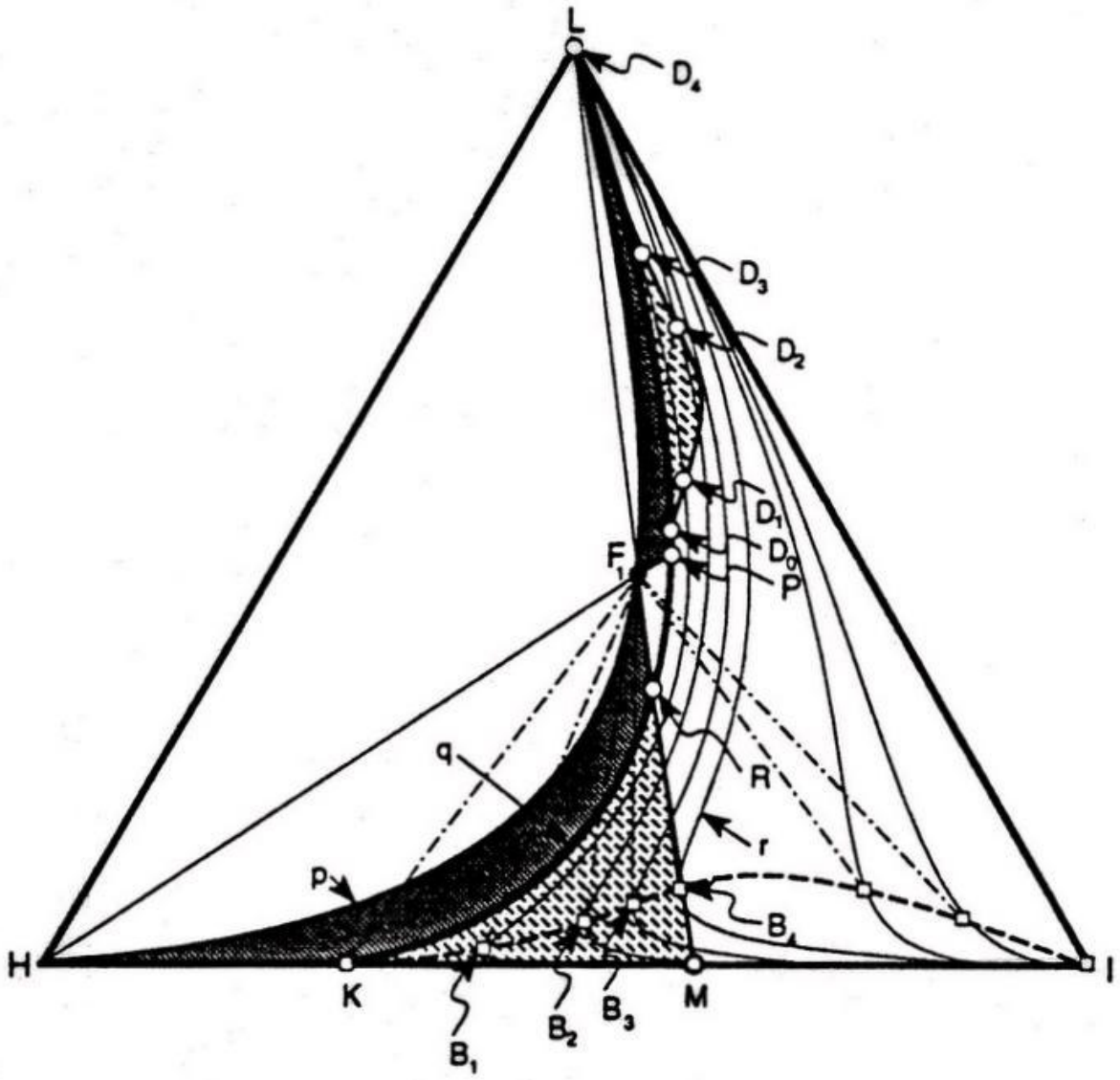
Find: Feasible product composition regions for Feed F_1.

Analysis: The solution to this exercise is given in detail by Widagdo and Seider in Ref. 19 of Chapter 11. Their figure 20, shown below, shows the bow-tie regions. Because the distillation boundary is highly curved, as discussed in Section 11.1, feasible product compositions lie on both sides of the distillation boundary when the feed is at F_1. The two dark-shaded feasible regions are on the feed side of the distillation boundary, while the two lightly shaded regions are on the other side of the distillation boundary. As stated by Widagdo and Seider, "The region of feasible compositions on the feed side is bounded by the distillation line *p* that passes through the feed, the distillation boundary (curve *q*), and the two overall mass-balance lines through pure species *H* and *L*. The bottoms products lie in the shaded portion of the F_1RKHF_1 region, and the distillates lie in the shaded portion of the F_1PLF_1 region. On the other side of the distillation boundary, the region of feasible bottoms-product compositions is bounded by the distillation boundary (curve *q*) and the overall mass-balance line that passes through pure species *L* (line LF_1M); that is, the lightly shaded region *RMKR*. The region of distillate compositions is also bounded by the distillation boundary (curve *q*). In addition, it is bounded by the end points of the chords (B_iD_i) that are tangent to the distillation lines at the tangent points (K, B_1,…, B_4 ,..., I) forming the dashed curve in the figure below. Because the distillate and bottoms-product compositions must lie on the same distillation line, for the feed composition at F_1, the distillate compositions must lie to the left of the overall mass-balance lines through the tangent points at B_i (D_i F_1 B_i).

It follows that, for the feed at F_1, the regions of feasible distillate and bottoms-product compositions, are the shaded portions of the union of F_1PLF_1 and LD_0 ... D_3L regions, and the F_1MHF_1 regions, respectively."

Exercise 11.7 (continued)

Analysis: (continued)



Exercise 11.8

Subject: Regions of feasible product composition on a ternary diagram

Given: Residue curve map and distillation curve map of Fig. 11.10 for the ternary system, acetone, methanol, and chloroform, which has one maximum-boiling binary azeotrope, two minimum-boiling azeotropes and one ternary azeotrope, all homogeneous.

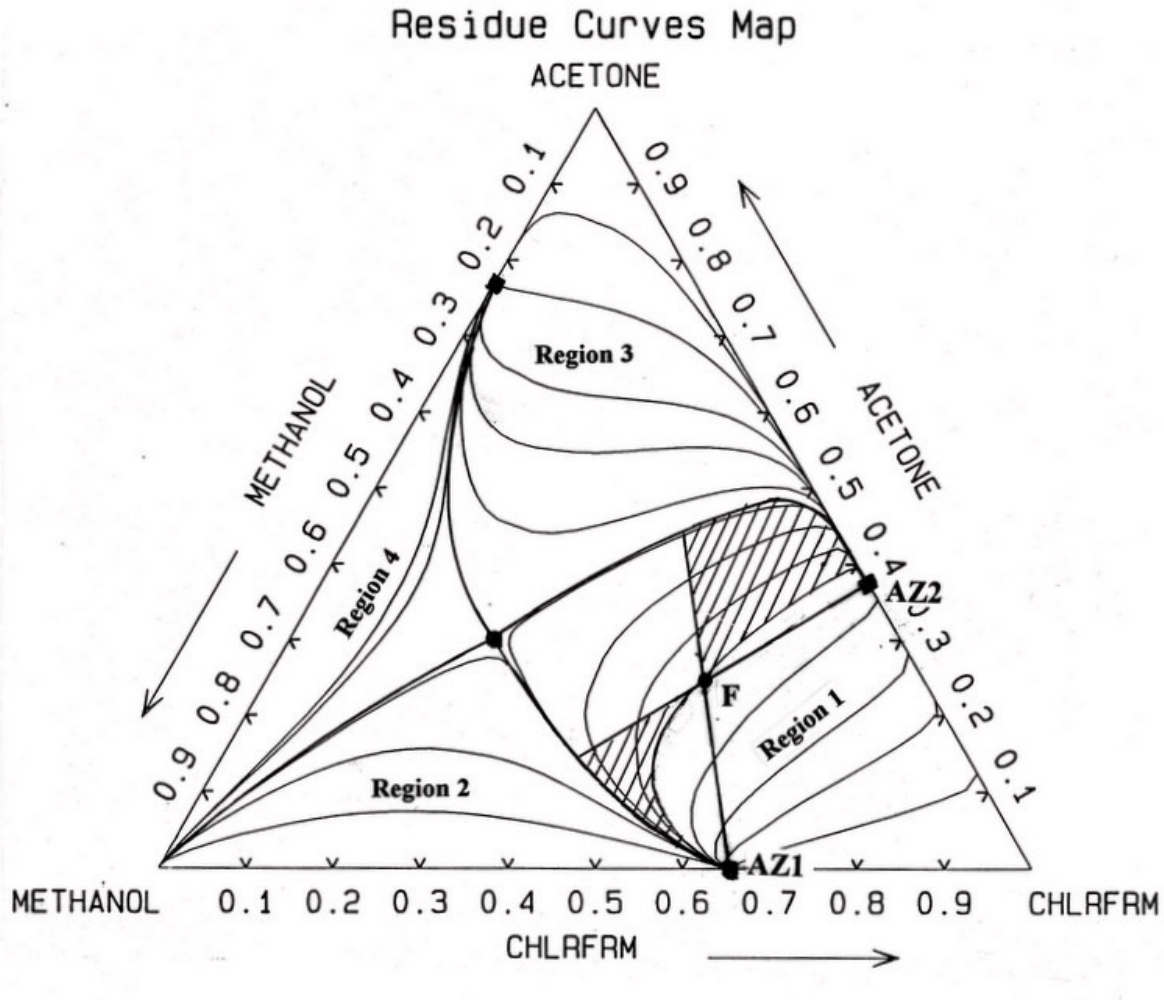
Find: Feasible product composition regions for a feed of 50 mol% chloroform, 25 mol% acetone, and 25 mol% methanol.

Analysis:

In the right-triangle diagram on the next page, the feed composition is shown at F. Thus, the feed is in Region 1, which is bounded by distillation boundaries A and B, the binary mixture of chloroform and acetone from pure methanol to the azeotrope, and the binary mixture of chloroform and methanol from pure chloroform to the binary azeotrope. For Region 1, the minimum boiling product is AZ1, the azeotrope of chloroform and methanol, boiling at 53.9^{o}C, while the maximum boiling product is AZ2, the azeotrope of chloroform and acetone, boiling at 65.5^{o}C. To determine the feasible product compositions, one straight line is drawn from AZ1 to its intersection with distillation boundary B. Another straight line is drawn from AZ2 to its intersection with distillation boundary A. These two lines define an approximate bow-tie region through which a line from the feed point F to either pure chloroform and the ternary azeotrope (both infeasible products) does not pass. This approximate bow tie region is refined by adding a residue curve (or distillation curve) that passes through the feed point F. The final feasible product composition region is confined to the convex side of this added residue curve, as shown by the shaded bow-tie region. Typical bow-tie regions are shown for this system in the equilateral triangle diagram of Figure 11.12b. For the feed of this exercise, the feasible product composition regions are shown on an equilateral triangle residue curve map diagram, drawn by Aspen Plus, on the last page of this exercise.

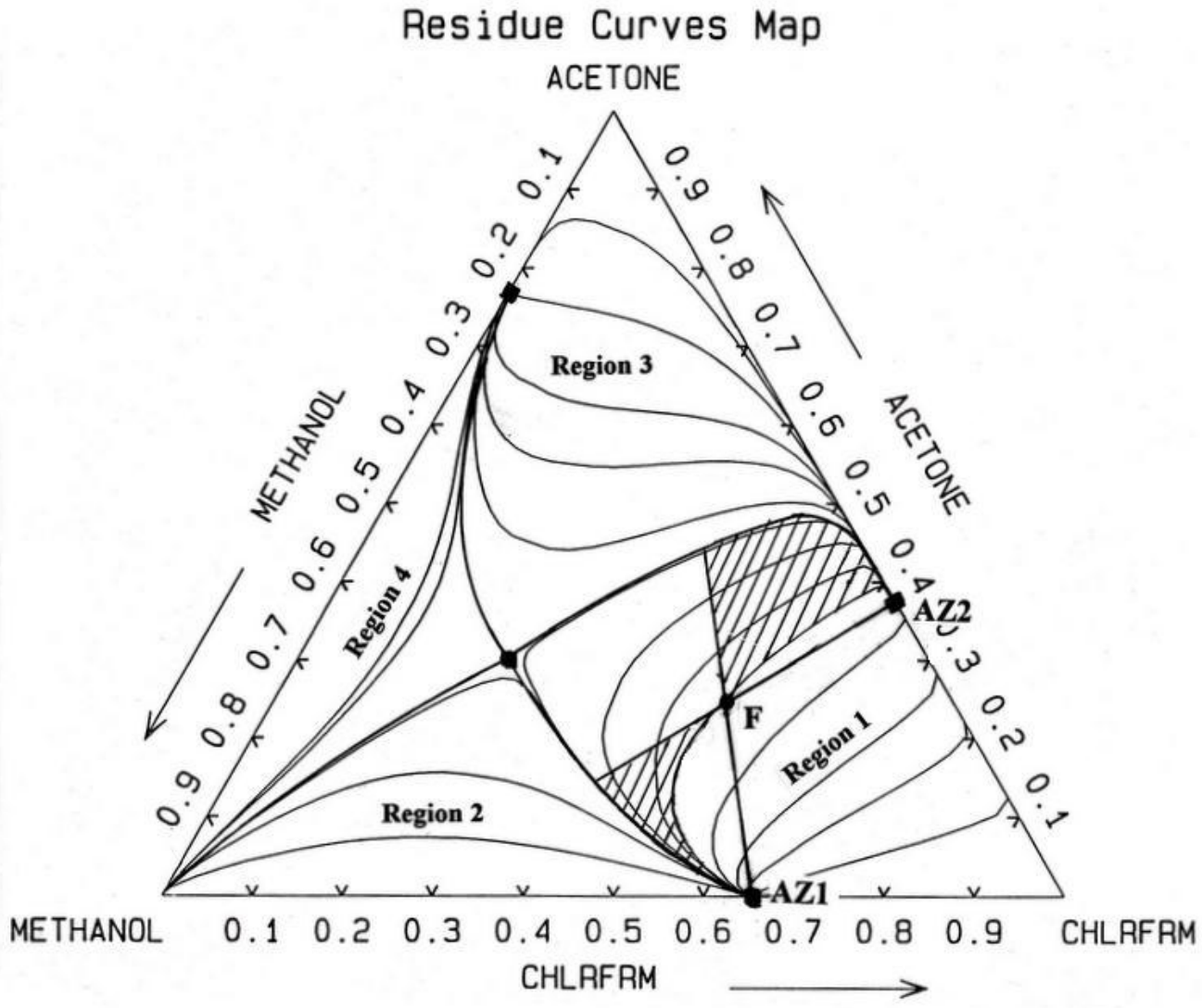
Exercise 11.8 (continued)

Analysis: (continued)



Exercise 11.8 (continued)

Analysis: (continued)



Exercise 11.9

Subject: Separation of acetone from methanol by extractive distillation with ethanol.

Given: Bubble-point feed of 30 mol/s acetone (A) and 10 mol/s methanol (M) at 1 atm. Ethanol (E) as the solvent. Results of Example 11.3 with a solvent of water.

Assumptions: Because the feed is close to the azeotropic composition of 22 mol% methanol, use a two-column system, with the first column being extractive distillation and the second ordinary distillation to recover the solvent. Column operations at 1 atm. UNIFAC for *K*-values. Negligible tray pressure drop. 100% tray efficiency.

Find: Suitable column designs to obtain an acetone product of at least 95 mol%, a methanol product of at least 98 mol%, and ethanol of 99.9 mol% purity for recycle.

Analysis: Extractive Distillation Column: First compute relative volatilities over a composition range to determine: (1) which of the two feed components is the most volatile in the presence of ethanol and (2) potential ease or difficulty of the separations. This is done with the LLVF three-phase flash model of Chemcad, which also detects any formation of a second liquid phase, by conducting a series of flashes at 1 atm and a $V/F = 0.0001$ (a near bubble-point condition), for different mole fractions of the two feed components. For all cases, the mole fraction of the solvent, ethanol, is fixed at 0.5 so as to have a strong effect on the liquid-phase activity coefficients of acetone and methanol. The flash model computes the *K*-values, from which the relative volatilities can be obtained. Since acetone and methanol boil at 56.5°C and 64.7°C, respectively, and methanol is closer in structure to ethanol than is acetone, it is expected that the volatility of acetone to methanol will be increased in the presence of ethanol The following results confirm this expectation:

x_A	K_A	K_M	K_E	$\alpha_{A\text{-}M}$	$\alpha_{A\text{-}E}$
0.475	1.444	1.043	0.576	1.38	2.51
0.375	1.579	1.019	0.561	1.55	2.81
0.250	1.832	1.032	0.568	1.78	3.23
0.125	2.234	1.105	0.613	2.02	3.64
0.025	2.746	1.233	0.692	2.23	3.97

Although these relative volatilities are favorable, they are not as high as those obtained when water is used as the solvent. Nevertheless, an initial run was made using the same arrangement of stages as in Example 11.3, a solvent rate equal to 60 mol/s, entering as a liquid at 60°C, and a reflux ratio of 4. The following results were obtained using the SCDS model of Chemcad, with an assumed bottoms rate of 68.774 mol/s, as computed in Example 11.3:

Exercise 11.9 (continued)

Analysis (continued)

	Mole fractions:	
Component	**Distillate**	**Bottoms**
Acetone, A	0.8801	0.0366
Methanol, M	0.0379	0.1282
Ethanol, E	0.0820	0.8352

The desired separation is not achieved. The distillate contains too much methanol and ethanol, while the bottoms contains too much acetone. The acetone recovery is only 70.3%. In Example 11.3, it is 99.5%. Therefore, the stage, reflux, and solvent rate were increased in increments until the specification for acetone purity, and a high acetone recovery were met. The following Chemcad SCDS results, for the listed conditions, satisfy the product specifications, but other combinations of stages, reflux, and solvent rate could also give satisfactory results:

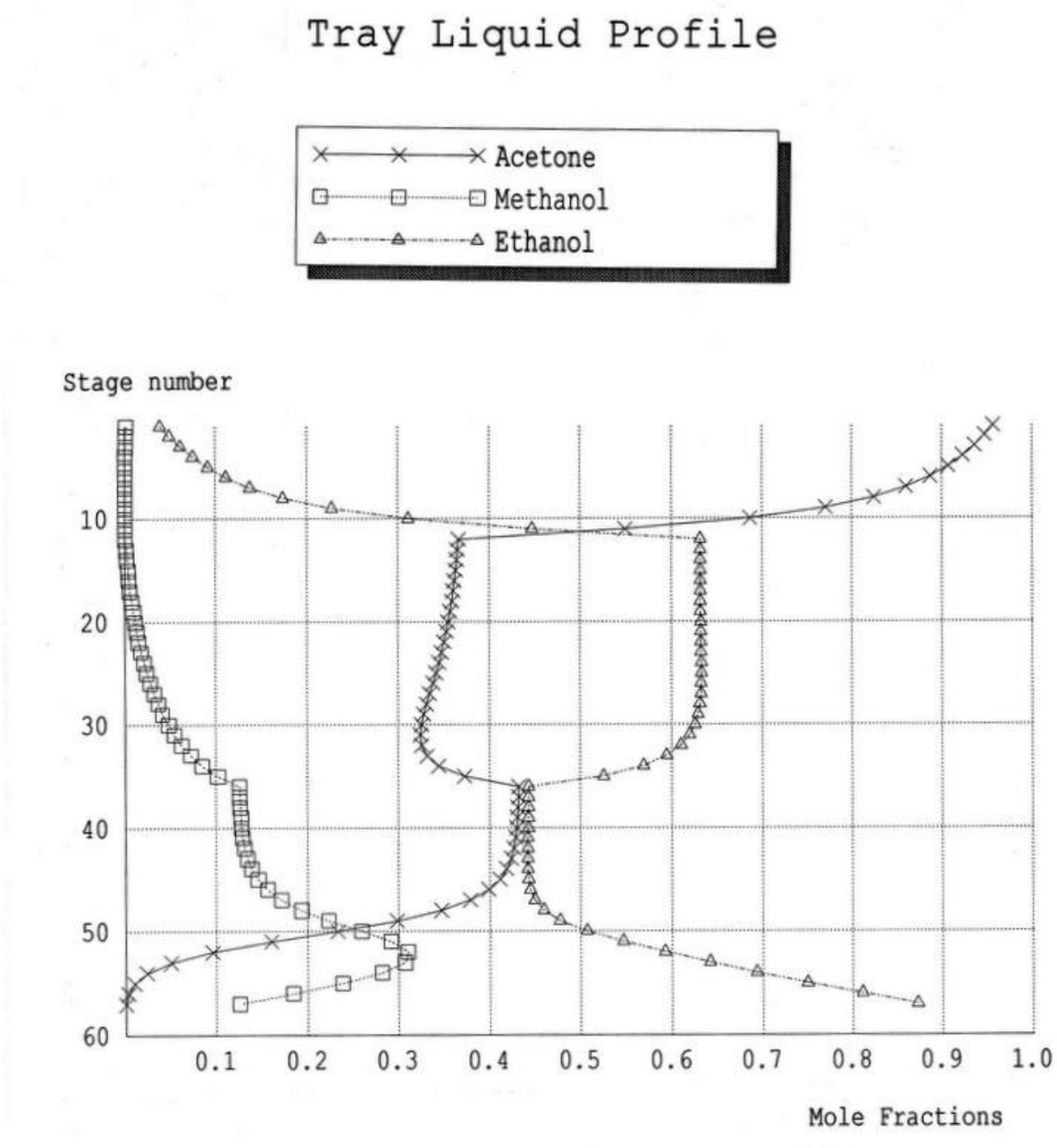
Number of stages = 57 (includes total condenser and partial reboiler)
Solvent enters stage 12 from the top
Feed enters stage 36 from the top Reflux ratio = 5
Bottoms flow rate = 78.774 mol/s Solvent flow rate = 70 mol/s
Initial guesses:
Distillate rate = 108 kmol/h Reflux rate = 540 kmol/h
Temperatures: Stage 1, 55°C Stage 57, 75°C Stage 2, 60°C Stage 56, 70°C
Convergence was achieved in 34 iterations with the following material balance:

	Solvent	**Feed**	**Distillate**	**Bottoms**
Temperature, °C	60	55.2	56.3	75.4
Flow rates, mol/s:				
Acetone	0	30	29.87	0.13
Methanol	0	10	0.11	9.89
Ethanol	70	0	1.24	68.76
Total:	70	40	31.22	78.78

The liquid phase composition profile is shown on the next page. The extractive distillation column was sized with Chemcad for sieve trays, with:
24-inch tray spacing 12% downcomer area 10% hole area
1/4-inch holes 80% of flooding
The resulting column inside diameter was determined to be 7 feet, which gives 79.5% of flooding at the top tray and 72.2% of flooding at the bottom.
The tray pressure drop averages 0.094 psi/tray, for a total of 5.2 psi or 0.35 atm for the 55 trays. Thus, the assumption of negligible tray pressure drop is not satisfactory. For a final design, the computations should be repeated taking into account tray pressure drop and tray efficiency.

Exercise 11.9 (continued)

Analysis (continued)



Exercise 11.9 (continued)

Analysis (continued)

Ordinary Distillation Column: This column separates the bottoms from the extractive distillation column to obtain 98 mol% methanol and 99.9 mol% ethanol. A starting point for this separation is obtained by using the ShortCut Column (FUG) model of Chemcad with an operating reflux ratio of 1.3 times the minimum ratio. The feed is assumed to be at the bubble point. To achieve the purity specifications, a preliminary material balance gives:

	mol/s:		
Component	**Feed**	**Distillate**	**Bottoms**
Acetone	0.13	0.13	0.00
Methanol	9.89	9.82	0.07
Ethanol	68.76	0.07	68.69
Total:	78.78	10.02	68.76

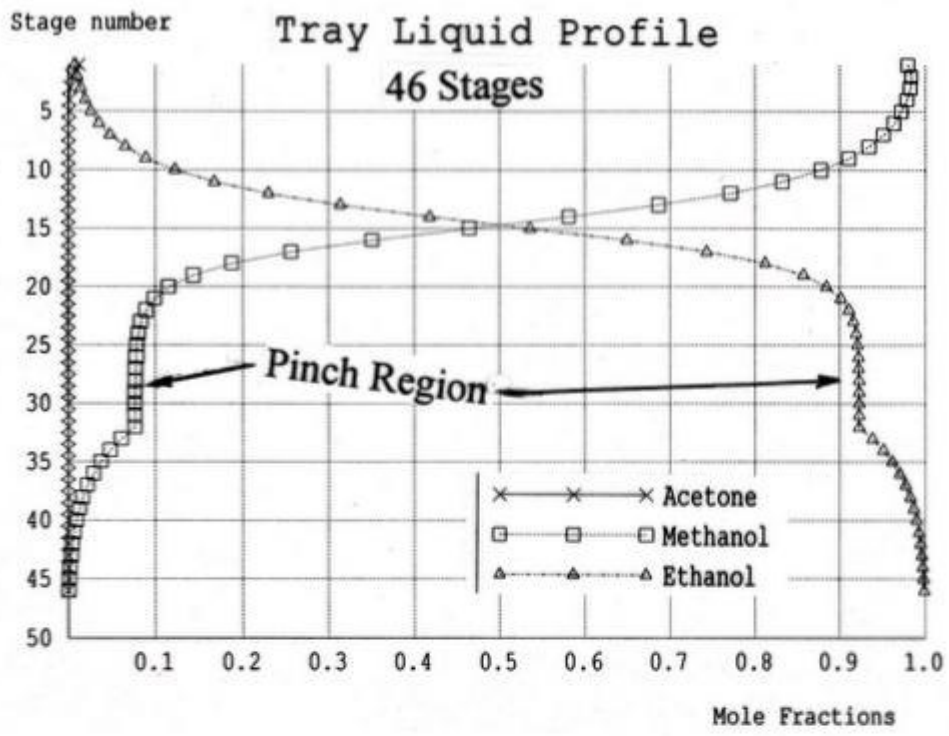
The specifications for the ShortCut Column model are 0.982/0.989 = 0.993 for the LK (methanol) and 0.07/68.76 = 0.001 for the HK (ethanol). The results are:
Minimum number of equilibrium stages = 24.6
Minimum reflux ratio = 11.9
Reflux ratio = 1.3(11.9) = 15.5
Number of equilibrium stages = 44.4
Feed stage location (Kirkbride equation) = 31 from the top

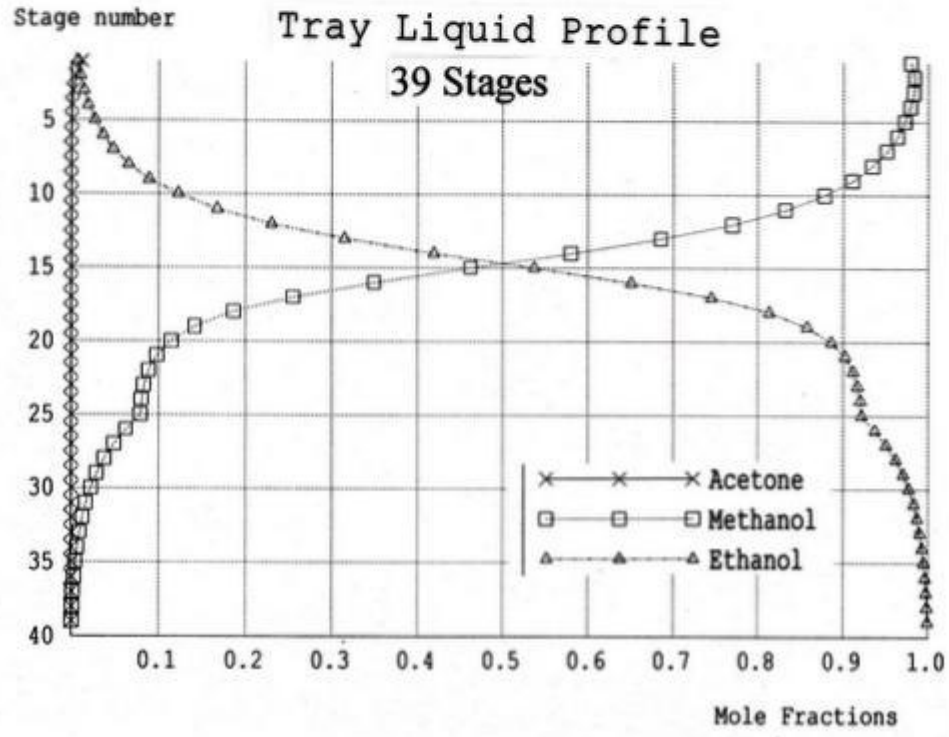
The SCDS Column model of the Chemcad program was then used to make a rigorous calculation based on the following input data:
Pressure constant at 1 atm
Number of stages = 46 (includes the total condenser and the partial reboiler)
Feed stage = 32
Methanol purity in the distillate = 98 mol%
Ethanol purity in the bottoms = 99.9 mol%
Estimated distillate rate = 36.1 kmol/h (10.03 mol/s)
Estimated reflux rate = 560 kmol/h (155.6 mol/s or a reflux ratio of 15.5)
Estimated temperatures: Stage 1, 64°C Stage 46, 78°C Stage 2, 65°C Stage 45, 75°C

A converged result was obtained in 6 iterations, with a computed reflux ratio of 14.9, compared to the above 15.5 estimate by the Underwood equations. However, as shown in the composition profile on the next page, a pinch region (where no composition changes occur) of approximately 7 stages is evident just above the feed stage. Accordingly, the calculations with the SCDS Column model were repeated by removing 7 stages above the feed, resulting in the following new input:
Number of stages = 39 (includes the total condenser and the partial reboiler)
Feed stage = 25
A converged result was obtained in 5 iterations, with a computed reflux ratio of 15.0, just slightly greater. The composition profile for this run also appears on the next page. No pinch is evident.

Exercise 11.9 (continued)

Analysis (continued)





Exercise 11.9 (continued)

Analysis (continued)

The ordinary distillation column for separating methanol from ethanol was sized with Chemcad for sieve trays, with:

24-inch tray spacing 12% downcomer area 10% hole area
1/4-inch holes 80% of flooding

The resulting column inside diameter was determined to be 6.5 feet, which gives 60.0% of flooding at the top tray and 72.4% of flooding at the bottom.

The tray pressure drop averages 0.091 psi/tray, for a total of 3.4 psi or 0.23 atm for the 37 trays. Thus, the assumption of negligible tray pressure drop is not satisfactory. For a final design, the computations should be repeated taking into account tray pressure drop and tray efficiency.

The final material balance for the ordinary distillation column was as follows:

	mol/s:		
Component	**Feed**	**Distillate**	**Bottoms**
Acetone	0.13	0.13	0.00
Methanol	9.89	9.82	0.07
Ethanol	68.76	0.07	68.69
Total:	78.78	10.02	68.76

Because the flow rate of ethanol in the bottoms is only 68.69 mol/s and 70.00 is needed for the extractive distillation column, the makeup ethanol rate is 70.00 - 68.69 = 1.31 mol/s.

Comparison with Example 11.3:

In Example 11.3, water is used as the solvent. It is much more effective than the ethanol solvent used in this exercise, as shown by the following comparison:

Item	**Water solvent**	**Ethanol solvent**
Solvent flow rate, mol/s	60	70
Solvent makeup rate, mol/s	1.4	1.31
Equilibrium stages in extractive distillation column	28	56
Equilibrium stages in ordinary distillation column	16	36
Diameter of extractive distillation column, feet	6	7
Diameter of ordinary distillation column, feet	2.5	6.5

Exercise 11.10

Subject: Separation of acetone from methanol by extractive distillation with methyl-ethyl-ketone (MEK)

Given: Bubble-point feed of 30 mol/s acetone (A) and 10 mol/s methanol (M) at 1 atm. MEK (K) as the solvent. Results of Example 11.3 with a solvent of water.

Assumptions: Because the feed is close to the azeotropic composition of 22 mol% methanol, use a two-column system, with the first column being extractive distillation and the second ordinary distillation to recover the solvent. UNIFAC for *K*-values. Negligible tray pressure drop. 100% tray efficiency.

Find: Suitable column designs to obtain an acetone product of at least 95 mol%, a methanol product of at least 98 mol%, and MEK of 99.9 mol% purity for recycle.

Analysis: Extractive Distillation Column: First compute relative volatilities over a composition range to determine: (1) which of the two feed components is the most volatile in the presence of MEK and (2) potential ease or difficulty of the separations. This is done with the LLVF three-phase flash model of Chemcad, which also detects any formation of a second liquid phase, by conducting a series of flashes at 1 atm and a $V/F = 0.0001$ (a near bubble-point condition), for different mole fractions of the two feed components. For all cases, the mole fraction of the solvent, MEK, is fixed at 0.5 so as to have a strong effect on the liquid-phase activity coefficients of acetone and methanol. The flash model computes the *K*-values, from which the relative volatilities can be obtained as given below. Since acetone and methanol boil at 56.5°C and 64.7°C, respectively, but acetone is closer in structure to MEK than is methanol, it is difficult to predict which of the two feed components will be the more volatile. At high concentrations of acetone, methanol is more volatile, while at high concentrations of methanol, acetone is more volatile.

x_A	K_A	K_M	K_K	$\alpha_{M\text{-}A}$	$\alpha_{M,K}$
0.475	1.345	1.877	0.629	1.40	2.98
0.375	1.310	1.616	0.613	1.23	2.64
0.250	1.331	1.415	0.627	1.06	2.26
0.125	1.413	1.301	0.671	0.92	1.94
0.025	1.524	1.255	0.731	0.82	1.72

Of greater importance, however, is the fact that UNIFAC predicts, at 1 atm, that MEK forms a minimum-boiling azeotrope with methanol at 64.0°C, with a mole fraction of methanol equal to 0.844. Thus, MEK is a questionable solvent for extractive distillation because on the ternary diagram for 1 atm pressure, a distillation boundary will connect the A-M azeotrope with the M-K azeotrope, similar to Fig. 11.5, where a distillation boundary connects the benzene-isopropanol

Exercise 11.10

Analysis: (Extractive Distillation Column continued)

azeotrope with the benzene-n-propanol azeotrope. For extractive distillation, a residue curve map similar to that in Fig. 11.14 is needed.

As shown in Fig. 11.22, some azeotropes are pressure sensitive, such that if the pressure is changed sufficiently the azeotrope disappears. As shown in the following table, based on the UNIFAC equation, the M-K azeotrope shows a favorable shift with pressure, while the A-M azeotrope does not. Above about 6 atm, the methanol-MEK azeotrope disappears.

Pressure, atm	0.3	1	3	5	10	15	25
	Mole% methanol in azeotrope:						
A-M azeotrope	6	22	40	50	62	70	80
M-K azeotrope	74	84	94	99	-	-	-

Thus, as shown by Knapp and Doherty in Ref. 34 of Chapter 11, a mixture of acetone and methanol can be separated by extractive distillation with MEK by operating the extractive distillation column (Column 1) at an elevated pressure so as eliminate the M-K azeotrope and to obtain, as will be shown, a distillate of 98 mol% methanol, followed by sending the bottoms to ordinary distillation (Column 2) at 1 atm to obtain a distillate of 95 mol% acetone and a bottoms of 99.9 mol% MEK for recycle. The two columns were designed with the SCDS (simultaneous correction) model of Chemcad leading to the following final material balance, which satisfies the product purity specifications:

	Mol/s:					
Component	**Feed**	**Solvent**	**Column 1 distillate**	**Column 1 bottoms**	**Column 2 distillate**	**Column 2 bottoms**
Acetone	30		0.016	29.984	29.924	0.060
Methanol	10		8.526	1.474	1.474	0.000
MEK		60	0.158	59.842	0.101	59.741
Total:	40	60	8.700	91.300	31.499	59.801
Temp, ^{o}C	144.9	145	144.6	169.5	55.8	79.1

The pressure of the extractive distillation column (Column 1) was set at 12 atm, with a solvent rate of 60 mol/s at 145^{o}C. The following Chemcad SCDS results, for the listed conditions, was obtained after 11 iterations. The resulting product compositions are those in the above table. Other combinations of stages, reflux, and solvent rate could also give satisfactory results:

Number of stages = 60 (includes total condenser and partial reboiler)
Solvent enters stage 20 from the top
Feed enters stage 40 from the top Acetone mole fraction in distillate = 0.98
Bottoms flow rate = 91.3 mol/s Solvent flow rate = 60 mol/s at 145^{o}C
Initial guesses: Distillate rate = 8 mol/s Reflux rate = 80 mol/s
Temperatures: Stage 1, 145^{o}C Stage 60, 170^{o}C Stage 2, 145^{o}C Stage 59, 160^{o}C

Exercise 11.10

Analysis: (Extractive Distillation Column continued)

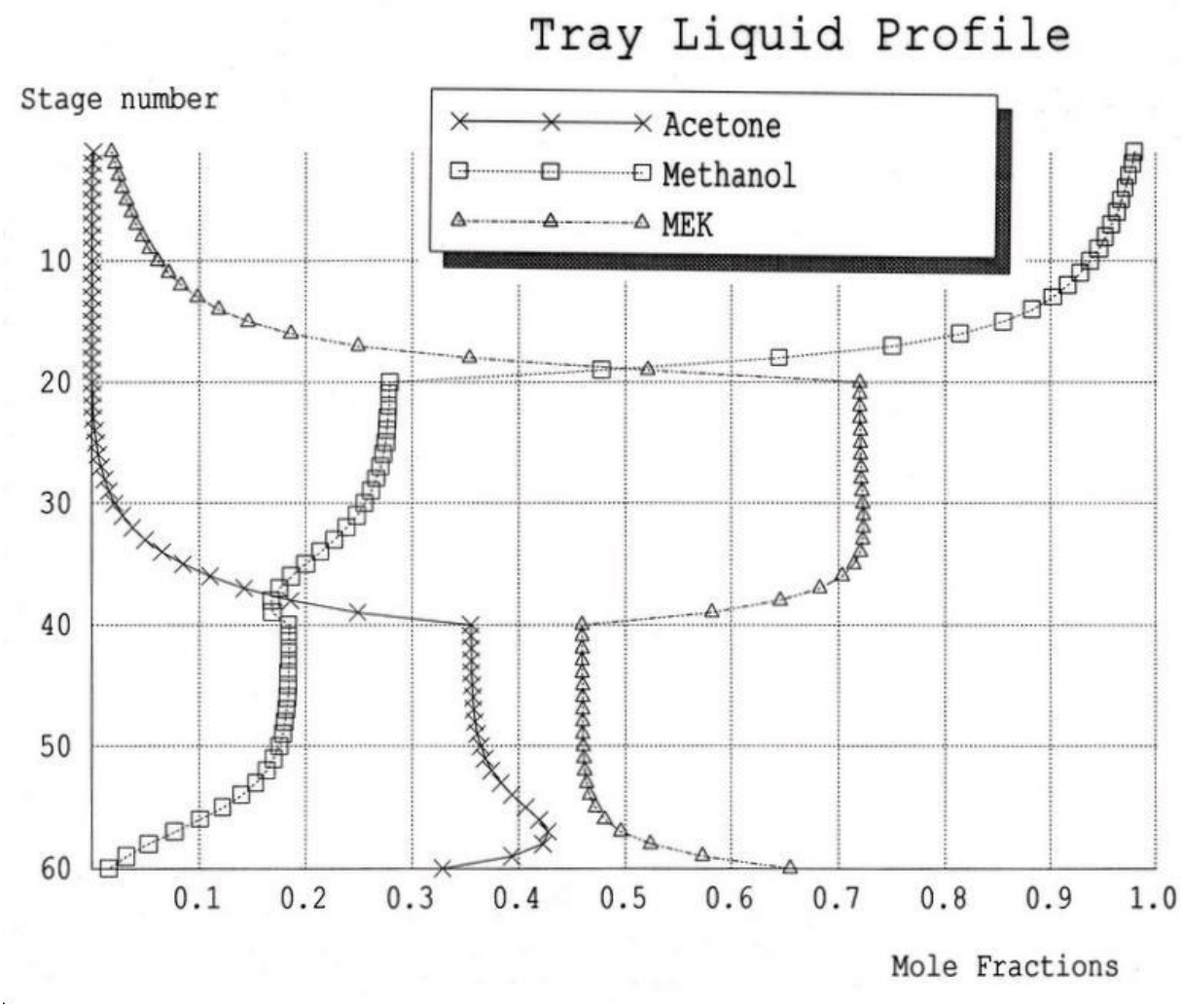
The reflux ratio was computed to be 8.083.

The liquid phase composition profile is shown below. The extractive distillation column was sized with Chemcad for sieve trays, with:

24-inch tray spacing 12% downcomer area 10% hole area

1/4-inch holes 80% of flooding

The resulting column inside diameter was determined to be 5 feet. For a final design, the computations should be repeated taking into account tray pressure drop, tray efficiency, and impurity in the MEK solvent.



Exercise 11.10 (continued)

Analysis: (continued)

Ordinary Distillation Column: This column, at a pressure of 1 atm, separates the bottoms from the extractive distillation column to obtain 95 mol% acetone and 99.9 mol% MEK. A starting point for this separation is obtained by using the ShortCut Column (FUG) model of Chemcad with an operating reflux ratio of 1.3 times the minimum ratio. The feed is assumed to be at the bubble point. Thus, the bottoms from Column 1 at 169.5°C and 12 atm is cooled and decompressed to 68.7°C and 1 atm. Using the above material balance table, the specifications for the ShortCut Column model are 29.924/29.984 = 0.998 for the recovery of the LK (methanol) to the distillate and 0.101/59.842 = 0.0169 for the recovery of the HK (MEK). The results are:
Minimum number of equilibrium stages = 17.7
Minimum reflux ratio = 2.52
Reflux ratio = 1.3(2.52) = 3.28
Number of equilibrium stages = 34.1
Feed stage location (Kirkbride equation) = 18 from the top

The SCDS Column model of the Chemcad program was then used to make a rigorous calculation based on the following input data:
Pressure constant at 1 atm
Number of stages = 35 (includes the total condenser and the partial reboiler)
Feed stage = 20 from the top
Acetone purity in the distillate = 95 mol%
MEK purity in the bottoms = 99.9 mol%
Estimated distillate rate = 31.4 mol/s
Estimated reflux rate = 109.9 mol/s (reflux ratio of 3.5)
Estimated temperatures: Stage 1, 64°C Stage 35, 78°C Stage 2, 65°C Stage 34, 75°C

A converged result was obtained in 5 iterations, with a computed reflux ratio of 3.69, compared to the above 3.5 estimate by the Underwood equations. The composition profile appears on the next page.
The ordinary distillation column for separating acetone from MEK was sized with Chemcad for sieve trays, with:
24-inch tray spacing 12% downcomer area 10% hole area
1/4-inch holes 80% of flooding
The resulting column inside diameter was determined to be 7.0 feet. For a final design, the computations should be repeated taking into account tray pressure drop and tray efficiency.

From the above material balance table, the flow rate of MEK in the bottoms of Column 2 is only 59.80 mol/s, while 60.00 is needed for the extractive distillation column, the makeup MEK rate is 60.00 - 59.74 = 0.26 mol/s.

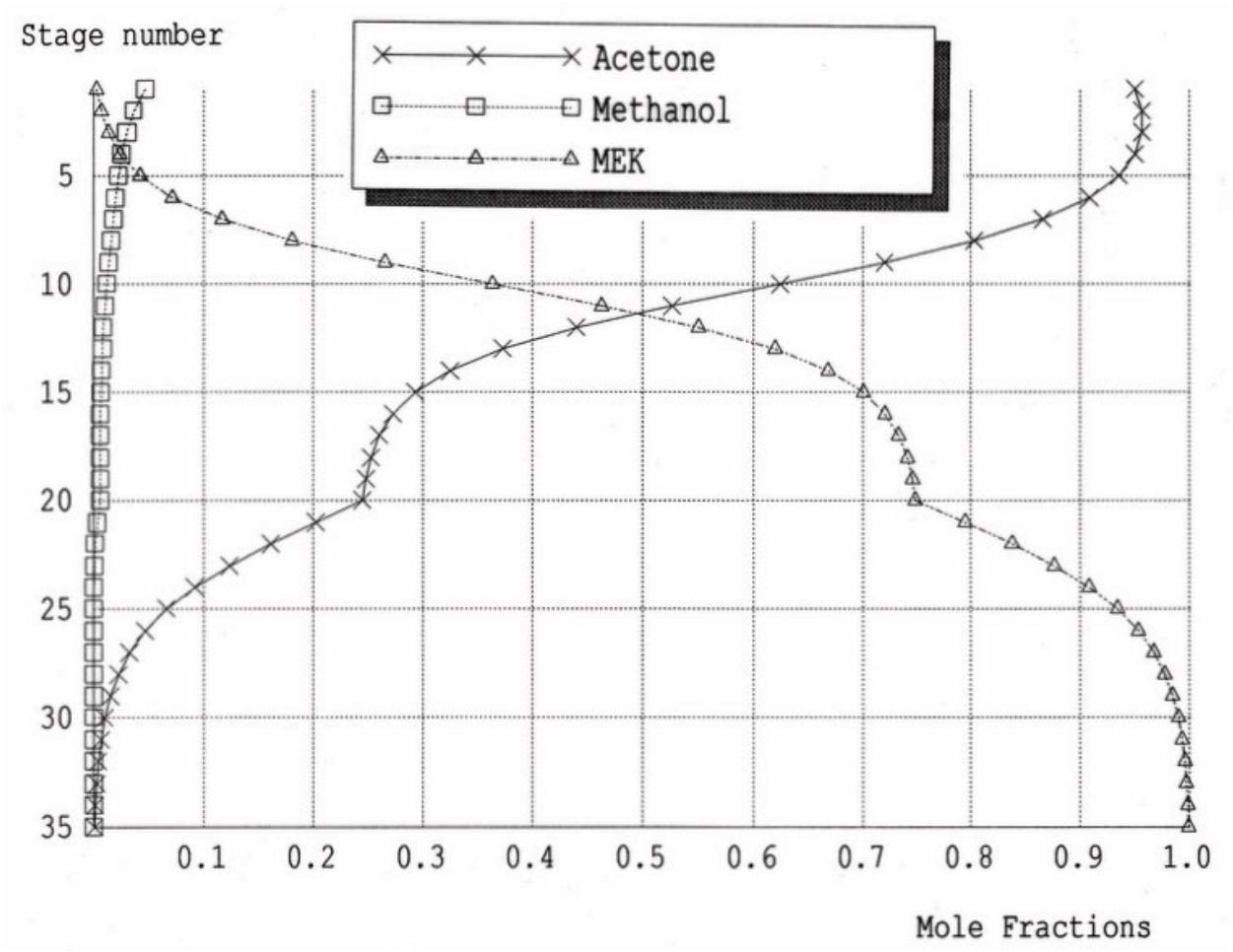
Exercise 11.10 (continued)

Analysis: (continued)

Comparison with Example 11.3:

In Example 11.3, water is used as the solvent. The following comparison shows that water is preferred over MEK.

Item	Water solvent	MEK solvent
Solvent flow rate, mol/s	60	60
Solvent makeup rate, mol/s	1.4	0.26
Equilibrium stages in extractive distillation column	28	59
Equilibrium stages in ordinary distillation column	16	34
Diameter of extractive distillation column, feet	6	5
Diameter of ordinary distillation column, feet	2.5	7
Operating pressure in extractive distillation	1	12



Exercise 11.11

Subject: Separation of acetone from methanol by extractive distillation with toluene

Given: Bubble-point feed of 30 mol/s acetone (A) and 10 mol/s methanol (M) at 1 atm. Toluene (T) as the solvent. Results of Example 11.3 with a solvent of water.

Assumptions: Because the feed is close to the azeotropic composition of 22 mol% methanol, use a two-column system, with the first column being extractive distillation and the second ordinary distillation to recover the solvent. UNIFAC for *K*-values. Negligible tray pressure drop. 100% tray efficiency.

Find: Suitable column designs to obtain an acetone product of at least 95 mol%, a methanol product of at least 98 mol%, and toluene of 99.9 mol% purity for recycle.

Analysis: Of great importance here is the fact that UNIFAC predicts, at 1 atm, that toluene forms a minimum-boiling azeotrope with methanol at 63.8°C, with a mole fraction of methanol equal to 0.891. Thus, toluene is a questionable solvent for extractive distillation because on the residue curve map for 1 atm pressure, shown on the next page, a distillation boundary connects the A-M azeotrope with the M-T azeotrope, similar to Fig. 11.5, where a distillation boundary connects the benzene-isopropanol azeotrope with the benzene-n-propanol azeotrope. For extractive distillation, a residue curve map similar to that in Fig. 11.14 is needed.

As shown in Fig. 11.22, some azeotropes are pressure sensitive, such that if the pressure is changed sufficiently the azeotrope disappears. Unfortunately, over the pressure range of 0.3 atm to 25 atm, neither the A-M azeotrope nor the M-T azeotrope disappears. Therefore, it is concluded that the use of toluene can not produce a distillate of either acetone or methanol by extractive distillation. To confirm this, two runs were made with the SCDS model of Chemcad for the conditions below. The runs differed only in the bottoms mole flow specification, with Case 1 being the sum of the toluene solvent and the acetone in the feed, in an attempt to obtain a distillate of methanol. For Case 2 the bottoms mole flow specification was the sum of the toluene and the methanol in the feed, in an attempt tot obtain a distillate of acetone. The results, given on the next page, confirm the effect of the distillation boundary. In Case 1, the distillate is not methanol, but is close to the distillation boundary near the M-T azeotrope. In Case 2, the distillate is not acetone, but is close to the distillation boundary and near the A-M azeotrope.

Solvent (toluene) flow rate = 60 mol/s 60°C
Pressure constant at 1 atm
Number of stages = 46 (includes the total condenser and the partial reboiler)
Solvent stage = 10 from the top
Feed stage = 30 from the top
Reflux ratio = 5
Bottoms mole flow rate: Case 1, 90 mol/s Case 2, 70 mol/s
Estimated distillate rate: Case 1, 10 mol/s Case 2, 30 mol/s
Estimated reflux rate: Case 1, 50 mol/s Case 2, 150mol/s (reflux ratio of 5)
Estimated temperatures: Stage 1, 55°C Stage 46, 75°C Stage 2, 60°C Stage 45, 70°C

Exercise 11.11 (continued)

Analysis: (continued)
Case 1 material balance:

	mol/s			
Component	**Solvent**	**Feed**	**Distillate**	**Bottoms**
Acetone		30	0.07	29.93
Methanol		10	8.74	1.26
Toluene	60		1.19	58.81
Total:	60	40	10.00	90.00

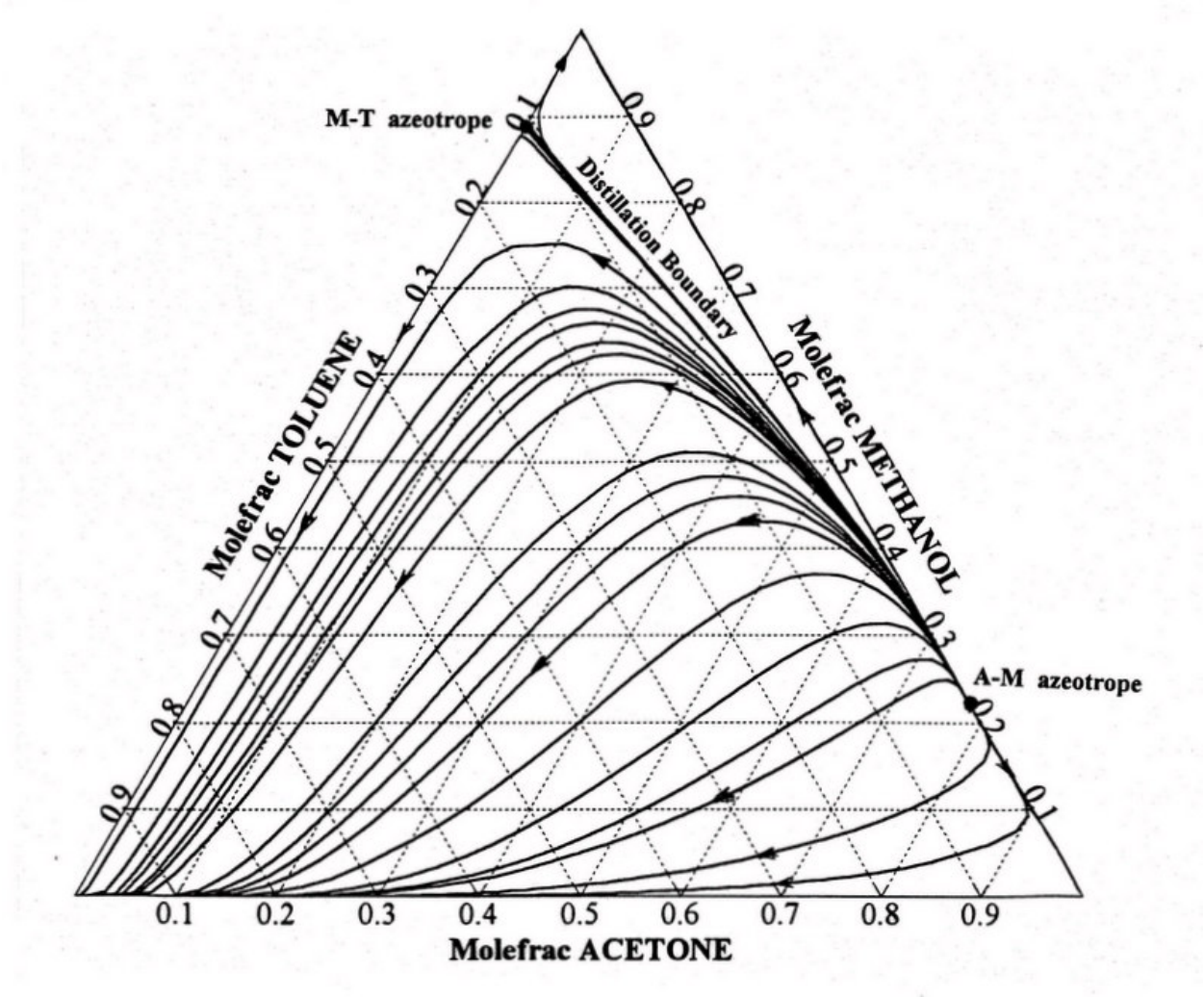
Case 2 material balance:

	mol/s			
Component	**Solvent**	**Feed**	**Distillate**	**Bottoms**
Acetone		30	19.98	10.02
Methanol		10	10.00	0.00
Toluene	60		0.02	59.98
Total:	60	40	30.00	70.00

For both cases, most of the methanol moves to the distillate because, in the presence of a substantial fraction of toluene, methanol is more volatile than acetone.

Exercise 11.11 (continued)

Analysis: (continued)



Exercise 11.12

Subject: Separation of n-heptane from toluene by extractive distillation with phenol.

Given: 400 lbmol/h of a feed of an equimolar mixture at 200°F and 20 psia of n-heptane and toluene. 1200 lbmol/h of phenol solvent at 20 psia and 220°F.

Assumptions: . Column operations at 20 psia UNIFAC for *K*-values. Negligible tray pressure drop. 100% tray efficiency.

Find: Suitable column designs to obtain reasonable product purities, with only a small loss of solvent.

Analysis:

Using the vapor pressure data in Chemcad, the boiling points at 20 psia are found to be: 229.1°F for n-heptane, 251.4°F for toluene, and 379.0°F for phenol. Thus, n-heptane appears to be the most volatile component. Although n-heptane and toluene do not form an azeotrope at 20 psia, their relative volatility at high concentrations of n-heptane is almost 1.0. Therefore, ordinary distillation of the mixture is not practical. Phenol does not form an azeotrope with either n-heptane or toluene, and with its higher boiling point is a possible solvent. Its selection is further enhanced because, as might be expected on molecular structure considerations, phenol at say a mole fraction in the liquid of 0.5 causes a larger liquid-phase activity coefficient for n-heptane than for toluene. For example, for 50 mol% phenol in the liquid and at low concentrations of toluene, the relative volatility of n-heptane with respect to toluene is about 1.7. At low concentrations of n-heptane and 50 mol% phenol in the liquid, the relative volatility of n-heptane with respect to toluene is even higher at about 2.8. Thus, phenol makes the separation of n-heptane and toluene quite favorable.

Extractive Distillation Column:

The following Chemcad results, using the Tower (inside-out) model, give a reasonable n-heptane distillate product. Convergence was achieved in 15 iterations. Other combinations of stages, reflux, and solvent and feed stage locations could also give satisfactory results.

Number of stages = 21 (includes total condenser and partial reboiler)

Solvent enters stage 6 from the top Feed enters stage 13 from the top

Reflux ratio = 5 Bottoms flow rate = 1400 lbmol/h (based on toluene + phenol)

Initial guesses: Distillate rate = 200 lbmol/h Reflux rate = 1000 lbmol/h

Temperatures: Stage 1, 200°F Stage 21, 300°F Stage 2, 220°F

Convergence was achieved in 34 iterations with the following material balance:

	Solvent	Feed	Distillate	Bottoms
Temperature, °F	220	200	229.2	323.4
Flow rates, lbmol/h:				
n-Heptane	0	200	198.2	1.8
Toluene	0	200	1.2	198.8
Phenol	1200	0	0.6	1199.4

Exercise 11.12 (continued)

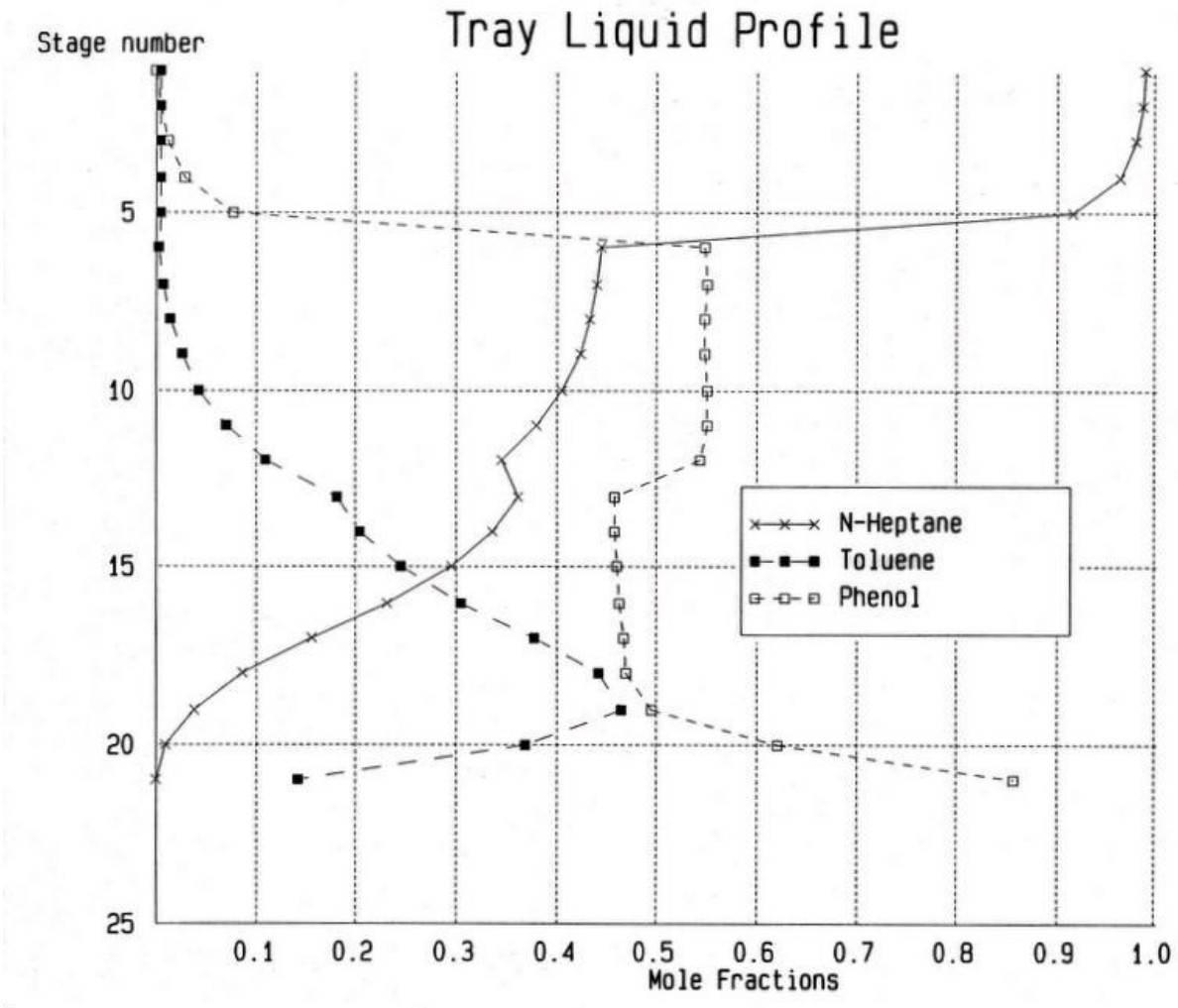
Analysis: Extractive Distillation Column (continued)

The liquid phase composition profile is shown below. The condenser and reboiler duties are 15.99 million Btu/h and 24.30 milllion Btu/h, respectively. The extractive distillation column was sized with Chemcad for sieve trays, with:

24-inch tray spacing	12% downcomer area	10% hole area
1/4-inch holes	80% of flooding	

The resulting column inside diameter was determined to be 8 feet

For a final design, the computations should be repeated taking into account tray pressure drop and tray efficiency.



Exercise 11.12 (continued)

Analysis: (continued)

Ordinary Distillation Column to separate toluene from phenol:

A starting point for this separation is obtained by using the ShortCut Column (FUG) model of Chemcad with an operating reflux ratio of 1.3 times the minimum ratio, with an operating pressure of 20 psia. The feed is assumed to be at the bubble point. To achieve reasonable product purities, the following material balance is assumed:

	lbmol/h:		
Component	**Feed**	**Distillate**	**Bottoms**
n-Heptane	1.8	1.8	0.00
Toluene	198.8	196.8	2.0
Phenol	1199.4	1.2	1198.2
Total:	1400.0	199.8	1200.2

The specifications for the ShortCut Column model are 196.8/198.8 = 0.99 for the recovery of toluene to the distillate, and 1.2/1199.4 = 0.001 for the recovery to the distillate of phenol.
The results are:
Minimum number of equilibrium stages = 7.7
Minimum reflux ratio = 1.50
Reflux ratio = 1.3(1.50) = 1.95
Number of equilibrium stages = 15.5
Feed stage location (Kirkbride equation) = 11.4 from the top

The Tower model of the Chemcad program is then used to make a rigorous calculation based on the following input data, using the FUG results:
Pressure constant at 20 psia.
Number of stages = 16 (includes the total condenser and the partial reboiler)
Feed stage = 12 from the top
Reflux ratio = 2
Bottoms mole flow rate = 1200 lbmol/h
Estimated distillate rate = 200 lbmol/h
Estimated reflux rate = 400 lbmol/h
Estimated temperatures: Stage 1, 200°F Stage 16, 300°F Stage 2, 220°F

A converged result, which showed a slightly better separation than specified for the FUG method, was obtained in 17 iterations: However, as shown in the composition profile on the next page, a pinch region (where no composition changes occur) of approximately 3 stages is evident just above the feed stage. Accordingly, the calculations with the Tower model were repeated by removing 3 stages above the feed, resulting in the following new input:
Number of stages = 13 (includes the total condenser and the partial reboiler)
Feed stage = 9

Exercise 11.12 (continued)

Analysis: Ordinary Distillation Column (continued)

A converged result was obtained in 17 iterations, with little change in the separation. The composition profile for this run appears on the next page. No pinch is evident.
The ordinary distillation column for separating methanol from ethanol was sized with Chemcad for sieve trays, with:

24-inch tray spacing	12% downcomer area	10% hole area
1/4-inch holes	80% of flooding	

The resulting column inside diameter was determined to be 5.5 feet. The condenser duty was computed to be 8.53 million Btu/h, with a reboiler duty of 11.70 million Btu/h. For a final design, the computations should be repeated taking into account tray pressure drop and tray efficiency.

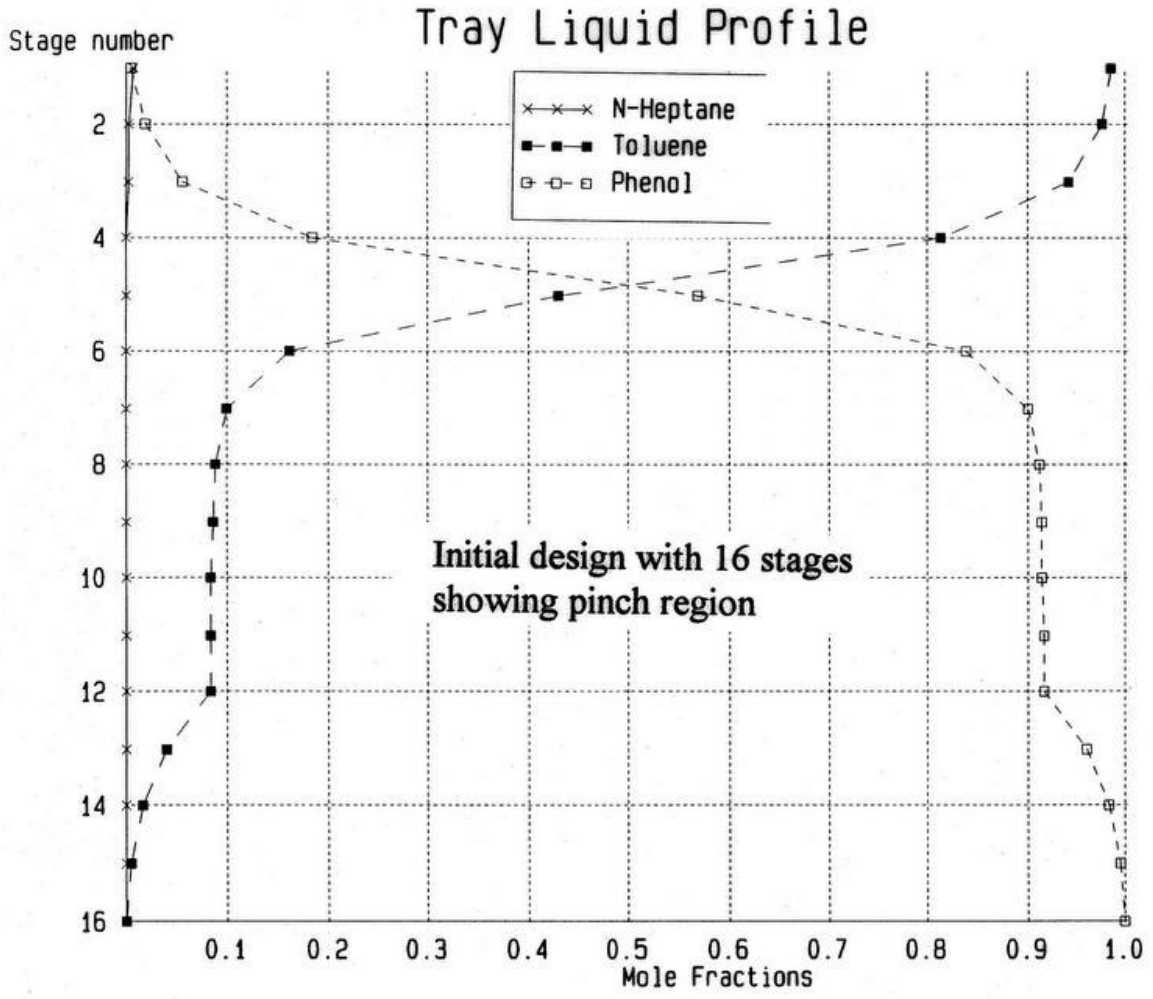
The final material balance for the ordinary distillation column was as follows:

	lbmol/h:		
Component	**Feed**	**Distillate**	**Bottoms**
n-Heptane	1.8	1.8	0.00
Toluene	198.8	197.0	1.8
Phenol	1199.4	1.2	1198.2
Total:	1400.0	200.0	1200.0
Temp., ^{o}F	323.3	251.0	378.2

Because the flow rate of phenol in the bottoms is only 1198.2 lbmol/h and 1200.0 is needed for the extractive distillation column, the makeup phenol rate is 1200.0 - 1198.2 = 1.8 lbmol/h.

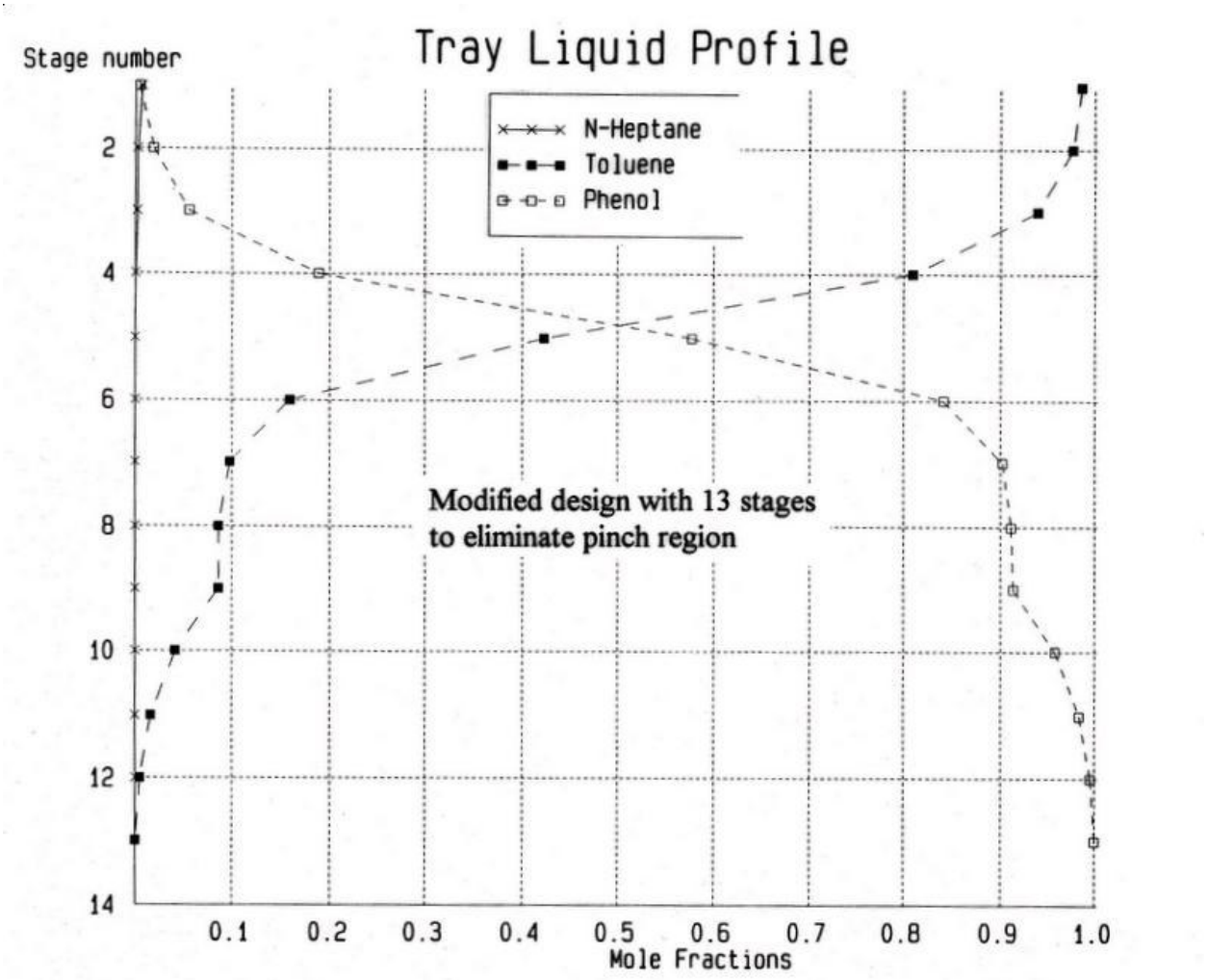
Exercise 11.12 (continued)

Analysis: Ordinary Distillation Column (continued)



Exercise 11.12 (continued)

Analysis: Ordinary Distillation Column (continued)



Exercise 11.13

Subject: Separation of a mixture of ethanol and benzene by pressure-swing distillation.

Given: Feed of 100 mol/s of 55 mol% ethanol and 45 mol% benzene at the bubble point at 101.3 kPa. Desired products are 99 mol% ethanol and 99 mol% benzene.

Assumptions: UNIFAC method for estimating *K*-values.

Find: Feasible design using pressure-swing distillation in the manner of Example 11.5 and Fig. 11.23(b).

Analysis: Use the two-column system of Fig. 11.23(b). Ethanol and benzene form a minimum-boiling azeotrope. Use the same column pressures as in Example 11.5. Therefore, in Column 1, the pressures are 26 kPa at the condenser outlet, 30 kPa at the top tray, and 40 kPa at the reboiler. The distillate product is the near azeotrope at 30 kPa and the bottoms product is 99 mol% ethanol. In Column 2, the pressures are 106kPa before the condenser, 101.3 kPa after the condenser, and 120 kPa at the reboiler. The distillate product is the near azeotrope at 101.3 kPa and the bottoms product is 99 mol% benzene. Using the Chemcad program with the UNIFAC method, the azeotrope compositions in mol% ethanol are 35.7 at 26 kPa, and 45.2 at 101.3 kPa.

A major factor in the design of a pressure-swing distillation system is the recycle-to-feed ratio, D_2/F in Fig. 11.23(b), which is related to compositions as follows:

Let x be the mole fraction of ethanol in any stream. Referring to Fig. 11.23(b), an overall system material balance for total flows gives: $F = B_1 + B_2$ (1)

An overall system balance on ethanol gives: $x_F F = x_{B_1} B_1 + x_{B_2} B_2$ (2)

A total material balance around Column 2 gives: $D_1 = D_2 + B_2$ (3)

An ethanol balance around Column 2 gives: $x_{D_1} D_1 = x_{D_2} D_2 + x_{B_2} B_2$ (4)

Substitute Eq. (1) into (2) to eliminate B_1. After rearrangement,

$$F = B_2 \left(\frac{x_{B_1} - x_{B_2}}{x_{B_1} - x_F} \right) \tag{5}$$

Substitute Eq. (3) into (4) to eliminate D_1. After rearrangement,

$$D_2 = B_2 \left(\frac{x_{D_1} - x_{B_2}}{x_{D_2} - x_{D_1}} \right) \tag{6}$$

Combine Eqs. (5) and (6) to eliminate B_1. After rearrangement, the recycle ratio is:

$$\frac{D_2}{F} = \left(\frac{x_{B_1} - x_F}{x_{B_1} - x_{B_2}} \right) \left(\frac{x_{D_1} - x_{B_2}}{x_{D_2} - x_{D_1}} \right) \tag{7}$$

In the limit, for pure bottoms products and azeotropic distillate products, Eq. (7) reduces to:

$$\frac{D_2}{F} = (1 - x_F) \left(\frac{x_{\mathrm{Az}_1}}{x_{\mathrm{Az}_2} - x_{\mathrm{Az}_1}} \right) \tag{8}$$

Exercise 11.13 (continued)

Analysis: (continued)

Eq. (8) shows that the recycle ratio is sensitive to the feed composition and the azeotropic compositions at the pressures of Columns 1 and 2. The smaller the difference between the two azeotropic compositions, the larger the recycle ratio.

For this exercise, $x_F = 0.55$, $x_{B_1} = 0.99$, and $x_{B_2} = 0.01$

Let $x_{D_1} = 0.37$, which is slightly greater than the azeotropic mole fraction of 0.357.

Let $x_{D_2} = 0.44$, which is slightly smaller than the azeotropic mole fraction of 0.452.

Substituting these 5 mole-fraction values into Eq. (7) gives $D_2/F = 2.309$. Therefore D_2 = 230.90 mol/s. Using Eqs. (1) to (6), the following material balance is obtained for the system:

Stream:	***F***	***D*$_2$**	***F*$_1$**	***B*$_1$**	***D*$_1$**	***B*$_2$**
Flow rate, mol/s:						
Ethanol	55	101.60	156.60	54.55	102.05	0.45
Benzene	45	129.30	174.30	0.55	173.75	44.45
Total:	100	230.90	330.90	55.10	275.80	44.90
mol% Ethanol:	55	44	47.33	99	37	1

The design of the two columns was made with the Chemcad program, using the Shortcut Column model (FUG method) to obtain initial estimates of stage and reflux requirements, followed by the SCDS Column or TOWER rigorous model to finalize the designs.

Column 1:

Using the above material balance, with a combined feed, F_1, the specifications for the ShortCut Column model are 173.75/174.3 = 0.997 for the recovery of benzene to the distillate, and 102.05/156.6 = 0.652 for the recovery to the distillate of ethanol. Thus, it is expected that little rectification is necessary.

The results are:

Minimum number of equilibrium stages = 6.23

Minimum reflux ratio = very small and probably in error. Therefore, the Gilliland correlation was not reliable.

The SCDS Column model of the Chemcad program was then used to make a rigorous calculation based initially on the following input data, using the FUG results, with $N = 2 \times N_{min}$.

A guess of R is made:

Pressures as stated above.

Number of stages = 12 (includes the total condenser and the partial reboiler)

Feed stage for recycle, D_2 = 4 from the top

Entry for feed, F = 6 from top

Reflux ratio = 0.5

Bottoms mole flow rate = 55.1 mol/s

Estimated distillate rate = 275.76 mol/s

Estimated reflux rate = 138 mol/s

Estimated temperatures: Stage 1, 35°C Stage 12, 40°C Stage 2, 36°C Stage 11, 39°C

Exercise 11.13 (continued)

Analysis: Column 1 (continued)

A converged result, which gave a 99.8 mol% purity of ethanol in the bottoms, was obtained in 10 iterations. A purity of only 99 mol% was needed. This indicated that the reflux could be reduced. Accordingly, using the profiles from the first rigorous run, a second run was made with a column top specification of D = 173.75 mol/s in place of the reflux specification. A converged result, with the desired 99 mol% ethanol purity in B_1, was obtained at a reflux ratio of 0.279 in 24 iterations. The material balance was in agreement with the above table. Although the feed locations could probably be improved, no pinch region is evident, as shown in the liquid-phase composition profile on the next page. Also included on the next page are the column profiles for temperature, liquid flow, and vapor flow.

Column 1 was sized with Chemcad for sieve trays, with:

24-inch tray spacing 12% downcomer area 10% hole area
1/4-inch holes 80% of flooding

The resulting column inside diameter was determined to be 12 feet. The condenser duty was computed to be 12.91 MW, with a reboiler duty of 11.58 MW. For the 10 theoretical plates, the total pressure drop was computed to be 8.2 kPa. For a final design, the computations should be repeated taking into account tray pressure drop and tray efficiency.

Column 2:

Using the above material balance table, the specifications for the ShortCut Column model are 101.60/102.05 = 0.9956 for the recovery of ethanol to the distillate, and 129.30/173.75 = 0.7442 for the recovery to the distillate of benzene. Thus, it is again expected that little rectification is necessary. The feed to Column 2 is the distillate from Column 1 after being pumped to a pressure of 120 kPa for entry into Column 2 and heating to the bubble point at that pressure.

The results are:

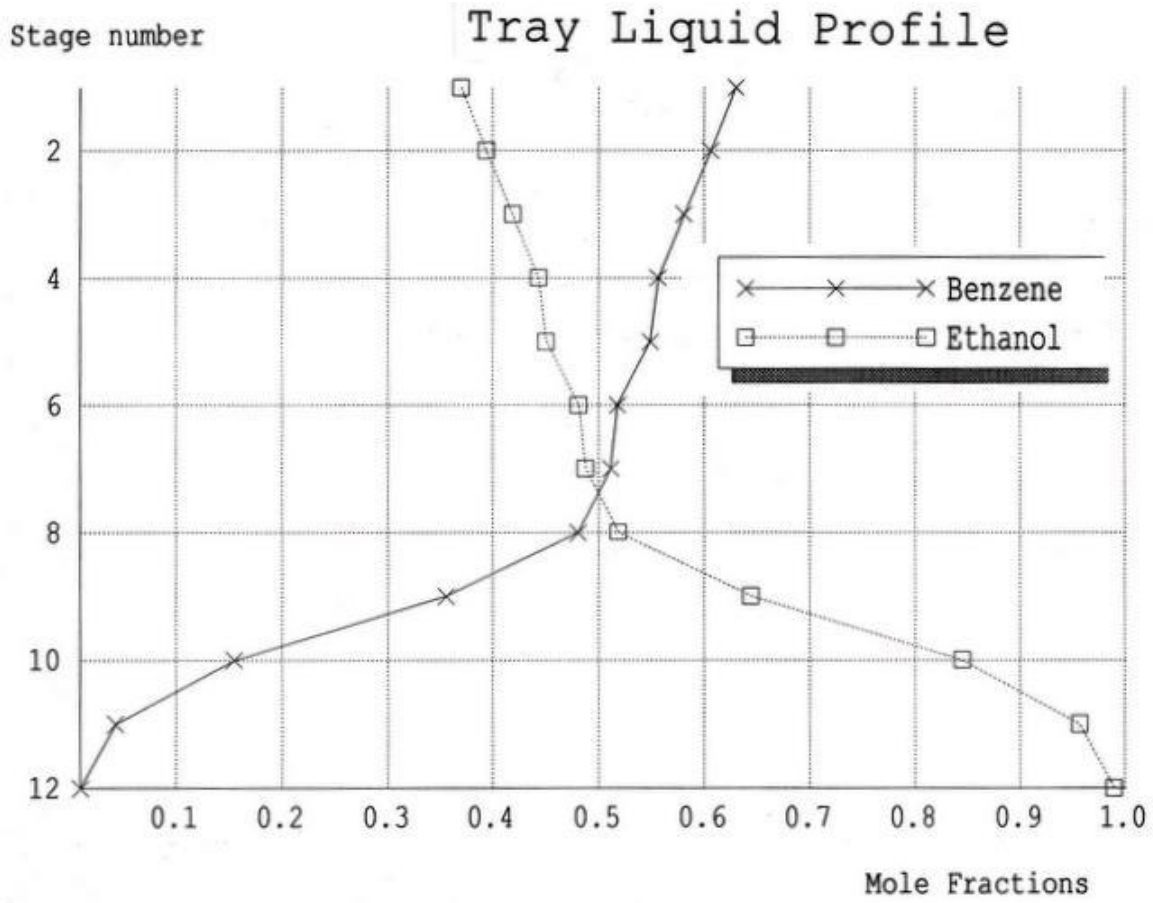
Minimum number of equilibrium stages = 5.0
Minimum reflux ratio = very small and probably in error. Therefore, the Gilliland correlation was not reliable.

The SCDS Column model of the Chemcad program experienced convergence difficulties and was replaced with the TOWER model, which also experienced difficulty until the following specifications were made with a damping factor of 0.7.

Pressures as stated above.
Number of stages = 6 (includes the total condenser and the partial reboiler)
Entry for feed = 2 from top (giving in effect a reboiled stripper with some reflux)
Distillate flow rate of ethanol = 101.60 mol/s
Bottoms mole flow rate = 44.9 mol/s
Estimated distillate rate = 230.90 mol/s
Estimated reflux rate = 23 mol/s (corresponding to a small reflux ratio of 0.1)
Estimated temperatures: Stage 1, 67°C Stage 6, 80°C Stage 2, 70°C

Exercise 11.13 (continued)

Analysis: Column 1 (continued)



Stg	Temp C	Pres kPa	* Net Flows * Liquid mol/sec	Vapor mol/sec	Feeds mol/sec	Product mol/sec
1	34.4	26.00	76.97			275.76
2	37.6	30.00	76.90	352.74		
3	38.4	31.00	76.16	352.66		
4	39.1	32.00	281.93	351.92	230.86	
5	39.8	33.00	281.67	326.83		
6	40.5	34.00	371.72	326.57	100.00	
7	41.2	35.00	371.63	316.62		
8	41.9	36.00	369.25	316.53		
9	43.0	37.00	358.43	314.15		
10	46.8	38.00	344.86	303.33		
11	52.4	39.00	341.62	289.76		
12	55.5	40.00		286.52		55.10

Exercise 11.13 (continued)

Analysis: Column 2 (continued)

A converged result was obtained in 21 iterations, with a small reflux ratio of 0.16 or 36.9 mol/s. The material balance was in agreement with the above table. Although the feed location could probably be improved, no pinch region is evident, as shown in the liquid-phase composition profile below. Also included are the column profiles for temperature, liquid flow, and vapor flow.

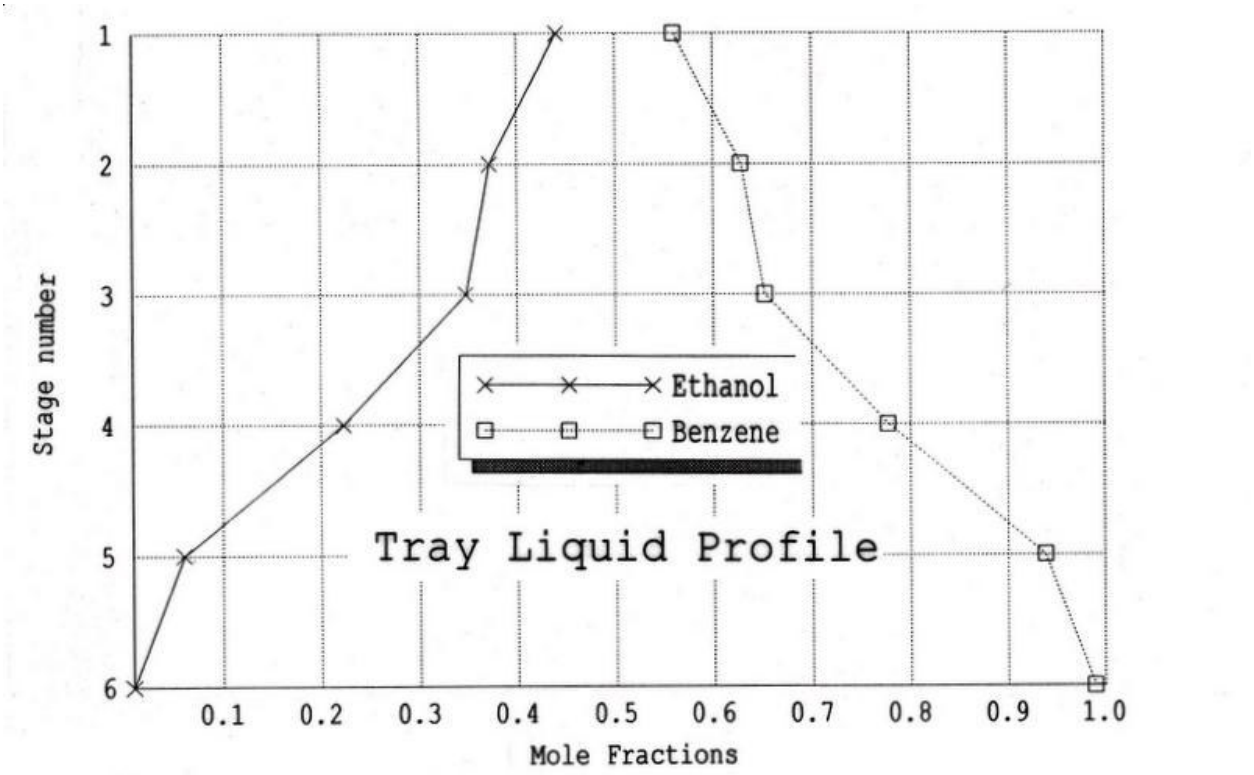
Column 2 was sized with Chemcad for sieve trays, with:

24-inch tray spacing	12% downcomer area	10% hole area
1/4-inch holes	80% of flooding	

The resulting column inside diameter was determined to be 9 feet. The condenser duty was computed to be 9.38 MW, with a reboiler duty of 9.30 MW. For the 4 theoretical plates, the total pressure drop was computed to be 3.9kPa. For a final design, the computations should be repeated taking into account tray pressure drop and tray efficiency.

Exercise 11.13 (continued)

Analysis: Column 2 (continued)



			* Net Flows *			
	Temp	Pres	Liquid	Vapor	Feeds	Product
Stg	C	kPa	mol/sec	mol/sec	mol/sec	mol/sec
1	67.6	101.30	36.91			230.90
2	68.9	106.00	308.51	267.80	275.80	
3	69.9	109.50	310.69	263.61		
4	71.3	113.00	317.86	265.79		
5	76.6	116.50	332.40	272.96		
6	83.6	120.00		287.50		44.90

Exercise 11.14

Subject: Separation of a mixture of ethanol and benzene by pressure-swing distillation.

Given: Feed of 100 mol/s of 20 mol% ethanol and 80 mol% benzene at the bubble point at 101.3 kPa. Desired products are 99 mol% ethanol and 99 mol% benzene.

Assumptions: UNIFAC method for estimating *K*-values.

Find: Feasible design using pressure-swing distillation in the manner of Example 11.5.

Analysis: Use the two-column system of Fig. 11.23(b). Ethanol and benzene form a minimum-boiling azeotrope. Use the same column pressures as in Example 11.5. Therefore, in Column 1, the pressures are 26 kPa at the condenser outlet, 30 kPa at the top tray, and 40 kPa at the reboiler. The distillate product is the near azeotrope at 30 kPa and the bottoms product is 99 mol% ethanol. In Column 2, the pressures are 106kPa before the condenser, 101.3 kPa after the condenser, and 120 kPa at the reboiler. The distillate product is the near azeotrope at 101.3 kPa and the bottoms product is 99 mol% benzene. Using the Chemcad program with the UNIFAC method, the azeotrope compositions in mol% ethanol are 35.7 at 26 kPa, and 45.2 at 101.3 kPa.

A major factor in the design of a pressure-swing distillation system is the recycle-to-feed ratio, D_2/F in Fig. 11.23(b), which is related to compositions as follows:

Let x be the mole fraction of ethanol in any stream. Referring to Fig. 11.23(b), an overall system material balance for total flows gives: $F = B_1 + B_2$ (1)

An overall system balance on ethanol gives: $x_F F = x_{B_1} B_1 + x_{B_2} B_2$ (2)

A total material balance around Column 2 gives: $D_1 = D_2 + B_2$ (3)

An ethanol balance around Column 2 gives: $x_{D_1} D_1 = x_{D_2} D_2 + x_{B_2} B_2$ (4)

Substitute Eq. (1) into (2) to eliminate B_1. After rearrangement,

$$F = B_2 \left(\frac{x_{B_1} - x_{B_2}}{x_{B_1} - x_F} \right) \tag{5}$$

Substitute Eq. (3) into (4) to eliminate D_1. After rearrangement,

$$D_2 = B_2 \left(\frac{x_{D_1} - x_{B_2}}{x_{D_2} - x_{D_1}} \right) \tag{6}$$

Combine Eqs. (5) and (6) to eliminate B_1. After rearrangement, the recycle ratio is:

$$\frac{D_2}{F} = \left(\frac{x_{B_1} - x_F}{x_{B_1} - x_{B_2}} \right) \left(\frac{x_{D_1} - x_{B_2}}{x_{D_2} - x_{D_1}} \right) \tag{7}$$

In the limit, for pure bottoms products and azeotropic distillate products, Eq. (7) reduces to:

$$\frac{D_2}{F} = (1 - x_F) \left(\frac{x_{\mathrm{Az}_1}}{x_{\mathrm{Az}_2} - x_{\mathrm{Az}_1}} \right) \tag{8}$$

Exercise 11.14 (continued)

Analysis: (continued)

Eq. (8) shows that the recycle ratio is sensitive to the feed composition and the azeotropic compositions at the pressures of Columns 1 and 2. The smaller the difference between the two azeotropic compositions, the larger the recycle ratio.

For this exercise, $x_F = 0.20$, $x_{B_1} = 0.99$, and $x_{B_2} = 0.01$

Let $x_{D_1} = 0.37$, which is slightly greater than the azeotropic mole fraction of 0.357.

Let $x_{D_2} = 0.44$, which is slightly smaller than the azeotropic mole fraction of 0.452.

Substituting these 5 mole-fraction values into Eq. (7) gives $D_2/F = 4.1457$. Therefore D_2 = 414.57 mol/s. This a very high recycle ratio. The system is technically feasible, but may not be economically attractive. Using Eqs. (1) to (6), the following material balance is obtained for the system:

Stream:	***F***	***D*₂**	***F*₁**	***B*₁**	***D*₁**	***B*₂**
Flow rate, mol/s:						
Ethanol	20	182.41	202.41	19.19	183.22	0.81
Benzene	80	232.16	312.16	0.20	311.96	79.80
Total:	100	414.57	514.57	19.39	495.18	80.61
mol% Ethanol:	20	44	39.3	99	37	1

The design of the two columns is made as follows with the Chemcad program, using the Shortcut Column model (FUG method) to obtain initial estimates of stage and reflux requirements, followed by the SCDS Column rigorous model to finalize the designs.

Column 1:

Using the above material balance, with a combined feed, F_1, the specifications for the ShortCut Column model are 311.96/312.96 = 0.9968 for the recovery of benzene to the distillate, and 183.22/202.41 = 0.9052 for the recovery to the distillate of ethanol. Thus, it is expected that little rectification is necessary. The results are:

Minimum number of equilibrium stages = 5.95

Minimum reflux ratio = very small and probably in error. Therefore, the Gilliland correlation was not reliable.

The SCDS Column model of the Chemcad program was then used to make a rigorous calculation. Based on several runs where the number of stages, the feed stage location, and the reflux ratio were varied, it was found that the separation was almost insensitive to the reflux ratio, indicating that little rectification was needed. However, attempts to configure the column as a reboiled stripper met with failure to converge. The following input data resulted in almost satisfying the specifications. Because the separation depended mainly on the number of stages, the specified separation could not be satisfied exactly.

Pressures as stated above.

Number of stages = 7 (includes the total condenser and the partial reboiler)

Feed stage for recycle, D_2 = 3 from the top

Entry for feed, F = 4 from top

Reflux ratio = 0.05

Bottoms mole flow rate = 19.39 mol/s

Exercise 11.14 (continued)

Analysis: Column 1 (continued)

Estimated distillate rate = 495.18 mol/s
Estimated reflux rate = 24.75 mol/s
Estimated temperatures: Stage 1, 35°C Stage 12, 55°C Stage 2, 40°C Stage 11, 50°C

A converged result, which gave just slightly less than the desired 99 mol% purity of ethanol in the bottoms, was obtained in 4 iterations. The material balance was almost in agreement with the above table. Although the feed locations could probably be improved, no pinch region is evident, as shown in the liquid-phase composition profile below. Also included on the this page are the column profiles for temperature, liquid flow, and vapor flow.

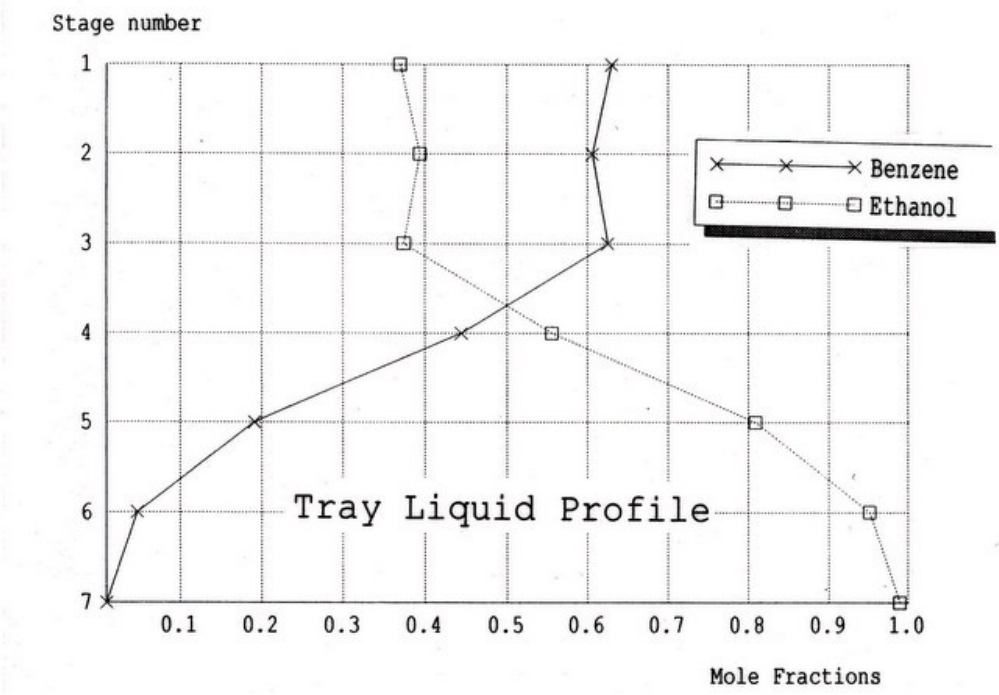
Column 1 was sized with Chemcad for sieve trays, with:

24-inch tray spacing	12% downcomer area	10% hole area
1/4-inch holes	80% of flooding	

The resulting column inside diameter was determined to be 14 feet. The condenser duty was computed to be 19.03 MW, with a reboiler duty of 16.42 MW. For the 5 theoretical plates, the total pressure drop was computed to be 4.9 kPa. For a final design, the computations should be repeated taking into account tray pressure drop and tray efficiency.

Exercise 11.14 (continued)

Analysis: Column 1 (continued)



			* Net Flows *			
Stg	Temp C	Pres kPa	Liquid mol/sec	Vapor mol/sec	Feeds mol/sec	Product mol/sec
1	34.4	26.00	24.76			495.18
2	37.6	30.00	23.39	519.94		
3	39.1	32.00	104.71	518.58	100.00	
4	40.7	34.00	454.08	499.89	414.57	
5	44.6	36.00	430.77	434.69		
6	51.5	38.00	424.89	411.38		
7	55.5	40.00		405.50		19.39

Exercise 11.14 (continued)

Analysis: (continued)

Column 2:

Using the above material balance table, the specifications for the ShortCut Column model are 182.41/183.22 = 0.9956 for the recovery of ethanol to the distillate, and 232.16/173.75 = 0.7442 for the recovery to the distillate of benzene. Thus, it is again expected that little rectification is necessary. The feed to Column 2 is the distillate from Column 1 after being pumped to a pressure of 120 kPa for entry into Column 2 and heating to the bubble point at that pressure.

The results are:

Minimum number of equilibrium stages = 5.0

Minimum reflux ratio = very small and probably in error. Therefore, the Gilliland correlation was not reliable.

The SCDS Column model of the Chemcad program experienced convergence difficulties and was replaced with the TOWER model, which also experienced difficulty until the following specifications were made with a damping factor of 0.7.

Pressures as stated above.

Number of stages = 6 (includes the total condenser and the partial reboiler)

Entry for feed = 2 from top (giving in effect a reboiled stripper with some reflux)

Distillate flow rate of ethanol = 182.41 mol/s

Bottoms mole flow rate = 80.61 mol/s

Estimated distillate rate = 414.57 mol/s

Estimated reflux rate = 41 mol/s (corresponding to a small reflux ratio of 0.1)

Estimated temperatures: Stage 1, 67°C Stage 6, 80°C Stage 2, 70°C

A converged result was obtained in 20 iterations, with a small reflux ratio of 0.155 or 64.1 mol/s. The material balance was in agreement with the above table. Although the feed location could probably be improved, no pinch region is evident, as shown in the liquid-phase composition profile on the next page. Also included on the next page are the column profiles for temperature, liquid flow, and vapor flow.

Column 2 was sized with Chemcad for sieve trays, with:

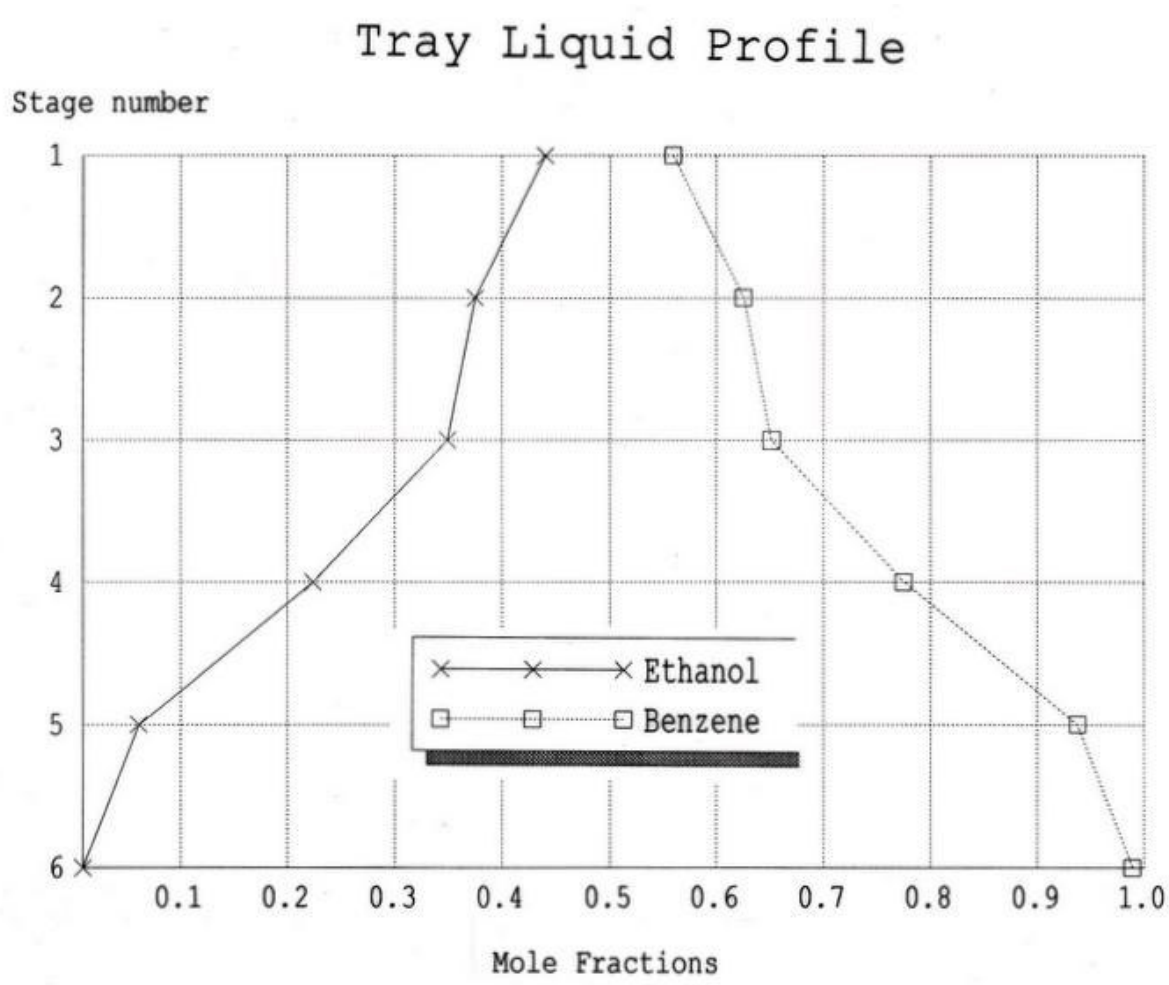
24-inch tray spacing 12% downcomer area 10% hole area

1/4-inch holes 80% of flooding

The resulting column inside diameter was determined to be 12 feet. The condenser duty was computed to be 16.76 MW, with a reboiler duty of 16.62 MW. For the 4 theoretical plates, the total pressure drop was computed to be 4.0 kPa. For a final design, the computations should be repeated taking into account tray pressure drop and tray efficiency.

Exercise 11.14 (continued)

Analysis: Column 2 (continued)



Stg	Temp C	Pres kPa	* Net Flows * Liquid mol/sec	Vapor mol/sec	Feeds mol/sec	Product mol/sec
1	67.6	101.30	64.09			414.57
2	68.9	106.00	551.74	478.66	495.18	
3	69.9	109.50	555.62	471.13		
4	71.3	113.00	568.42	475.01		
5	76.6	116.50	594.46	487.81		
6	83.6	120.00		513.85		80.61

Exercise 11.15

Subject: Separation of a mixture of ethanol and water by pressure-swing distillation.

Given: Feed of 100 mol/s of 30 mol% ethanol and 70 mol% water. Desired product is 99.8 mol% ethanol..

Assumptions: Feed at the bubble point at 120 kPa. Use of NRTL equation to obtain *K*-values using modified coefficients given below.

Find: Feasible design using pressure-swing distillation in the manner of Fig. 11.23(b).

Analysis: Use the two-column system of Fig. 11.23(b), except that for this system, the bottoms from Column 1 is nearly pure B (water), while the bottoms from Column 2 is nearly pure A (ethanol). Ethanol and water form a minimum-boiling azeotrope. Using Chemcad, the NRTL equation and the following binary interaction parameters, which were entered to override the stored parameters (I = ethanol, J= water, Bij = 246, Bji = -586, alpha = 0.3, Aij = -0.8, and Aji = 3.45), the predicted azeotropes are 89.3 mol% ethanol at 1 atm, 85.6 mol% ethanol at 300 kPa, and 94.3 mol% ethanol at 13 kPa. Agreement with experimental data is excellent at 1 atm, but not accurate at 13 kPa torr, where the azeotrope composition is about 97 mol%. Thus, the following calculations using the NRTL equation will not be as accurate as would be desired. For Column 1, set the pressures at 13 kPa at the condenser outlet, 15 kPa at the top tray, and 30 kPa at the reboiler. Specify a Column 1 distillation composition of 92.5 mol% ethanol compared to the predicted azeotropic composition of 94.3 mol%. Let the ethanol composition of the bottoms from Column 1 be 0.0001 mol% ethanol, because, as will be shown, it is easy to obtain a very high water purity. For Column 2, set the pressures at 300 kPa at the condenser outlet, 305 kPa at the top tray, and 375 kPa at the reboiler. Specify a distillation composition of 88 mol% ethanol compared to the predicted azeotrope of 85.6 mol% ethanol. The bottoms from Column 2 is specified as 99.8 mol% ethanol.

A major factor in the design of a pressure-swing distillation system is the recycle-to-feed ratio, D_2/F in Fig. 11.23(b), which is related to compositions as follows:

Let x be the mole fraction of ethanol in any stream. Referring to Fig. 11.23(b), an overall system material balance for total flows gives: $F = B_1 + B_2$ (1)

An overall system balance on ethanol gives: $x_F F = x_{B_1} B_1 + x_{B_2} B_2$ (2)

A total material balance around Column 2 gives: $D_1 = D_2 + B_2$ (3)

An ethanol balance around Column 2 gives: $x_{D_1} D_1 = x_{D_2} D_2 + x_{B_2} B_2$ (4)

Substitute Eq. (1) into (2) to eliminate B_1. After rearrangement,

$$F = B_2 \left(\frac{x_{B_1} - x_{B_2}}{x_{B_1} - x_F} \right) \qquad (5)$$

Exercise 11.15 (continued)

Analysis: (continued)

Substitute Eq. (3) into (4) to eliminate D_1. After rearrangement,

$$D_2 = B_2\left(\frac{x_{D_1} - x_{B_2}}{x_{D_2} - x_{D_1}}\right) \qquad (6)$$

Combine Eqs. (5) and (6) to eliminate B_1. After rearrangement, the recycle ratio is:

$$\frac{D_2}{F} = \left(\frac{x_{B_1} - x_F}{x_{B_1} - x_{B_2}}\right)\left(\frac{x_{D_1} - x_{B_2}}{x_{D_2} - x_{D_1}}\right) \qquad (7)$$

In the limit, for pure bottoms products and azeotropic distillate products, Eq. (7) reduces to:

$$\frac{D_2}{F} = x_F\left(\frac{1 - x_{\mathrm{Az}_1}}{x_{\mathrm{Az}_1} - x_{\mathrm{Az}_2}}\right) \qquad (8)$$

Eq. (8) shows that the recycle ratio is sensitive to the feed composition and the azeotropic compositions at the pressures of Columns 1 and 2. The smaller the difference between the two azeotropic compositions, the larger the recycle ratio.

For this exercise, $x_F = 0.30$, $x_{B_1} = 0.0001$, and $x_{B_2} = 0.998$

$x_{D_1} = 0.925$, which is slightly greater than the azeotropic mole fraction of 0.943.

$x_{D_2} = 0.88$, which is slightly smaller than the azeotropic mole fraction of 0.856.

Substituting these 5 mole-fraction values into Eq. (7) gives $D_2/F = 0.4876$. Therefore D_2 = 48.76 mol/s. This a modest recycle ratio. Using Eqs. (1) to (6), the following material balance is obtained for the system:

Stream:	***F***	***D*₂**	***F*₁**	***B*₁**	***D*₁**	***B*₂**
Flow rate, mol/s:						
Ethanol	30	42.91	72.91	0.00007	72.91	30.00
Water	70	5.85	75.85	69.94	5.91	0.06
Total:	100	48.76	148.76	69.94	78.82	30.06
mol% Ethanol:	30	88	49.0	0.0001	92.5	99.8

The design of the two columns was made as follows with the Chemcad program, by making rough estimates of tray and reflux requirements, followed by use of the SCDS Column or Tower rigorous models to finalize the designs.

Column 1:

Using the TPXY plot feature of Chemcad, it was found that the relative volatility, α, for ethanol with respect to water, at 13 kPa, varies widely over the composition range, from 1.020 at 92.5 mol% ethanol to 12.0 at 0.0001 mol% ethanol, both mole fractions in the liquid phase. Accordingly, it was believed that the FUG method would not give reliable estimates of stages and reflux. To obtain rough estimates of the stage requirements and feed locations, the Fenske equation (9-11) was applied to each of the three sections of the column, as summarized in the following table, using a pressure of 13 kPa rather than taking into account pressure drop.

Exercise 11.15 (continued)

Analysis: Column 1 (continued)

Location or Column section	Mole fraction ethanol in liquid	Relative volatility ethanol to water	Geometric average relative volatility	Minimum stages by Fenske equation
Overhead	0.925	1.020		
Overhead to Feed 1			1.05	10.7
Feed 1	0.88	1.086		
Feed 1 to Feed 2			1.97	2.2
Feed 2	0.30	3.587		
Feed 2 to Bottoms			6.56	5.2
Bottoms	0.000001	12.0		

The minimum stages were multiplied by about 2 to obtain the following estimates of equilibrium stages for input to the SCDS model:
Total number of stages = 2(10.7 + 2.2 + 5.2) = 36.2. This was increased to 41 + total condenser = 42 to be on the conservative side.
Feed 1, the recycle from Column 2, entering at 2(10.7) = 21.4, increased to Stage 23.
Feed 2, the fresh feed, entering at 2(2.2) = 4.4 stages further down, changed to Stage 35 after it was found that the section between the two feeds was dominated by the lower end of the range of relative volatility.
Determination of a reasonable estimate for the reflux ratio was difficult. A rough estimate was made with the Class I Underwood equation (9-20), using Feed 1, with x = ethanol mole fraction

$$R = 1.3R_{\min} = \frac{1.3\left[\left(\frac{x_D}{x_{F_1}}\right) - \alpha_{\mathrm{EtOH,H_2O}}\left(\frac{1-x_D}{1-x_{F_1}}\right)\right]}{\alpha_{\mathrm{EtOH,H_2O}} - 1} = \frac{1.3\left[\left(\frac{0.925}{0.88}\right) - 1.05\left(\frac{1-0.925}{1-0.88}\right)\right]}{1.05-1} = 10.3$$

Since the relative volatility in the section between the overhead and the Feed 1 entry is close to one, the reflux ratio is sensitive to relative volatility. Accordingly, a conservative reflux ratio estimate of 15 was used.
The specifications for running Chemcad with the SCDS model were as follows:
Feed 1 at the bubble point at 120 kPa. Feed 2 at the bubble point at 120 kPa. Thus, both feeds would become partially vaporized upon entry into Column 1 operating under vacuum.
Top pressure = 13 kPa Condenser ΔP = 2 kPa Column ΔP = 15 kPa
No. of stages = 42 (includes total condenser and partial reboiler)
1st feed stage = 23 2nd feed stage = 35
Distillate flow rate = 78.82 mol/s (from above material balance)
Molar flow rate of ethanol in bottoms = 0.00007 mol/s
Estimated distillate rate = 78.82 mol/s (specified value)
Estimated reflux rate = 15D = 15(78.82) = 1182 mol/s
Estimated temperatures: Stage 1, 35°C Stage 12, 60°C Stage 2, 40°C Stage 11, 55°C

Exercise 11.15 (continued)

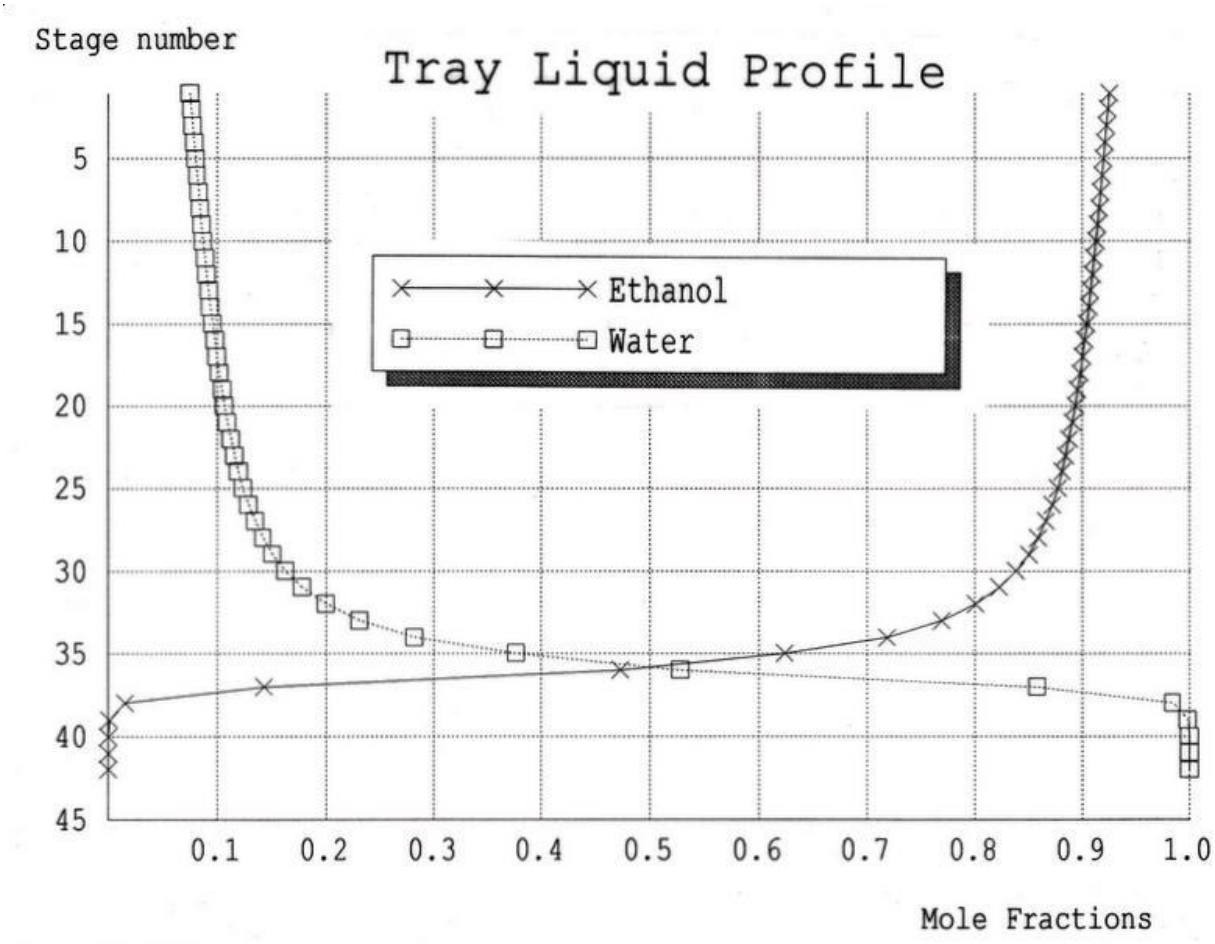
Analysis: Column 1 (continued)

A converged result, was obtained in 5 iterations, with a resulting reflux ratio of 13.47. The material balance was in agreement with the above material balance table for the system. Although the feed locations could probably be improved, no pinch region is evident, as shown in the liquid-phase composition profile below. Also included on the next page are the column profiles for temperature, liquid flow, and vapor flow, as well as the stage compositions at the bottom of the column, which show rapid changes, making the high bottoms purity easy to attain.

Column 1 was sized with Chemcad for valve trays, with a 30-inch tray spacing. The resulting column inside diameter was determined to be 24.5 feet, which is large of the high reflux ratio and vacuum conditions. The percent of flooding varied from 86% at the top to 38% at the bottom. The condenser duty was computed to be 48.11 MW, with a reboiler duty of 47.42 MW. For the 40 theoretical plates, the total pressure drop was computed to be 32 kPa. For a final design, the computations should be repeated taking into account tray pressure drop and tray efficiency.

Exercise 11.15 (continued)

Analysis: Column 1 (continued)



Exercise 11.15 (continued)

Analysis: Column 1 (continued)

			* Net Flows *			
	Temp	Pres	Liquid	Vapor	Feeds	Product
Stg	C	kPa	mol/sec	mol/sec	mol/sec	mol/sec
1	33.8	13.00	1061.81			78.82
2	36.5	15.00	1068.44	1140.63		
3	36.9	15.37	1069.09	1147.26		
4	37.4	15.75	1069.74	1147.91		
5	37.8	16.12	1070.36	1148.56		
6	38.3	16.50	1070.98	1149.18		
7	38.7	16.87	1071.58	1149.80		
8	39.1	17.25	1072.17	1150.40		
9	39.5	17.62	1072.74	1150.99		
10	40.0	18.00	1073.30	1151.56		
11	40.4	18.37	1073.85	1152.12		
12	40.7	18.75	1074.38	1152.67		
13	41.1	19.12	1074.91	1153.20		
14	41.5	19.50	1075.41	1153.72		
15	41.9	19.87	1075.91	1154.23		
16	42.3	20.25	1076.39	1154.73		
17	42.6	20.62	1076.85	1155.21		
18	43.0	21.00	1077.30	1155.67		
19	43.3	21.37	1077.73	1156.12		
20	43.7	21.75	1078.14	1156.55		
21	44.0	22.12	1078.54	1156.96		
22	44.3	22.50	1078.91	1157.36		
23	44.7	22.87	1122.52	1157.73	48.76	
24	45.0	23.25	1122.89	1152.58		
25	45.3	23.62	1123.21	1152.95		
26	45.7	24.00	1123.48	1153.27		
27	46.0	24.37	1123.69	1153.54		
28	46.3	24.75	1123.81	1153.75		
29	46.6	25.12	1123.81	1153.87		
30	46.9	25.50	1123.67	1153.88		
31	47.3	25.87	1123.29	1153.73		
32	47.6	26.25	1122.56	1153.35		
33	48.0	26.62	1121.24	1152.62		
34	48.5	27.00	1118.66	1151.30		
35	49.2	27.37	1207.10	1148.72	100.00	
36	50.3	27.75	1195.29	1137.16		
37	54.7	28.12	1176.91	1125.35		
38	64.5	28.50	1187.20	1106.97		
39	67.8	28.87	1192.38	1117.26		
40	68.5	29.25	1193.27	1122.44		
41	68.8	29.62	1193.67	1123.33		
42	69.1	30.00		1123.73		69.94

Exercise 11.15 (continued)

Analysis: Column 1 (continued)

Stage # 35	49.15 C	27.37 kPa	
	V Mole frac	L Mole frac	K
Ethanol	0.72538	0.62372	1.16298
Water	0.27462	0.37628	0.72983
Total mol/sec	1148.7212	1207.1020	
Stage # 36	50.30 C	27.75 kPa	
	V Mole frac	L Mole frac	K
Ethanol	0.66208	0.47252	1.40118
Water	0.33792	0.52748	0.64062
Total mol/sec	1137.1619	1195.2858	
Stage # 37	54.73 C	28.12 kPa	
	V Mole frac	L Mole frac	K
Ethanol	0.50189	0.14221	3.52922
Water	0.49811	0.85779	0.58069
Total mol/sec	1125.3456	1176.9087	
Stage # 38	64.53 C	28.50 kPa	
	V Mole frac	L Mole frac	K
Ethanol	0.15119	0.01599	9.45826
Water	0.84881	0.98401	0.86260
Total mol/sec	1106.9684	1187.1993	
Stage # 39	67.84 C	28.87 kPa	
	V Mole frac	L Mole frac	K
Ethanol	0.01699	0.00145	11.71352
Water	0.98301	0.99855	0.98444
Total mol/sec	1117.2590	1192.3821	
Stage # 40	68.46 C	29.25 kPa	
	V Mole frac	L Mole frac	K
Ethanol	0.00154	0.00013	11.97733
Water	0.99846	0.99987	0.99859
Total mol/sec	1122.4418	1193.2744	
Stage # 41	68.78 C	29.62 kPa	
	V Mole frac	L Mole frac	K
Ethanol	0.00014	0.00001	12.00499
Water	0.99986	0.99999	0.99987
Total mol/sec	1123.3341	1193.6679	
Stage # 42	69.07 C	30.00 kPa	
	V Mole frac	L Mole frac	K
Ethanol	0.00001	0.00000	12.01035
Water	0.99999	1.00000	0.99999
Total mol/sec	1123.7275	69.9404	

Exercise 11.15 (continued)

Analysis: (continued)

Column 2:

Using the TPXY plot feature of Chemcad, it was found that the relative volatility, α, for water with respect to ethanol, at 300 kPa, is close to one, but does not vary widely over the composition range, from 1.027 at 88 mol% ethanol at the distillate to 1.149 at 99.8 mol% ethanol at the bottoms, both mole fractions in the liquid phase. Accordingly, it was believed that the FUG method, the ShortCut Column of Chemcad, could give good estimates. Using the above material balance table, the specifications were 5.85/5.91 = 0.9898 for the recovery of water to the distillate, and 42.91/72.91 = 0.5885 for the recovery to the distillate of ethanol. The feed to Column 2 is the distillate from Column 1 after being pumped to a pressure of 350 kPa for entry into Column 2 and heating to the bubble point at that pressure.

The results are:

Minimum number of equilibrium stages = 47.2

Minimum reflux ratio = 5.85

Operating reflux ratio = 1.3(5.85) = 7.6

Number of equilibrium stages from Gilliland correlation = 86.9

Feed stage = 9

Using some small modifications to these values, the input data to the Tower model of Chemcad was as follows:

Top pressure = 300 kPa Condenser ΔP = 5 kPa Column ΔP = 70 kPa

No. of stages = 88 (includes total condenser and partial reboiler)

Feed stage = 10 from the top

Reflux ratio = 7.6

Bottoms molar flow rate = 30.06

Estimated distillate rate = 48.76 mol/s (specified value)

Estimated reflux rate = 15D = 7.6(48.76) = 370.6 mol/s

Estimated temperatures: Stage 1, 10835°C Stage 12, 116°C Stage 2, 110°C

With these input data, a converged solution was obtained, but an ethanol bottoms product of only 98.8 mol% purity was obtained compared to the desired 99.8 mol%. Also a pinch region of about 10 stages was evident just below the feed. Therefore, a second run was made with the following changes:

Feed stage = 20 from the top (moved down 10 stages)

Distillate flow rate = 78.82 mol/s, in place of reflux ratio

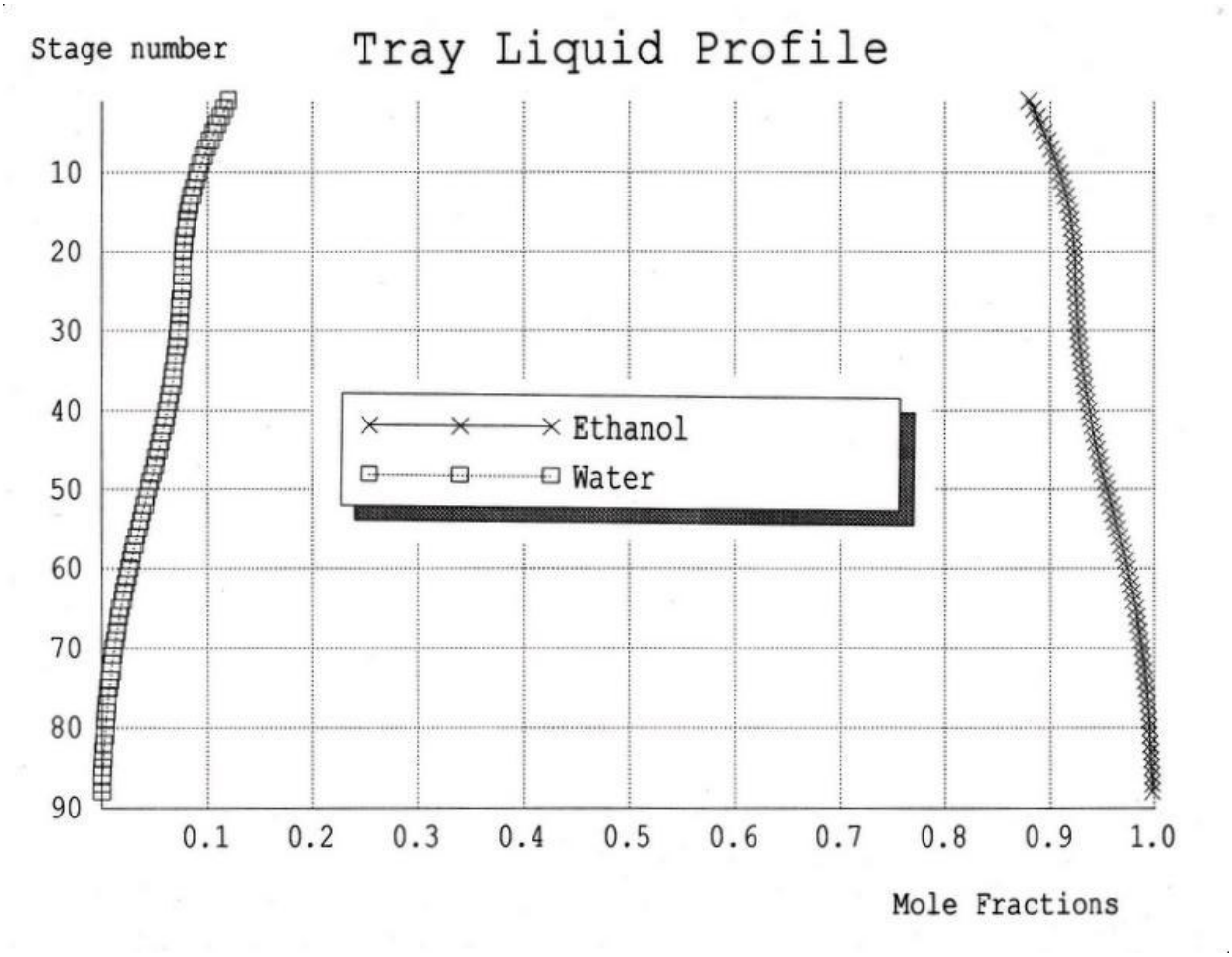
Mole fraction of ethanol in bottoms = 0.998, in place of bottoms flow rate

Convergence was achieved in 7 iterations, with a reflux ratio = 7.34. The material balance was in agreement with the above material balance table for the system. Although the feed location could probably be improved, no pinch region was now evident, as shown in the liquid-phase composition profile on the next page.

Column 2 was sized with Chemcad for valve trays, with a 24-inch tray spacing. The resulting column inside diameter was determined to be 7.5 feet for a nominal 85% of flooding. The condenser duty was computed to be 14.88 MW, with a reboiler duty of 14.86 MW. For the 86 theoretical plates, the total pressure drop was computed to be 74.6 kPa. For a final design, the computations should be repeated taking into account tray pressure drop and tray efficiency

Exercise 11.15 (continued)

Analysis: Column 2 (continued)



Exercise 11.16

Subject: Feasibility of the separation of benzene (B) from cyclohexane (C) using homogeneous azeotropic distillation with methanol (M) as the entrainer.

Given: Fresh feed of 100 kmol/h of 25 mol% B and 75 mol% C. Reference to an article by Ratliff and Strobel.

Assumptions: Feed is at the bubble point at 1 atm. Homogeneous azeotropic distillation at 1 atm using M.

Find: Whether M can make possible the separation of B from C.

Analysis: The normal boiling points of the three components are:

Component	B	C	M
Normal b. pt., ^{o}C	80.24	80.64	64.48

From the "Handbook of Chemistry and Physics" and use of the Wilson equation for activity coefficients with the Chemcad program, the following experimental and predicted binary azeotropes, respectively, are found, with reasonably good agreement.

	Handbook, expt.		**Wilson, predic.**	
Binary mixture:	***T*, ^{o}C**	**Mol%**	***T*, ^{o}C**	**Mol%**
B	77.56	53.7	77.62	54.7
C		46.3		45.3
B	57.5	39.0	58.59	40.9
M		61.0		59.1
C	53.9	40.0	54.97	39.0
M		60.0		61.0

No ternary azeotrope is known.

In the reference article by Ratliff and Strobel of Continental Oil, they describe the use of homogeneous azeotropic distillation with methanol to purify a benzene-rich stream. The feed to the tower, including the methanol entrainer, is in vol%, 9.1 M, 86.3 B, 2.4 paraffins-napthenes (including C), and 2.2 olefins. The amount of C in the feed is not known. From the azeotropic tower, a bottoms product of 99.0 vol% benzene is obtained, together with 0.3 vol% paraffins-naphthenes and 0.7 vol% olefins. The distillate in vol% is 36.0 M, 48.6 B, 8.7 paraffins-naphthenes, and 6.7 olefins. Thus, compared to the design with acetone in Example 11.6, Ratliff and Strobel report the use of only a small amount of M and a recovery of benzene of only 85%.

Exercise 11.16 (continued)

Analysis: (continued)

A residue curve map, produced by the Aspen Plus program with the Wilson equation, for the B-C-M system at 1 atm is shown on the next page, where the three binary azeotropes are marked with dots. Note that Aspen Plus predicts the B-M azeotrope at about 39 mol% B, which is in agreement with experiment. There are two distillation boundaries, one from the C-M azeotrope to the B-M azeotrope with little curvature, and one from the C-M azeotrope to the B-C azeotrope, with much curvature. These two boundaries divide the diagram into three distillation regions. Also included on the diagram are two straight lines, one from the B-C feed of 75 mol% C to pure M. The composition of the combined feed and entrainer lies somewhere on this line. Assume that ideally the bottoms product is pure benzene and that the distillate is the C-M azeotrope. Another straight line connects these two product points. The intersection of the two lines is the mixing point. By the inverse lever-arm rule or by material balance, the following preliminary, ideal material balance is obtained:

	kmol/h:			
Component	**Feed**	**Entrainer**	**Distillate**	**Bottoms**
B	25	0	0	25
C	75	0	75	0
M	0	192	117	0
Total:	100	192	192	25

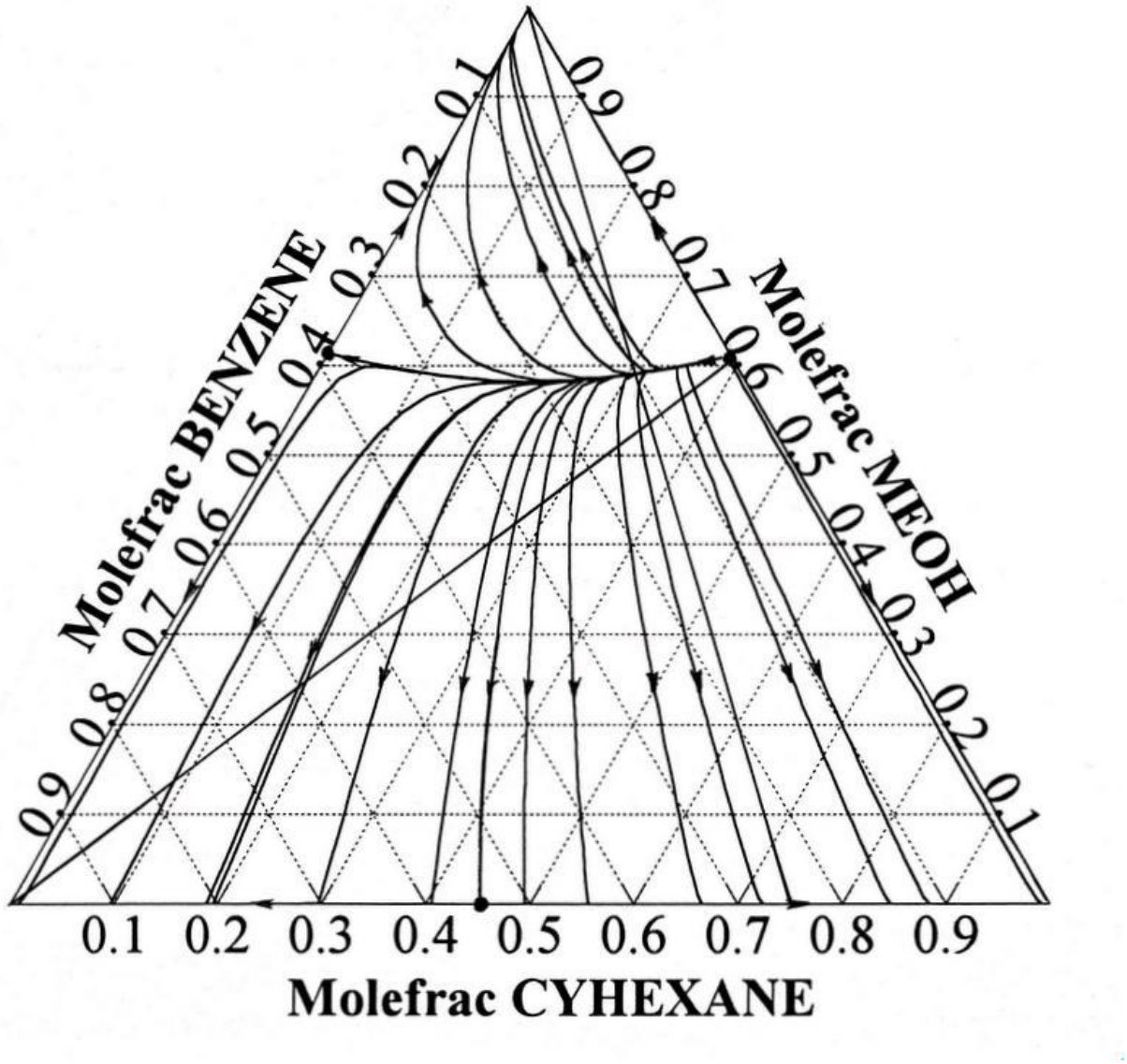
Even though the distillate and bottoms compositions appear to lie in a region different from the combined feed and entrainer, the separation is considered possible because of the strong curvature of the boundary from the C-M azeotrope to the B-M azeotrope, as discussed on pages 602-604. However, many stages may be necessary to achieve the products. As a first try, assume a reflux ratio of 5 and 100 equilibrium stages. Mix the feed and entrainer together and send the combined feed, as a bubble-point liquid, to stage 40 from the top. Specify a bottoms flow rate of 25 kmol/h. The calculations were made with the Chemsep program, using the continuation option because of convergence difficulties due to the non-ideality of the system. A good separation was not achieved since the bottoms was only 79.2 mol% B. Several of the parameters, including total stages, methanol entry stage, feed entry stage, reflux ratio, methanol flow rate, reflux ratio, and bottoms flow rate. The best result was obtained with the following specifications:

Number of equilibrium stages = 100 + total condenser = 101
Methanol flow rate = 115 kmol/h sent to stage 56 from the top, counting the total condenser.
Feed sent to stage 71 from the top, counting the total condenser.
Reflux ratio = 10
Bottoms flow rate = 24.0 kmol/h
Products were as follows, with 99.58 mol% benzene bottoms, but only a 95.6% recovery of benzene:

Component	**Feed**	**Entrainer**	**Distillate**	**Bottoms**
B	25	0	1.1	23.9
C	75	0	75.0	0.0
M	0	115	114.9	0.1
Total:	100	115	191.0	24.0

Exercise 11.16 (continued)

Analysis: (continued)



Exercise 11.17

Subject: Separation of toluene (T) from 2,5-dimethylhexane (H) by a sequence that includes homogeneous azeotropic distillation with methanol (M) as the entrainer.

Given: Feed of 100 mol/s of 50 mol% T and 50 mol% H. Reference to an article by Benedict and Rubin.

Find: A separation sequence that includes homogeneous azeotropic distillation with M as the entrainer. A feasible design for the azeotropic distillation column.

Analysis:
The normal boiling points of the three components are:

Component	T	H	M
Normal b. pt., ^{o}C	110.64	109.15	64.48

From use of the UNIFAC equation for activity coefficients with the Chemcad program, the following predicted minimum boiling binary azeotropes are found for a pressure of 1 atm.

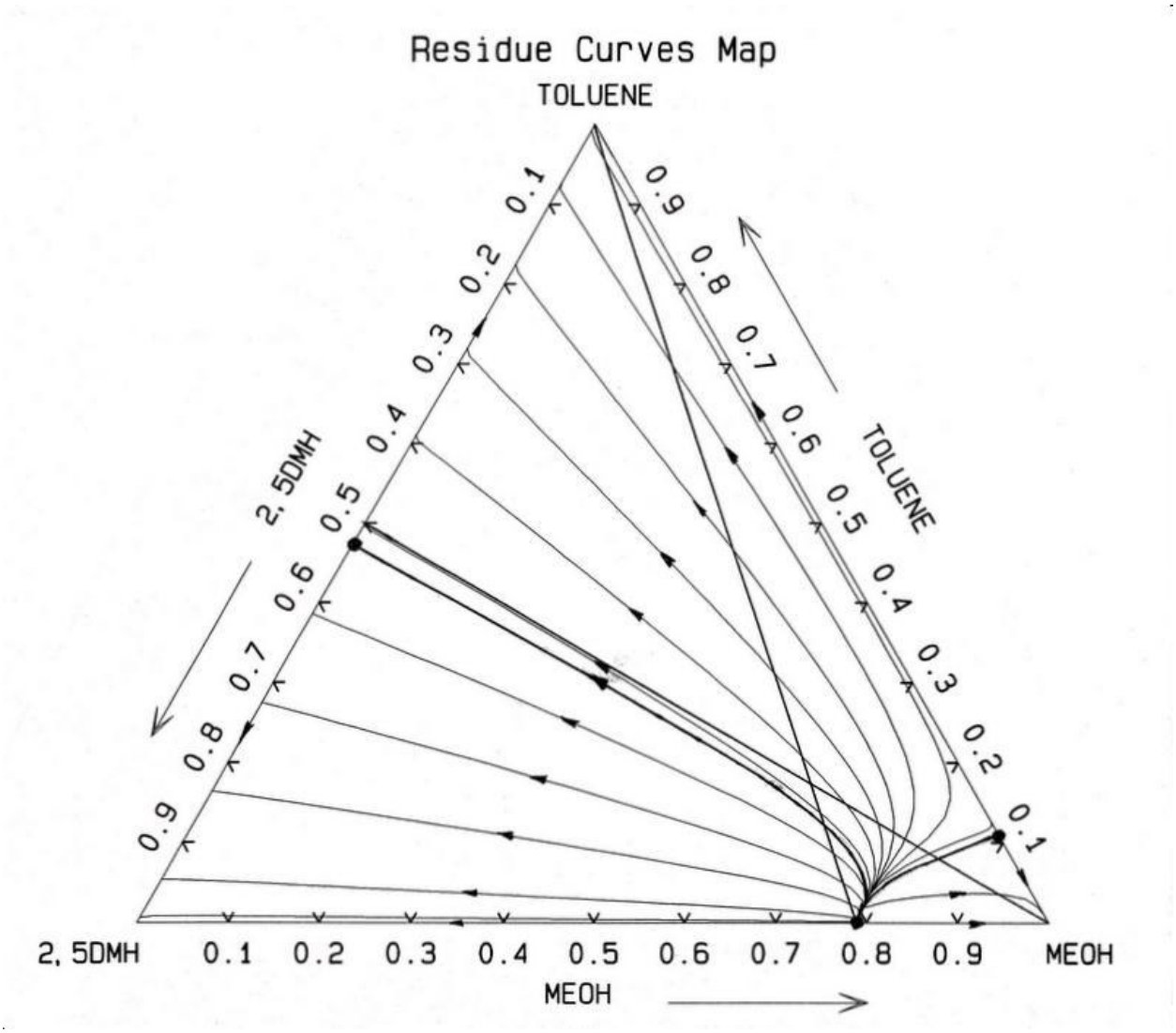
	UNIFAC, prediction	
Binary mixture:	***T*, ^{o}C**	**Mol%**
T	106.9	47.5
H		52.5
T	63.8	11.2
M		88.8
H	60.3	20.7
M		79.3

No ternary azeotrope is known.

A residue curve map, produced by the Aspen Plus program with the UNIFAC equation, for the T-H-M system at 1 atm is shown on the next page, where the three binary azeotropes are marked with dots. There are two distillation boundaries, one from the T-M azeotrope to the H-M azeotrope with little curvature, and one from the T-H azeotrope to the H-M azeotrope, with much curvature. These two boundaries divide the diagram into three distillation regions. Also included on the diagram are two straight lines, one from the T-M feed of 50 mol% H to pure M. The composition of the combined feed and entrainer must lie somewhere on this line. If we take advantage of the high degree of curvature of the second distillation boundary, we can assume that ideally the bottoms product can be pure toluene, with a distillate of the H-M azeotrope. Another straight line connects these two product points. The intersection of the two lines is the mixing

Exercise 11.17 (continued)

Analysis: (continued)



Exercise 11.17 (continued)

Analysis: (continued)

point. By the inverse lever-arm rule or by material balance, the following preliminary, ideal material balance is obtained:

	mol/s:			
Component	**Feed**	**Entrainer**	**Distillate**	**Bottoms**
T	50	0	0	50
H	50	0	50	0
M	0	192	192	0
Total:	100	192	242	50

An initial run is made with the Chemcad SCDS model using the following specifications:
Combined feed and entrainer at 1 atm and the bubble point.
Top pressure = 1 atm Condenser $\Delta P = 0$ Column $\Delta P = 0$
No. of stages = 31 (includes total condenser and partial reboiler)
Combined feed stage = 16 from the condenser
Reflux ratio =3
Bottoms flow rate = 50 mol/s (from above material balance)
Estimated (actual) distillate rate = 192 mol/s
Estimated (actual) reflux rate = 576 mol/s
Estimated temperatures: Stage 1, 60°C Stage 31, 60°C Stage 2, 60°C Stage 30, 60°C

This column was difficult to converge, but with the above specifications, plus a 0.50 damping factor, converge was achieved in 25 iterations. The calculated material balance was as follows:

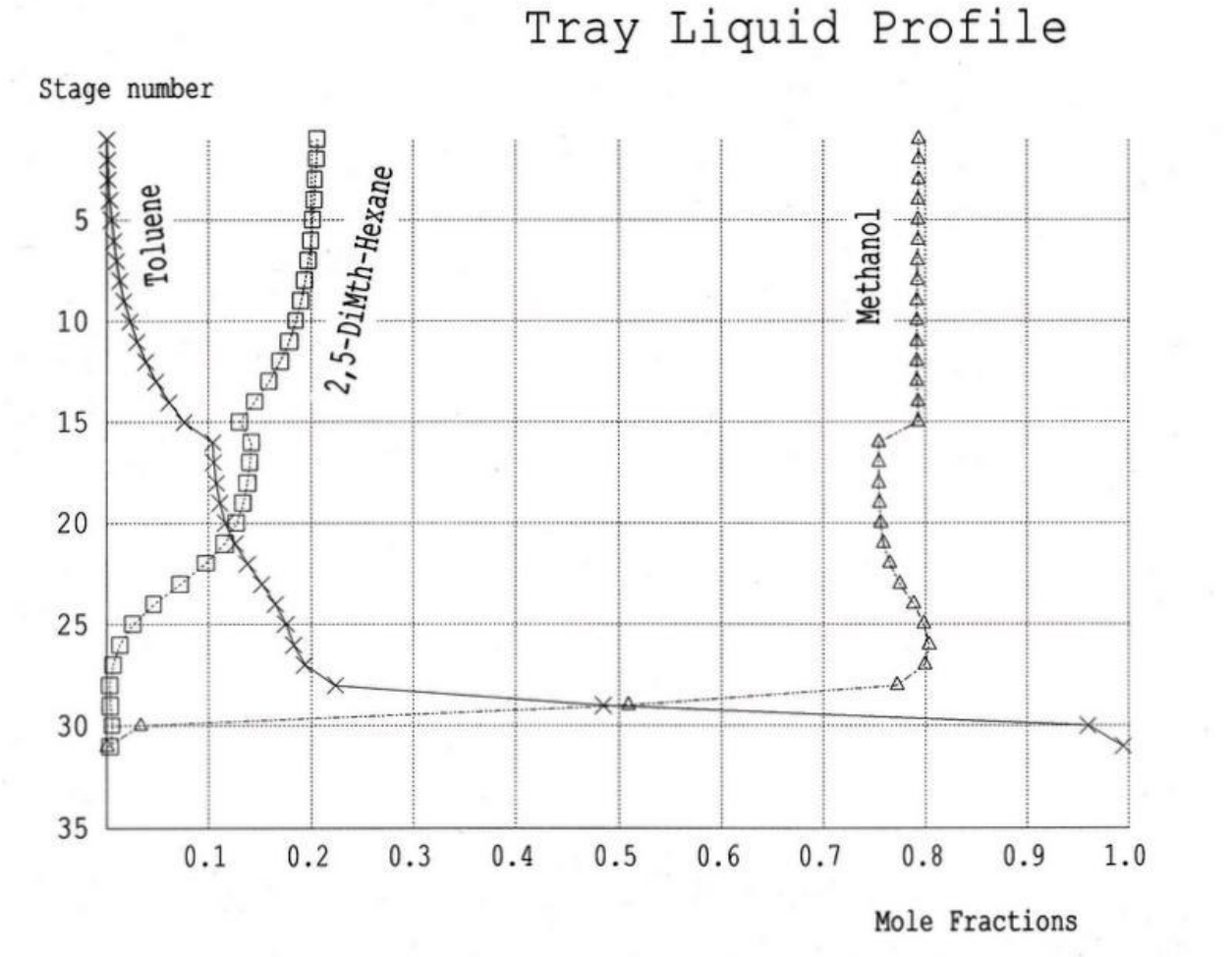
	mol/s:			
Component	**Feed**	**Entrainer**	**Distillate**	**Bottoms**
T	50	0	0.3	49.7
H	50	0	49.8	0.2
M	0	192	191.9	0.1
Total:	100	192	242.0	50.0

The liquid phase composition profile is on the following page. The condenser and reboiler duties are 12.37 x 10^4 MJ/h and 12.50 MJ/h respectively. The column profiles are given on a following page. The azeotropic distillation column was sized with Chemcad for sieve trays, with:
24-inch tray spacing 12% downcomer area 10% hole area
1/4-inch holes 80% of flooding
The resulting column inside diameter was determined to be 16 feet
For a final design, the computations should be repeated taking into account tray pressure drop and tray efficiency.

Exercise 11.17 (continued)

Analysis: (continued)

A feasible separation sequence would include the azeotropic distillation column, considered above, to separate the feed into 99.5 mol% toluene and a near azeotropic mixture of methanol and 2,5 dimethylhexane. The M-H azeotrope would be separated by liquid-liquid extraction with water to give nearly pur H and a methanol-water mixture. The latter would be separated by ordinary distillation to recover the methanol for recycle to the azeotropic tower, and water for recycle to the extraction section.



Exercise 11.17 (continued)

Analysis: (continued)

			* Net Flows *			
Stg	Temp C	Pres psia	Liquid kmol/hr	Vapor kmol/hr	Feeds kmol/hr	Product kmol/hr
1	60.3	14.70	2613.60			871.20
2	60.3	14.70	2613.58	3484.80		
3	60.3	14.70	2613.55	3484.78		
4	60.3	14.70	2613.50	3484.75		
5	60.3	14.70	2613.45	3484.70		
6	60.3	14.70	2613.39	3484.65		
7	60.4	14.70	2613.31	3484.59		
8	60.4	14.70	2613.20	3484.51		
9	60.5	14.70	2613.07	3484.40		
10	60.5	14.70	2612.90	3484.27		
11	60.6	14.70	2612.70	3484.10		
12	60.7	14.70	2612.45	3483.90		
13	60.8	14.70	2612.16	3483.65		
14	61.0	14.70	2611.87	3483.36		
15	61.2	14.70	2611.54	3483.07		
16	61.4	14.70	3663.08	3482.74	1051.20	
17	61.4	14.70	3663.03	3483.08		
18	61.4	14.70	3662.97	3483.04		
19	61.5	14.70	3662.87	3482.97		
20	61.6	14.70	3662.75	3482.87		
21	61.7	14.70	3662.65	3482.75		
22	61.9	14.70	3662.81	3482.65		
23	62.3	14.70	3663.71	3482.81		
24	62.7	14.70	3665.77	3483.71		
25	63.1	14.70	3668.54	3485.77		
26	63.5	14.70	3670.92	3488.54		
27	63.8	14.70	3671.96	3490.92		
28	64.0	14.70	3667.68	3491.96		
29	64.9	14.70	3499.45	3487.68		
30	86.5	14.70	3495.99	3319.45		
31	109.4	14.70		3315.99		180.00

Mole Reflux ratio 3.000

Exercise 11.18

Subject: Feasibility of the separation of a mixture of methyl acetate (A) and methanol (M) by a sequence that includes homogeneous azeotropic distillation using as the entrainer either n-hexane (H), cyclohexane (C), or toluene (T).

Given: Feed rate of 16,500 kg/h of 55 wt% A and 45 wt% M. Desired products are 99.5 wt% A and 99 wt% M. H, C, and T as potential entrainers.

Find: Feasibility of a separation sequence that includes homogeneous azeotropic distillation with one the three potential entrainers. If not feasible, find an alternative feasible process.

Analysis:
The molecular weights and normal boiling points of the five components of interest are:

Component	Molecular Weight	Normal boiling point, ^{o}C
Methyl acetate, A	74.08	57.1
Methanol, M	32.04	64.7
n-Hexane, H	86.17	69.0
Cyclohexane, C	84.16	80.7
Toluene, T	92.13	110.8

Convert the feed specification from a weight to a mole basis.

Component	Feed, kg/h	Feed, kmol/h	Feed, mol%
Methyl acetate, A	9,075	122.5	34.58
Methanol, M	7,425	231.7	65.42
Total:	16,500	354.2	100.00

From the Handbook of Chemistry and Physics, the homogeneous binary azeotropes are:

Binary pair	Normal boiling pt., ^{o}C	Mol%
A-M	54.0	65.3, 34.7
A-H	51.8	64.2, 35.8
A-C	55.5	80.1, 19.9
M-T	63.7	88.3, 11.7

Also, heterogeneous binary azeotropes are formed by the pairs M-H and M-C. No azeotrope is formed with the pair A-T.
The following two homogeneous ternary azeotropes are formed. No ternary azeotrope is formed by A-M-T.

Ternary system	Normal boiling pt., ^{o}C	Mol%
A-M-H	45.0	24.5, 29.4, 46.1
A-M-C	50.8	40.7, 34.5, 24.8

Exercise 11.18 (continued)

Analysis: (continued)

The calculations can be made with the ChemCad program, using the SCDS model. The results will depend on the method used to compute *K*-values. Because neither the NRTL nor the UNIQUAC methods in ChemCad include parameters for the methanol-normal hexane pair, use the UNIFAC method. Consider the use of n-hexane as the entrainer. A two-column method used successfully by Laroche, Bekiaris, Andersen, and Morari in Ind. Eng. Chem. Res., 31, 2190-2209 (1992), sends to the first column the feed and a recycle of near ternary azeotrope from the second column. The bottoms is nearly pure methanol. The distillate is fed to the second column, where the bottoms is nearly pure methyl acetate and the distillate is the near ternary azeotrope, which is recycled to the first column. Care is needed in using n-hexane because as noted above, it forms a two-liquid-phase system over part of the composition space as shown in the triangular diagram on the following page. Operation of both columns must be outside the two-liquid-phase region. Included on the diagram are the composition points for the azeotropes and approximate distillation boundary curves. For a first approximation, assume that the recycle distillate from the second column is 1500 kmol/h of 29 mol% A, 34.5 mol% M, and 36.5 mol% H. With a reflux ratio of 0.5 and 22 stages (including total condenser and partial reboiler) in the first column, with the feed and recycle distillate sent to stage 11 from the condenser, a very pure M is obtained. A 99.97 mol% M bottoms is produced with 14 stages, with stage 7 as the feed stage. With a reflux ratio of 4 and 42 stages (including total condenser and partial reboiler) in the second column, with the feed (distillate from the second column) sent to stage 21 from the condenser, a bottoms of 98.6 mol% A is obtained. This could not be improved by increasing the reflux, increasing the number of stages, or shifting the feed stage. The liquid composition profiles are shown on subsequent pages, where it is seen that no pinch zones are evident. The material balance is as follows:

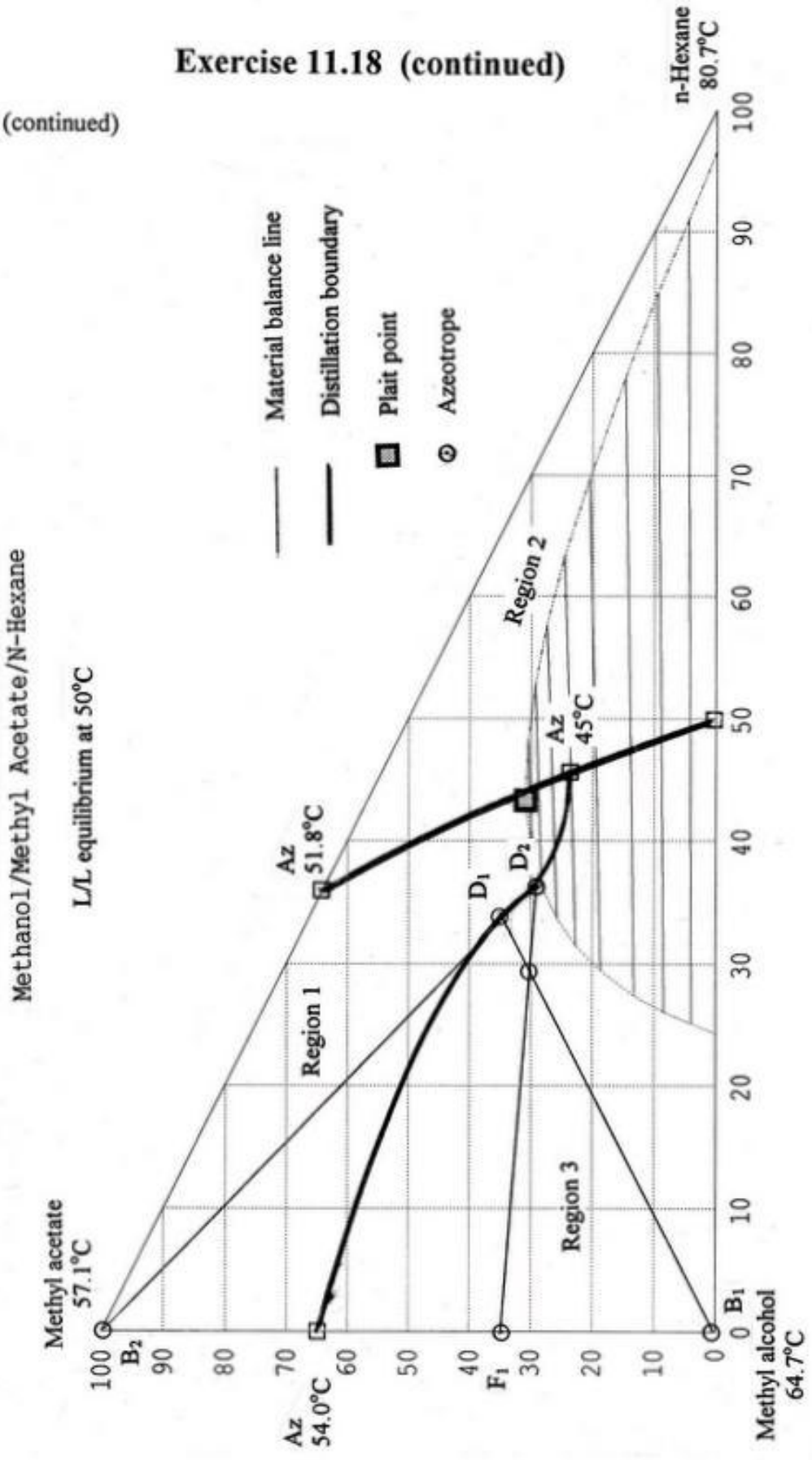
kmol/h:

Component	**Feed F_1**	**Entrainer, D_2**	**B_1**	**$D_1 = F_2$**	**B_2**
Methanol, M	231.7	516.4	230.0	518.1	1.7
Methyl acetate, A	122.5	436.6	0.1	559.0	122.4
n-Hexane, H	0.0	547.0	0.0	547.0	0.0
Total	354.2	1500.0	230.1	1624.1	124.1

The material balance lines are included on the triangular diagram on the next page.

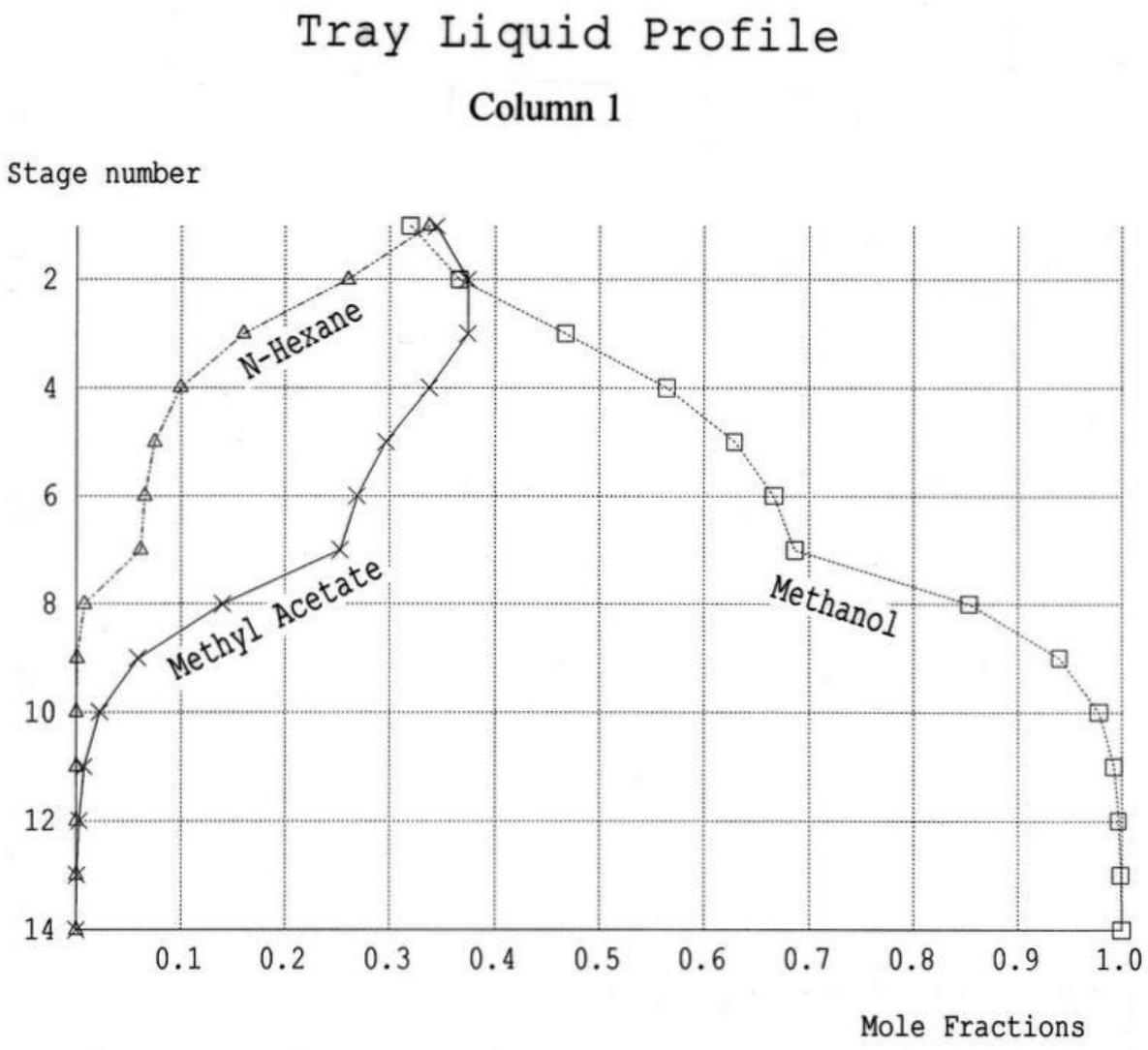
Exercise 11.18 (continued)

Analysis: (continued)



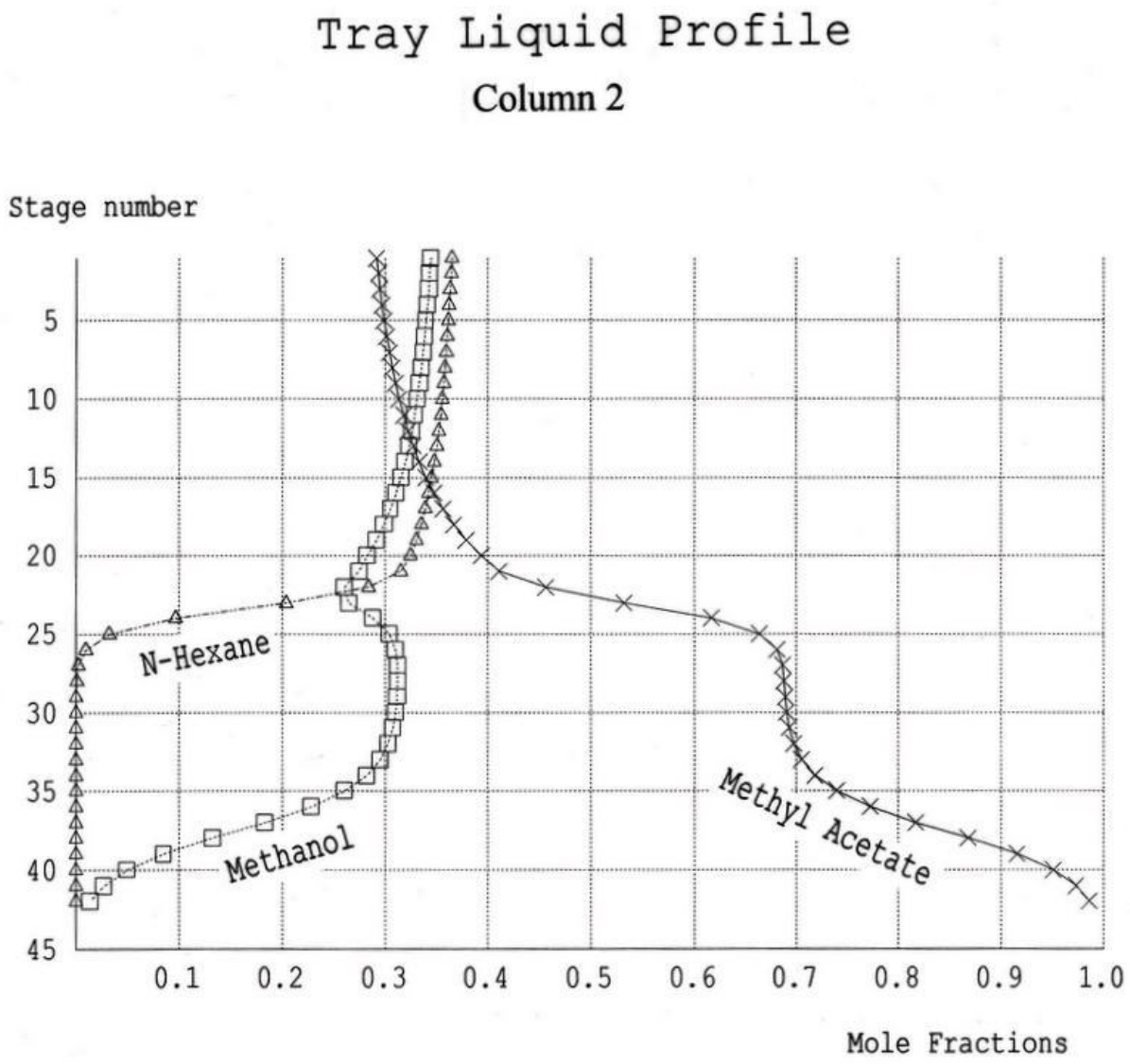
Exercise 11.18 (continued)

Analysis: (continued)



Exercise 11.18 (continued)

Analysis: (continued)



Exercise 11.19

Subject: Separation of a mixture of ethanol and water into nearly pure ethanol and pure water, using a three-column sequence that includes heterogeneous azeotropic distillation with benzene.

Given: 150 mol/s of the ethanol-water azeotrope at 1 atm. Benzene as the entrainer for heterogeneous azeotropic distillation.

Find: A suitable three-column design. However, because the feed is at near-azeotropic composition, the first (Preconcentrator) column is not needed.

Analysis:

The molecular weights and normal boiling points of the three components of interest are:

Component	Molecular Weight	Normal boiling Point, ^{o}C
Water, W	18.02	100.0
Benzene, B	78.11	80.1
Ethyl alcohol, E	46.07	78.5

From the Handbook of Chemistry and Physics, the binary azeotropes are:

Binary pair	Normal boiling pt., ^{o}C	Type Azeotrope	Mol% overall	Mol% upper liquid phase	Mol% lower liquid phase
W-B	69.4	Heterogeneous	29.8% W 70.2% B	0.26% W 99.74% B	99.98% W 0.02% B
W-E	78.2	Homogeneous	10.5% W 89.5% E		
B-E	67.8	Homogeneous	55.2% B 44.8% E		

Also, the following heterogeneous ternary azeotrope is formed:

Ternary System	Normal boiling pt., ^{o}C	Type Azeotrope	Mol% overall	Mol% upper liquid phase	Mol% lower liquid phase
W-B-E	64.6	Heterogeneous	23.3% W 53.9% B 22.8% E	5.0% W 76.0% B 19.0% E	66.7% W 1.7% B 31.6% E

The column calculations were made with the ChemCad program. Important decisions were the choice of activity coefficient method for the liquid and the binary interaction parameters for the selected method because these decisions can have a significant influence on the results of the calculations. The UNIQUAC method was selected, with values of the binary interaction parameters taken from the Appendix of the article by Bekiaris, Meski, and Morari, IEC Res., 35, 207-227 (1996). They give the parameters as values of $(u_{ij} - u_{jj})/R$ in K. For the ChemCad program, the parameters must be given as $(u_{ij} - u_{jj})$ in cal/mol. Therefore, the Bekiaris, Meski,

Exercise 11.19 (continued)

Analysis: (continued)

and Morari values were multiplied by 1.987 cal/mol-K, giving the following values of (u_{ij} - u_{jj}) for input to ChemCad:

i *j*	**Water**	**Benzene**	**Ethanol**
Water	----	719.890	405.036
Benzene	1795.85	----	764.780
Ethanol	-65.995	-85.507	----

With these values, the computed azeotropes at 1 atm, which deviate somewhat from the above experimental values, were as follows, where the homogeneous azeotropes were determined with the TPYX plot feature and the heterogeneous azeotropes were determined by running three-phase flash calculations with the LLVF model until the vapor and overall liquid compositions were equal. The most serious deviation is the lower liquid phase composition of the ternary azeotrope. From the built-in vapor pressure correlations in ChemCad, the normal boiling points of water and benzene are the same as the above literature values, but the ethanol value is 78.3°C.

Binary pair	**Normal boiling pt., °C**	**Type Azeotrope**	**Mol% overall**	**Mol% upper liquid phase**	**Mol% lower liquid phase**
W-B	69.2	Heterogeneous	29.8% W 70.2% B	0.47% W 99.53% B	99.94% W 0.06% B
W-E	78.2	Homogeneous	9.7% W 90.3% E		
B-E	67.8	Homogeneous	55.0% B 45.0% E		

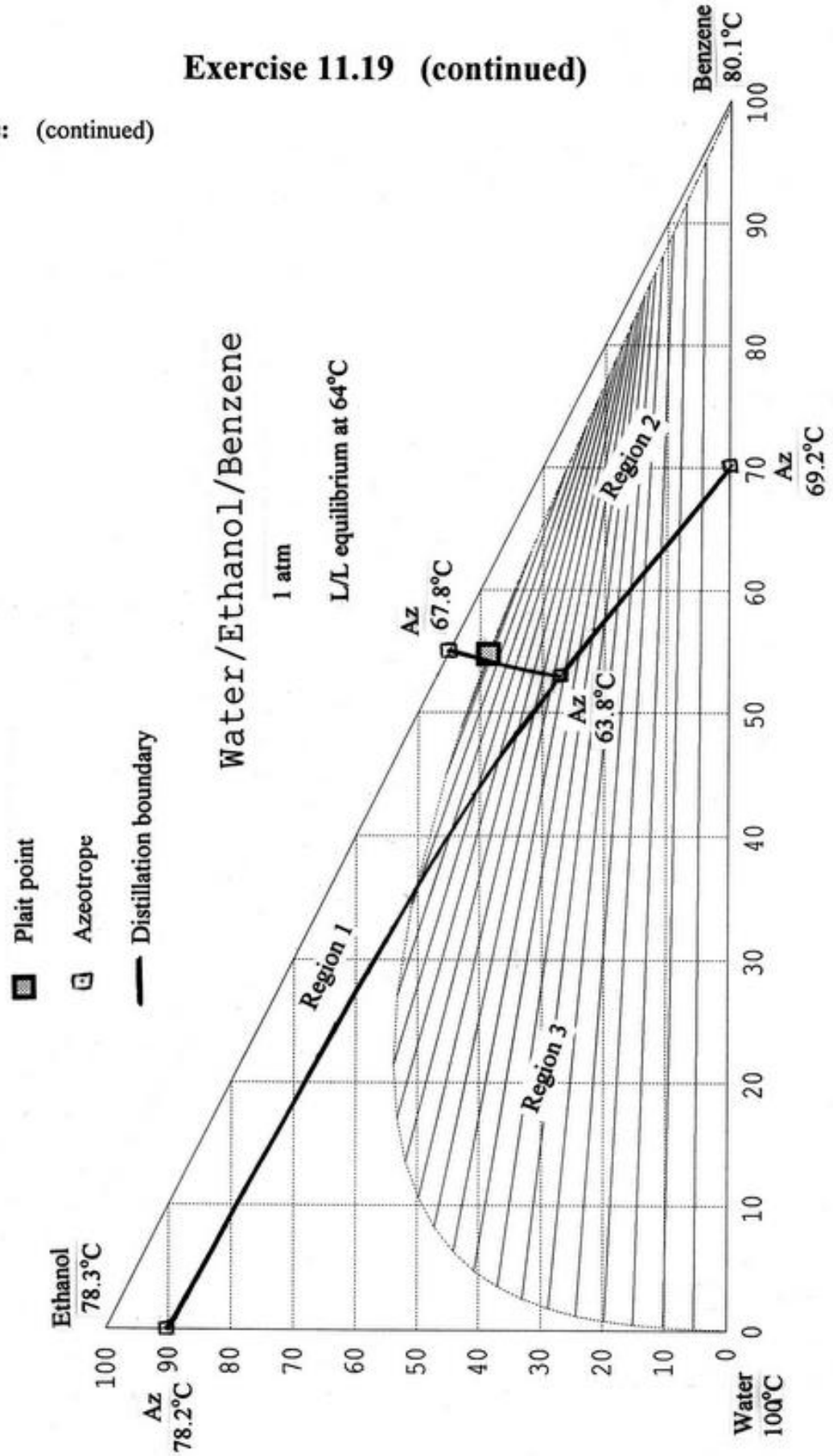
Ternary System	**Normal boiling pt., °C**	**Type Azeotrope**	**Mol% overall**	**Mol% upper liquid phase**	**Mol% lower liquid phase**
W-B-E	63.8	Heterogeneous	19.7% W 53.1% B 27.2% E	2.4% W 81.7% B 15.9% E	47.7% W 7.0% B 45.3% E

The above values also differ somewhat from the values cited in Section 11.6.

A binodal plot for the liquid-liquid equilibrium of the ternary system, as computed with ChemCad at a temperature of 64°C, is given on the next page. Many liquid-liquid phase equilibrium tie lines are shown. Added to the diagram are the above computed temperatures and compositions for the azeotropes, and estimates of the distillation boundary lines taken from the above-cited Bekiaris, Meski, and Morari article

Exercise 11.19 (continued)

Analysis: (continued)



Exercise 11.19 (continued)

Analysis: (continued)

The plot on the previous page differs somewhat from the residue curve map in Figure 11.29, but the same three distillation regions are evident. Therefore, as discussed in Section 11.6, it appears possible, using the three column scheme of Fig. 11.31 (without the first column because the feed is already close to the azeotropic composition of the ethanol-water mixture), to obtain nearly pure ethanol from the bottom of the second column and nearly pure water from the bottom of the third column.

Runs with ChemCad were made by sending the feed at the bubble point temperature directly to the azeotropic column in Fig. 1131a. Unfortunately, repeated attempts to achieve nearly pure ethanol, using different combinations of entrainer flow rates and compositions were unsuccessful. The best ethanol purity achieved was 95 mol%. For that case, 14 equilibrium stages were used in the azeotropic column plus a decanter-condenser combination and a partial reboiler, with the feed to stage 4 from the top. The entrainer recovery column had a reflux ratio of two and 15 stages, including a total condenser and a partial reboiler, with the feed to stage 5 from the condenser. The distillate from the third column and the benzene-rich liquid phase from the decanter were recycled to the top of the azeotropic column. Convergence of both the column calculations and the recycle streams was difficult. A reasonably converged material balance, keyed to the three-column diagram of Fig. 11.31 is as follows:

Mol/sec:

Stream in Fig. 11.31a	**D1**	**D3**	**L2**	**V2**	**B2**	**D2**	**B3**
Component							
Water	15	11.4	3.8	23.3	6.9	19.5	8.1
Benzene	0	20.0	88.8	108.8	0.2	20.0	0.0
Ethanol	135	46.2	25.7	71.9	135.0	46.3	0.1
Total:	150	77.6	118.3	204.0	142.1	85.8	8.2

Exercise 11.20

Subject: Separation of a mixture of isopropanol and water into nearly pure isopropanol and pure water, using a three-column sequence that includes heterogeneous azeotropic distillation with benzene.

Given: 120 mol/s of the isopropanol-water azeotrope at 1 atm. Benzene as the entrainer for the heterogeneous azeotropic distillation step.

Find: A suitable three-column design.

The molecular weights and normal boiling points of the three components of interest are:

Component	Molecular Weight	Normal boiling point, °C
Water, W	18.02	100.0
Benzene, B	78.11	80.1
Isopropyl alcohol, P	60.09	82.3

From the Handbook of Chemistry and Physics, the experimental binary azeotropes are:

Binary pair	Normal boiling pt., °C	Type Azeotrope	Mol% overall	Mol% upper Liquid phase	Mol% lower liquid phase
W-B	69.4	Heterogeneous	29.8% W 70.2% B	0.26% W 99.74% B	99.98% W 0.02% B
W-P	80.4	Homogeneous	31.7% W 68.3% P		
B-P	71.5	Homogeneous	60.6% B 39.4% P		

Also, the following heterogeneous ternary azeotrope is formed:

Ternary System	Normal boiling pt., °C	Type Azeotrope	Mol% overall	Mol% upper liquid phase	Mol% lower liquid phase
W-B-P	65.7	Heterogeneous	26.7% W 54.0% B 19.3% P	8.8% W 68.5% B 22.7% P	95.1% W 0.1% B 4.8% P

The column calculations were made with the ChemCad program. Important decisions were the choice of activity coefficient method for the liquid and the binary interaction parameters for the selected method, because these decisions can have a significant influence on the results of the calculations. The UNIQUAC method was selected, with built-in values of the binary interaction parameters for pairs with isopropanol; but for the benzene-water pair, values were taken from the Appendix of the article by Bekiaris, Meski, and Morari, IEC Res., 35, 207-227 (1996). They give the parameters as values of $(u_{ij} - u_{jj})/R$ in K. For the ChemCad program, the parameters

Exercise 11.20 (continued)

Analysis: (continued)
must be given as (u_{ij} - u_{jj}) in cal/mol. Therefore, the Bekiaris, Meski, and Morari values were multiplied by 1.987 cal/mol-K. In summary, the following values of (u_{ij} - u_{jj}) were used for the ChemCad runs:

i ***j***	**Water**	**Benzene**	**Isopropanol**
Water	----	719.890	109.550
Benzene	1795.85	----	319.618
Isopropanol	300.190	54.883	----

With these values, the computed azeotropes at 1 atm, which deviate somewhat from the above experimental values, were as follows, where the homogeneous azeotropes were determined with the TPYX plot feature of ChemCad and the heterogeneous azeotropes were determined by running three-phase flash calculations with the LLVF model of ChemCad until the assumed feed composition gave vapor and overall liquid compositions that were equal. The most serious deviations are for the ternary heterogeneous azeotrope. From the built-in vapor pressure correlations in ChemCad, the normal boiling points of water and benzene are the same as the above literature values, but the isopropanol value is 82.5°C.

Binary pair	**Normal boiling pt., °C**	**Type Azeotrope**	**Mol% overall**	**Mol% upper liquid phase**	**Mol% lower liquid phase**
W-B	69.2	Heterogeneous	29.8% W 70.2% B	0.47% W 99.53% B	99.94% W 0.06% B
W-P	80.2	Homogeneous	32.6% W 67.4% P		
B-P	71.6	Homogeneous	58.5% B 41.5% P		

Ternary System	Normal boiling pt., °C	Type Azeotrope	Mol% overall	Mol% upper liquid phase	Mol% lower liquid phase
W-B-P	60.6	Heterogeneous	23.8% W 52.3% B 23.9% P	4.6% W 67.6% B 27.8% P	89.3% W 0.3% B 10.4% P

A binodal plot for the liquid-liquid equilibrium of the ternary system, as computed with ChemCad at a temperature of 66°C, is given on the next page. Many liquid-liquid phase equilibrium tie lines are shown. Added to the diagram are the above computed temperatures and compositions for the azeotropes, and estimates of the distillation boundary lines, which divide the composition plot into three distillation regions.

Exercise 11.20 (continued)

Analysis: (continued)

As discussed in Section 11.6, it appears possible, using the three column scheme of Fig. 11.31a (without the first column because the feed is already at or near the azeotropic composition of the isopropanol-water mixture), to obtain nearly pure isopropanol from the bottom of the second column and nearly pure water from the bottom of the third column.

Runs with ChemCad were made with a feed of 120 mol/s of near-azeotropic composition of 67 mol% P and 33 mol% W at the bubble point temperature, sent directly to the azeotropic column in Fig. 11.31a. An estimate of the total entrainer flow rate and composition (streams L_2 and D_3 combined) was made by locating a composition point near the distillation boundary between Regions 1 and 2 and near the binodal curve separating the two-liquid-phase region from the one-liquid-phase region. The composition was taken as 8.5 mol% W, 56 mol% B, and 35.5 mol% P. To determine an initial approximation of the total flow rate of the entrainer, the overhead vapor from the azeotropic column was assumed to be near the ternary azeotropic composition. By material balance, the entrainer flow rate was computed to be 240 mol/s. The azeotropic column (column 2 in Fig. 11.31a) was then computed with the SCDS model in ChemCad, using the following specifications, with the pressure = 1 atm everywhere:

Total number of equilibrium stages (including partial reboiler) = 20
Feed stage = stage 5 from the top
No condenser
Bottoms flow rate = 80.4 mol/s (the flow rate of P in the feed)
Assumed distillate rate = 239.6 mol/s
Assumed reflux rate = 200 mol/s
Assumed stage temperatures = 61, 82, 62, and 78^{O}C

The converged results showed a large pinch region where little or no separation occurred, and the bottoms purity with respect to isopropanol was not acceptable. Accordingly, a number of additional runs were made with varying conditions for the total number of stages, feed stage location, and total entrainer flow rate. A bottoms product of isopropanol purity of better than 99.5 mol/s at a flow rate of 80.4 mol/s was achieved with 20 equilibrium stages, feed to the top stage, and a total entrainer flow rate of 300 mol/s. The entire separation process was then simulated with Chemcad, according to the flowsheet in Fig. 11.31a, but without the first column (Preconcentration). The flowsheet included the azeotropic column (column 2) with recycle entrainer from the entrainer recovery column (column 3), and a condenser-decanter to condense the overhead vapor from column 2 and split the condensate into two liquid phases, with the organic-rich phase sent as entrainer reflux to the top of column 2 and the water-rich phase sent to column 3. To achieve a nearly pure water bottoms product from column 3, only 4 equilibrium stages (including a total condenser and partial reboiler) were needed with the feed to stage 2 (the top stage of the column) and a reflux ratio of 1. The distillate from column 3 was recycled to the top of column 2. Several loops were needed to converge the material balance for the recycle process.

Exercise 11.20 (continued)

Analysis: (continued)

The resulting material balance was as follows:

Mol/sec:

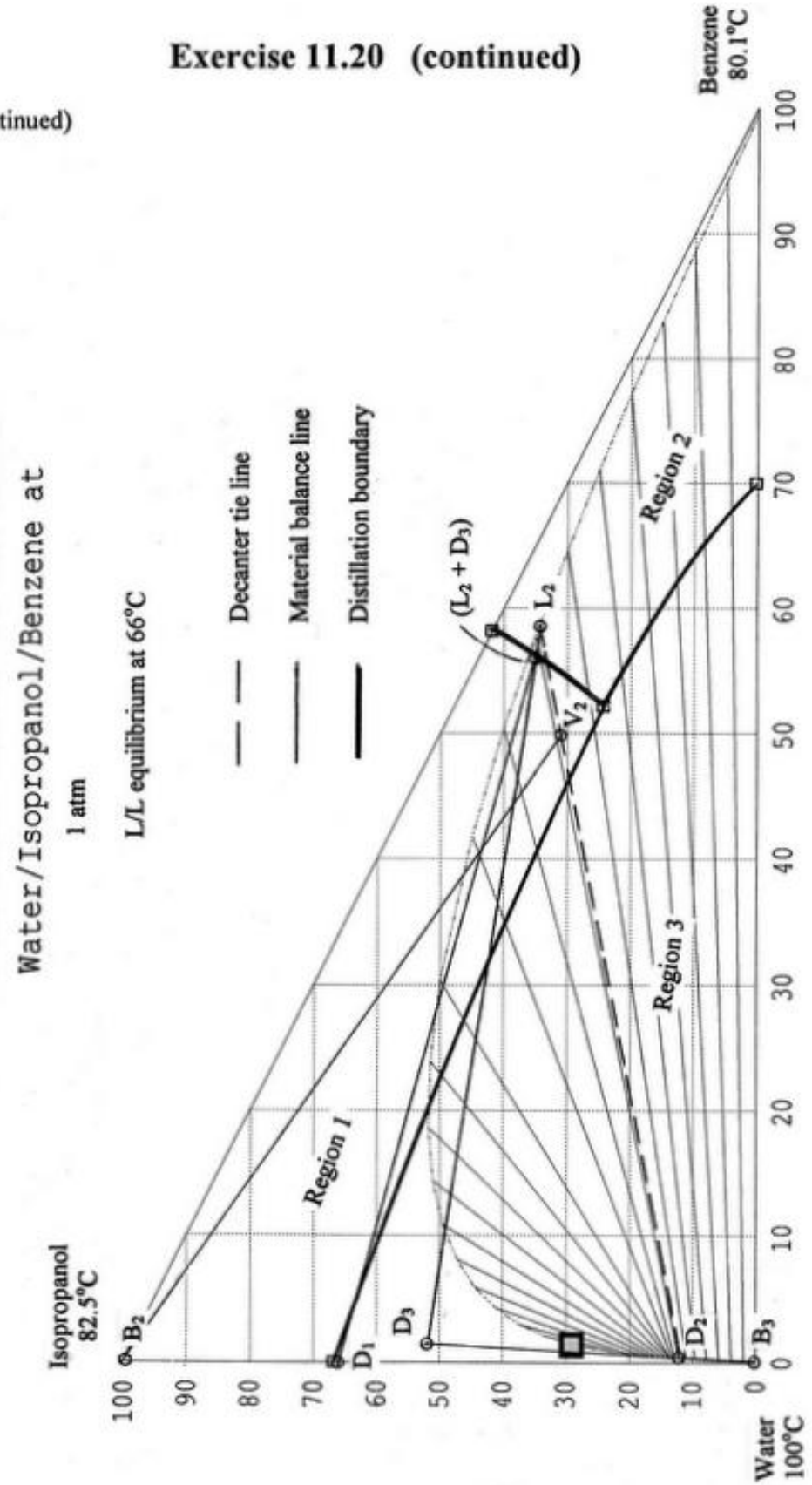
Stream in Fig. 11.31a	**D1**	**D3**	**L2**	**V2**	**B2**	**D2**	**B3**
Component							
Water	39.6	5.8	19.9	65.2	0.1	45.3	39.5
Benzene	0	0.2	169.3	169.5	0.0	0.2	0.0
Isopropanol	80.4	6.1	99.5	105.8	80.2	6.3	0.2
Total:	120.0	12.1	288.7	340.5	80.3	51.8	39.7

From the above material balance, the isopropanol product purity is 99.9 mol% and the water product purity is 99.6 mol%. The benzene loss is negligible. The material balance lines are shown on the triangular diagram on the following page. The separation in column 1 is in distillation region 1, but the decanter sends the distillate, D_2, into region 2 where the separation in column 3 occurs.

The composition profiles for columns 2 and 3 are shown in two subsequent pages, where it is seen that no pinch zones are evident.

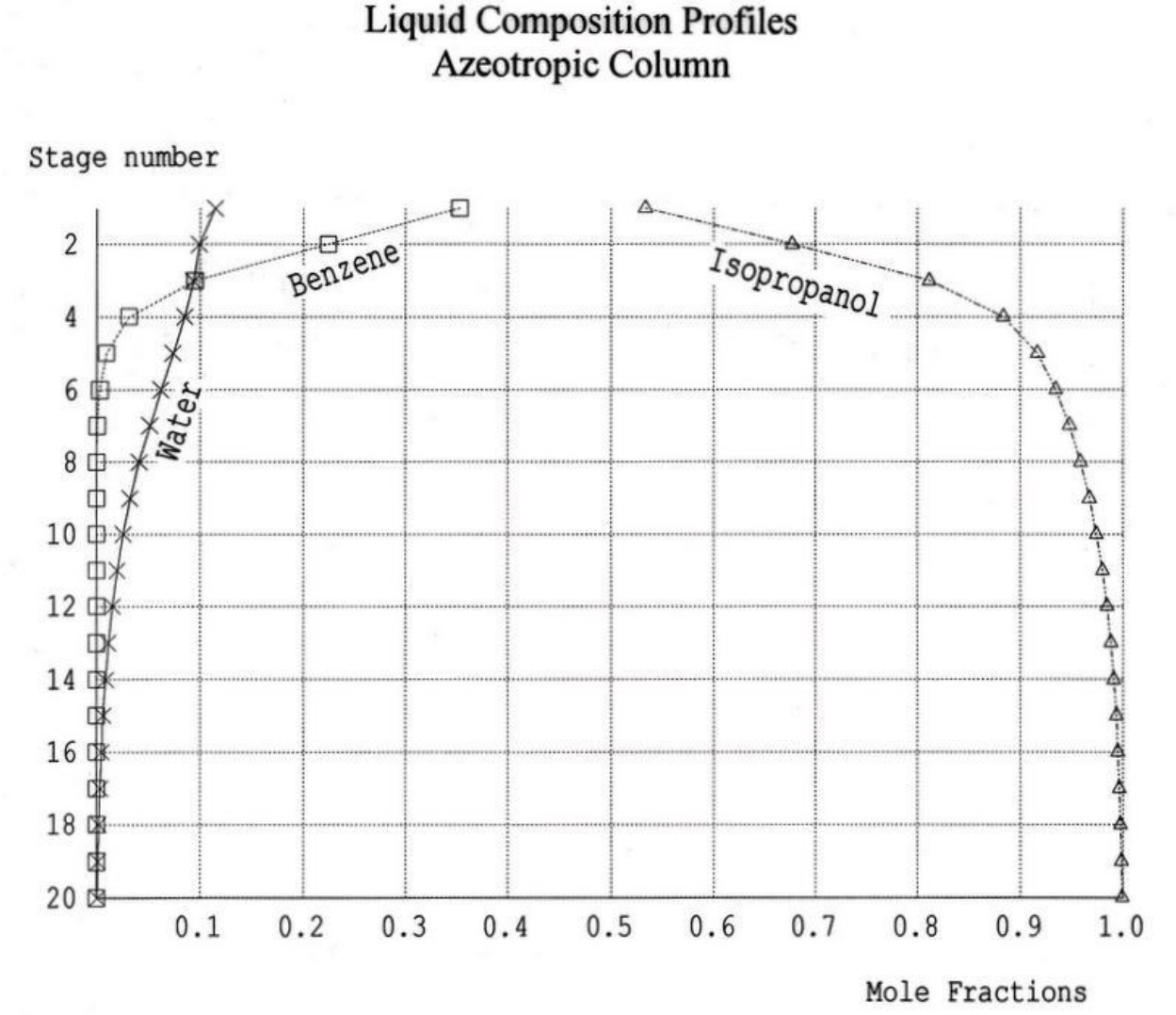
Exercise 11.20 (continued)

Analysis: (continued)



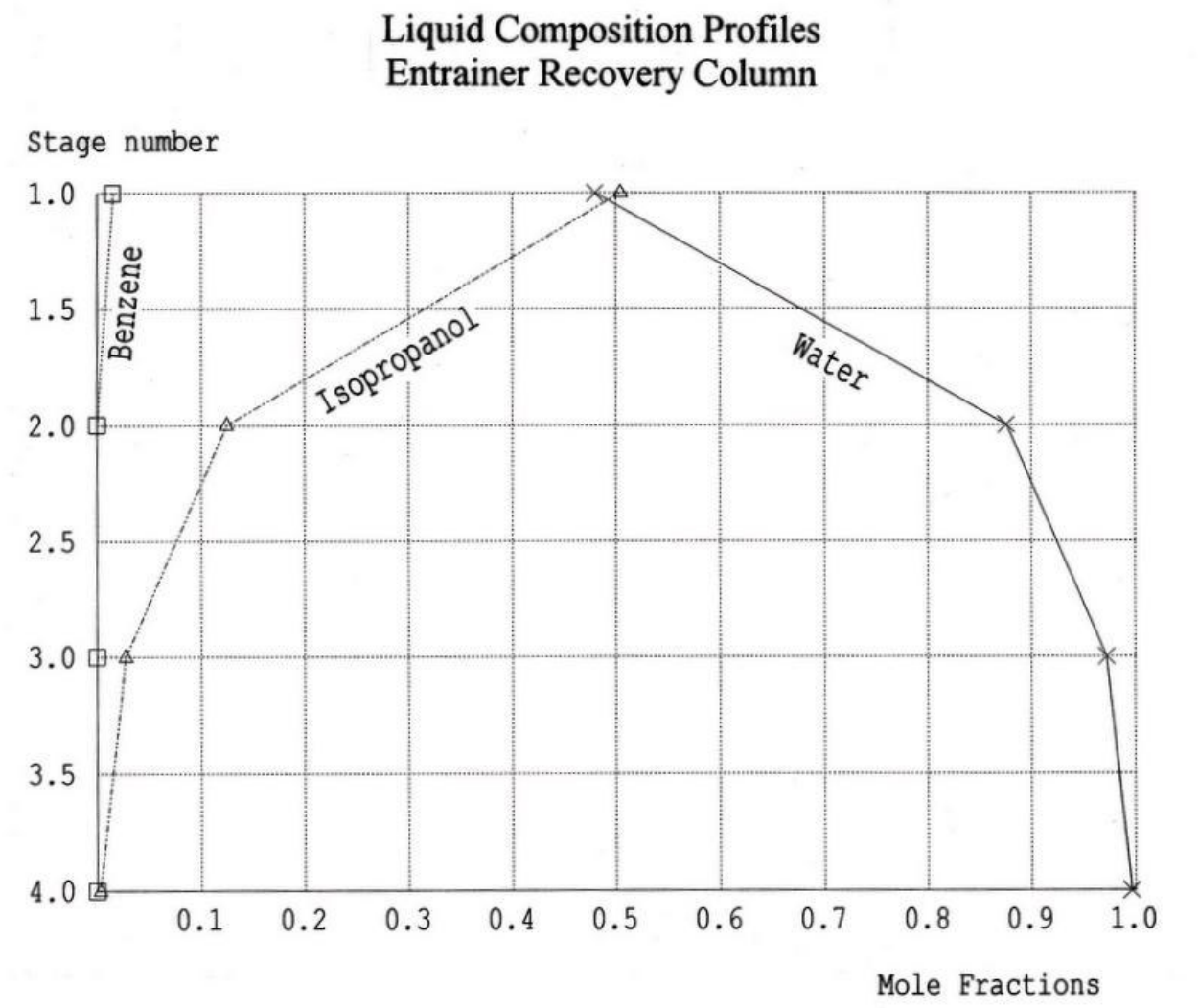
Exercise 11.20 (continued)

Analysis: (continued)



Exercise 11.20 (continued)

Analysis: (continued)



Exercise 11.21

Subject: Separation of a mixture of acetic acid (A) and water (W) into nearly pure acetic acid and pure water, using a two-column sequence that includes heterogeneous azeotropic distillation with n-propyl acetate (NPA).

Given: 1,000 kmol/h of 20 mol% acetic acid in water.

Find: A suitable two-column design.

Analysis: The phase behavior of the acetic acid/water/n-propyl acetate system at 1 atm was explored with the UNIQUAC equation for liquid-phase activity coefficients, noting that the normal boiling points in ^{o}C are 118.1 for A, 100 for water, and 101.4 for NPA. Using the ChemCad and Aspen Plus programs, the following data were obtained, including a residue curve map for the vapor-liquid system at 1 atm and a ternary liquid-liquid diagram for the system at 80^{o}C, both shown on the next page. Acetic acid and water form a minimum-boiling azeotrope at 90 mol% water that boils at 99.47^{o}C. Acetic acid and n-propyl acetate do not form an azeotrope. Water and n-propyl acetate form a heterogeneous azeotrope at approximately 40 mol% NPA and 80^{o}C. This azeotrope separates into a mixture of almost pure water and 83 mol% NPA. The two diagrams show that a ternary mixture, when distilled will tend to give a bottoms of almost pure acetic acid and an overhead that when condensed will split into two liquid phases, one of near pure water, and the other of concentrated NPA that can be recycled to the column as entrainer.

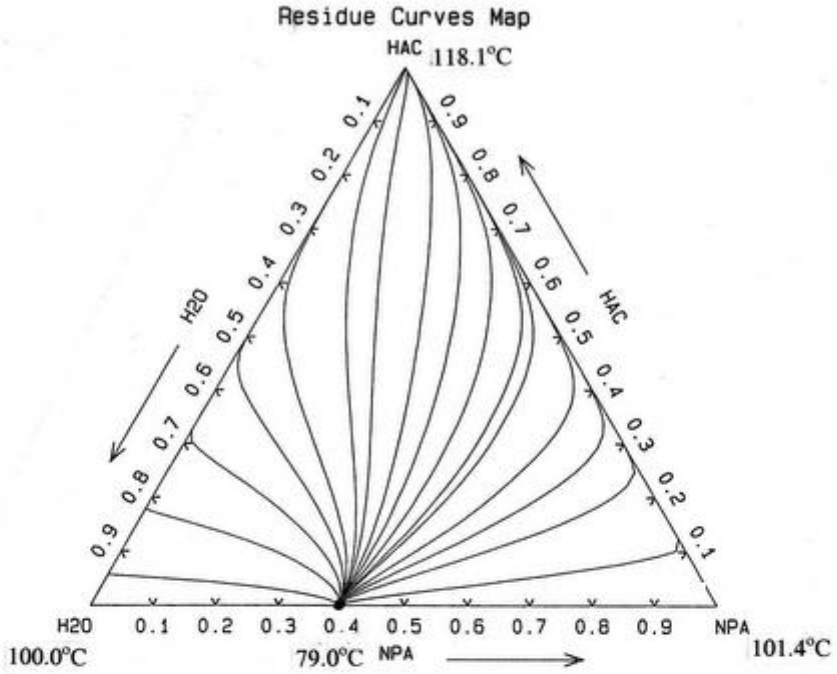
Consider a separation sequence that omits the preconcentator column shown in Fig. 11.31 because the feed is already concentrated in water. The feed is sent directly into the heterogeneous azeotropic distillation column with a decanter to split the two liquid phases resulting from the condensation of the overhead vapor. An initial geometrical construction for determining the separation in that column is included in the ternary diagram on the next page. The feed, F, of 800 kmol/h of W and 200 kmol/h of A enters the column along with an entrainer, R, of saturated NPA-rich phase containing 18 mol% W, 10 mol% A, and 72 mol% NPA in equilibrium with a saturated water-rich phase containing 97.5 mol% W, 2 mol% A, and 0.5 mol% NPA, which becomes the distillate. The amount of entrainer reflux is fixed so as to give the mixing point, M, such that a line through that point and about 99 mol% A in W will intersect a liquid-liquid tie line that connects the reflux and the nearly pure liquid water distillate in the region close to the binary heterogeneous azeotrope of W and NPA. From this construction, the amount of reflux is determined as 1,000 kmol/h. An initial material balance was then computed, from the feed and mole fraction compositions, with the following result:

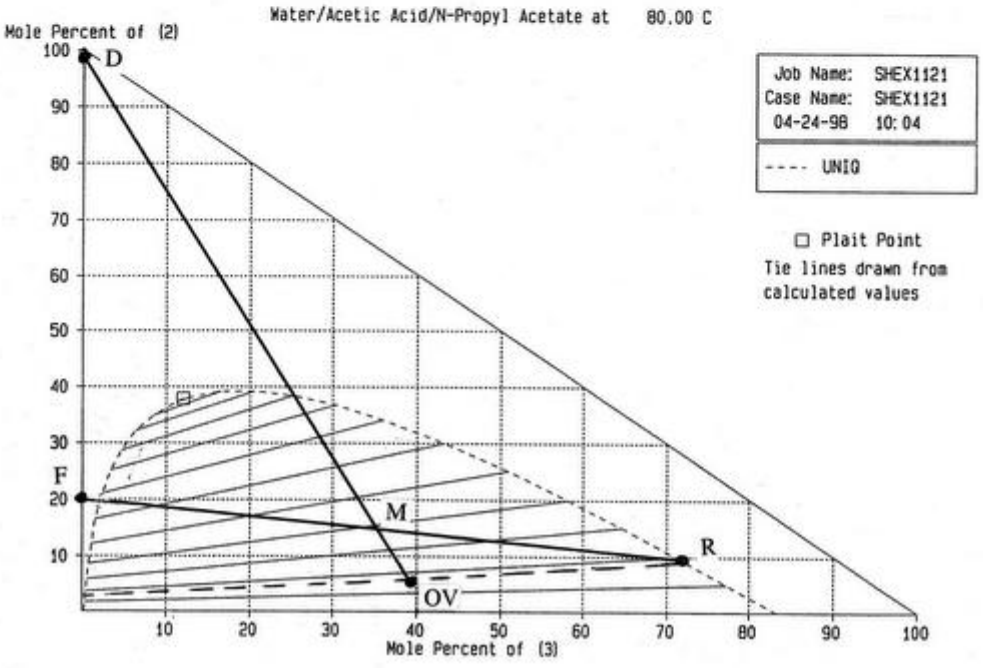
kmol/h:

Component	Feed	Entrainer w/o makeup	Make-up NPA	Bottoms	Overhead vapor	Distillate
Water	800	180	0	2	978	798
Acetic acid	200	100	0	185	115	15
NPA	0	720	4	0	720	4
Total:	1000	1000	4	187	1813	817

Exercise 11.21 (continued)

Analysis: (continued)





Exercise 11.21 (continued)

Analysis: (continued)

The SCDS distillation model of Chemcad was used with no condenser and a partial reboiler. The overhead vapor was sent a three-phase flash condenser (decanter) operating at the bubble point, modeled with the LLVF unit. The NPA-rich phase would be recycled to the column as entrainer reflux entering the top stage, but in the calculation the guessed amount of 1,000 kmol/h at the above composition was used and then converged by trial and error, accounting for the necessary makeup NPA. An initial guess was made of 20 stages, including the reboiler, with the feed entering stage 6 from the top. Other specifications were 1 atm for the column, feed and entrainer at the bubble-point temperature at 1 atm, 187 kmol/h of bottoms, estimates of 1800 kmol/h for the distillate, 1000 kmol/h for the reflux; 80, 110, 90, and 100 ^{o}C for the four temperatures; and a damping factor of 0.3. The calculations converged without difficulty in 14 iterations, but the entrainer flows minus the makeup NPA did not equal the NPA-rich liquid from the decanter. Also 10 of stages appeared to be pinched. Therefore, the number of stages was reduced to 10, the feed stage was moved to stage 4 from the top, and the component flow rates in the entrainer were revised by trial and error until a reasonable closure of the material balance was obtained. The final material balance was as follows:

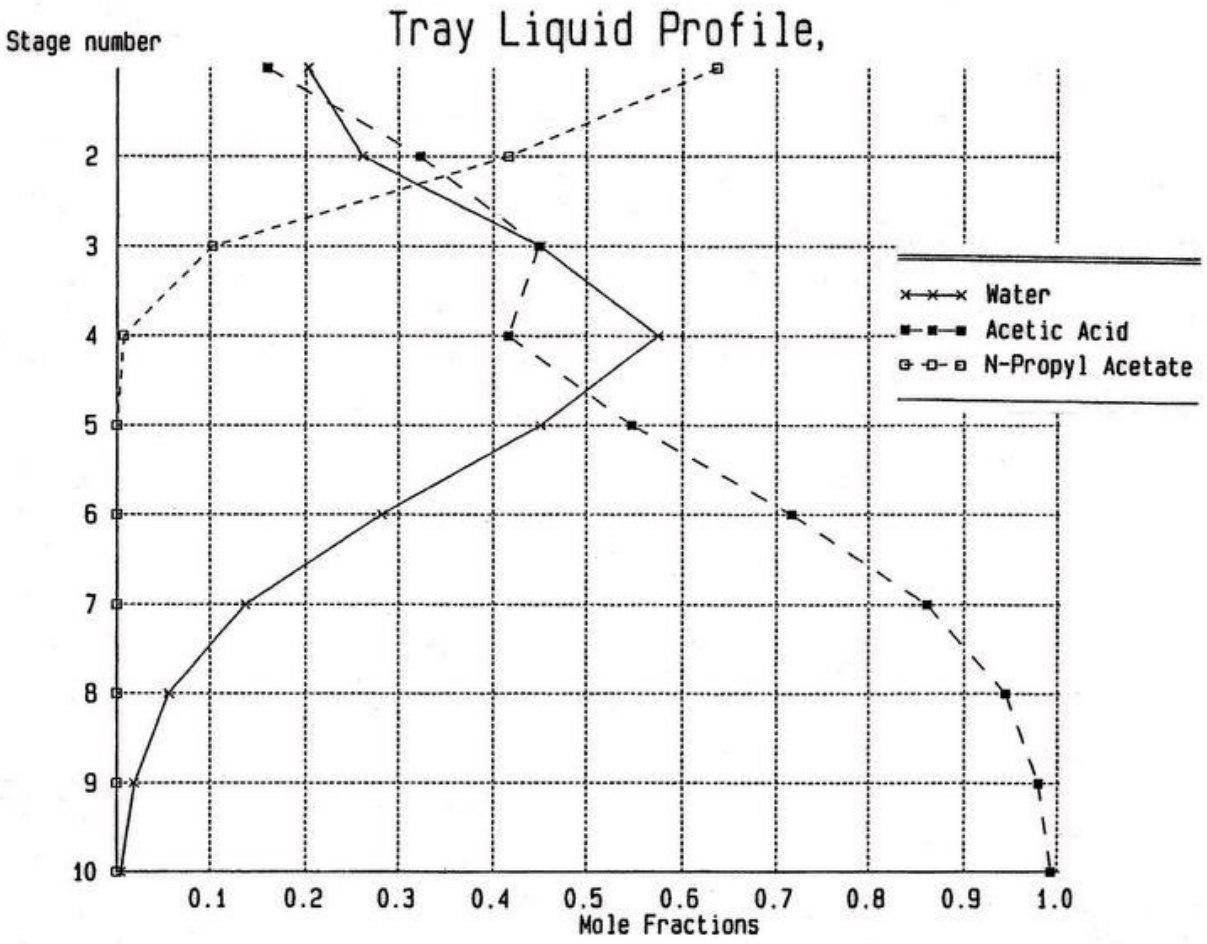
kmol/h:

Component	Feed	Entrainer w/o makeup	Make-up NPA	Bottoms	Overhead vapor	Distillate
Water	800	184	0	1.3	982.7	798.4
Acetic acid	200	58	0	183.6	74.4	16.0
NPA	0	760	3.6	0.1	763.5	3.5
Total:	1000	1002	3.6	185.0	1820.6	817.9

Temperatures in the column varied from 85.6^{o}C at the top to 117.5^{o} C at the bottom. The temperature in the decanter was 83.9^{o}C. The following is a plot of the liquid-phase composition profile showing that no pinch existed in the column. The acetic acid product is 99.2 mol% acetic acid, while the bottoms water product is 97.6 mol% water. This could be further purified in a second column, with the small amount of acetic acid-rich product recycled.

Exercise 11.21 (continued)

Analysis: (continued)



Exercise 11.22

Subject: Reactive distillation of isobutene (IB) with methanol (M), in the presence of n-butene (NB) to produce MTBE. Effect of the feed stage location for methanol.

Given: Mixed butenes feed of 195.44 mol/s of IB and 353.56 mol/s of NB entering stage 11 as a vapor at 350 K and 11 bar. Methanol feed of 215.5 mol/s at 320 K and 11 bar. Column operates at 11 atm and has 15 equilibrium stages, with a total condenser and partial reboiler. Reflux ratio = 7 and bottoms flow rate is set at 197 mol/s. Catalyst for the reaction is provided in the amount of 204.1 kg/stage only at stages 4 through 11. Kinetic data are given in Example 11.9. Use UNIQUAC method for liquid-phase activity coefficients, with the binary interaction parameters in Example 11.9, and RK EOS for vapor-phase fugacities.

Find: Distillate and bottoms products as a function of feed stage location for methanol.

Analysis: Chemcad can be used, but here, the calculations were made with Aspen Plus version 10.1, but convergence was not easy to achieve. The initial case was run with the methanol fed to stage 7 from the top, counting the total condenser as the first stage. The input data, which are given on the next two pages, differ slightly from the listing for Example 11.9. With this feed stage, the overall material balance in mol/s are:

Component	Feed 1	Feed 2	Distillate	Bottoms
Methanol	215.50	0.00	31.26	0.13
Isobutene	0.00	195.44	8.25	3.08
n-butene	0.00	353.56	343.69	9.87
MTBE	0.00	0.00	0.19	183.92
Total:	215.50	549.00	383.39	197.00

To obtain the results for the other methanol feed-stage locations, the following procedure was used. Starting from Stage 7 and using the previous results to start each new run, results were obtained for methanol feed stages of 8, 9, 10, and 11. Working backward from Stage 7, results were obtained for methanol feed stages of 6 and 5. Then, results were obtained, starting from Stage 2, for methanol feed stages of 2, 3, and 4, where the input on the next two pages were modified under BLOCK B1 RADFRAC to:

X-EST 17 MEOH 0.01 / 17 MTBE 0.95

Y-EST 17 MEOH 0.02 / 17 MTBE 0.875

To obtain results for methanol feed stages 12 to 16, the input data on the next two pages were first modified under BLOCK B1 RADFRAC to:

X-EST 17 MEOH 0.90 / 17 MTBE 0.00

Y-EST 17 MEOH 0.90 / 17 MTBE 0.00

This gave results for methanol feed stages of 12, 13, 14, 15, and 16; and 12 back to 11.

The values for % conversion of isobutene were as follows, and compare well with Fig. 11.39.

Stage	2	3	4	5	6	7	8	9	10	11	11	12	13	14	15	16
%Conv	89	91	92	93	94	94	95	95	96	96	0.7	0.7	0.6	0.6	0.6	0.6

Exercise 11.22 (continued)

Analysis: (continued)

```
TITLE 'SHEX1122'

IN-UNITS MET VOLUME-FLOW='cum/hr' ENTHALPY-FLO='MMkcal/hr'    &
        HEAT-TRANS-C='kcal/hr-sqm-K' PRESSURE=bar TEMPERATURE=C  &
        VOLUME=cum DELTA-T=C HEAD=meter MOLE-DENSITY='kmol/cum'  &
        MASS-DENSITY='kg/cum' MOLE-ENTHALP='kcal/mol'  &
        MASS-ENTHALP='kcal/kg' HEAT=MMkcal MOLE-CONC='mol/l'  &
        PDROP=bar

OUT-UNITS MET TEMPERATURE=K MOLE-FLOW='mol/sec'

DEF-STREAMS CONVEN ALL

DATABANKS PURE10  / AQUEOUS  / SOLIDS  / INORGANIC  /  &
        NOASPENPCD

PROP-SOURCES PURE10  / AQUEOUS  / SOLIDS  / INORGANIC

COMPONENTS
    MEOH CH4O MEOH /
    IB C4H8-5 IB /
    NB C4H8-1 NB /
    MTBE C5H12O-D2 MTBE

FLOWSHEET
    BLOCK B1 IN=1 2 OUT=3 4

PROPERTIES SYSOP11

PROP-REPLACE SYSOP11 UNIQ-RK
      PROP PHILMX PHILMX11
      PROP HLMX HLMX11
      PROP GLMX GLMX11
      PROP SLMX SLMX11
      PROP MUVMX MUVMX02
      PROP MULMX MULMX02
      PROP KVMX KVMX02
      PROP DV DV01

PROP-DATA UNIQ-1
    IN-UNITS MET VOLUME-FLOW='cum/hr' ENTHALPY-FLO='MMkcal/hr'    &
        HEAT-TRANS-C='kcal/hr-sqm-K' PRESSURE=bar TEMPERATURE=K  &
        VOLUME=cum DELTA-T=C HEAD=meter MOLE-DENSITY='kmol/cum'  &
        MASS-DENSITY='kg/cum' MOLE-ENTHALP='kcal/mol'  &
        MASS-ENTHALP='kcal/kg' HEAT=MMkcal MOLE-CONC='mol/l'  &
        PDROP=bar
    PROP-LIST UNIQ
    BPVAL MEOH IB 0.0 35.38 0.0 0.0 0.0 1000.000
    BPVAL IB MEOH 0.0 -706.34 0.0 0.0 0.0 1000.000
    BPVAL MEOH MTBE 0.0 88.04 0.0 0.0 0.0 1000.000
    BPVAL MTBE MEOH 0.0 -468.76 0.0 0.0 0.0 1000.000
    BPVAL IB MTBE 0.0 -52.2 0.0 0.0 0.0 1000.000
    BPVAL MTBE IB 0.0 24.63 0.0 0.0 0.0 1000.000
```

Exercise 11.22 (continued)

Analysis: (continued)

```
    BPVAL MEOH NB 0.0 35.38 0.0 0.0 0.0 1000.000
    BPVAL NB MEOH 0.0 -706.34 0.0 0.0 0.0 1000.000
    BPVAL NB MTBE 0.0 -52.2 0.0 0.0 0.0 1000.000
    BPVAL MTBE NB 0.0 24.63 0.0 0.0 0.0 1000.000

PROP-SET VLE PHIMX GAMMA PL SUBSTREAM=MIXED PHASE=V L

STREAM 1
    SUBSTREAM MIXED TEMP=320. <K> PRES=11. <bar> NPHASE=1 PHASE=L
    MOLE-FLOW MEOH 215.5 <mol/sec> / IB 0. <mol/sec> / NB  &
        0. <mol/sec> / MTBE 0. <mol/sec>

STREAM 2
    SUBSTREAM MIXED TEMP=350. <K> PRES=11. <bar> NPHASE=1
    MOLE-FLOW MEOH 0. <mol/sec> / IB 195.44 <mol/sec> / NB  &
        353.56 <mol/sec> / MTBE 0. <mol/sec>

BLOCK B1 RADFRAC
    PARAM NSTAGE=17 ALGORITHM=NONIDEAL MAXOL=99 DAMPING=MEDIUM
    COL-CONFIG CONDENSER=TOTAL
    FEEDS 1 7 ON-STAGE / 2 11 ON-STAGE
    PRODUCTS 3 1 L / 4 17 L
    P-SPEC 1 11. <bar> / 2 11. <bar>
    COL-SPECS DP-STAGE=0. <bar> MOLE-B=197. <mol/sec> MOLE-RR=7.
    REAC-STAGES 4 11 R-1
    HOLD-UP 4 11 MASS-LHLDP=8000.
    T-EST 1 350 <K> / 17 420 <K>
    X-EST 17 MEOH 0.05 / 17 MTBE 0.95
    Y-EST 17 MEOH 0.125 / 17 MTBE 0.875
    TRAY-REPORT TRAY-OPTION=ALL-TRAYS PROPERTIES=VLE

STREAM-REPOR PROPERTIES=VLE

REACTIONS R-1 REAC-DIST
    REAC-DATA 1 KINETIC CBASIS=MOLEFRAC
    REAC-DATA 2 KINETIC CBASIS=MOLEFRAC
    RATE-CON 1 PRE-EXP=3.67E+012 ACT-ENERGY=92400. <kJ/kmol>
    RATE-CON 2 PRE-EXP=2.67E+017 ACT-ENERGY=134454. <kJ/kmol>
    STOIC 1 MEOH -1. / IB -1. / NB 0. / MTBE 1.
    STOIC 2 MTBE -1. / NB 0. / MEOH 1. / IB 1.
    POWLAW-EXP 1 MEOH -1. / IB 1. / NB 0. / MTBE 0.
    POWLAW-EXP 2 MTBE 1. / NB 0. / MEOH -2. / IB 0.
```

Exercise 11.23

Subject: Reactive distillation of isobutene (IB) with methanol (M), in the presence of n-butene (NB) to produce MTBE. Use of activities instead of mole fractions in the kinetic equations.

Given: Mixed butenes feed of 195.44 mol/s of IB and 353.56 mol/s of NB entering stage 11 as a vapor at 350 K and 11 bar. Methanol feed of 215.5 mol/s at 320 K and 11 bar to stage 10. Column operates at 11 atm and has 15 equilibrium stages, with a total condenser and partial reboiler. Reflux ratio = 7 and bottoms flow rate is set at 197 mol/s. Catalyst for the reaction is provided in the amount of 204.1 kg/stage only at stages 4 through 11. Kinetic data is given in Example 11.9, but substitute activities for mole fractions in the kinetic equations. Use UNIQUAC method for liquid-phase activity coefficients, with the binary interaction parameters in Example 11.9, and RK EOS for vapor-phase fugacities.

Find: Distillate and bottoms products, and comparison of results with those of Example 11.9.

Analysis: Kinetic equations for the reaction rates are most often written in terms of component concentrations, component mole fractions, or component partial pressures (in the case of gas-phase reactions). However for liquid-phase reactions when the components form a non-ideal solution, chemical equilibrium can only be satisfied when the rate equation is written in terms of activities (product of mole fraction times liquid-phase activity coefficient). For the formation of MTBE from isobutene and methanol, the Rehfinger and Hoffmann article was developed in terms of component activities. However, in Example 11.9, component mole fractions are used, as seen in Eqs. (1) and (2). This assumes that all component activity coefficients are equal to one. With Aspen Plus, built-in kinetic rate-law expressions are not available in terms of activities. Therefore, a FORTRAN subroutine for the rate-law must be provided. On the following four pages, the Aspen Plus input data are listed for solving this exercise. Under the Aspen Plus paragraph REACTIONS R-MTBE-U REAC-DIST, reference is made to the user-supplied subroutine RAMTBE. This subroutine is listed on the subsequent five pages, where the kinetic rate equation is written in terms of activities. The Aspen Plus input data are written to explore the variation of methanol feed stage. For methanol fed to stage 10, the conversion of isobutene, when using activities, is 99.5% compared to a 95.6% conversion in Example 11.9, where mole fractions are used.

Exercise 11.23 (continued)

Analysis: (continued)

ASPEN PLUS INPUT DATA

```
TITLE 'REACTIVE DISTILLATION FOR THE PRODUCTION OF MTBE'

IN-UNITS SI ENTHALPY-FLO=KW POWER=KW PRESSURE=BAR TEMPERATURE=C &
    DELTA-T=C PDROP=BAR

DEF-STREAMS CONVEN ALL

DIAGNOSTICS
  TERMINAL SIM-LEVEL=0 CONV-LEVEL=0 COST-LEVEL=0 PROP-LEVEL=0 &
    ECON-LEVEL=0 STREAM-LEVEL=0 SYS-LEVEL=0

DESCRIPTION "Reactive distillation for MTBE production.
    Added data for the regression of UNIQUAC parameters from UNIFAC flash curve.
    Addition of a kinetic routine using activities in the RADFRAC model. "

DATABANKS PURE856 / ASPENPCD

PROP-SOURCES PURE856 / ASPENPCD

COMPONENTS
  CH3OH CH4O CH3OH /
  "IC4=" C4H8-5 "IC4=" /
  "NC4=" C4H8-1 "NC4=" /
  MTBE C5H12O-D2 MTBE

FLOWSHEET
  BLOCK B-DIST IN=B-MEF B-C4F OUT=B-C4M B-MTBE

PROPERTIES UNIFAC
  PROPERTIES UNIQ-RK

PROP-REPLACE UNIQ-RK UNIQ-RK
  MODEL GMUQUAC 2

ESTIMATE ALL

PROP-DATA UNIQ-2
  IN-UNITS SI ENTHALPY-FLO=KW POWER=KW PRESSURE=BAR &
    TEMPERATURE=C DELTA-T=C PDROP=BAR
  PROP-LIST UNIQ 2
  BPVAL CH3OH "IC4=" 0.0 35.80000 0.0 0.0 0.0 1000.000
  BPVAL "IC4=" CH3OH 0.0 -706.3400 0.0 0.0 0.0 1000.000
  BPVAL CH3OH MTBE 0.0 88.04 0.0 0.0 0.0 1000.000
  BPVAL MTBE CH3OH 0.0 -468.76 0.0 0.0 0.0 1000.000
  BPVAL "IC4=" MTBE 0.0 -52.20 0.0 0.0 0.0 1000.000
  BPVAL MTBE "IC4=" 0.0 24.630 0.0 0.0 0.0 1000.000
  BPVAL "NC4=" MTBE 0.0 -52.2 0.0 0.0 0.0 1000.000
  BPVAL MTBE "NC4=" 0.0 24.63 0.0 0.0 0.0 1000.000
  BPVAL CH3OH "NC4=" 0 35.8 0.0 0.0 0.0 1000.000
  BPVAL "NC4=" CH3OH 0 -706.34 0.0 0.0 0.0 1000.000
```

Exercise 11.23 (continued)

Analysis: (continued)

```
PROP-SET PS-1
  IN-UNITS SI
  PROPNAME-LIS TEMP MOLEFRAC SUBSTREAM=MIXED PHASE=L V

STREAM B-C4F
  SUBSTREAM MIXED TEMP=76.85000 PRES=12.00 &
    MOLE-FLOW=0.5490
  MOLE-FRAC "IC4=" 0.356 / "NC4=" 0.644

STREAM B-MEF
  SUBSTREAM MIXED TEMP=46.85 PRES=12.00
  MOLE-FLOW CH3OH 0.206

BLOCK B-DIST RADFRAC
  PARAM NSTAGE=18 ALGORITHM=NONIDEAL INIT-OPTION=STANDARD &
    MAXOL=100 DAMPING=MEDIUM
  FEEDS B-MEF 10 ON-STAGE / B-C4F 11 ON-STAGE
  PRODUCTS B-C4M 1 L / B-MTBE 18 L
  P-SPEC 1 11
  COL-SPECS MOLE-RDV=0 MOLE-B=0.197 MOLE-RR=7
  REAC-STAGES 4 11 R-MTBE-U
  HOLD-UP 4 11 MASS-LHLDP=800.00
  T-EST 1 73 / 11 83 / 18 154
  TRAY-SIZE 1 2 3 FLOAT
  TRAY-SIZE 2 12 17 FLOAT
  TRAY-RATE 1 2 17 FLOAT DIAM=5.5 P-UPDATE=NO
  PROPERTIES UNIQ-RK

SENSITIVITY S-4
  PARAM BASE-CASE=NO
  DEFINE F MOLE-FLOW STREAM=B-C4F SUBSTREAM=MIXED &
    COMPONENT="IC4="
  DEFINE T MOLE-FLOW STREAM=B-C4M SUBSTREAM=MIXED &
    COMPONENT="IC4="
  DEFINE B MOLE-FLOW STREAM=B-MTBE SUBSTREAM=MIXED &
    COMPONENT="IC4="
  DEFINE XMTBE MOLE-FRAC STREAM=B-MTBE SUBSTREAM=MIXED &
    COMPONENT=MTBE
  DEFINE QC BLOCK-VAR BLOCK=B-DIST VARIABLE=COND-DUTY &
    SENTENCE=RESULTS
  DEFINE QB BLOCK-VAR BLOCK=B-DIST VARIABLE=REB-DUTY &
    SENTENCE=RESULTS
  DEFINE TMEOH MOLE-FRAC STREAM=B-C4M SUBSTREAM=MIXED &
    COMPONENT=CH3OH
  DEFINE TNC4 MOLE-FRAC STREAM=B-C4M SUBSTREAM=MIXED &
    COMPONENT="NC4="
  DEFINE TMTBE MOLE-FRAC STREAM=B-C4M SUBSTREAM=MIXED &
    COMPONENT=MTBE
```

Exercise 11.23 (continued)

Analysis: (continued)

```
    TABULATE 1 "(F-T-B)/F" COL-LABEL="CNV"
    TABULATE 2 "XMTBE" COL-LABEL="MTBE"
    TABULATE 3 "QC" COL-LABEL="QC"
    TABULATE 4 "QB" COL-LABEL="QB"
    TABULATE 5 "TMEOH" COL-LABEL="MEOH"
    TABULATE 6 "TNC4" COL-LABEL="NC4"
    TABULATE 7 "TMTBE" COL-LABEL="MTBE TOP"
    VARY BLOCK-VAR BLOCK=B-DIST VARIABLE=PRES SENTENCE=P-SPEC &
      ID1=1
    RANGE LOWER="7  " UPPER="15 " INCR="0.5  "

  PROPERTY-REP PCES NOPROP-DATA

  REACTIONS R-MTBE REAC-DIST
    REAC-DATA 1 KINETIC CBASIS=MOLEFRAC
    REAC-DATA 2 KINETIC CBASIS=MOLEFRAC
    RATE-CON 1 PRE-EXP=1.7983E13 ACT-ENERGY=9.239E7
    RATE-CON 2 PRE-EXP=9.014E-15 ACT-ENERGY=1.023E8  &
      TEMP-EXPONEN=10.52
    STOIC 1 CH3OH -1 / "IC4=" -1 / MTBE 1
    STOIC 2 MTBE -1 / CH3OH 1 / "IC4=" 1
    POWLAW-EXP 1 CH3OH -1 / "IC4=" 1 / MTBE 0
    POWLAW-EXP 2 MTBE 1 / CH3OH -2 / "IC4=" 0

  REACTIONS R-MTBE-U REAC-DIST
    PARAM SUBROUTINE=RAMTBE
    REAC-DATA 1 KINETIC
    STOIC 1 CH3OH -1 / "IC4=" -1 / MTBE 1

  PROP-TABLE 12-UNIF FLASHCURVE
    DESCRIPTION "Flash for CH3OH/IC4= with UNIFAC model"
    MOLE-FLOW CH3OH 1 / "IC4=" 1
    STATE PRES=12 VFRAC=0
    VARY MOLE-FRAC COMP=CH3OH
    RANGE LOWER=0 UPPER=1 INCR=0.05
    TABULATE PROPERTIES=PS-1

  PROP-TABLE 12-UNIQ FLASHCURVE
    DESCRIPTION "Flash CH3OH/MTBE using UNIQUAC/RK"
    PROPERTIES UNIQ-RK
    MOLE-FLOW CH3OH 1 / "IC4=" 1
    STATE PRES=12 VFRAC=0
    VARY MOLE-FRAC COMP=CH3OH
    RANGE LOWER=0 UPPER=1 INCR=0.05
    TABULATE PROPERTIES=PS-1
```

Exercise 11.23 (continued)

Analysis: (continued)

```
PROP-TABLE 13-UNIF FLASHCURVE
   DESCRIPTION "Flash CH3OH/NC4="
   MOLE-FLOW CH3OH 1 / "NC4=" 1
   STATE PRES=12 VFRAC=0
   VARY MOLE-FRAC COMP=CH3OH
   RANGE LOWER=0 UPPER=1 INCR=0.05
   TABULATE PROPERTIES=PS-1

PROP-TABLE 14-UNIF FLASHCURVE
   DESCRIPTION "Flash CH3OH/MTBE with UNIFAC model"
   MOLE-FLOW CH3OH 0.1 / MTBE 0.1
   STATE PRES=12 VFRAC=0
   VARY MOLE-FRAC COMP=CH3OH
   RANGE LOWER=0 UPPER=1 INCR=0.05
   TABULATE PROPERTIES=PS-1

PROP-TABLE 14-UNIQ FLASHCURVE
   DESCRIPTION "Flash CH3OH/MTBE using UNIQUAC/REDLICH KWONG"
   PROPERTIES UNIQ-RK
   MOLE-FLOW CH3OH 0.1 / MTBE 0.1
   STATE PRES=12 VFRAC=0
   VARY MOLE-FRAC COMP=CH3OH
   RANGE LOWER=0 UPPER=1 INCR=0.05
   TABULATE PROPERTIES=PS-1

PROP-TABLE 24-UNIF FLASHCURVE
   DESCRIPTION "Flash IC4=/MTBE using UNIFAC"
   MOLE-FLOW "IC4=" 1 / MTBE 1
   STATE PRES=12 VFRAC=0
   VARY MOLE-FRAC COMP="IC4="
   RANGE LOWER=0 UPPER=1 INCR=0.05
   TABULATE PROPERTIES=PS-1
```

Exercise 11.23 (continued)

Analysis: (continued)

ASPEN PLUS KINETICS SUBROUTINE

```
C     Calculation of MTBE synthesis reaction rate using activities.
C     User Kinetics Subroutine for RADFRAC
C
      SUBROUTINE RAMTBE (NSTAGE, NCOMP,  NR,     NRL,    NRV,
     2                   T,      TLIQ,   TVAP,   P,      VF,
     3                   F,      X,      Y,      IDX,    NBOPST,
     4                   KDIAG,  STOIC,  IHLBAS, HLDLIQ, TIMLIQ,
     5                   IHVBAS, HLDVAP, TIMVAP, NINT,   INT,
     6                   NREAL,  REAL,   RATES,  RATEL,  RATEV,
     7                   NINTB,  INTB,   NREALB, REALB,  NIWORK,
     8                   IWORK,  NWORK,  WORK)
C
C       VARIABLES IN ARGUMENT LIST
C
C        VARIABLE  I/O  TYPE     DIMENSION     DESCRIPTION AND RANGE
C        NSTAGE     I    I          -          STAGE NUMBER
C        NCOMP      I    I          -          NUMBER OF COMPONENTS
C        NR         I    I          -          TOTAL NUMBER OF KINETIC
C                                               REACTIONS
C        NRL        I    I          -          NUMBER OF LIQUID PHASE
C                                               KINETIC REACTIONS
C        NRV        I    I          -          NUMBER OF VAPOR PHASE
C                                               KINETIC REACTIONS
C        T          I    R          -          STAGE TEMPERATURE (K)
C        TLIQ       I    R          -          LIQUID TEMPERATURE (K)
C                                               * USED ONLY BY RATEFRAC **
C        TVAP       I    R          -          VAPOR TEMPERATURE (K)
C                                               * USED ONLY BY RATEFRAC **
C        P          I    R          -          STAGE PRESSURE (N/SQ.M)
C        VF         I    R          -          VAPOR FRACTION
C        F          I    R          -          TOTAL FLOW ON STAGE
C                                               (VAPOR+LIQUID) (KMOL/SEC)
C        X          I    R        NCOMP,3      LIQUID MOLE FRACTION
C        Y          I    R        NCOMP        VAPOR MOLE FRACTION
C        IDX        I    I        NCOMP        COMPONENT INDEX VECTOR
C        NBOPST     I    I         6           OPTION SET BEAD POINTER
C        KDIAG      I    I         -           LOCAL DIAGNOSTIC LEVEL
C        STOIC      I    R        NCOMP,NR     REACTION STOICHIOMETRY
C        IHLBAS     I    I         -           BASIS FOR LIQUID
C                                               HOLDUP SPECIFICATION
C                                               1:VOLUME,2:MASS,3:MOLE
C        HLDLIQ     I    R         -           LIQUID HOLDUP
C                                               IHLBAS    UNITS
C                                               1         CU.M.
C                                               2         KG
C                                               3         KMOL
C        TIMLIQ     I    R         -           LIQUID RESIDENCE TIME
C                                               (SEC)
```

Exercise 11.23 (continued)

Analysis: (continued)

```
C       IHVBAS     I    I          -          BASIS FOR VAPOR
C                                              HOLDUP SPECIFICATION
C                                              1:VOLUME,2:MASS,3:MOLE
C       HLDVAP     I    R          -          VAPOR HOLDUP
C                                              IHVBAS    UNITS
C                                              1         CU.M.
C                                              2         KG
C                                              3         KMOL
C       TIMVAP     I    R          -          VAPOR RESIDENCE TIME (SEC)
C       NINT       I    I          -          LENGTH OF INTEGER VECTOR
C       INT       I/O   I         NINT        INTEGER VECTOR
C       NREAL      I    I          -          LENGTH OF REAL VECTOR
C       REAL      I/O   R         NREAL       REAL VECTOR
C       RATES      O    R         NCOMP       COMPONENT REACTION RATES
C                                              (KMOL/SEC)
C       RATEL      O    R         NRL         INDIVIDUAL REACTION RATES
C                                              IN THE LIQUID PHASE
C                                              (KMOL/SEC)
C                                              * USED ONLY BY RATEFRAC **
C       RATEV      O    R         NRV         INDIVIDUAL REACTION RATES
C                                              IN THE VAPOR PHASE
C                                              (KMOL/SEC)
C                                              * USED ONLY BY RATEFRAC **
C       NINTB      I    I          -          LENGTH OF INTEGER VECTOR
C                                              (FROM UOS BLOCK)
C       INTB      I/O   I         NINTB       INTEGER VECTOR
C                                              (FROM UOS BLOCK)
C       NREALB     I    I          -          LENGTH OF REAL VECTOR
C                                              (FROM UOS BLOCK)
C       REALB     I/O   R         NREALB      REAL VECTOR
C                                              (FROM UOS BLOCK)
C       NIWORK     I    I          -          LENGTH OF INTEGER WORK
C                                              VECTOR
C       IWORK     I/O   I         NIWORK      INTEGER WORK VECTOR
C       NWORK      I    I          -          LENGTH OF REAL WORK VECTOR
C       WORK      I/O   R         NWORK       REAL WORK VECTOR
C
C*******************************************************************************
C
```

Exercise 11.23 (continued)

Analysis: (continued)

```
      IMPLICIT REAL*8 (A-H, O-Z)

C     Component order
C     ===============
C     This routine assumes that the components are in this order :
      PARAMETER(K_MEOH=1)
      PARAMETER(K_IC4=2)
      PARAMETER(K_NC4=3)
      PARAMETER(K_MTBE=4)

      PARAMETER(N_COMP=4)

      REAL*8 PHI(N_COMP)
      REAL*8 DPHI(N_COMP)
      REAL*8 ACTIV(N_COMP)

C
      COMMON /USER/ RMISS,  IMISS,  NGBAL, IPASS, IRESTR,
     2              ICONVG, LMSG,   LPMSG, KFLAG, NHSTRY,
     3              NRPT,   NTRMNL, ISIZE
C
C
      COMMON /MAXWRT/ MAXBUF
      CHARACTER*80 MAXBUF(20)

      DIMENSION X(NCOMP,3), Y(NCOMP), IDX(NCOMP), NBOPST(6),
     2          STOIC(NCOMP,NR), INT(NINT), REAL(NREAL),
     3          RATES(NCOMP), RATEL(NRL), RATEV(NRV), INTB(NINTB),
     4          REALB(NREALB), IWORK(NIWORK), WORK(NWORK)

      COMMON /IPOFF3/IPOFF3(1)

      COMMON /PLEX/IB(1)
      DIMENSION B(1)
      EQUIVALENCE(B(1),IB(1))

      DATA IDBG/0/
```

Exercise 11.23 (continued)

Analysis: (continued)

```
C     Thermodynamic rate constant DKA
C     ===============================
      TZERO=298.15D+00
      C1=-1493.D+00
      C2=-77.4D+00
      C3=0.508D+00
      C4=-0.913D-03
      C5=1.11D-06
      C6=-0.628D-09
      FT=C1*(1.D+00/T-1.D+00/TZERO)
     *  +C2*DLOG(T/TZERO)
     *  +C3*(T-TZERO)
     *  +C4*(T*T-TZERO*TZERO)
     *  +C5*(T**3-TZERO**3)
     *  +C6*(T**4-TZERO**4)

      DKA=284D+00*DEXP(FT)

C     Reaction rate constant
C     ======================
      DKR=3.67D+12*DEXP(-11110.D+00/T)

      IF(IDBG.GE.1)THEN
        WRITE(MAXBUF(1),9010) FT,DKA,DKR
        CALL WRTTRM(1)
      ENDIF
 9010 FORMAT(1X,3(G13.6,1X))

C     Calculation of components activities
C     ====================================
C     Calculate only fugacity coefficient
      KPHI=1

C     Fugacity coefficient of components in the mixture
      CALL FUGLY(T,P,X(1,1),Y,NCOMP,IDX,NBOPST,KDIAG,KPHI,PHI,DPHI,KER)
      IF(KER.NE.0)THEN
        WRITE(MAXBUF(1),9000) T,P,KER
        CALL WRTTRM(1)
      ENDIF
 9000 FORMAT(' fugly failed at T=',G12.5,' P=',G12.5,' ker=',I4)

C     Set offset to get activity coefficients
      L_GAMMA=IPOFF3(24)
```

Exercise 11.23 (continued)

Analysis: (continued)

```
C     Calculate activities for plex data
      DO J=1,NCOMP
        ACTIV(J)=DEXP(B(L_GAMMA+J))*X(J,1)
      END DO
      IF(IDBG.GE.1)THEN
        DO J=1,NCOMP
          WRITE(MAXBUF(1),9020) J,X(J,1),ACTIV(J)
          CALL WRTTRM(1)
        END DO
      ENDIF
 9020 FORMAT(' compo ',I3,' mole-frac=',G12.5,' activity=',G12.5)

C     Reaction rate
C     =============
C     RATE : mol/s/kgcata
C     Q    : equiv/kgcata
C     DKR  : mol/s/equiv
      Q=4.9D+00
      RATE=Q*DKR*
     *      (ACTIV(K_IC4)/ACTIV(K_MEOH)
     *     -ACTIV(K_MTBE)/DKA/ACTIV(K_MEOH)**2)
C     Use mass holdup as kgcata
      RATNET=RATE*HLDLIQ*1.D-03

      RATES(K_IC4)=-RATNET
      RATES(K_MEOH)=-RATNET
      RATES(K_MTBE)=RATNET
      RATES(K_NC4)=0.D+00

      IF(IDBG.GE.1)THEN
        WRITE(MAXBUF(1),9030) NSTAGE,RATE,RATNET
        CALL WRTTRM(1)
      ENDIF
 9030 FORMAT(' stage=',I4,' spec-rate=',G12.5,' net-rate=',G12.5)
      RETURN
      END
```

Exercise 11.24

Subject: Reactive distillation of isobutene (IB) with methanol (M), in the presence of n-butene (NB) to produce MTBE. Chemical equilibrium at each stage that has catalyst.

Given: Mixed butenes feed of 195.44 mol/s of IB and 353.56 mol/s of NB entering stage 11 as a vapor at 350 K and 11 bar. Methanol feed of 215.5 mol/s at 320 K and 11 bar to stage 10. Column operates at 11 atm and has 15 equilibrium stages, with a total condenser and partial reboiler. Reflux ratio = 7 and bottoms flow rate is set at 197 mol/s. Chemical equilibrium is achieved at stages 4 through 11. RK EOS for vapor-phase fugacities.

Assumptions: Use UNIFAC method for liquid-phase activity coefficients.

Find: Distillate and bottoms products, and comparison of results with those of Example 11.9.

Analysis: The ChemCad program, with the SCDS model and reactive distillation option, was used to make the equilibrium stage calculations. To do this, it is assumed that the required chemical equilibrium constant can be computed by taking the ratio of the forward to the backward rate constant. From Eqs. (1) and (2) in Example 11.9,

$$K = 1.375 \times 10^{-5} \exp(42014/(RT)) \qquad (1)$$

From Fig. 11.38(a), all of the reaction takes place at a temperature of about 350 K. From Eq. (1), at T = 350 K, with R = 8.314 J/mol-K, K = 25.6. In ChemCad, let ln$K$ = A. Therefore, A = 3.24.

Input data for ChemCad, included:
No. of stages = 17, with M fed to stage 10, and the butenes fed to stage 11.
Estimated temperatures in K were 350, 340, 400, and 420 for stages 1, 2, 16, and 17.
A damping factor of 0.25 was used with a maximum of 50 iterations.
A single reaction was specified for the equilibrium option and stages 1-3 and 12-17 were disabled.
The problem was very slow to converge, taking almost the maximum number of iterations. The overall material balance is as follows:

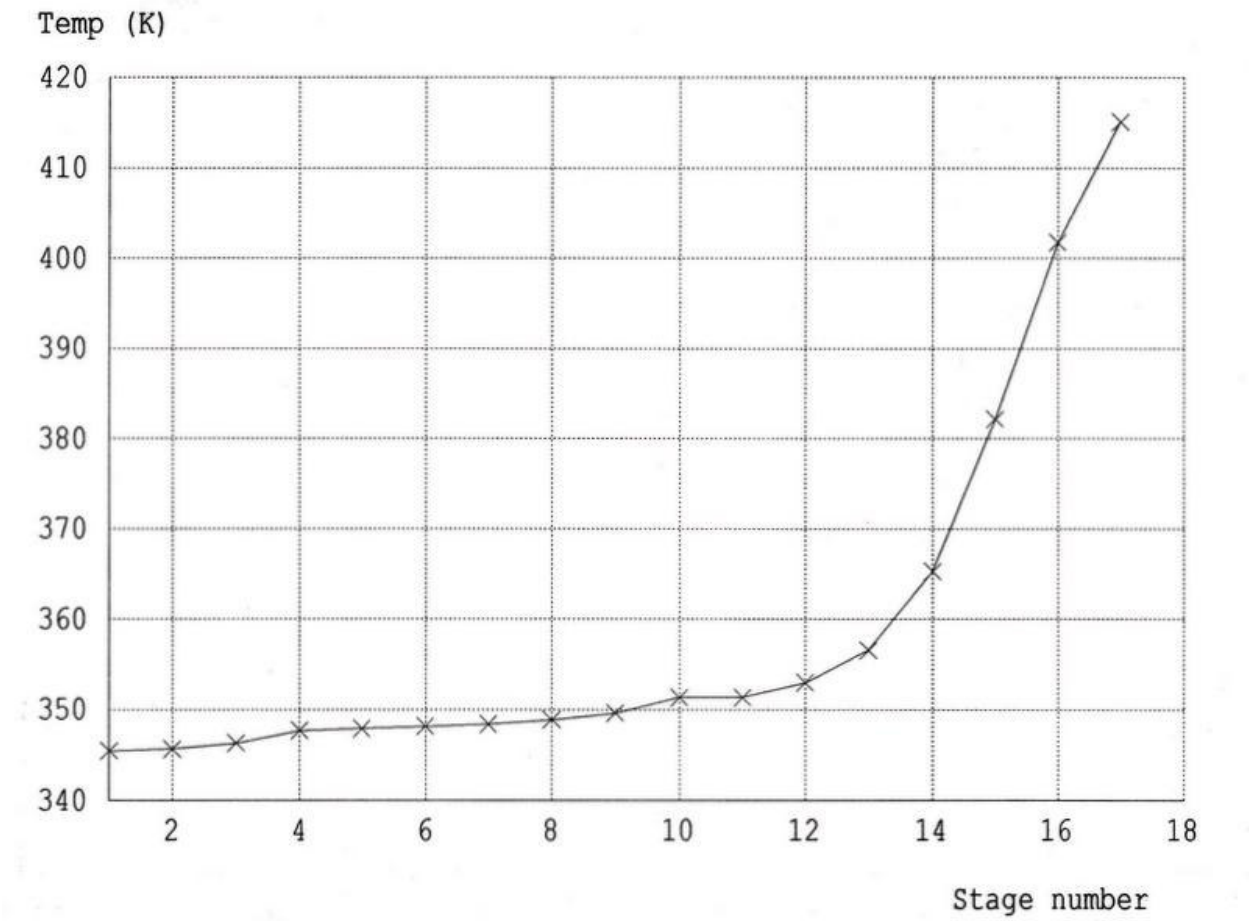
Mol/s:

Component	Feed 1	Feed 2	Distillate	Bottoms
Methanol	215.50	0.00	36.28	0.12
Isobutene	0.00	195.44	13.58	2.76
n-butene	0.00	353.56	338.39	15.17
MTBE	0.00	0.00	0.15	178.95
Total:	215.50	549.00	388.40	197.00

The % conversion of isobutene to MTBE = 91.64%. This compares to 95.6% in Example 11.9.
The profiles are shown on the next three pages and compare favorably to Figs. 11.38(a to c).

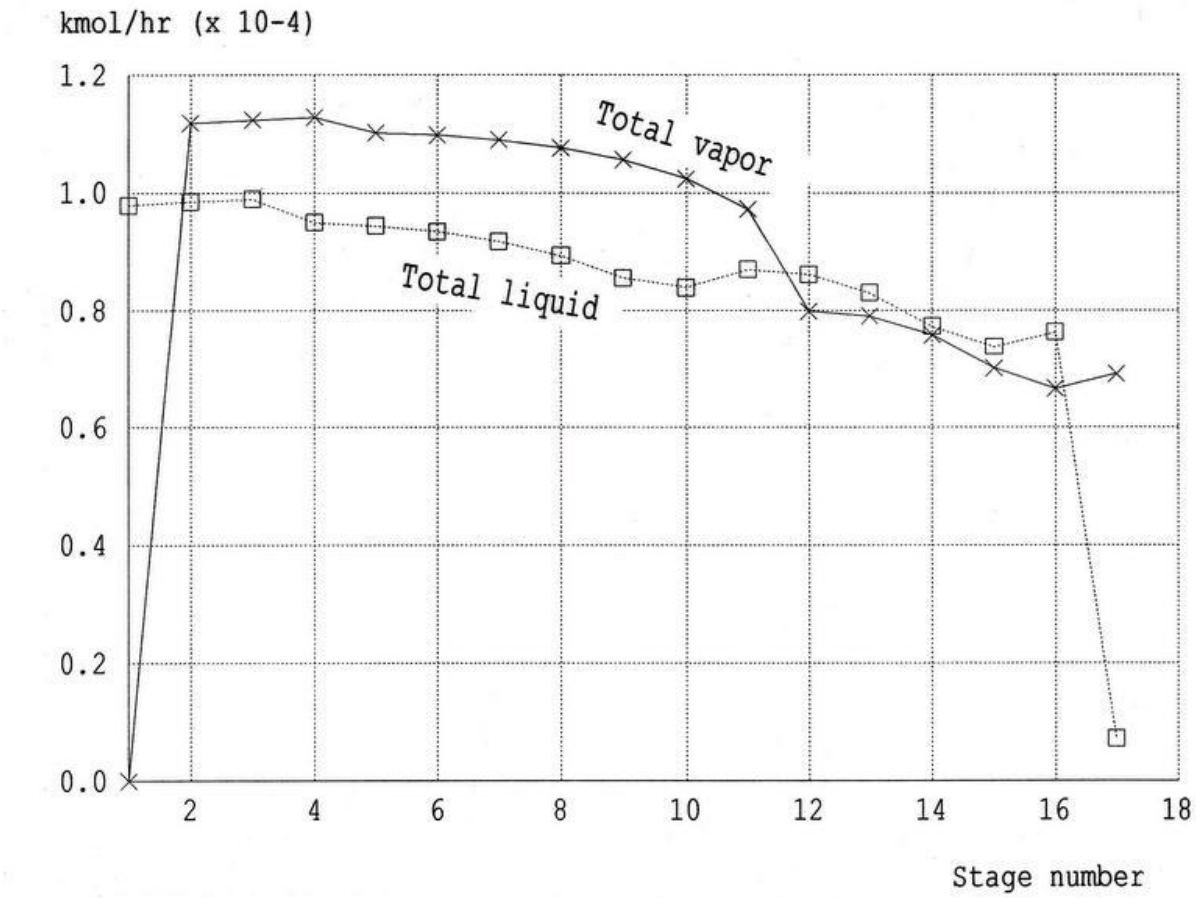
Exercise 11.24 (continued)

Analysis: (continued)



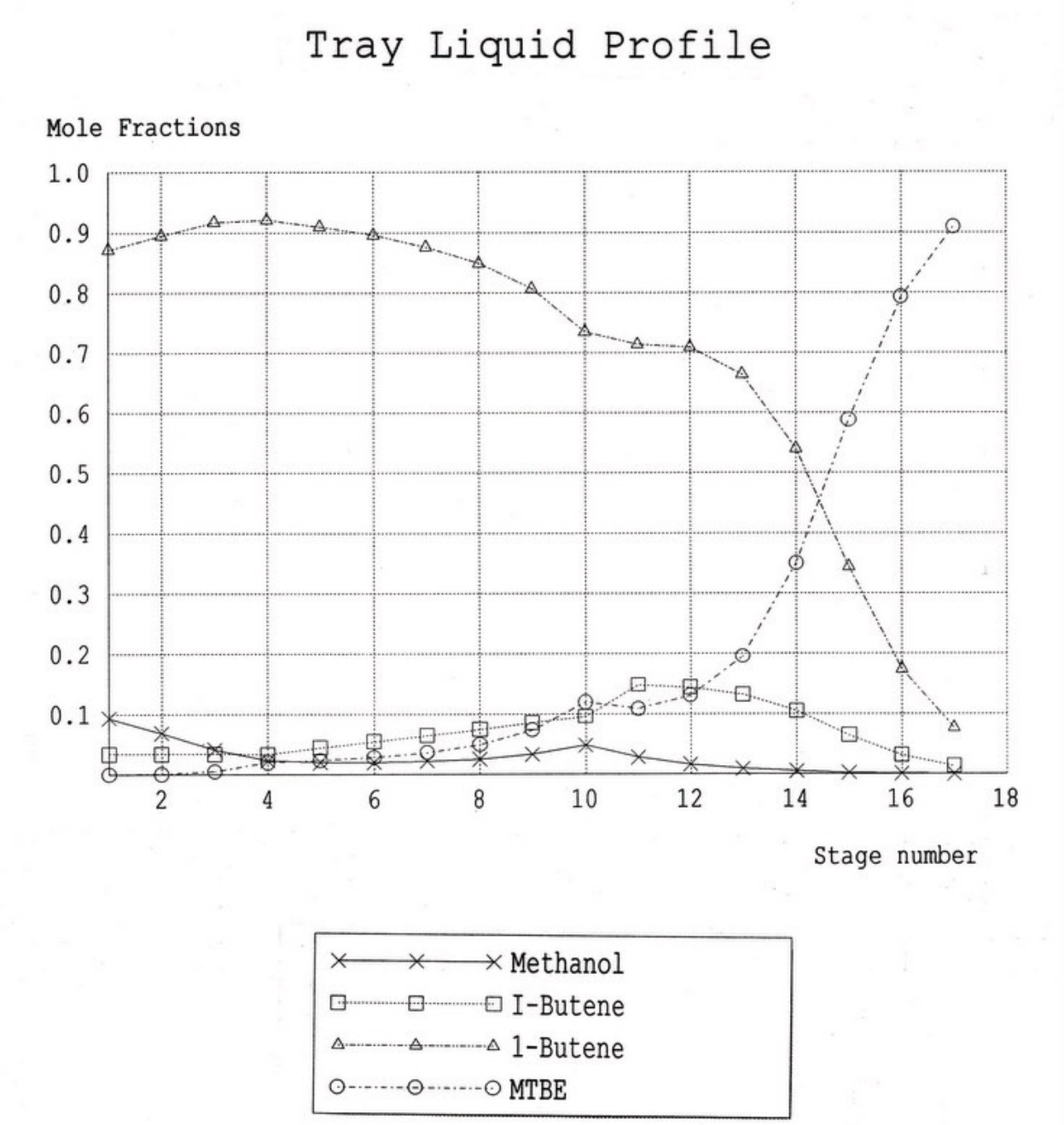
Exercise 11.24 (continued)

Analysis: (continued)



Exercise 11.24 (continued)

Analysis: (continued)



Exercise 11.25

Subject: Supercritical extraction of 1 mol/s of 10 wt% ethanol in water by 3 mol/s of carbon dioxide at 305 K and 9.86 MPa in a staged contactor.

Given: 10 equilibrium stages. *K*-values from Example 11.10.

Find: Flow rates and compositions of the exiting extract and raffinate. Compare results to those of Example 11.10.

Analysis: The ChemCad program with the Tower Plus model was used to make the calculations, as in Example 11.10. Isothermal conditions were employed by allowing heat transfer at each stage. The polynomial *K*-value option was used to supply the constant *K*-values given in Example 11.10 (0.115 for ethanol, 0.00575 for water, and 34.5 for CO_2) The calculations converged in 7 iterations. The overall material balance was as follows:

Mol/s:

Component	Feed	Solvent	Raffinate	Extract
Carbon dioxide	0.0000	3.0000	0.0287	2.9713
Ethanol	0.0417	0.0000	0.0277	0.0140
Water	0.9583	0.0000	0.9422	0.0161
Total:	1.0000	3.0000	0.9986	3.0014

These results are almost identical to those for Example 11.10, which used just 5 equilibrium stages.

This should not be surprising! Supercritical extraction is analogous to stripping or liquid-liquid extraction. Thus, an approximate calculation can be made with the Kremser method based on stripping factors for ethanol and water, and an absorption factor for carbon dioxide.

For ethanol, the stripping factor is $S = KV/L = 0.115(3)/1 = 0.345$. From the Kremser plot in Fig. 5.9, the fraction extracted is approximately 35%, independent of the number of stages above 3. For water, $S = 0.00575(3)/1 = 0.0173$, and the Kremser plot gives approximately 1.7% extracted, again independent of the number of stages above 3. For carbon dioxide, an absorption factor is used, where $A = L/KV = 1/[34.5(3)] = 0.00966$. From the Kremser plot, approximately 1% of the carbon dioxide is transferred to the raffinate. These values are very close to the following values computed from the above material balance:

% extraction of ethanol = 0.0140/0.0417 x 100% = 33.6%

% extraction of water = 0.0161/0.9583 x 100% = 1.68%

% loss of carbon dioxide to raffinate = 0.0287/3.0 x 100% = 0.957%

Exercise 11.26

Subject: Development of a mathematical model for the supercritical extraction of a solute from particles of natural material. An example is the extraction of caffeine from coffee beans by supercritical CO_2.

Given: Rate of extraction is independent of the flow rate of CO_2 past the particles, but dependent on the particle size.

Find: A mathematical model for the rate of extraction. The parameter in the model that must be determined by experiment.

Analysis: In the extraction of a solute from a natural material by a fluid solvent, the following mechanism may be considered. It is discussed in several places in the literature, including an article by Goto, Roy, and Hirose in The Journal of Supercritical Fluids, 9, 128-133 (1996), entitled "Shrinking-Core Leaching Model for Supercritical-Fluid Extraction". The particle of natural material is soaked in the solvent so that the solvent penetrates into the particle, usually causing it to swell. The material may be thought of as a porous or cellular matrix that fixes or traps the solute in the matrix. However, in the presence of the solvent, the solute is released and can diffuse from the interior of the material to the surface of the particle, and from there into the bulk of the solvent. Thus, the solute mass-transfer process can be viewed as taking place in two steps, one (internal mass-transfer resistance) by diffusion in the interior of the material and the other (external mass-transfer resistance) by convection in the exterior solvent surrounding the material. Assuming that the solvent flows past the particles so as to sweep away the solute as it leaves the surface of the particles, it can be assumed that the external mass-transfer resistance is negligible because the rate of extraction is given as independent of the solvent flow rate past the particle. This is so because it is recalled from Chapter 3 that for forced convection past a spherical particle, Eq. (3-170), the mass-transfer coefficient is proportional to the fluid mass velocity or velocity past the particle to the 0.6 exponent and inversely proportional to the particle diameter to the 0.4 exponent. Since there is no effect of velocity, all of the mass transfer resistance resides in the interior of the particle, where a Fickian diffusion process can be assumed.

As suggested by the Goto, Roy, and Hirose (cited above), the interior diffusion process can be viewed as one in which the rate of diffusion in the non-extracted interior core of the particle is much slower than in the outer shell of the particle where most of the solute has been extracted. This results in a sharp boundary or interface between the inner core and outer shell. In the inner core, the concentration of solute is at its initial value. With time, the core region shrinks as the sharp boundary progresses toward the center of the particle. This is the basis for the so-called shrinking-core model widely used in modeling leaching operations. The model was first conceived by Yagi and Kunii in 1955 ["Fifth Symposium (International) on Combustion," Reinhold Publishing Corp., NY (1955), pp. 231-244] for application to gas-solid combustion, and extended to liquid-solid leaching by Roman, Benner, and Becker in 1974 [Trans. Soc. Mining Engineering of AIME, 256, 247-256 (1974)]. In its general form, takes into account both

Exercise 11.26 (continued)

Analysis: (continued)

internal and external mass-transfer resistances. Let us develop the model for the case of negligible mass-transfer resistance in the liquid external to the particle.

Assume that dr_c/dt, the rate of movement of the interface at the particle radius, r_c, is small with respect to the diffusion velocity of solute A, through the outer shell of the particle. This is referred to as the *pseudo-steady-state* assumption. The importance of this assumption is that it allows us to neglect the accumulation of solute as a function of time in the outer shell layer as that layer increases in thickness, with the result that the model can be formulated as an ordinary differential equation rather than as a partial differential equation. Thus, the rate of diffusion of solute A through the outer shell is given by Fick's second law, (3-74), ignoring the term on the left-hand side and replacing the molecular diffusivity with an effective diffusivity, D_e, for the solute through the solvent in the complex matrix of natural material:

$$\frac{D_e}{r^2}\frac{d}{dr}\left(r^2\frac{dc_A}{dr}\right)=0 \qquad (1)$$

where c_A is the concentration of solute in the outer shell of the particle and r is the radial distance from the center of the particle. The boundary conditions are:

$$c_A = c_{A_s} = c_{A_b} \text{ at } r = r_s$$

$$c_A = c_{A_0} \text{ at } r = r_c$$

where the subcripts are s for the particle surface, b for the bulk, 0 for initial condition, and c for the interface between the outer shell and core of the particle. These boundary conditions hold because the mass-transfer resistance in the liquid film or boundary layer is assumed negligible and the concentration of solute in the core remains at its initial value as the core shrinks.

If Eq. (1) is integrated twice and the boundary conditions are applied, the result after simplification is:

$$c_A = c_{A_0} - \left(c_{A_0} - c_{A_b}\right)\left[\frac{1-\frac{r_c}{r}}{1-\frac{r_c}{r_s}}\right] \qquad (2)$$

To obtain a relationship between the location of the interface r_c and time t, differentiate Eq. (2) with respect to r and evaluate the differential at $r = r_c$. This gives:

$$\left.\frac{dc_A}{dr}\right|_{r=r_c} = \frac{-\left(c_{A_0} - c_{A_b}\right)}{r_c\left(1-\frac{r_c}{r_s}\right)} \qquad (3)$$

The rate of diffusion at $r = r_c$ is given by Fick's first law, e.g. Eq. (3-66):

$$-\frac{d\mathcal{N}_A}{dt} = 4\pi r_c^2 D_e\left(\frac{dc_A}{dr}\right)_{r=r_c} \qquad (4)$$

Exercise 11.26 (continued)

Analysis: (continued)
Where,

$\mathcal{N}_A$ is the amount of *A* diffused. Combining Eqs. (3) and (4):

$$\frac{d\mathcal{N}_A}{dt} = \frac{4\pi r_c D_e \left(c_{A_0} - c_{A_b}\right)}{\left(1 - \frac{r_c}{r_s}\right)} \tag{5}$$

By material balance for the solute in the core:

$$\frac{d\mathcal{N}_A}{dt} = -\frac{\rho_A}{M_A}\frac{d}{dt}\left(\frac{4}{3}\pi r_c^3\right) = -\frac{4\pi r_c^2 \rho_A}{M_A}\frac{dr_c}{dt} \tag{6}$$

where:

ρ_A = initial mass of *s*olute per unit volume of solid particle

M_A = molecular weight of *s*olute

Combining Eqs. (5) and (6):

$$\frac{-\rho_A}{M_A}\left(\frac{1}{r_c} - \frac{1}{r_s}\right) r_c^2 dr_c = D_e\left(c_{A_0} - c_{A_b}\right)dt \tag{7}$$

Integrating Eq. (7) and applying the boundary condition: $r_c = r_s$ at $t = 0$ gives:

$$t = \frac{\rho_A r_s^2}{6 D_e M_A \left(c_{A_0} - c_{A_b}\right)}\left[1 - 3\left(\frac{r_c}{r_s}\right)^2 + 2\left(\frac{r_c}{r_s}\right)^3\right] \tag{8}$$

For complete extraction, $r_s = 0$, and Eq. (8) becomes:

$$t = \frac{\rho_A r_s^2}{6 D_e M_A \left(c_{A_0} - c_{A_b}\right)} \tag{9}$$

Equations (5) and (9) indicate that both the rate of extraction and time for extraction depend on the effective diffusivity of the solute in the particle, which must be measured experimentally.

Exercise 11.27

Subject: Supercritical extraction of a slurry of 0.002 kmol/h of solid β-carotene in 0.20 kmol/h of water with a solvent of recycle carbon dioxide in a single-stage contactor operating in the supercritical region to extract 99% of the carotene.

Given: Design of a supercritical extractor using the Group-Contribution EOS of Skjold-Jorgensen, at 353 K and 1013 bar, as shown in Fig. 1 of the cited article by Cygnarowicz and Seider.

Find: Design of a similar extractor using the Peng-Robinson EOS with the Wang-Sandler mixing rules.

Analysis: In the Cygnarowicz and Seider (C-S) article, the solubility of the carotene in water is neglected and a fit of experiment data for the solubility of carotene in CO_2 is given in Fig. 2 of the C-S article. Thus, it was only necessary here to model a single-stage flash of CO_2 and water. An initial run was made with the Aspen Plus program with the FLASH2 model under the following conditions, based on the PR EOS with the Wang-Sandler mixing rules (PRWS):

Feed of 0.2 kmol/h of water.
Solvent of 0.8004 kmol of CO_2 and 0.0081 kmol/h of water.
Single-stage extraction at 353 K and 1013 bar.

The result of the flash was only a single phase containing both the feed and the solvent. Thus, use of the PR EOS with Wang-Sandler mixing rule did not give the required two equilibrium phases shown in the C-S article. When the extraction pressure was reduced to 101.3 bar (100 atm), the following results, which are close to the C-S results, were obtained:

kmol/h:

Component	Feed	Solvent	Raffinate	Extract
CO_2	0.0	0.8004	0.0275	0.7729
Water	0.2	0.0081	0.1950	0.0131
Total:	0.2	0.8085	0.2225	0.7860

However, at this much lower pressure, Fig. 2 of the C-S article shows that the mole fraction of carotene in the extract is an unacceptable 4×10^{-8} instead of the desired value of 0.0025. This is a huge difference and illustrates the importance of using reliable methods for estimating *K*-values in the supercritical region. In this case, the PR EOS with the Wang-Sandler mixing rules does not appear to be applicable.

Exercise 11.28

Subject: Supercritical extraction of 100 mol/min of 10 mol% acetone in water by carbon dioxide in a staged contactor operating in the supercritical region to recover 98% of the acetone

Given: Design of a supercritical extractor using the Group-Contribution EOS of Skjold-Jorgensen, which is in good agreement with the experimental VLE data for acetone-CO_2 at 313 K, as shown in the cited article by Cygnarowicz and Seider.

Find: Design of a similar extractor using the Peng-Robinson EOS with the Wang-Sandler mixing rules.

Analysis: In the Cygnarowicz and Seider (C-S) article, the experimental phase equilibria data for the acetone-CO_2 system at 313 K is shown in their Fig. 1. The Aspen Plus program was used to prepare a similar plot based on the PR EOS with the Wang-Sandler mixing rules (PRWS). The result is shown on the next page. Comparison of that plot with Fig. 1 in the C-S article shows that the liquid composition is not predicted well. For example, when the pressure is 70 atm, Fig. 1 in the C-S article gives a carbon dioxide mole fraction of 0.84 in the liquid phase, while the PRWS prediction in the figure on the next page gives a mole fraction of 0.94. Therefore, the design given in Fig. 3 of the C-S article may not give the desired results for PRWS. Consequently, a new design was sought based on the following specifications in the C-S article:

Extractor pressure > 70 atm — Extractor temperature > 310 K
CO_2 feed rate > 200 mol/min — Acetone recovery of at least 98%
Water recovery of at least 6%.

The Aspen Plus program was applied with the RADFRAC model, using the non-ideal algorithm with severe damping because of the difficulty in converging the calculations. However, initially, a single-stage isothermal flash was used to establish preliminary conditions of extractor pressure and temperature, and CO_2 feed rate that would insure the presence of both vapor and liquid phases. One set of conditions that accomplished this was 350 K, 70 atm, and 300 mol/min of CO_2. However, when these feed conditions were used with a 10-stage column, an acetone recovery of only 68.8% was achieved. Consequently, other combinations of feed conditions were tried, with some of the results as follows, where a solvent feed rate of 300 mol/min of CO_2 was used in all cases:

Pressure, atm	Feed temperatures, K	% Extraction of acetone	% Extraction of water
70	350	68.8	4.53
70	360	79.1	5.64
70	370	89.7	6.97
80	370	97.9	7.37

The last result is the best, because it satisfies the specifications, except that not quite 98% of the acetone is extracted. The material balance for this case is given on the next page.

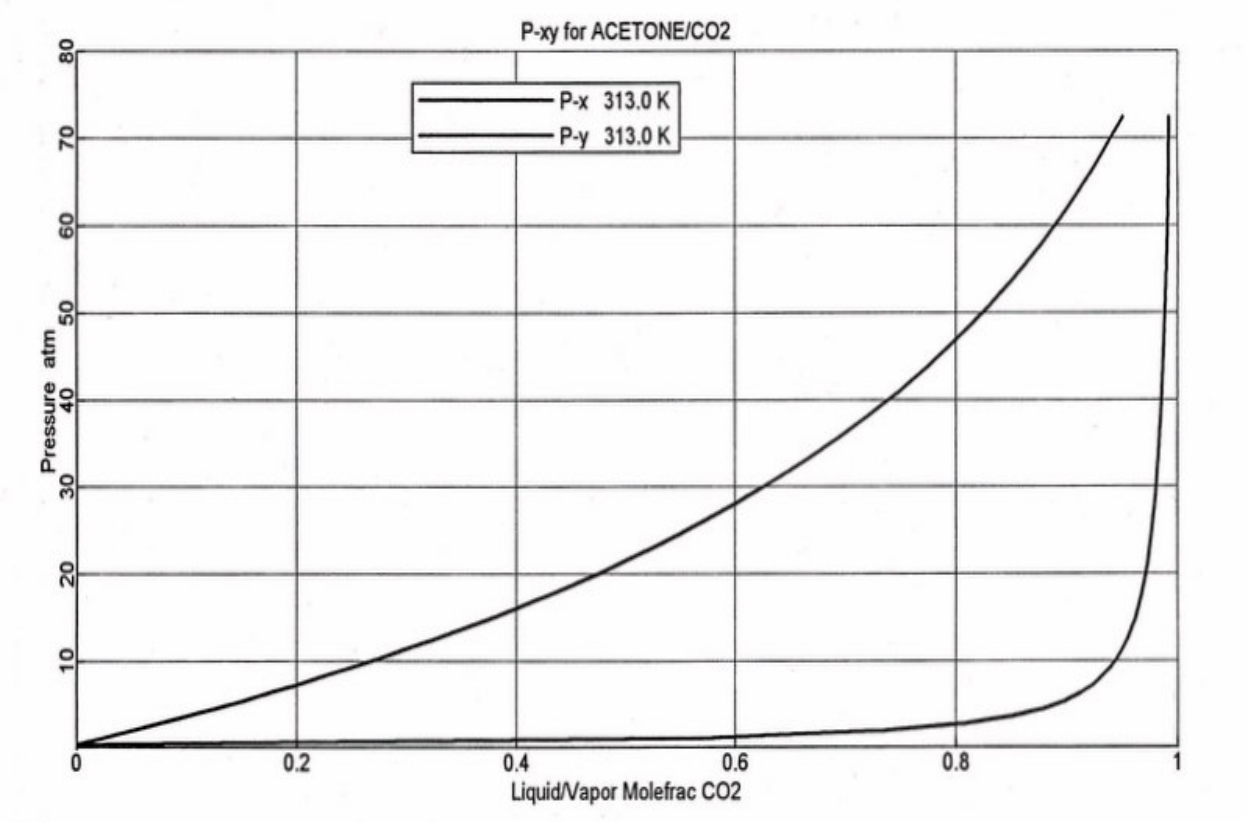
Exercise 11.28 (continued)

Analysis: (continued)

Mol/min:

Component	Feed	Solvent	Raffinate	Extract
Carbon dioxide	0.0	300.0	8.62	291.38
Acetone	10.0	0.0	0.21	9.79
Water	90.0	0.1	83.47	6.63
Total:	100.0	300.1	92.30	307.80

Compared to the C-S results, a higher temperature, lower pressure, smaller CO_2 flow rate, and higher number of equilibrium stages are required. Unlike the C-S result, the above is not the optimal result, but is feasible depending on the reliability of the PR EOS with the WS mixing rules. Energy balances were made around each stage, resulting in stage temperatures varying from 355 to 365 K.



Exercise 12.1

Subject: Revision of rate-based equations to account for entrainment and occlusion.

Given:. Rate-based model Eqs. (12-4) to (12-18).

Find: Modified equations

Analysis: Entrainment:

Let ϕ_j = ratio of entrained liquid (in the exiting vapor) that leaves Stage *j* to the liquid leaving Stage *j*, $y_{i,n}$ and $y^{I}_{i,n}$. Then, the entrained component liquid flow rate leaving Stage *j* = $\phi_j x_{i,} (1+r_j^L) L_j$.

Correspondingly, the entrained component liquid flow rate entering Stage *j* = $\phi_{j+1} x_{i,j+1} (1+r_{j+1}^L) L_{j+1}$.

Occlusion:

Let θ_j = ratio of occluded vapor (in the exiting liquid) that leaves Stage *j* to the vapor leaving Stage *j*, $(1+r_j^V)V_j$. Then the occluded component vapor flow rate leaving Stage *j* = $\theta_j\, y_{i,j}\, (1+r_j^V)V_j$.

Correspondingly, the occluded component vapor flow rate entering Stage *j* = $\theta_{j-1}\, y_{i,j-1} (1+r_{j-1}^V)V_{j-1}$.

The liquid-phase component material balance, Eq. (12-4), and vapor-phase component material balance, Eq. (12-5), become, respectively,

$$M_{i,j}^L \equiv (1+r_j^L+\phi_j)L_j x_{i,j} - L_{j-1}x_{i,j-1} - \phi_{j+1}(1+r_{j+1}^L)L_{j+1}x_{i,j+1} - f_{i,j}^L - N_{i,j}^L = 0, \quad i = 1,\ 2,\ \ldots,\ C$$

$$M_{i,j}^V \equiv (1+r_j^V+\theta_j)V_j y_{i,j} - V_{j+1}y_{i,j+1} - \theta_{j-1}(1+r_{j-1}^V)V_{j-1}y_{i,j-1} - f_{i,j}^V + N_{i,j}^V = 0, \quad i = 1,\ 2,\ \ldots.,\ C$$

The liquid-phase energy balance, Eq. (12-6), and vapor-phase energy balance, Eq. (12-7), become , respectively,

$$E_j^L \equiv (1+r_j^L+\phi_j)L_j H_j^L - L_{j-1}H_{j-1}^L - \phi_{j+1}(1+r_{j+1}^L)L_{j+1}H_{j+1}^L - H_j^{LF}\sum_{i=1}^{C} f_{i,j}^L + Q_j^L - e_j^L = 0$$

$$E_j^V \equiv (1+r_j^V+\theta_j)V_j H_j^V - V_{j+1}H_{j+1}^V - \theta_{j-1}(1+r_{j-1}^V)V_{j-1}H_{j-1}^V - H_j^{VF}\sum_{i=1}^{C} f_{i,j}^V + Q_j^V + e_j^V = 0$$

The total phase material balances, Eqs. (12-16) and (12-17), become, respectively,

$$M_{T,j}^L \equiv (1+r_j^L+\phi_j)L_j - L_{j-1} - \phi_{j+1}(1+r_{j+1}^L)L_{j+1} - \sum_{i=1}^{C} f_{i,j}^L - N_{T,j} = 0$$

$$M_{T,j}^V \equiv (1+r_j^V+\theta_j)V_j - V_{j+1} - \theta_{j-1}(1+r_{j-1}^V)V_{j-1} - \sum_{i=1}^{C} f_{i,j}^V + N_{T,j} = 0$$

Exercise 12.2

Subject: Revision of rate-based equations to account for a chemical reaction in the liquid phase.

Given:. Rate-based model Eqs. (12-4) to (12-18).

Assumption: Perfect mixing in the liquid on a stage.

Find: Modified equations for:
(a) chemical equilibrium
(b) kinetic rate law

Analysis: Let the chemical reaction be:

$$\nu_A A + \nu_B B \Leftrightarrow \nu_R R + \nu_S S$$

where: ν_i = stoichiometric coefficient of component i where it is (+) for products R and S, and (-) for reactants A and B.

Let the change in flow rate of component i in the liquid on stage j due to reaction be:

$$\Delta n_{i,j} = -M_j \left(\frac{\nu_i}{\nu_k} \right) r_{k,j} \qquad (1)$$

where: M_j = volumetric holdup of liquid on stage j.

$r_{k,j}$ = chemical reaction rate, $dc_{k,j}/dt$, for the limiting reactant, k, on stage j.

Let the rate law be a power-law expression, in terms of the reference limiting reactant, k,

$$-\frac{dc_{k,j}}{dt} = k_{f,j} \left[\prod_{i=1}^{C} c_{i,j}^{n_i} - \frac{\prod_{i=1}^{C} c_{i,j}^{m_i}}{K_{C,j}} \right]$$

where: $k_{f,j} = A_f e^{-\frac{E_f}{RT_j}}$

$c_{i,j} = x_{i,j} c_{T,j}$

$c_{T,j}$ = total concentration of all components in the liquid on stage j

$K_{C,j}$ = chemical equilibrium constant in terms of concentrations on stage j

superscripts n, m = reaction orders for forward and backward reactions, respectively, which are related to the stoichiometric coefficients by $\nu_i = m_i - n_i$

Exercise 12-2 (continued)

Analysis (a): (continued)

(a) Chemical equilibrium

Eqs. (12-5), (12-7) to (12-15), and (12-17) to (12-18) apply . In Eq. (12-4), liquid mole fractions $x_{i,j}$ are in chemical equilibrium as governed by the chemical equilibrium constant and the stoichiometry, such that:

$$M_{i,j}^{L} \equiv (1+r_j^L) L_j x_{i,j} - L_{j-1} x_{i,j-1} - \Delta n_{i,j} - f_{i,j}^{L} - N_{i,j}^{L} = 0, \quad i = 1,\ 2,\ \ldots,\ C$$

In energy balance, Eq. (12-6), liquid enthalpies include heats of formation. Eq. (12-16) becomes:

$$M_{T,j}^{L} \equiv (1+r_j^L) L_j - L_{j-1} - \Delta n_{k,j} \sum_{i=1}^{C} \left(\frac{\nu_i}{\nu_k} \right) - \sum_{i=1}^{C} f_{i,j}^{L} - N_{T,j} = 0$$

(b) Kinetic rate law

Eqs. (12-5), (12-7) to (12-15), and (12-17) to (12-18) apply. Eq. (12-4) becomes:

$$M_{i,j}^{L} \equiv (1+r_j^L) L_j x_{i,j} - L_{j-1} x_{i,j-1} - \Delta n_{i,j} - f_{i,j}^{L} - N_{i,j}^{L} = 0, \quad i = 1,\ 2,\ \ldots,\ C$$

where $\Delta n_{i,j}$ is computed from the reaction rate equation, Eq. (1), above.

In Eq. (12-6), enthalpies must include heat of formation.

Eq. (12-16) becomes:

$$M_{T,j}^{L} \equiv (1+r_j^L) L_j - L_{j-1} - \Delta n_{k,j} \sum_{i=1}^{C} \left(\frac{\nu_i}{\nu_k} \right) - \sum_{i=1}^{C} f_{i,j}^{L} - N_{T,j} = 0$$

Exercise 12.3

Subject: Reduction of the number of equations in the rate-based model.

Given:. Rate-based model based on Eqs. (12-4) to (12-18).

Find: Method to reduce the number of equations.

Analysis:

In Chapter 10, equilibrium-stage models are written for each equilibrium stage in terms of either:

Case 1: $x_{i,j}, y_{i,j}, L_j, V_j,$ and T_j $(2C+3)$ variables

Case 2: $l_{i,j}, v_{i,j},$ and T_j $(2C+1)$ variables

In Section 12.1, the rate-based model is written in terms of :

$$x_{i,j}, y_{i,j}, x^{\mathrm{I}}_{i,j}, y^{\mathrm{I}}_{i,j}, N_{i,j}, T^L_j, T^V_j, T^{\mathrm{I}}_j, L_j, \text{ and } V_j \qquad (5C+5) \text{ variables}$$

The equations could be rewritten to replace:

$$x_{i,j}, y_{i,j}, L_j, \text{ and } V_j \quad \text{by} \quad l_{i,j} \text{ and } v_{i,j} \text{ to give } (5C+3) \text{ variables.}$$

For example, Eq. (12-4) would become:

$$M^L_{i,j} \equiv (1+r^L_j) l_{i,j} - l_{i,j-1} - f^L_{i,j} - N^L_{i,j} = 0, \quad i = 1,\ 2,\ \ldots,\ C$$

This would eliminate Eqs. (12-11) and (12-12).

In Ref. 16, Taylor and his colleagues use component flow rates. This has the advantage that the component material balances are linear and fewer equations are needed because there are two fewer variables per stage. In Ref. 17, Taylor and his colleagues use component mole fractions and total flow rates. This choice is preferable when total flow rates are useful, such as when taking into account entrainment, occlusion, backmixing, weeping, and tray hydraulics.

The percentage reduction in the number of variables and equations for the rate-based model is not nearly as great as for the equilibrium model because, at least not for many components, that number is dominated by the $5C$ term.

Exercise 12.4

Subject: Mass-transfer rates and tray efficiencies from data for a perfectly mixed tray.

Given: Vapor-liquid traffic, component mole fractions, and mass-transfer coefficients for a tray in a column separating acetone (1), methanol (2), and water (3) at 14.7 psia

Find: (a) Component molar diffusion rates.
(b) Component mass-transfer rates.
(c) Murphree vapor tray efficiencies.

Analysis:

Because mass-transfer coefficients are given for the gas phase, work with the values of $y_{i,n}$ and $y^{\mathrm{I}}_{i,n}$. Because rates instead of fluxes are given, the equations developed in this section are used with rates rather than fluxes.

(a) Compute the reciprocal rate functions, R, from Eqs. (12-31) and (12-32), assuming linear mole fraction gradients such that z_i can be replaced by $(y_i + y_i^{\mathrm{I}})/2$. Thus,

$$z_1 = (0.4913 + 0.5291)/2 = 0.5102$$
$$z_2 = (0.4203 + 0.4070)/2 = 0.4136$$
$$z_3 = (0.0884 + 0.0639)/2 = 0.0762$$

$$R^V_{11} = \frac{z_1}{k_{13}} + \frac{z_2}{k_{12}} + \frac{z_3}{k_{13}} = \frac{0.5102}{2154} + \frac{0.4136}{1750} + \frac{0.0762}{2154} = 0.000509 \text{ h/lbmol}$$

$$R^V_{22} = \frac{z_2}{k_{23}} + \frac{z_1}{k_{21}} + \frac{z_3}{k_{23}} = \frac{0.4136}{2503} + \frac{0.5102}{1750} + \frac{0.0762}{2503} = 0.000487 \text{ h/lbmol}$$

$$R^V_{12} = -z_1\left(\frac{1}{k_{12}} - \frac{1}{k_{13}}\right) = -0.5102\left(\frac{1}{1750} - \frac{1}{2154}\right) = -0.000055 \text{ h/lbmol}$$

$$R^V_{21} = -z_2\left(\frac{1}{k_{21}} - \frac{1}{k_{23}}\right) = -0.4136\left(\frac{1}{1750} - \frac{1}{2503}\right) = -0.000071 \text{ h/lbmol}$$

In matrix form: $\left[\boldsymbol{R}^V\right] = \begin{bmatrix} 0.000509 & -0.000055 \\ -0.000071 & 0.000487 \end{bmatrix}$

From Eq. (12-29), by matrix inversion, $\left[\boldsymbol{\kappa}^V\right] = \left[\boldsymbol{R}^V\right]^{-1} = \begin{bmatrix} 1996 & 225.4 \\ 291 & 2086 \end{bmatrix}$

Because the off-diagonal terms in the above 2 x 2 matrix are much smaller that the diagonal terms, the effect of coupling in this example is small, approximately 10%.

Exercise 12.4 (continued)

Analysis: (continued)

From Eq. (12-27) with units of J^V in lbmol/h

$$\begin{bmatrix} J_1^V \\ J_2^V \end{bmatrix} = \begin{bmatrix} \kappa_{11}^V & \kappa_{12}^V \\ \kappa_{21}^V & \kappa_{22}^V \end{bmatrix} \begin{bmatrix} \left(y_1 - y_1^{\mathrm{I}}\right) \\ \left(y_2 - y_2^{\mathrm{I}}\right) \end{bmatrix}$$

$$J_1^V = \kappa_{11}^V \left(y_1 - y_1^{\mathrm{I}}\right) + \kappa_{12}^V \left(y_2 - y_2^{\mathrm{I}}\right)$$

$$= 1996\left(0.4913 - 0.5291\right) + 225.4(0.4203 - 0.4070) = -72.45 \text{ lbmol/h}$$

$$J_2^V = \kappa_{21}^V \left(y_1 - y_1^{\mathrm{I}}\right) + \kappa_{22}^V \left(y_2 - y_2^{\mathrm{I}}\right)$$

$$= 291(0.4913 - 0.5291) + 2086(0.4203 - 0.4070) = 16.74 \text{ lbmol/h}$$

From Eq. (12-23):

$$J_3^V = -J_1^V - J_2^V = 72.45 - 16.74 = 55.71 \text{ lbmol/h}$$

(b) $N_T = V_{n+1} - V_n = 1164 - 1200 = -36$ lbmol/h.

From Eq. (12-19), but with diffusion and mass-transfer rates instead of fluxes,

$$N_1^V = J_1^V + z_1 N_T^V = -72.45 + 0.5102(-36) = -90.8 \text{ lbmol/h}$$

$$N_2^V = J_2^V + z_2 N_T^V = 16.74 + 0.4136(-36) = 1.9 \text{ lbmol/h}$$

$$N_3^V = J_3^V + z_3 N_T^V = 55.71 + 0.0762(-36) = 53.0 \text{ lbmol/h}$$

(c) Approximate values of the Murphree vapor tray efficiency are obtained from (12-3), with *K*-values at phase interface conditions:

$$E_{MV_i} = \left(y_{i,n} - y_{i,n+1}\right) / \left(K_{i,n}^{\mathrm{I}} x_{i,n} - y_{i,n+1}\right)$$

Accordingly:

$$E_{MV_1} = \frac{\left(0.4913 - 0.4106\right)}{\left[\left(1.507\right)\left(0.3683\right) - 0.4106\right]} = 0.559 = 55.\ 9\%$$

$$E_{MV_2} = \frac{\left(0.4203 - 0.4389\right)}{\left[\left(0.900\right)\left(0.4487\right) - 0.4389\right]} = 0.530 = 53.\ 0\%$$

$$E_{MV_3} = \frac{\left(0.0884 - 0.1505\right)}{\left[\left(0.3247\right)\left(0.1830\right) - 0.1505\right]} = 0.682 = 68.2\%$$

Exercise 12.5

Subject: Reciprocal rate functions for a five-component system.

Given:. Eqs. (12-31) and (12-32) for a general *C*-component system.

Find: Expanded forms of Eqs. (12-31) and Eq. (12-32).

Analysis: From Eq. (12-31):

$$R_{11}^P = \frac{z_1}{k_{15}^P} + \frac{z_2}{k_{12}^P} + \frac{z_3}{k_{13}^P} + \frac{z_4}{k_{14}^P} + \frac{z_5}{k_{15}^P}$$

$$R_{22}^P = \frac{z_2}{k_{25}^P} + \frac{z_1}{k_{21}^P} + \frac{z_3}{k_{23}^P} + \frac{z_4}{k_{24}^P} + \frac{z_5}{k_{25}^P}$$

$$R_{33}^P = \frac{z_3}{k_{35}^P} + \frac{z_1}{k_{31}^P} + \frac{z_2}{k_{32}^P} + \frac{z_4}{k_{34}^P} + \frac{z_5}{k_{35}^P}$$

$$R_{44}^P = \frac{z_4}{k_{45}^P} + \frac{z_1}{k_{41}^P} + \frac{z_2}{k_{42}^P} + \frac{z_3}{k_{43}^P} + \frac{z_5}{k_{45}^P}$$

$$R_{12}^P = -z_1\left(\frac{1}{k_{12}^P} - \frac{1}{k_{15}^P}\right) \qquad R_{13}^P = -z_1\left(\frac{1}{k_{13}^P} - \frac{1}{k_{15}^P}\right)$$

$$R_{14}^P = -z_1\left(\frac{1}{k_{14}^P} - \frac{1}{k_{15}^P}\right) \qquad R_{21}^P = -z_2\left(\frac{1}{k_{21}^P} - \frac{1}{k_{25}^P}\right)$$

$$R_{23}^P = -z_2\left(\frac{1}{k_{23}^P} - \frac{1}{k_{25}^P}\right) \qquad R_{24}^P = -z_2\left(\frac{1}{k_{24}^P} - \frac{1}{k_{25}^P}\right)$$

$$R_{31}^P = -z_3\left(\frac{1}{k_{31}^P} - \frac{1}{k_{35}^P}\right) \qquad R_{32}^P = -z_3\left(\frac{1}{k_{32}^P} - \frac{1}{k_{35}^P}\right)$$

$$R_{34}^P = -z_3\left(\frac{1}{k_{34}^P} - \frac{1}{k_{35}^P}\right) \qquad R_{41}^P = -z_4\left(\frac{1}{k_{41}^P} - \frac{1}{k_{45}^P}\right)$$

$$R_{42}^P = -z_4\left(\frac{1}{k_{42}^P} - \frac{1}{k_{45}^P}\right) \qquad R_{43}^P = -z_4\left(\frac{1}{k_{43}^P} - \frac{1}{k_{45}^P}\right)$$

Exercise 12.6

Subject: Mass-transfer rates and tray efficiencies from data for a perfectly mixed tray.

Given: Vapor-liquid traffic, component mole fractions, and mass-transfer coefficients for a tray in a column separating methanol (1), water (2), and acetone (3) at 14.7 psia from Example 12.1, but with the designations 1, 2, 3 changed to see if different results are obtained.

Find: (a) Component molar diffusion rates.
(b) Component mass-transfer rates.
(c) Murphree vapor tray efficiencies.

Analysis:

Because mass-transfer coefficients are given for the gas phase, work with the values of $y_{i,n}$ and $y_{i,n}^{\mathrm{I}}$. Because rates instead of fluxes are given, the equations developed in this section are used with rates rather than fluxes.

(a) Compute the reciprocal rate functions, *R*, from Eqs. (12-31) and (12-32), assuming linear mole fraction gradients such that z_i can be replaced by $(y_i + y_i^{\mathrm{I}})/2$. Thus, with the new designations for 1, 2, 3, the values from Example 12.1 become:

$$z_1 = 0.4654$$
$$z_2 = 0.2100$$
$$z_3 = 0.3246$$

$$R_{11}^V = \frac{z_1}{k_{13}} + \frac{z_2}{k_{12}} + \frac{z_3}{k_{13}} = \frac{0.4654}{1955} + \frac{0.2100}{2797} + \frac{0.3246}{1955} = 0.000479 \text{ h/lbmol}$$

$$R_{22}^V = \frac{z_2}{k_{23}} + \frac{z_1}{k_{21}} + \frac{z_3}{k_{23}} = \frac{0.2100}{2407} + \frac{0.4654}{2797} + \frac{0.3246}{2407} = 0.000388 \text{ h/lbmol}$$

$$R_{12}^V = -z_1\left(\frac{1}{k_{12}} - \frac{1}{k_{13}}\right) = -0.4654\left(\frac{1}{2797} - \frac{1}{1955}\right) = -0.0000717 \text{ h/lbmol}$$

$$R_{21}^V = -z_2\left(\frac{1}{k_{21}} - \frac{1}{k_{23}}\right) = -0.2100\left(\frac{1}{2797} - \frac{1}{2407}\right) = -0.0000122 \text{ h/lbmol}$$

In matrix form: $\left[\boldsymbol{R}^V\right] = \begin{bmatrix} 0.000497 & 0.0000717 \\ 0.0000122 & 0.000388 \end{bmatrix}$

From Eq. (12-29), by matrix inversion, $\left[\boldsymbol{\kappa}^V\right] = \left[\boldsymbol{R}^V\right]^{-1} = \begin{bmatrix} 2021 & -373.5 \\ -63.6 & 2589 \end{bmatrix}$

Exercise 12.6 (continued)

Analysis: (continued)
Because the off-diagonal terms in the above 2 x 2 matrix are much smaller that the diagonal terms, the effect of coupling in this example is small, approximately 10%.

From Eq. (12-27) with units of J^V in lbmol/h

$$\begin{bmatrix} J_1^V \\ J_2^V \end{bmatrix} = \begin{bmatrix} \kappa_{11}^V & \kappa_{12}^V \\ \kappa_{21}^V & \kappa_{22}^V \end{bmatrix} \begin{bmatrix} \left(y_1 - y_1^{\mathrm{I}}\right) \\ \left(y_2 - y_2^{\mathrm{I}}\right) \end{bmatrix}$$

$$J_1^V = \kappa_{11}^V \left(y_1 - y_1^{\mathrm{I}}\right) + \kappa_{12}^V \left(y_2 - y_2^{\mathrm{I}}\right)$$
$$= 2021(0.4631 - 0.4677) - 373.5(0.2398 - 0.1802) = -31.6 \text{ lbmol/h}$$

$$J_2^V = \kappa_{21}^V \left(y_1 - y_1^{\mathrm{I}}\right) + \kappa_{22}^V \left(y_2 - y_2^{\mathrm{I}}\right)$$
$$= -63.6(0.4631 - 0.4677) + 2589(0.2398 - 0.1802) = 154.6 \text{ lbmol/h}$$

From Eq. (12-23):

$$J_3^V = -J_1^V - J_2^V = 31.6 - 154.6 = -123.0 \text{ lbmol/h}$$

These three values are very close to those in Example 12.1: -32.7, 154.5, -121.8

(b) From Example 12.1, $N_T = V_{n+1} - V_n =$ -54 lbmol/h

From Eq. (12-19), but with diffusion and mass-transfer rates instead of fluxes,

$$N_1^V = J_1^V + z_1 N_T^V = -31.6 + 0.4654(-54) = \text{-56.7 lbmol/h}$$
$$N_2^V = J_2^V + z_2 N_T^V = 154.6 + 0.2100(-54) = 143.3 \text{ lbmol/h}$$
$$N_3^V = J_3^V + z_3 N_T^V = -123.0 + 0.3246(-54) = -140.5 \text{ lbmol/h}$$

These three values are very close to those in Example 12.1: -57/8, 143.2, -139.4

(c) Approximate values of the Murphree vapor tray efficiency are obtained from (12-3), with K-values at phase interface conditions:

$$E_{MV_i} = \left(y_{i,n} - y_{i,n+1}\right) / \left(K_{i,n}^{\mathrm{I}} x_{i,n} - y_{i,n+1}\right)$$

The three values are identical to those in Example 12.1 because they only involve the given mole fractions and K-values.

In summary, the values calculated are the same as those computed in Example 12.1. The small differences are caused by round-off error. As would be expected, it makes no difference how the components are ordered.

Exercise 12.7

Subject: Correlations for estimating binary-pair mass-transfer coefficients for trayed columns.

Find: Advantages and disadvantages of the correlations

Analysis: In Section 12.3, methods for trayed columns are mentioned as those of AIChE, Harris, Hughmark, Zuiderweg, Chan and Fair, and Chen and Chuang. To these may be added the method of Young and Stewart [AIChE J., 38, 592-602 (1992)] for sieve trays, and the method of Scheffe and Weiland [Ind. Eng. Chem. Res., 26, 228-236 (1987) for valve trays, but they are not considered here because they are not compared to other methods.

The AIChE correlation, Ref. 20, was published in a book in 1958. The method is based on separate empirical equations for the individual number of transfer units, N_V and N_L, developed from experimental data on small bubble-cap columns of 2-ft diameter with a 2-ft tray spacing. The method gave favorable results when used to predict efficiencies of four commercial bubble-cap columns of 4-ft, 5.5-ft, 8-ft, and 13-ft diameter. The method also gave favorable results for a commercial sieve-tray column of 13-ft diameter. The experimental data for the 2-ft diameter columns cover weir heights from 1 to 5 inches, F-factors from 0.2 to 2.6 (93% of flooding), liquid rates of 5-25 gpm/ft of average width, a vapor Schmidt number of 0.61, and a liquid diffusivity of 2.42×10^{-5} to 7.5×10^{-5} cm^2/s. No bubble-cap design features were incorporated into the correlation. Round bubble-cap diameters ranged from 1.5 to 4 inches. Slot velocity in and cap-spacing for the bubble caps were varied widely.

The transfer-unit correlation for the gas phase was developed from data on the absorption of ammonia from air into water at 1 atm and 20°C , which is controlled by mass-transfer in the gas phase because of the high solubility of ammonia in water. The correlation gives N_V as a function only of the weir height, a superficial F-factor (see p. 313), the volumetric liquid rate per average width of flow path, and the vapor Schmidt number, which however was not varied. The effect of pressure was determined from data on the acetone-benzene system over a range from 20 to 92 psia. This system was largely gas-phase controlling because the slope, m, in Eq. (7-50) was kept small. After correcting for a small mass-transfer resistance in the liquid phase and mixing, the results for the acetone-benzene system were in reasonable agreement with the correlation developed from the ammonia-air-water system at 1 atm.

The transfer-unit correlation for the liquid phase is a function only of the liquid diffusivity, the contact time of the liquid on the tray, and the F-factor. The correlation was developed from data on the desorption of small amounts of oxygen from water into air. Because of the small solubility of oxygen in air, the mass-transfer resistance is almost wholly in the liquid phase. To check the difference between an aqueous system and an organic system, the normal pentane-paraxylene system was used at very low concentrations of normal pentane such that λ in Eq. (7-48) was very large and, thus, the system was controlled by mass transfer in the liquid phase. Corrections for gas-phase resistance and mixing were more difficult, but the results compared well with the correlation based on the oxygen-air-water system.

Exercise 12.7 (continued)

Analysis: (continued)

For both AIChE correlations, the effect of physical properties was not explored over any significant range. Based on previous published work, the Schmidt number exponent was assumed to be -0.5 in the N_V correlation and the liquid diffusivity exponent was assumed to be 0.5 in the N_L correlation. Because it was not found necessary to incorporate any bubble-cap geometry into the correlation, it was assumed by others that the AIChE method could be applied to sieve and valve trays as well. This was fortunate because soon after the AIChE program, bubble-cap trays fell into disfavor for new installations because of the good efficiency and capacity, together with lower pressure drop, for the less expensive sieve and valve trays.

An advantage in the application of the AIChE method is that it is independent of tray design features such as bubble-cap size and spacing or hole diameter and hole area for sieve trays. However, it has received the following criticisms:

1. It is based on a very narrow range of Schmidt number in the gas phase.
2. It is based on data for absorption and desorption, and not for distillation (Chen and Chuang, 1994).
3. It overpredicts point efficiencies for liquid-phase controlled systems operating at low liquid flow rates (Dribika and Biddulph, 1992).
4. It is based on systems where the mass-transfer resistance is confined entirely to either the gas phase or the liquid phase (Chen and Chuang, 1995).
5. It greatly overpredicts N_L for distillation systems (Chen and Chuang, 1995).
6. It underpredicts point efficiencies for sieve trays with small holes (Dribika and Biddulph, 1992).
7. It significantly underpredicts point efficiencies of distillation systems (Korchinsky, Ehsani, and Plaka, 1994).

The method of Harris (Ref. 21) has received little attention and will not be considered here. The method of Hughmark (Ref. 22) has received much attention. It was developed as an improvement over the AIChE method for systems controlled by mass transfer in the liquid phase. It considers the interfacial area for mass transfer in a separate correlation that depends on the F factor, weir height, liquid head flowing over the weir, gas and liquid densities, liquid viscosity, and surface tension. Other factors required are gas and liquid diffusivities, froth height, liquid holdup, and superficial gas velocity. Thus, the disadvantage of the Hughmark method is that it requires more information than the AIChE method. The advantage of the Hughmark method is that it is more accurate for systems controlled by mass transfer in the liquid phase. It predicts three chemical systems for sieve trays well (Korchinsky, Ehsani, and Plaka, 1994). However, it is not accurate for sieve trays with small holes (Dribika and Biddulph, 1992).

Unlike the AIChE and Hughmark methods, which are based on AIChE bubble-cap data, the Zuiderweg method (Ref. 23) is based on published sieve-tray efficiency data of FRI. The correlations for the mass-transfer coefficients are very simple, with the only factors being the gas density and liquid diffusivity. However, correlations for the interfacial area depend on the flow regime (spray or mixed emulsion). These depend on the F factor, liquid holdup, flow parameter,

Exercise 12.7 (continued)

Analysis: (continued)
weir height, surface tension, hole pitch, weir length, and liquid density. Although based on distillation data, those data cover only a narrow range of slope of the equilibrium line. Thus, for other distillation systems, the use of the method is questionable. Another disadvantage of the Zuiderweg method is the need for more information than the AIChE method. An advantage of the Zuiderweg method is that it considers the flow regime for sieve-tray columns. Unfortunately, the method greatly underestimates point efficiency for sieve trays with small holes (Dribika and Biddulph, 1992) and also does very poorly on three chemical systems distilled in sieve trays (Korchinsky, Ehsani, and Plaka, 1994). It is difficult to see how the Zuiderweg method could be recommended over other methods.

The Chan and Fair method (Ref. 24) for sieve trays has received much attention because it is based on a large amount of experimental data for large sieve-tray columns. It utilizes volumetric mass-transfer coefficients that depend on the *F* factor, liquid diffusivity, gas diffusivity, gas velocity as a fraction of flooding, and liquid holdup. The correlation for the volumetric mass-transfer coefficient in the liquid phase is not new, but is close to that of the AIChE method. The correlation for the volumetric mass-transfer coefficient in the gas phase is based on distillation data, rather than on absorption data as in the AIChE method. Like the AIChE method, the Chan and Fair method is relatively easy to apply. For sieve trays with small holes (Dribika and Biddulph, 1992), point efficiencies are mostly overpredicted, but no method gives consistently good predictions. For two of three chemical systems (Korchinsky, Ehsani, and Plaka, 1994), the Chan and Fair method gives the best predictions.

Chen and Chuang, in presenting their method (Ref. 25), criticize methods based on absorption and desorption data because they may involve different interfacial areas. Their method is based on separating the interfacial area from the mass-transfer coefficients. The former is determined from a force balance suggested in a book by Levich (1962), and depends on liquid viscosity, % hole area, *F* factor, liquid density, and surface tension. The mass-transfer coefficients are both based on Higbe's penetration theory. Thus, they depend on diffusivities and contact times. The Chen and Chuang method compares very well with FRI data on three hydrocarbon systems over a very wide pressure range of 13.3 to 2758 kPa. No comparisons are given for non-ideal organic or aqueous systems.

Finally, Koziol and Mackowiak [Chem. Eng. Technol., 15, 103-113 (1992)] criticize methods for predicting mass-transfer coefficients in trayed columns with downcomers because they ignore effects of entrainment and weeping. An exception, as discussed by Kooijman and Taylor (Ref. 31) is the Chan and Fair method, which accounts for both weeping and entrainment by using an empirical quadratic function of fraction of flooding to correlate gas-phase mass transfer. Kooijman and Taylor also point out that although mass transfer in distillation is largely controlled by the gas phase, the liquid-phase resistance may contribute up to 30% of the total mass-transfer resistance.

Exercise 12.8

Subject: Correlations for estimating binary-pair mass-transfer coefficients for packed columns.

Find: Advantages and disadvantages of the correlations for random and structured packings

Analysis:

Random Packings:

In Section 12.3, the following correlations are listed:
1. Onda, Takeuchi, and Okumoto, Ref. 26, (1968).
2. Bravo and Fair, Ref. 27 (1982).

The correlations of Onda, Takeuchi, and Okumoto were developed from data on absorption and desorption in columns packed with Raschig rings and Berl saddles. Separate correlations are presented for the wetted area, the gas-phase mass-transfer coefficient, and the liquid-phase mass-transfer coefficient. The wetted area depends on the packing surface area, the surface tension, critical surface tension of the packing, and Reynolds, Froude, and Weber numbers for the liquid. The gas-phase mass-transfer coefficient depends on the packing surface area density, the gas diffusivity, the nominal packing size, and the Reynolds and Schmidt numbers for the gas phase. The liquid-phase mass-transfer coefficient, obtained from aqueous and organic solvent systems, depends on the liquid density and viscosity, packing surface area density, nominal packing size, and Reynolds and Schmidt numbers for the liquid. The liquid phase is correlated much better than the gas phase. This is unfortunate because the overall resistance in distillation is often dominated by the gas phase.

Bravo and Fair use the mass-transfer coefficient equations of Onda, Takeuchi, and Okumoto, but present a new correlation for the mass-transfer area, which accounts for mass-transfer area other than the packing wetted area. The use of the packing wetted area as the area for mass transfer is criticized by Bravo and Fair because it ignores the area provided by suspended and falling droplets, gas bubbles within liquid, ripples on the liquid film surface, and wall films. Their area depends on the packing area, a capillary number, a Reynolds number for the vapor, the surface tension, and the height of the packing. Because the liquid-phase Reynolds number is a function of the area density for mass transfer, Bravo and Fair compute values of the liquid-phase mass transfer coefficient different from Onda, Takeuchi, and Okumoto. The correlation of Bravo and Fair is based on data for Pall rings as well as Raschig rings and Berl saddles. It is also recommended for Intalox saddles. As discussed by Shariat and Kunesh, 1995, the efficiency of the reflux distributor can have a large effect on mass transfer. As discussed by Brierley, 1994, the efficiency of random packings for high pressure operation may be lower than predicted. Data and correlations are needed for the newer high void-fraction packings.

Exercise 12.8 (continued)

Analysis: (continued)

Structured Packings:

In Section 12.3, the following correlations are listed:
1. Bravo, Rocha, and Fair, Ref. 28 (1985).
2. Bravo, Rocha, and Fair, Ref. 29 (1992).
3. Billet and Schultes, Ref. 30 (1992).

Reference 28 presents a method for estimating HETP for distillation in columns with structured packing of the gauze type, such as Sulzer BX and Gempak 4BG. The correlations consist of: (a) gas-phase mass-transfer coefficient in terms of an equivalent flow channel diameter, gas diffusivity, vapor density and viscosity, vapor and liquid velocities, and vapor Schmidt number; (b) liquid-phase mass-transfer coefficient in terms of liquid diffusivity, liquid channel velocity, and channel side dimension; and (c) area for mass transfer equal to the packing surface area. The equivalent flow channel diameter is based on the hydraulic radius concept. The correlation was tested on four chemical systems distilled in columns ranging in diameter from 0.07 to 1.0 m, and at pressures from 10 to 760 torr. Good agreement was obtained with measured HETP, computed from equations in Table 6.7 and 7.6.

Reference 29, and a more recent article by the same authors, Rocha, Bravo, and Fair, Ind. Eng. Chem. Res., 35, 1660-1667 (1996), extend the study of Ref. 28 to more structured packings (Fexipac, Intalox 2T, Maxpak, and Mellapak) and to other binary systems, covering a wide pressure range of 0.021 to 20.4 bar, and column diameters of 0.07 to 1.2 m. The gas-phase mass-transfer coefficient uses a modified hydraulic diameter and is a function of a Reynolds number that involves both liquid and gas velocities, the Schmidt number, and the gas diffusivity. The liquid-phase mass-transfer coefficient uses a modified exposure time to take into account slower surface renewal in certain parts of the packing, the liquid diffusivity, liquid velocity, and the side dimension of the packing. The biggest change is to the interfacial area for mass transfer, which uses an empirical surface enhancement factor to characterize each type of packing. The area depends on the geometric area and other geometrical factors, in addition to the Weber, Froude, and Reynolds numbers.

In Ref. 30, Billet and Schultes present a semi-theoretical treatment that combines the interfacial area for mass transfer with expressions for the gas-side and the liquid-side mass-transfer coefficients. An advantage of their method is accuracy, but a disadvantage is that the expressions for the coefficients include a total of three constants that must be determined experimentally for each packing type and size from holdup, absorption, and desorption tests.

Exercise 12.9

Subject: Modeling flow patterns in a rate-based model.

Given:. The rate-based models described in Chapter 12.

Find: How the method of Fair, Null, and Bolles (Ref. 32) might be used to model flow patterns in a rate-based model. How the mole-fraction driving forces can be calculated.

Analysis: In the first comprehensive rate-based model for distillation (Krishnamurthy and Taylor, Ref. 16), the simplest flow patterns were assumed: (1) Perfect mixing in both the liquid and vapor phases. In Ref. 31 by Kooijman and Taylor, the Taylor et al. model is developed for three other flow patterns:

2. Plug flow of vapor up through perfectly mixed liquid, assuming that the vapor entering the tray is well mixed.
3. Plug flow of vapor up through plug flow of liquid across the tray in the flow direction, assuming that the vapor entering the tray is well mixed. At any location moving across the tray, the liquid is of uniform concentration in the vertical direction through the froth on the tray.
4. Plug flow of vapor up through liquid that is dispersed by eddy diffusion in the liquid flow direction across the tray, assuming that the vapor entering the tray is well mixed. At any location moving across the tray, the liquid is of uniform concentration in the vertical direction through the froth on the tray. The extent of eddy diffusion in the liquid phase depends on the Peclet number in the net liquid flow direction. The Peclet number is inversely proportional to the eddy diffusivity, as given in Eq. (6-36).

The method of Fair, Null, and Bolles (Ref. 32) is designed to take experimental tray efficiency data, obtained with a small Oldershaw perforated-plate column, of the type shown in Fig. 6.20, and scale the results up to a large column by correcting for the flow patterns. The most general model is number 4 above, which reduces to model 1 for a small Peclet number, and to model 3 for a large Peclet number. Ref. 32 gives an empirical correlation for estimating the Peclet number. The average mole-fraction driving force is obtained by integration over the tray, as derived in Ref. 31.

Exercise 12.10

Subject: Separation of methanol (M) from a mixture containing isopropanol (P) and water (W) by distillation in a sieve-tray column, using a rate-based method.

Given: A bubble-point feed of 100 kmol/h of M, 50 kmol/h of P, and 100 kmol/h of W at 1 atm is sent to tray 25 from the top tray of a column containing 40 trays, operating at 1 atm. Reflux ratio is 5 and bottoms mole flow rate = 150 kmol/h. Use UNIFAC method for liquid-phase activity coefficients and the Chan-Fair method for mass-transfer coefficients and interfacial area.

Assumptions: Assume both phases are perfectly mixed on each tray. Operation is at about 80% of flooding.

Find: The separation achieved.

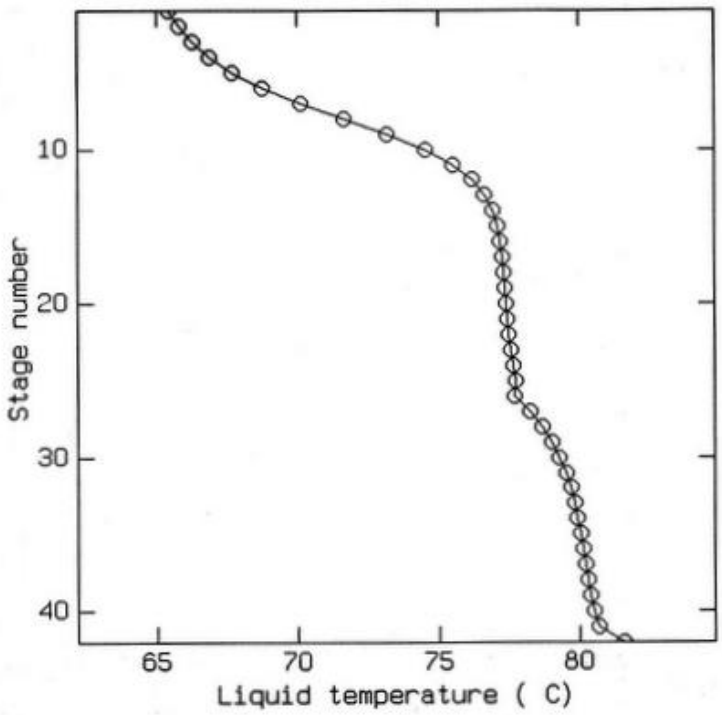
Analysis: The Chemsep method is applied with the Simple Distillation option, a total condenser, a partial reboiler, and 42 stages (counting the condenser and the reboiler). Thus, the feed is sent to stage 26 from the top. To estimate *K*-values, the ideal gas law is assumed with DIPPR vapor pressure, and excess enthalpy for the liquid phase.
For physical properties necessary to size the column diameter and compute mass-transfer coefficients and interfacial area, the following options were chosen:
Rackett equation for liquid density. Wilke and DIPPR for vapor viscosity.
Molar averaging of DIPPR pure component liquid viscosity, vapor thermal conductivity, liquid thermal conductivity, and surface tension. Binary liquid diffusivities from Wilke-Chang method.
Neglect pressure drop. Automatic initialization.
Newton's method, but maximum change of liquid or vapor flow rate of only 10% and maximum temperature change of only 2^{o}C.
Problem converged in 10 iterations. The separation achieved is as follows:

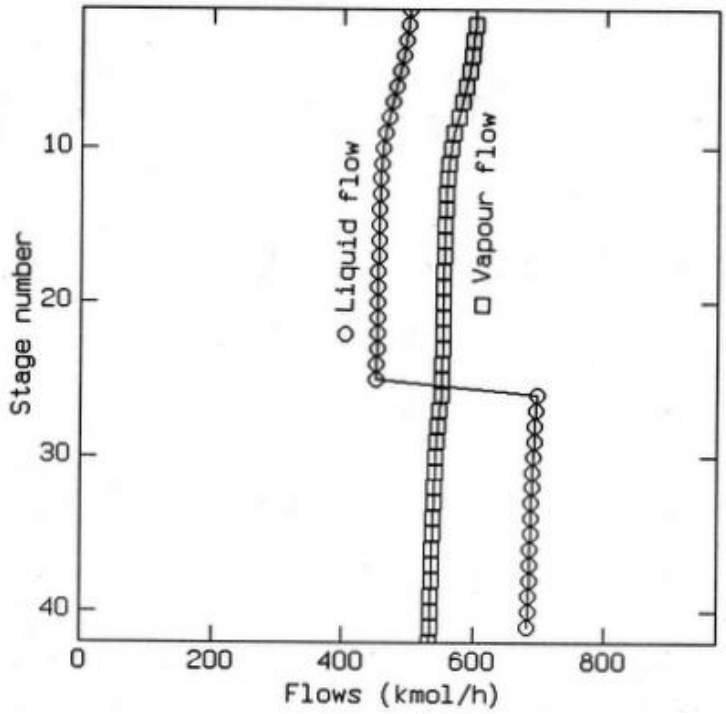
Component	Feed	Distillate	Bottoms
Flow, kmol/h:			
Methanol	100.0	90.76	9.24
Isopropanol	50.0	9.17	40.83
Water	100.0	0.07	99.93
Total:	250.0	100.0	150.0
Mole fraction:			
Methanol	0.4000	0.9076	0.0616
Isopropanol	0.2000	0.0917	0.2722
Water	0.4000	0.0007	0.6662

Exercise 12.10 (continued)

Analysis: (continued)

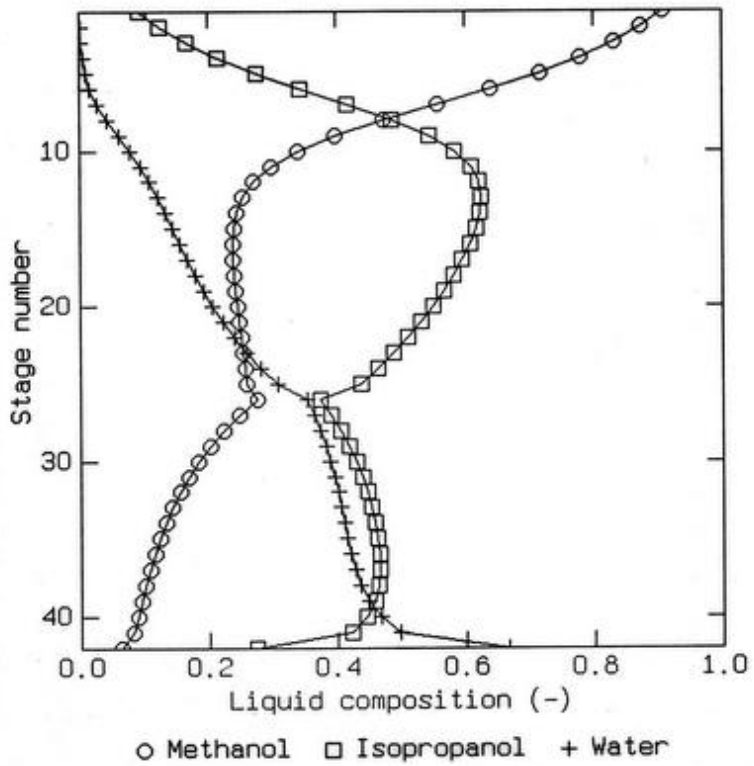
Shown below and on the next page are plots of tray liquid temperatures, vapor and liquid traffic, liquid composition profile, and mass-transfer rate profile from the Chemsep run.

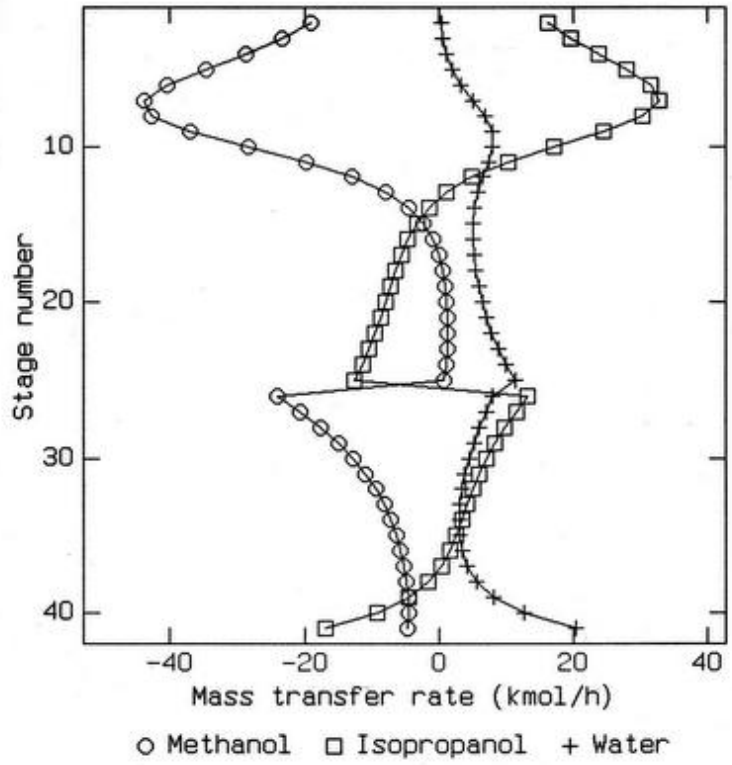




Exercise 12.10 (continued)

Analysis: (continued)

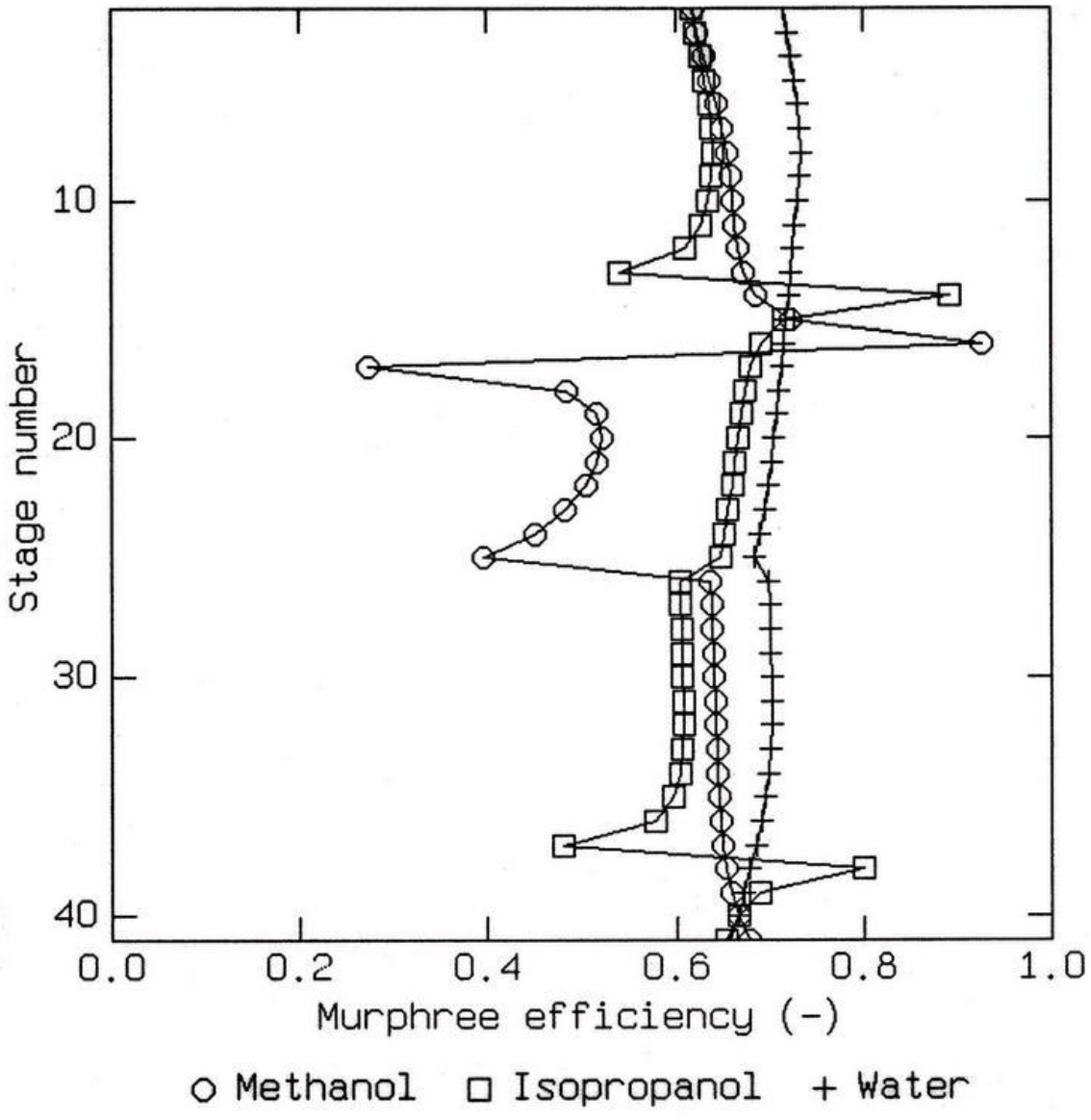




Exercise 12.10 (continued)

Analysis: (continued)

Shown below are the component profiles for the Murphree vapor tray efficiencies. For methanol, they range mainly from 39.5% to 92.61%, with most efficiencies in the range from 60 to 68%. For isopropanol, the efficiencies range mainly from 60.4% to 69.0%. For water, the efficiencies range from 65.8% to 73.4%. These values seem reasonable for perfect mixing on the trays.



Exercise 12.11

Subject: Separation of a mixture of acetone (A) and methanol (M) by extractive distillation with water (W) in a sieve-tray column, using a rate-based method.

Given: A feed of 50 kmol/h of A and 150 kmol/h of M at 1 atm and 60°C is sent to tray 35 from the top of a column containing 40 trays. 50 kmol/h of W at 1 atm and 65°C is sent to tray 5 from the top tray. Column operates at 1 atm. Reflux ratio is 10 and bottoms mole flow rate = 200 kmol/h. Use UNIFAC method for liquid-phase activity coefficients and the AIChE method for mass-transfer coefficients and interfacial area.

Assumptions: Assume the liquid phase is perfectly mixed and the vapor phase is in plug flow on each tray. Operation is at about 80% of flooding.

Find: Separation achieved. The number of equilibrium stages to achieve the same separation.

Analysis: The Chemsep method is applied with the Extractive Distillation option, a total condenser, a partial reboiler, and 42 stages (counting the condenser and the reboiler). Thus, the feeds are sent to stages 6 and 36 from the top. To estimate *K*-values, the ideal gas law is assumed with DIPPR vapor pressure, and excess enthalpy for the liquid phase.
For physical properties necessary to size the column diameter and compute mass-transfer coefficients and interfacial area, the following options were chosen:
Rackett equation for liquid density. Wilke and DIPPR for vapor viscosity.
Molar averaging of DIPPR pure component liquid viscosity, vapor thermal conductivity, liquid thermal conductivity, and surface tension. Binary liquid diffusivities from Wilke-Chang method.
Neglect pressure drop. Automatic initialization.
Newton's method, but maximum change of liquid or vapor flow rate of only 10% and maximum temperature change of only 2°C.
Problem converged in 9 iterations in 8 seconds with a Pentium 90. The separation achieved is:

Component	2 Feeds	Distillate	Bottoms
Flow, kmol/h:			
Acetone	50.0	47.59	2.41
Methanol	150.0	0.20	149.80
Water	50.0	2.20	47.80
Total:	250.0	49.99	200.01
Mole fraction:			
Acetone	0.2000	0.9519	0.0120
Methanol	0.6000	0.0040	0.7490
Water	0.2000	0.0441	0.2390

Exercise 12.11 (continued)

Analysis: (continued)

The back-calculated Murphree vapor tray efficiencies are computed by Chemsep to be:
From about 62.6 to 78.5% for acetone
From about 60.4 to 84.1% for methanol
A wide range of 20 to 172% for water

On the basis of these values, assume an overall average tray efficiency of 75%. Therefore, for an equilibrium stage calculation, take 0.75(40) = 30 equilibrium stages or 32 total stages (including the condenser and reboiler). Try feeding the water to stage 5 from the top and the main feed to stage 1+0.75(35) = 27. However, a separation closer to the one for the rate-based result above was achieved by sending the main feed to stage 23. The result is as follows with convergence in 7 iterations in 2 seconds with a Pentium 90:

Component	2 Feeds	Distillate	Bottoms
Flow, kmol/h:			
Acetone	50.0	47.20	2.80
Methanol	150.0	0.22	149.80
Water	50.0	2.58	47.42
Total:	250.0	50.00	200.02
Mole fraction:			
Acetone	0.2000	0.9439	0.0140
Methanol	0.6000	0.0045	0.7489
Water	0.2000	0.0516	0.2371

Exercise 12.12

Subject: Separation of methanol (M) from a mixture containing isopropanol (P) and water (W) by distillation in a packed column with a dumped packing, using a rate-based method.

Given: A bubble-point feed of 100 kmol/h of M, 50 kmol/h of P, and 100 kmol/h of W at 1 atm. Column contains 40 ft of 2-inch stainless steel Pall rings in two sections (one above the feed and one below the feed). Feed entry is 25 ft from the top of the packing. Reflux ratio = 5 and bottoms mole flow rate = 150 kmol/h

Assumptions: Use 100 segments (called stages in the Chemsep program, when solving a packed column) to simulate each of the two sections of packing, with perfectly mixed vapor and liquid in each segment. Operation at about 75% of flooding.

Find: The separation achieved.

Analysis: The calculations were made with the Chemsep program. The properties chosen were:

Gamma-Phi K model UNIFAC Activity coefficient
Ideal gas law Equation of State DIPPR Vapour pressure
Excess Enthalpy

Other physical properties were by default with Wilke-Chang for liquid diffusivities.
Bravo-Fair 1982 method for mass-transfer coefficients and interfacial area.
Generalized pressure drop correlation of Leva for pressure drop.
Newton's method to converge calculations with maximum of 10% change in vapor rate and 2^{o}C change in temperature between iterations.

Calculations converged in 11 iterations and 30 seconds with a Pentium 90 PC, giving the following distillate and bottoms compositions:

Component	Feed	Distillate	Bottoms
Flow, kmol/h:			
Methanol	100.0	90.00	10.00
Isopropanol	50.0	9.91	40.09
Water	100.0	0.08	99.92
Total:	250.0	99.99	150.01
Mole fraction:			
Methanol	0.4000	0.9000	0.0666
Isopropanol	0.2000	0.0991	0.2672
Water	0.4000	0.0008	0.6661

Back-calculated values of HETP ranged from about 1.5 to 3 ft for M and P, and 1.5 to 2 ft for W.
Column diameter was computed to be 5.1 ft with a column pressure drop of 0.84 psi.

Exercise 12.13

Subject: Separation of methanol (M) from a mixture containing isopropanol (P) and water (W) by distillation in a packed column with a structured packing, using a rate-based method.

Given: A bubble-point feed of 100 kmol/h of M, 50 kmol/h of P, and 100 kmol/h of W at 1 atm. Column contains 40 ft of structured packing in two sections (one above the feed and one below the feed). Feed entry is 25 ft from the top of the packing. Reflux ratio = 5 and bottoms mole flow rate = 150 kmol/h

Assumptions: Use 100 segments (called stages in the Chemsep program, when solving a packed column) to simulate each of the two sections of packing, with perfectly mixed vapor and liquid in each segment. Operation at about 75% of flooding.

Find: The separation achieved.

Analysis: The calculations were made with the Chemsep program. The properties chosen were:

Gamma-Phi K model UNIFAC Activity coefficient
Ideal gas law Equation of State DIPPR Vapour pressure
Excess Enthalpy

Other physical properties were by default with Wilke-Chang for liquid diffusivities.
Several different structured packings could used. Flexipac 2 in stainless steel was selected.
Bravo-Rocha-Fair 1985 method for mass-transfer coefficients and interfacial area.
Bravo-Rocha-Fair 1986 method for pressure drop.
Newton's method to converge calculations with maximum of 10% change in vapor rate and 2°C change in temperature between iterations.
Calculations converged in 10 iterations and 28 seconds with a Pentium 90 PC, giving the following distillate and bottoms compositions:

Component	Feed	Distillate	Bottoms
Flow, kmol/h:			
Methanol	100.0	90.09	8.91
Isopropanol	50.0	8.89	41.11
Water	100.0	0.02	99.98
Total:	250.0	100.00	150.00
Mole fraction:			
Methanol	0.4000	0.9109	0.0594
Isopropanol	0.2000	0.0889	0.2740
Water	0.4000	0.0002	0.6666

Back-calculated values of HETP ranged from about 1.3 to 2 ft for M and P, and 1.1 to 1.4 ft for W. Column diameter was computed to be 5.1 ft with a column pressure drop of 0.43 psi.

Exercise 12.14

Subject: Separation of a mixture of methanol (M) from a mixture containing isopropanol (P) and water (W) by distillation in a sieve-tray column for various conditions of % flood, weir height, and % hole area, using a rate-based method.

Given: A bubble-point feed of 100 kmol/h of M, 50 kmol/h of P, and 100 kmol/h of W at 1 atm is sent to tray 25 from the top tray of a column containing 40 trays, operating at 1 atm. Reflux ratio is 5 and bottoms mole flow rate = 150 kmol/h. Use UNIFAC method for liquid-phase activity coefficients and the Chan-Fair method for mass-transfer coefficients and interfacial area.

Consider combinations of:
80%, 60%, and 40% of flooding.
3, 2, and 1 inch weir heights.
14%, 10%, and 6% hole area.

Assumptions: Assume both phases are perfectly mixed on each tray.

Find: The separations achieved.

Analysis: The Chemsep method is applied with the Simple Distillation option, a total condenser, a partial reboiler, and 42 stages (counting the condenser and the reboiler). Thus, the feed is sent to stage 26 from the top. To estimate *K*-values from the UNIFAC method, the ideal gas law is assumed with DIPPR vapor pressure, and excess enthalpy for the liquid phase.
For physical properties necessary to size the column diameter and compute mass-transfer coefficients and interfacial area, the following options were chosen:
Rackett equation for liquid density. Wilke and DIPPR for vapor viscosity.
Molar averaging of DIPPR pure component liquid viscosity, vapor thermal conductivity, liquid thermal conductivity, and surface tension. Binary liquid diffusivities from Wilke-Chang method.
Neglect pressure drop. Automatic initialization.
Newton's method, but maximum change of liquid or vapor flow rate of only 10% and maximum temperature change of only 2°C.

It was found that the % hole area had a negligible effect on the purity of methanol in the distillate. Therefore, only combinations of % flood and weir height are reported here. The separations achieved are given below in terms of the methanol purity in the distillate in mole%.

% Flood	80	80	80	60	60	60	40	40	40
Weir height, in.	1	2	3	1	2	3	1	2	3
Mole % M in distillate	90.54	90.76	90.86	90.03	90.34	90.71	89.32	89.81	90.17

For this problem, the separation achieved is not significantly affected by the % flood or weir height.

Exercise 12.15

Subject: Effect of % flood on the Murphree efficiency for oxygen and the separation of air in the upper column of an air separation system, using a rate-based method.

Given: A sieve-tray column with 48 plates, no condenser, and a split reboiler that gives 50 mol% liquid bottoms and 50 mol% vapor bottoms. A feed at 80 K, 131.7 kPa, and 1349 lbmol/h, with a composition of 97.868 mol% N_2, 0.365 mol% A, and 1.767 mol% O_2, entering the top tray. A feed at 83 K, 131.7 kPa, and 1832 lbmol/h, with a composition of 59.70 mol% N_2, 1.47 mol% A, and 38.83 mol% O_2, entering tray 12 from the top. Column operates at 131.7 kPa, with a vapor distillate flow rate = 2487 lbmol/h.

Assumptions: Ideal solutions and ideal gas law. Raoult's law *K*-values.

Find: Effect of % flooding on the Murphree vapor tray efficiency for oxygen and the separation.

Analysis: The rate-based calculations were made with the Chemsep program using the reboiled absorber/stripper option, no condenser, a partial reboiler, and 49 stages (48 trays + reboiler). To simulate the split reboiler, a vapor sidestream was withdrawn from stage 49. Antoine vapor pressure and default properties were used. A total material balance around the column gives: $F_1 + F_2 = D + B_V + B_L$ with $B_V = B_L$. Thus, the bottoms flow rate, B_L, was specified as: (1349 + 1832 - 2487)/2 = 347 lbmol/h. The vapor sidestream flow rate from stage 49, B_V, was also specified as 347 lbmol/h. The Chan-Fair method was used to estimate mass-transfer coefficients and interfacial area. Mixed flow was specified for vapor and liquid phases. Defaults were used for solving the problem. The feed to tray 1 was computed to be 69 mol% vaporized, while the feed to tray 12 was all liquid. Convergence of the calculations was achieved without difficulty, with the following results:

% Flood	Mole fraction of O_2 in the vapor distillate	Mole fraction of N_2 in the liquid bottoms	Median Murphree efficiency for O_2, %
25	0.0317	0.0063	50
50	0.0314	0.0059	54
75	0.0313	0.0060	53
85	0.0313	0.0064	48
95	0.0314	0.0072	40

Exercise 12.15 (continued)

The peak efficiency was achieved in the neighborhood of 50% flooding, but the separation was little affected over the range of 25 to 85% of flooding. The complete material balance for 85% of flooding was as follows:

Component	Feed to tray 1	Feed to tray 12	Vapor Distillate	Vapor bottoms	Liquid bottoms
Nitrogen	1320	1094	2398.83	12.95	2.22
Argon	5	27	10.36	12.69	8.95
Oxygen	24	711	77.81	321.36	335.83
Total:	1349	1832	2487.00	347.00	347.00

Exercise 12.16

Subject: Separation of methanol (M), n-hexane (HX) , and n-heptane (HP), from toluene (T) by extractive distillation with phenol (P), using a rate-based method.

Given: Bubble-point feed of 50 kmol/h of M, 20 kmol/h of HX, 180 kmol/h of HP, and 150 kmol/h of T at 1.4 atm. Entrainer of 10 kmol/h of T and 800 kmol/h of P, at 1.4 atm and same temperature as the feed. Sieve-tray column with 30 trays, a total condenser, and partial reboiler. Thus, 32 stages are needed. Entrainer to tray 5 from top {Stage 6) and feed to tray 15 from top (Stage 16). Condenser outlet pressure = 1.1 atm. Condenser inlet pressure = 1.2 atm. Bottom tray pressure = 1.4 atm. Reflux ratio = 5 and bottoms rate = 960 kmol/h. Use UNIFAC method with Antoine equation for liquid phase and SRK EOS for the vapor phase. Vapor and liquid on each tray are well mixed. Use Chan-Fair for mass-transfer coefficients and interfacial area. Operation at about 75% of flooding.

Find: The separation and average Murphree vapor tray efficiencies. Any improvement in the separation by moving the entrainer and feed trays. Any improvement in the separation by changing other parameters.

Analysis: The Chemsep methods was applied with the Extractive Distillation option. For physical properties necessary to size the column diameter and compute mass-transfer coefficients and interfacial area, the following default options were chosen except that binary liquid diffusivities were estimated from the Wilke-Chang method.
Used automatic initialization with Newton's method, but max. change of liquid or vapor flow rate of only 5% and max. temperature change of only 2°C. The problem was difficult to converge. The separation achieved is:

Component	2 Feeds	Distillate	Bottoms
Flow, kmol/h:			
Methanol	50.0	50.00	0.00
n-Hexane	20.0	20.00	0.00
n-Heptane	180.0	172.23	7.77
Toluene	160.0	6.55	153.45
Phenol	800.0	1.22	798.78
Total:	1210.0	250.00	960.00
Mole fraction:			
Methanol	0.0413	0.2000	0.0000
n-Hexane	0.0165	0.0800	0.0000
n-Heptane	0.1488	0.6889	0.0081
Toluene	0.1322	0.0262	0.1598
Phenol	0.6612	0.0049	0.8321

Exercise 12.16 (continued)

Analysis: (continued)

The above separation that was achieved for the problem specifications indicates that the separation between n-heptane and toluene is not sharp. Also, it is desirable to try to reduce the amount of phenol in the distillate. The average back-calculated Murphree vapor tray efficiencies are approximately:

Methyl alcohol:	50%
n-Hexane	50%
n-Heptane	55%
Toluene	55%
Phenol	Constantly changing over a wide range from negative to 65%

To reduce the amount of phenol in the distillate, might lower the entrainer feed entry from tray 5 to 6. This reduced the phenol rate in the distillate from 1.22 to 0.78 kmol/h, but the toluene in the distillate increased. The separation could not be significantly improved by changing the entrainer and feed tray entries.

To improve the separation, might increase the number of trays and/or the reflux ratio. When the number of trays was doubled to 60 (62 stages), with the entrainer fed to stage 13 and the feed to stage 35, the separation was improved, but not dramatically, to the following:

Component	2 Feeds	Distillate	Bottoms
Flow, kmol/h:			
Methanol	50.0	50.00	0.00
n-Hexane	20.0	20.00	0.00
n-Heptane	180.0	176.94	3.06
Toluene	160.0	2.97	157.03
Phenol	800.0	0.09	799.91
Total:	1210.0	250.00	960.00

Increasing the reflux ratio from 5 to 6 had a negligible effect on the separation.

Increasing the entrainer flow rate by 20% had a negligible effect on the separation.

Thus, a sharp separation is difficult to achieve and is best accomplished by using a large number of trays.

Exercise 12.17

Subject: Absorption of light hydrocarbons in a rich gas with an absorber oil in a bubble-cap column, using both equilibrium-stage and rate-based methods.

Given: Temperature, pressure, and component flow rates of the rich gas and absorber oil.

Find: (a) Number of equilibrium stages and splits of all components for 40% absorption of propane.

(b) Actual number of trays, the splits, and Murphree vapor tray efficiencies, with a rate-based method

(c) Comparison and discussion.

Analysis: The ChemSep program was applied to both cases, using the SRK method for *K*-values and enthalpies.

(a) It was determined for the equilibrium stage method that the average *K*-value for propane was about 3.0. Therefore, the approximate absorption factor is $A = L/KV = 11/[(3)(11)] = 0.33$ For this small an absorption factor, using the Kremser plot in Fig. 5.9, the fraction of propane absorbed is independent of the number of equilibrium stages above about 3. However, the effect of stages on n-butane and n-pentane is significant. Therefore, one possible specification was 20 trays with a 75% overall efficiency or the equivalent of 15 equilibrium stages. This gave almost 40% absorption of propane, 94% absorption of n-butane, and 96% absorption of n-pentane. The splits were as follows:

Flow rate, kmol/s:

Component	Absorber oil	Rich gas	Lean gas	Rich oil
Methane	0.00	3.146	3.050	0.096
Ethane	0.00	1.727	1.503	0.224
Propane	0.00	2.640	1.618	1.022
n-Butane	0.22	1.859	0.121	1.958
n-Pentane	0.55	1.628	0.084	2.094
n-Dodecane	10.23	0.000	0.001	10.229
Total	11.00	11.000	6.377	15.623

(b) Difficulty was experienced in converging the rate-based method for this exercise, probably because of the tray design calculations for a bubble-cap column, which led to a very large diameter column with many liquid passes. Accordingly, the following procedure was employed. The number of actual trays was fixed at 20. The profiles of temperature, vapor and liquid flow rates, and vapor and liquid compositions from the equilibrium-stage calculations in part (a) were saved and used as "old results" to initialize the rate-based calculations. Default physical properties were chosen, along with the AIChE method for mass-transfer coefficients and interfacial area. Mixed flow was assumed for both vapor and liquid phases and 85% of flooding

Exercise 12.17 (continued)

Analysis: (continued)

was chosen, along with a system factor for foaming of 0.75. The calculations for a bubble-cap column terminated with an error before completing even one iteration, probably because of difficulty in determining an initial estimate of column diameter. A sieve-tray column was then specified and the system factor was reduced to 0.1. The calculations converged. The system factor was then increased to 0.2 and then to 0.3, with convergence both times using profiles from the previous run. A column diameter of about 13 m was then computed by taking the diameter calculated for a system factor of 0.3 and scaling it to a system factor, F_F, of 0.75, using Eqs. (6-42), (6-40), and (6-44). A bubble-cap column was then attempted with a specified column diameter of 13 m. This time the calculations converged, with the following splits:

Flow rate, kmol/s:

Component	Absorber oil	Rich gas	Lean gas	Rich oil
Methane	0.00	3.146	3.050	0.096
Ethane	0.00	1.727	1.501	0.226
Propane	0.00	2.640	1.605	1.035
n-Butane	0.22	1.859	0.120	1.959
n-Pentane	0.55	1.628	0.081	2.097
n-Dodecane	10.23	0.000	0.001	10.229
Total	11.00	11.000	6.358	15.642

These results are almost identical to those above for the equilibrium-stage calculations. However, the % absorption of propane is now 39.2%. Five passes were needed to handle the high liquid flow rate.

The back-calculated Murphree vapor tray efficiencies were mainly in the following ranges:

Methane:	54 to 80%
Ethane:	55 to 75%
Propane:	46 to 77%
n-Butane:	65 to 77%
n-Pentane:	74 to 80%
n-Dodecane:	73 to 78%

(c) The tray efficiencies were higher than anticipated, probably due to somewhat higher temperatures at the elevated pressure, which reduces the liquid viscosity. The rate-based method has the advantage of predicting the efficiency. However, in this exercise, as pointed out above, the near 40% absorption of propane is independent of the number of equilibrium stages above three. A column diameter of 13 m is probably too large. Two or more columns in parallel should be considered.

Exercise 12.18

Subject: Separation of methanol (M) from a mixture with ethanol (E) and water (W) by distillation, using equilibrium-stage and rate-based methods with a trayed column.

Given: A feed at 1.3 atm and 316 K of 142.46 kmol/h of 65.36 mol% M, 3.51 mol% E, and 31.13 mol% W. Column is equipped with a total condenser (1.1 atm in and 1.0 atm out) and a partial reboiler. Reflux ratio = 1.2 and distillate rate = 93.10 kmol/h (almost equal to the M feed rate). Distillate is to have a mole fraction of W less than or equal to 0.0001. UNIFAC method for activity coefficients. Sieve-tray efficiency of 85%.

Find: (a) Number of equilibrium stages, optimal feed stage location, and the split of all components.

(b) Actual number of sieve trays, the split of all components, and the Murphree vapor tray efficiencies. Comparison and discussion of results.

Analysis: The ChemSep method was applied to both parts, using the ideal gas law, Antoine vapor pressure, and excess enthalpy with UNIFAC. A column bottoms pressure of 1.3 atm was assumed. The calculations used automatic initialization with Newton's method and defaults for step limits on flows, temperature, and composition. The bottoms flow rate was specified as 142.46 - 93.10 = 49.36 kmol/h.

(a) For the equilibrium-stage case, the total number of stages and the optimal feed stage were varied, starting with 42 stages (including the condenser and reboiler) and a feed stage of 21 from the condenser, until the water mol% specification in the distillate was met. A satisfactory result was achieved for 24 stages (including the condenser and reboiler) with the feed to stage 20 from the condenser. The splits were as follows:

Component	Feed	Distillate	Bottoms
Flow, kmol/h:			
Methanol	93.11	89.49	3.62
Ethanol	5.00	3.60	1.40
Water	44.35	0.01	44.34
Total:	142.46	93.10	49.36
Mole fraction:			
Methanol	0.6536	0.9612	0.0734
Ethanol	0.0351	0.0387	0.0283
Water	0.3113	0.000087	0.8983

Exercise 12.18 (continued)

Analysis: (continued)

(b) For the rate-based case, a sieve-tray column was used, with default properties and the Wilke-Chang method for liquid diffusivities. The Chan-Fair method was used to estimate mass-transfer coefficients and interfacial area. Plug flow was used for the vapor and the mixed flow option was applied to the liquid. Initially, a tray efficiency of 80% was used to obtain an initial estimate of the number of actual trays and feed tray location. These values were then varied to meet the mol% water specification in the distillate. The result was 25 trays plus a condenser and reboiler, with the feed to tray 21 from the top. The splits were as follows:

Component	Feed	Distillate	Bottoms
Flow, kmol/h:			
Methanol	93.11	89.45	3.66
Ethanol	5.00	3.64	1.36
Water	44.35	0.01	44.34
Total:	142.46	93.10	49.36
Mole fraction:			
Methanol	0.6536	0.9607	0.0743
Ethanol	0.0351	0.0392	0.0274
Water	0.3113	0.0001	0.8983

These results for the rate-based case compare well with the equilibrium-stage case. They indicate an overall tray efficiency of approximately 22/25 = 0.88 or 88%.

The computed Murphree vapor tray efficiencies were as follows:

Methyl alcohol: 78.2 to 88.5%
Ethyl alcohol: 44.0 to 127.8%, a very wide range, with most values between 44 and 128%
Water: 82.4 to 90.4%

Computing time was 2 s with 3 iterations for the equilibrium-stage calculation.
Computing time was 5 s with 5 iterations for the rate-based method of calculation.

Exercise 12.19

Subject: Separation of methanol (M) from a mixture with ethanol (E) and water (W) by distillation in a packed bed, using a rate-based method.

Given: A feed at 1.3 atm and 316 K of 142.46 kmol/h of 65.36 mol% M, 3.51 mol% E, and 31.13 mol% W. Column is equipped with a total condenser (1.1 atm in and 1.0 atm out) and a partial reboiler. Reflux ratio = 1.2 and distillate rate = 93.10 kmol/h (almost equal to the M feed rate). Distillate is to have a mole fraction of W less than or equal to 0.0001. UNIFAC method for activity coefficients. 2-inch metal Pall-ring packing.

Assumptions: Operation at about 75% of flooding.

Find: Height of packing above and below the feed entry.

Analysis: The ChemSep method was applied, using the ideal gas law, Antoine vapor pressure, and excess enthalpy with UNIFAC. Default properties were selected with the Wilke-Chang method for liquid diffusivities. In section above the feed, 80 segments (called stages) were used. In the section below the feed, 20 segments were used. A column bottoms pressure of 1.3 atm was assumed, but the actual pressure drop was estimated using the Billet-Schultes method of 1992. Mass-transfer coefficients and interfacial area were estimated with the Billet-Schultes method of 1992. The calculations used automatic initialization with Newton's method and defaults for step limits on flows, temperature, and composition. The bottoms flow rate was specified as 142.46 - 93.10 = 49.36 kmol/h. To determine an initial estimate of the packed heights above and below the feed, an HETP of 0.6 m was assumed giving 12.8 m above the feed and 2.4 m below. These heights were then varied to meet the mol% water specification in the distillate. The final result, which was achieved in 14 s with 8 iterations, was 23 m above the feed and 4 m below. The split was:

Component	Feed	Distillate	Bottoms
Flow, kmol/h:			
Methanol	93.11	89.28	3.84
Ethanol	5.00	3.82	1.18
Water	44.35	0.01	44.34
Total:	142.46	93.10	49.36
Mole fraction:			
Methanol	0.6536	0.9589	0.0777
Ethanol	0.0351	0.0410	0.0240
Water	0.3113	0.0001	0.8983

Calculated values of HETP were:

Methanol: 1.1 to 1.8 m Ethanol: Very wide range Water: 0.8 to 1.25 m

A pressure drop of 0.06 atm was estimated. Estimated column diameters were 1 m above and 1.28 m below the feed entry.

Exercise 12.20

Subject: Absorption of benzene from a near-air stream by n-tridecane in a sieve-tray tower using the rate-based method.

Given: A gas feed at 1 atm, 300 K, and 0.01487 kmol/s, with 75.05 mol% nitrogen, 19.95 mol% oxygen, and 5.0 mol% benzene. Absorption oil at 1 atm, 300K, and 0.005 kmol/s of 99.5 mol% n-tridecane and 0.5 mol% benzene. Tray geometry with 0.5 m tray spacing, 0.05 m weir height, 0.003 m hole diameter, and 0.002 m tray thickness. 80% of flooding.

Find: Number of actual trays required, column diameter, and Murphree vapor tray efficiency of benzene for all possible combinations of vapor and liquid flow patterns.

Analysis: The Chemsep program was used with non-equilibrium, absorber options and the SRK EOS was applied for *K*-values and enthalpies. Default properties and the Hayduk-Minhas method for liquid diffusivities were specified. The Chan-Fair method was used to estimate mass-transfer coefficients and interfacial area. For each combination of flow patterns, the number of actual trays was varied to achieve close to 96% absorption of benzene. In all cases the material balance for the other components was essentially the same as follows:

Flow rate, kmol/h	Feed gas	Absorbent	Lean gas	Rich oil
Nitrogen	40.18	0.00	40.15	0.03
Oxygen	10.66	0.00	10.65	0.01
Benzene	2.68	0.09	0.19	2.58
n-Tridecane	0.00	17.91	0.0038	17.91
Total:	53.52	18.00	50.99	20.53

The number of actual trays and the Murphree vapor tray efficiency for the combinations of flow patterns were as follows. For all three cases, the column diameter was 0.63 to 0.65 m.

Vapor flow	Liquid flow	Number of trays	Benzene tray efficiency, %
Mixed	Mixed	11	49 to 55
Plug	Mixed	8	64 to 67
Plug	Plug	7.5	73 to 75

The number of equilibrium stages was determined to be about 6. In this exercise, with only one component (benzene) undergoing any significant mass transfer, an equilibrium-stage method is adequate, but only if a good estimate of the tray efficiency is available. For the relative small column diameter, the mixed-mixed flow-pattern case is probably best.

Exercise 13.1

Subject: Evaporation of a small amount of n-heptane (C7) from a drum of toluene (T).

Given: A drum of toluene containing 2 mol% C7. Simple batch differential (Rayleigh) distillation at 1 atm. Vapor-liquid equilibrium data for the C7-toluene system at 1 atm.

Assumptions: Perfect mixing in the still. Exiting vapor in equilibrium with the liquid.

Find: (a) Composition of the residue in the pot as a function of wt% distilled. Composition of residue and the cumulative distillate at 50 wt% distilled.
(b) Composition of the cumulative distillate and the residue when 50% of the C7 has been distilled. Weight percent of the original charge distilled.

Analysis: The vapor-liquid equilibrium data indicate that C7 is more volatile than T. Therefore, make the calculations in terms of C7. Because the initial concentration of C7 in the charge is low (2 mol%), assume that the distillation takes place at constant relative volatility, $\alpha = \alpha_{C7\text{-}T}$. Alternatively, the y - x data in the low concentration region could be fitted to a quadratic equation and used with Eq. (13-2). The lowest concentration in the data table is 2.5 mol% C7, where x = 0.025 and y = 0.048. Therefore, for the binary system, using Eqs. (2-19) and (2-21),

$K_{C7} = y/x = 0.048/0.025 = 1.92$ $\quad K_T = (1\text{-}y)/(1\text{-}x) = (1 - 0.048)/(1 - 0.025) = 0.976$

$\alpha_{C7\text{-}T} = K_{C7}/K_T = 1.92/0.976 = 1.97$

A similar calculation at the next point in the data table, x = 0.062 and y = 0.107, gives $\alpha_{C7\text{-}T}$ = 1.81. Therefore the relative volatility increases as x drops to zero. Take $\alpha_{C7\text{-}T} = 2$ for the region of interest.

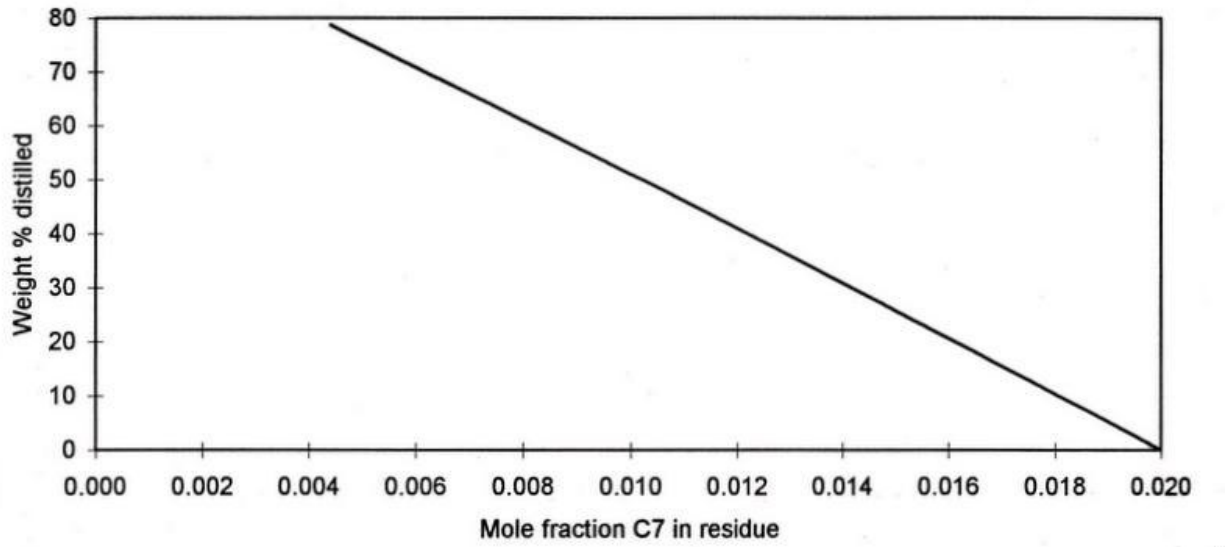
From Eq. (13-5), $$\ln\left(\frac{W_0}{W}\right) = \frac{1}{\alpha - 1}\left[\ln\left(\frac{x_0}{x}\right) + \alpha \ln\left(\frac{1-x}{1-x_0}\right)\right] = \ln\left(\frac{0.025}{x}\right) + 2\ln\left(\frac{1-x}{1-0.025}\right) \qquad (1)$$

Taking a basis of W_0 = 1 lbmole, this equation can be solved with a spreadsheet for W for a series of values of x from 0.020 to 0.0. For each value of x, a material balance on C7 gives Eq. (13-6) for the mole fraction of C7 in the cumulative distillate, $$\left(y_D\right)_{avg} = \frac{W_0 x_0 - W x}{W_0 - W} \qquad (2)$$

With values of W, x, and $\left(y_D\right)_{avg}$, together with the molecular weights of 100.21 for C7 and 92.14 for T, amounts in mass units can be computed, using Eqs. (1) and (2). The spreadsheet is given on the following page, from which the following results are obtained.
(a) Initial residue = 92.29 lb. At 50 wt% distilled, residue = 46.145 lb. From the spreadsheet, the mole fraction of C7 in the residue = 0.0102, the mass fraction of C7 in the residue = 0.0110. The mass fraction of C7 in the cumulative distillate = 0.0324.
(b) When 50% of the C7 has distilled, the mole fraction of C7 in the residue = 0.0142, the mass fraction of C7 in the cumulative distillate = 0.0365, and the wt% of charge distilled = 29.9%.

Exercise 13.1 (continued)

x	ln(*Wo*/*W*)	*W*	mols C7 in residue	lb C7 in residue	mols T in residue	lb T in residue	Total lb residue	wt% distilled	C7 mass fraction in residue	lb cum. distillate	C7 mass fraction in cum. distillate
0.0200	0.000	1.000	0.0200	2.0040	0.980	90.29	92.29	0.000	0.0217	0.00	
0.0196	0.021	0.979	0.0192	1.9231	0.960	88.45	90.37	2.083	0.0213	1.92	0.0421
0.0192	0.042	0.958	0.0184	1.8439	0.940	86.61	88.45	4.163	0.0208	3.84	0.0417
0.0188	0.064	0.938	0.0176	1.7664	0.920	84.77	86.53	6.240	0.0204	5.76	0.0413
0.0184	0.087	0.917	0.0169	1.6907	0.900	82.93	84.62	8.313	0.0200	7.67	0.0408
0.0180	0.109	0.896	0.0161	1.6166	0.880	81.09	82.71	10.382	0.0195	9.58	0.0404
0.0176	0.133	0.876	0.0154	1.5443	0.860	79.26	80.80	12.448	0.0191	11.49	0.0400
0.0172	0.157	0.855	0.0147	1.4737	0.840	77.43	78.90	14.510	0.0187	13.39	0.0396
0.0168	0.181	0.835	0.0140	1.4048	0.821	75.59	77.00	16.569	0.0182	15.29	0.0392
0.0164	0.206	0.814	0.0133	1.3376	0.801	73.76	75.10	18.625	0.0178	17.19	0.0388
0.0160	0.231	0.794	0.0127	1.2722	0.781	71.94	73.21	20.677	0.0174	19.08	0.0384
0.0156	0.257	0.773	0.0121	1.2084	0.761	70.11	71.32	22.725	0.0169	20.97	0.0379
0.0152	0.284	0.753	0.0114	1.1463	0.741	68.28	69.43	24.771	0.0165	22.86	0.0375
0.0148	0.312	0.732	0.0108	1.0858	0.721	66.46	67.55	26.812	0.0161	24.75	0.0371
0.0144	0.340	0.712	0.0103	1.0271	0.702	64.64	65.66	28.851	0.0156	26.63	0.0367
0.0140	0.369	0.692	0.0097	0.9700	0.682	62.82	63.79	30.886	0.0152	28.50	0.0363
0.0136	0.399	0.671	0.0091	0.9147	0.662	61.00	61.91	32.917	0.0148	30.38	0.0359
0.0132	0.429	0.651	0.0086	0.8610	0.642	59.18	60.04	34.945	0.0143	32.25	0.0354
0.0128	0.461	0.631	0.0081	0.8089	0.623	57.36	58.17	36.970	0.0139	34.12	0.0350
0.0124	0.493	0.610	0.0076	0.7585	0.603	55.55	56.31	38.991	0.0135	35.99	0.0346
0.0120	0.527	0.590	0.0071	0.7098	0.583	53.73	54.44	41.009	0.0130	37.85	0.0342
0.0116	0.562	0.570	0.0066	0.6627	0.564	51.92	52.58	43.024	0.0126	39.71	0.0338
0.0112	0.598	0.550	0.0062	0.6173	0.544	50.11	50.73	45.035	0.0122	41.56	0.0334
0.0108	0.635	0.530	0.0057	0.5735	0.524	48.30	48.88	47.042	0.0117	43.42	0.0329
0.0104	0.673	0.510	0.0053	0.5314	0.505	46.49	47.03	49.047	0.0113	45.27	0.0325
0.0100	0.713	0.490	0.0049	0.4909	0.485	44.69	45.18	51.048	0.0109	47.11	0.0321



Exercise 13.2

Subject: Simple differential batch (Rayleigh) distillation of a mixture of isopropanol and water.

Given: Charge of 40 mol% isopropanol (P) and 60 mol% water (W). Distillation at 1 atm until 70 mol% of the charge is distilled. Vapor-liquid equilibrium data in Exercise 7.33.

Assumptions: Perfect mixing in the still. Exiting vapor in equilibrium with the liquid.

Find: Compositions of residue in still and cumulative distillate.

Analysis: Because the vapor-liquid equilibrium data indicate that P is the more volatile component below 40 mol% P in the liquid, base the calculations on P. Use Eq. (13-3), with x_0 = 0.4 and W/W_0 = 0.3 (70 mol% vaporized). Thus, Eq. (13-3) becomes:

$$\int_{0.4}^{x} \frac{dx}{y-x} = \ln 0.3 = -1.204 \quad \text{or} \quad \int_{x}^{0.4} \frac{dx}{y-x} = 1.204 \qquad (1)$$

where x is the mole fraction of P in the residue at 70 mol% distilled and y is in equilibrium with x.
Equilibrium data from Exercise 7.33 that are in the potential range of this exercise are:

y	0.4620	0.5242	0.5686	0.5926
x	0.0841	0.1978	0.3496	0.4525

A perfect fit of these data to a cubic equation gives:

$$y = 0.38858 + 1.04439x - 2.20358x^2 + 1.97113x^3 \qquad (2)$$

Substitute Eq. (2) into Eq. (1) and, using a spreadsheet, integrate the resulting equation using the trapezoidal rule with a Δx increment of 0.01 starting from x = 0.4 with decreasing values of x until the integral equals 1.204. As an example, using this method for the first four increments, the integral is equal to $\Delta x[\ 0.5f_{x=0.40} + f_{x=0.39} + f_{x=0.38} + f_{x=0.37} + 0.5f_{x=0.36}\ ]$, where $f = 1/(y-x)$.
The complete spreadsheet is given on the following page. From it, the following result is obtained: Mole fraction of P in the residue at 70 mol% distilled = 0.0575.
For this value of x, a material balance on P gives Eq. (13-6) for the mole fraction of C7 in the cumulative distillate,

$$(y_D)_{\text{avg}} = \frac{W_0 x_0 - Wx}{W_0 - W} \qquad (3)$$

Therefore, for a basis of W_0 = 1 mole, $(y_D)_{\text{avg}} = \dfrac{1(0.4) - 0.3(0.0575)}{1 - 0.3} = 0.547$

Exercise 13.2 (continued)

x	y	$f = 1/(y-x)$	Value of Integral
0.40	0.580	5.558	
0.39	0.578	5.329	0.054
0.38	0.575	5.117	0.107
0.37	0.573	4.922	0.157
0.36	0.571	4.741	0.205
0.35	0.569	4.573	0.252
0.34	0.566	4.417	0.297
0.33	0.564	4.272	0.340
0.32	0.562	4.137	0.382
0.31	0.559	4.011	0.423
0.30	0.557	3.894	0.462
0.29	0.554	3.785	0.501
0.28	0.552	3.683	0.538
0.27	0.549	3.588	0.575
0.26	0.546	3.499	0.610
0.25	0.543	3.416	0.645
0.24	0.540	3.338	0.678
0.23	0.536	3.266	0.711
0.22	0.533	3.198	0.744
0.21	0.529	3.135	0.775
0.20	0.525	3.076	0.806
0.19	0.521	3.021	0.837
0.18	0.517	2.970	0.867
0.17	0.512	2.923	0.896
0.16	0.507	2.879	0.925
0.15	0.502	2.838	0.954
0.14	0.497	2.801	0.982
0.13	0.491	2.767	1.010
0.12	0.486	2.735	1.037
0.11	0.479	2.707	1.065
0.10	0.473	2.681	1.092
0.09	0.466	2.658	1.118
0.08	0.459	2.638	1.145
0.07	0.452	2.621	1.171
0.06	0.444	2.606	1.197
0.05	0.436	2.594	1.223
0.04	0.427	2.584	1.249

Exercise 13.3

Subject: Simple differential batch (Rayleigh) distillation of a mixture of benzene and toluene.

Given: Charge of 100 moles of 30 mol% benzene (B) and 70 mol% toluene (T). Distillation until the cumulative distillate contains 45 mol% benzene.

Assumptions: Relative volatility = $\alpha = \alpha_{B\text{-}T} = 2.5$. Perfect mixing in the still. Exiting vapor in equilibrium with the liquid.

Find: Moles of residue.

Analysis: For constant relative volatility, Eq. (13-5) applies with $\alpha = 2.5$, $W_0 = 100$, $x_0 = 0.30$.

Thus,
$$\ln\left(\frac{100}{W}\right) = \frac{2}{3}\left[\ln\left(\frac{0.30}{x}\right) + 2.5\ln\left(\frac{1-x}{0.70}\right)\right] \qquad (1)$$

From Eq. (13-6), the mole fraction of benzene in the cumulative distillate is given by:

$$\left(y_D\right)_{\text{avg}} = 0.45 = \frac{30 - Wx}{100 - W} \qquad (2)$$

Eqs. (1) and (2) are solved by first solving Eq. (2) for x in terms of W to obtain

$$x = 0.45 - \frac{15}{W} \qquad (3)$$

Substituting Eq. (3) into Eq. (1) and solving the resulting nonlinear equation gives $W = 57.9$ moles.

In lieu of a nonlinear equation solver, a spreadsheet can be used by assuming a value of W and solving Eq. (3) for x. Then substitute this value into Eq. (1) and solve for W. Repeat until the assumed value of W equals the calculated value. This is readily done by setting up a table in W, working in increments from $W = 100$ moles down to a low value of W.

Exercise 13.4

Subject: Simple differential batch (Rayleigh) distillation of a mixture of benzene and toluene.

Given: Charge of 250 lb of 70 mol% benzene (B) and 30 mol% toluene (T). Distillation at 1 atm until 1/3 of the original charge is distilled.

Assumptions: Ideal *K*-values. Perfect mixing in still. Exiting vapor in equilibrium with liquid.

Find: Compositions of the residue and distillate.

Analysis: Using molecular weights of 78.11 for benzene and 92.14 for toluene, the average molecular weight of the charge = 0.7(78.11) + 0.3(92.14) = 82.32. Therefore, the charge contains 250/82.32 = 3.037 lbmol. Final mass of the residue = 0.667(250) = 166.7 lb.
Benzene is the more volatile component. Therefore, base the calculations on B. Use Eq. (13-3), with $x_0 = 0.7$ and $W_0 = 3.037$ lbmol. Thus, Eq. (13-3) becomes:

$$\int_{0.7}^{x} \frac{dx}{y-x} = \ln\left(\frac{W}{3.037}\right) \quad \text{or} \quad \int_{x}^{0.7} \frac{dx}{y-x} = \ln\left(\frac{3.037}{W}\right) \qquad (1)$$

where x is the mole fraction of B in the final residue and y is in equilibrium with x.
Equilibrium data at 1 atm are conveniently obtained from a simulation program. For example, data from the Chemcad program are included below for the range of interest, based on Raoult's law (ideal *K* values).
Using a spreadsheet with the equilibrium y-x data, integrate Eq. (1) using the trapezoidal rule with a Δx increment of 0.02 starting from $x = 0.70$ with decreasing values of x. As an example, using this method for the first four increments, the integral is equal to $\Delta x[\ 0.5f_{x=0.40} + f_{x=0.39} + f_{x=0.38} + f_{x=0.37} + 0.5f_{x=0.36}\ ]$, where $f = 1/(y\text{-}x)$. At each step , W is computed and then the mass in pounds
until 166.7 lb of residue is reached.
The complete spreadsheet is given below From it, the following result is obtained:
By interpolation, mole fraction of B in the residue = 0.630, corresponding to $W = 2.005$ lbmol.
Using these values, a material balance on B gives for Eq. (13-6),

$$(y_D)_{avg} = \frac{3.037(0.7) - 2.005(0.63)}{3.037 - 2.005} = 0.836$$

x	*y*	*f* =1/(*y* -*x*)	Value of Integral	*W*, lbmol	*W*, lb
0.70	0.8550	6.452		3.307	250.0
0.68	0.8428	6.143	0.1259	2.678	221.2
0.66	0.8302	5.875	0.2461	2.374	196.8
0.64	0.8172	5.643	0.3613	2.116	176.0
62	0.8037	5.444	0.4722	1.894	158.0

Exercise 13.5

Subject: Simple differential batch (Rayleigh) distillation of a mixture of benzene and toluene.

Given: Mixture of 60 mol% benzene (B) and 40 mol% toluene (T). Distillation at 1 atm at the conditions below.

Assumptions: Relative volatility = $\alpha = \alpha_{B\text{-}T} = 2.43$, a constant. Perfect mixing in the still. Exiting vapor in equilibrium with the liquid.

Find: (a) Number of moles in the distillate for 100 moles of feed
(b) Compositions of distillate and residue.
for:
(1) A (cumulative) distillate of 70 mol% B.
(2) 40 mol% of the feed distilled.
(3) 60 percent of B distilled.

Analysis: Calculations are made in terms of benzene, the more volatile component. Because the relative volatility is assumed constant, Eq. (13-5) applies, which for $x_0 = 0.60$, $W_0 = 100$ moles, and $\alpha = 2.43$ is:

$$\ln\left(\frac{100}{W}\right) = 0.6993\left[\ln\left(\frac{0.60}{x}\right) + 2.43\ln\left(\frac{1-x}{0.40}\right)\right] \qquad (1)$$

The composition of the cumulative distillate is given by Eq. (13-6), which becomes:

$$\left(y_D\right)_{\text{avg}} = \frac{60 - Wx}{100 - W} \qquad (2)$$

Case 1: From Eq. (2), $\left(y_D\right)_{\text{avg}} = 0.70 = \dfrac{60 - Wx}{100 - W}$ or $W = \dfrac{10}{0.7 - x}$ (3)

Substituting Eq. (3) into Eq. (1) and solving the resulting nonlinear equation gives $x = 0.33$. Then from Eq. (3), $W = 27.0$ moles. The distillate = W_0 - W = 100 - 27 = 73 moles.
In lieu of a nonlinear equation solver, a spreadsheet can be used by assuming a value of W and solving Eq. (3) for x. Then substitute this value into Eq. (1) and solve for W. Repeat until the assumed value of W equals the calculated value. This is readily done by setting up a table in W, and working in increments from $W = 100$ moles down to a low value of W.

Exercise 13.5 (continued)

Analysis: (continued)

Case 2: For 40 mol% distilled, $W = 100 - 40 = 60$ moles. Substitute this value into Eq. (1)

$$\ln\left(\frac{100}{W}\right) = \ln\left(\frac{100}{60}\right) = 0.5108 = 0.6993\left[\ln\left(\frac{0.60}{x}\right) + 2.43\ln\left(\frac{1-x}{0.40}\right)\right]$$

This is a nonlinear equation in x. Solving with a spreadsheet or a nonlinear equation solver, $x = 0.50$. Substituting this value for x and $W = 60$ moles into Eq. (2) gives:

$$(y_D)_{\text{avg}} = \frac{60 - Wx}{100 - W} = \frac{60 - 60(0.5)}{100 - 60} = 0.75$$

Case 3: The original charge contains 60 moles of B per 100 moles of charge. If 60% of the benzene is distilled, then 36 moles of benzene are in the cumulative distillate and 60 - 36 = 24 moles of benzene are in the residue. To find the number of moles of distillate = 100 - W, and the residue and cumulative distillate benzene mole fractions, use a spreadsheet. Solve Eq. (1) for W using a series of decreasing values of x, starting from $x_0 = 0.6$. For each value of x, compute the moles of benzene in the residue from Wx, until a value of 24 moles is obtained. Then compute the cumulative distillate mole fraction from Eq. (2). The spreadsheet result is:

x	*W*	*Wx*
0.60	100.00	60.00
0.58	89.87	52.13
0.56	81.03	45.38
0.54	73.25	39.55
0.52	66.36	34.51
0.50	60.24	30.12
0.48	54.77	26.29
0.46	49.86	22.94
0.44	45.44	19.99

By interpolation, for $Wx = 24$ moles, $x = 0.466$ and $W = 51.47$ moles.
From Eq. (2),

$$(y_D)_{\text{avg}} = \frac{60 - Wx}{100 - W} = \frac{60 - 24}{100 - 51.47} = 0.742$$

Exercise 13.6

Subject: Simple differential batch (Rayleigh) distillation of a mixture of phenol and water.

Given: Mixture of 15 mol% phenol (P) and 85 mol% water (W). Distillation at 260 torr at the conditions below. Vapor-liquid equilibrium data given in wt% water

Assumptions: Perfect mixing in the still. Exiting vapor in equilibrium with the liquid.

Find: Fraction of original charge that remains as residue and the residue concentration when the cumulative distillate contains 98 mol% water.

Analysis: Make the calculations in terms of water because it is the more volatile component. First convert the given equilibrium data from wt% to mol% using molecular weights of 18.016 for water and 94.108 for phenol. Using a spreadsheet, the results are:

wt% W in liquid	wt% P in liquid	wt% W in vapor	wt% P in vapor	*x*, water	*y*, water
1.54	98.46	41.10	58.90	0.0755	0.7847
4.95	95.05	79.72	20.28	0.2139	0.9536
6.87	93.13	82.79	17.21	0.2782	0.9617
7.73	92.27	84.45	15.55	0.3044	0.9659
19.63	80.37	89.91	10.09	0.5606	0.9790
28.44	71.56	91.05	8.95	0.6749	0.9815
39.73	60.27	91.15	8.85	0.7749	0.9818
82.99	17.01	91.86	8.14	0.9622	0.9833
89.95	10.05	92.77	7.23	0.9791	0.9853
93.38	6.62	94.19	5.81	0.9866	0.9883
95.74	4.26	95.64	4.36	0.9916	0.9913

For 98 mol% W in the cumulative distillate, Eq. (13-6) becomes:

$$\left(y_D\right)_{\text{avg}} = 0.98 = \frac{W_0 x_0 - Wx}{W_0 - W} = \frac{x_0 - \left(\frac{W}{W_0}\right)x}{1-\left(\frac{W}{W_0}\right)} = \frac{0.85 - \left(\frac{W}{W_0}\right)x}{1-\left(\frac{W}{W_0}\right)} \qquad (1)$$

From Eq. (13-3), $$\int_{x_0}^{x} \frac{dx}{y-x} = \ln\left(\frac{W}{W_0}\right) \quad \text{or} \quad \int_{x}^{0.85} \frac{dx}{y-x} = \ln\left(\frac{W_0}{W}\right) \qquad (2)$$

Exercise 13.6 (continued)

Analysis:

Eqs. (1) and (2) together with the y-x table are solved for x and W/W_0. Eq. (2) must be integrated numerically. One way to do this is to fit the equilibrium data to a polynomial equation. Using the data from $x = 0.2782$ to 0.9622, the fit to a cubic equation is:

$$y = 0.913992 + 0.25125x - 0.315062x^2 + 0.133892x^3 \qquad (3)$$

Substitute Eq. (3) into Eq. (2) and integrate using a spreadsheet with the trapezoidal rule for a Δx increment of 0.01 starting from $x = 0.85$ with decreasing values of x. As an example, using this method for the first four increments, the integral is equal to $\Delta x[\ 0.5f_{x=0.40} + f_{x=0.39} + f_{x=0.38} + f_{x=0.37} + 0.5f_{x=0.36}\ ]$, where $f = 1/(y\text{-}x)$. At each step , W/W_0 is computed and then the mole fraction of water in the cumulative distillate from Eq. (1), repeating until a value for the latter of 0.98 is achieved.

The complete spreadsheet is given below. From it, the following result is obtained:

$x = 0.22$ and $W/W_0 = 0.1711$.

x	y	$f = 1/(y\text{-}x)$	Value of Integral	W/W_0	y in cum distillate
0.85	0.98215	7.567			
0.84	0.98209	7.038	0.0730	0.9296	0.9820
0.83	0.98204	6.577	0.1411	0.8684	0.9820
0.82	0.98199	6.173	0.2049	0.8148	0.9820
0.81	0.98195	5.816	0.2648	0.7674	0.9819
0.80	0.98191	5.497	0.3214	0.7252	0.9819
0.79	0.98186	5.212	0.3749	0.6874	0.9819
0.78	0.98182	4.955	0.4257	0.6533	0.9819
0.77	0.98178	4.722	0.4741	0.6224	0.9819
0.76	0.98174	4.510	0.5203	0.5944	0.9819
0.75	0.98169	4.316	0.5644	0.5687	0.9819
0.74	0.98165	4.138	0.6067	0.5452	0.9818
0.73	0.98159	3.975	0.6472	0.5235	0.9818
0.72	0.98154	3.824	0.6862	0.5035	0.9818
0.71	0.98148	3.684	0.7238	0.4849	0.9818
0.70	0.98141	3.554	0.7600	0.4677	0.9818
0.69	0.98134	3.432	0.7949	0.4516	0.9818
0.68	0.98126	3.319	0.8286	0.4366	0.9818
0.67	0.98117	3.214	0.8613	0.4226	0.9817
0.66	0.98107	3.115	0.8930	0.4094	0.9817
0.65	0.98096	3.022	0.9236	0.3971	0.9817
0.64	0.98084	2.934	0.9534	0.3854	0.9817
0.63	0.98071	2.851	0.9823	0.3744	0.9817
0.62	0.98057	2.773	1.0105	0.3640	0.9817
0.61	0.98041	2.700	1.0378	0.3542	0.9816

0.60	0.98024	2.630	1.0645	0.3449	0.9816
0.59	0.98006	2.564	1.0904	0.3361	0.9816
0.58	0.97985	2.501	1.1158	0.3277	0.9816
0.57	0.97964	2.441	1.1405	0.3197	0.9816
0.56	0.97940	2.384	1.1646	0.3120	0.9815
0.55	0.97915	2.330	1.1882	0.3048	0.9815
0.54	0.97888	2.279	1.2112	0.2978	0.9815
0.53	0.97859	2.229	1.2338	0.2912	0.9815
0.52	0.97828	2.182	1.2558	0.2848	0.9814
0.51	0.97794	2.137	1.2774	0.2788	0.9814
0.50	0.97759	2.094	1.2986	0.2729	0.9814
0.49	0.97721	2.053	1.3193	0.2673	0.9813
0.48	0.97681	2.013	1.3396	0.2619	0.9813
0.47	0.97638	1.975	1.3596	0.2568	0.9813
0.46	0.97593	1.938	1.3791	0.2518	0.9812
0.45	0.97546	1.903	1.3983	0.2470	0.9812
0.44	0.97495	1.869	1.4172	0.2424	0.9812
0.43	0.97442	1.837	1.4357	0.2379	0.9811
0.42	0.97386	1.806	1.4539	0.2336	0.9811
0.41	0.97327	1.775	1.4718	0.2295	0.9811
0.40	0.97265	1.746	1.4895	0.2255	0.9810
0.39	0.97200	1.718	1.5068	0.2216	0.9810
0.38	0.97132	1.691	1.5238	0.2179	0.9809
0.37	0.97060	1.665	1.5406	0.2143	0.9809
0.36	0.96986	1.640	1.5571	0.2107	0.9808
0.35	0.96908	1.615	1.5734	0.2073	0.9808
0.34	0.96826	1.592	1.5894	0.2040	0.9807
0.33	0.96741	1.569	1.6052	0.2008	0.9807
0.32	0.96652	1.547	1.6208	0.1977	0.9806
0.31	0.96559	1.525	1.6362	0.1947	0.9806
0.30	0.96463	1.505	1.6513	0.1918	0.9805
0.29	0.96362	1.485	1.6663	0.1889	0.9805
0.28	0.96258	1.465	1.6810	0.1862	0.9804
0.27	0.96150	1.446	1.6956	0.1835	0.9803
0.26	0.96037	1.428	1.7099	0.1809	0.9803
0.25	0.95921	1.410	1.7241	0.1783	0.9802
0.24	0.95800	1.393	1.7382	0.1758	0.9802
0.23	0.95674	1.376	1.7520	0.1734	0.9801
0.22	0.95544	1.360	1.7657	0.1711	0.9800
0.21	0.95410	1.344	1.7792	0.1688	0.9799
0.20	0.95271	1.329	1.7926	0.1665	0.9799

Exercise 13.7

Subject: Simple differential batch (Rayleigh) distillation of a mixture of benzene and toluene, but with the continual supply of feed of the same composition, while heat is supplied at a rate that maintains the liquid level in the still.

Given: Charge of 25 mol of 35 mol% benzene (B) and 65 mol% toluene (T). Continuous feed of 7 mol/h of the same composition as the charge. Constant relative volatility = 2.5.

Assumptions: Perfect mixing in the still. Exiting vapor in equilibrium with the liquid. No change in molar density of the mixture as the composition changes.

Find: Time for the benzene mole fraction of the instantaneous distillate to fall to 0.45.

Analysis: Base the calculations on benzene, which is the more volatile component. Initially, the distillate mole fraction in equilibrium with the initial charge is obtained from Eq. (4-8) for constant relative volatility, α:

$$y = \frac{\alpha x}{1 + x(\alpha - 1)} = \frac{2.5(0.35)}{1 + 0.35(2.5 - 1)} = 0.574 \qquad (1)$$

When the benzene mole fraction in the instantaneous distillate = $y_D = 0.45$, the mole fraction of benzene in the liquid in the still is obtained form a rearrangement of Eq. (1),

$$x = \frac{y}{\alpha + y(1 - \alpha)} = \frac{0.45}{2.5 + 0.45(1 - 2.5)} = 0.2466$$

Modify Eq. (13-1) to include the constant feed added to the still, noting that, with the above assumptions, W = total moles in the still = constant = W_0 = 25 moles, $dW/dt = 0$, and the distillate rate, call it D = molar feed rate, F:

$$Fx_F - W\frac{dx}{dt} = Dy_D = Fy_D \qquad \text{Rearranging,} \quad \frac{dx}{dt} = \frac{F(x_F - y_D)}{W_0} \qquad (2)$$

Eq. (2) is integrated as follows, noting that $y_D = y$. Substituting Eq. (1) into Eq. (2) gives,

$$\frac{F}{W_0}dt = \frac{7}{25}dt = \frac{dx}{x_F - \dfrac{\alpha x}{1 + x(\alpha - 1)}} = \frac{dx}{0.35 - \dfrac{2.5x}{1 + 1.5x}} = \frac{(1 + 1.5x)dx}{0.35 - 1.975x}$$

$$\frac{7}{25}\int_0^t dt = 0.28t = \int_{0.35}^{0.2466} \frac{(1 + 1.5x)dx)}{0.35 - 1.975x} = 0.599 \qquad \text{Therefore, } t = 0.599/0.28 = 2.14 \text{ h}$$

Exercise 13.8

Subject: Simple differential batch (Rayleigh) distillation of a mixture of A and B, but with a continual supply of feed, while heat is supplied at a rate that maintains the liquid level in the still.

Given: Charge of 20 lbmol of 30 mol% A and 70 mol% B. Continuous feed of 10 lbmol/h. Constant relative volatility = 2.5.

Assumptions: Perfect mixing in the still. Exiting vapor in equilibrium with the liquid. No change in molar density of the mixture as the composition changes. Composition of the feed is the same as the initial charge. Overhead product is the instantaneous distillate.

Find: Time for the mole fraction of A in the instantaneous distillate to fall to 0.40.

Analysis: Base the calculations on A, which is the more volatile component. Initially, the distillate mole fraction in equilibrium with the initial charge is obtained from Eq. (4-8) for constant relative volatility, α:

$$y = \frac{\alpha x}{1 + x(\alpha - 1)} = \frac{2.5(0.30)}{1 + 0.30(2.5 - 1)} = 0.5172 \qquad (1)$$

When the mole fraction of A in the instantaneous distillate = $y_D = 0.40$, the mole fraction of A in the liquid in the still is obtained form a rearrangement of Eq. (1),

$$x = \frac{y}{\alpha + y(1 - \alpha)} = \frac{0.40}{2.5 + 0.40(1 - 2.5)} = 0.2105$$

Modify Eq. (13-1) to include the constant feed added to the still, noting that, with the above assumptions, W = total moles in the still = constant = W_0 = 20 lbmole, $dW/dt = 0$, and the distillate rate, call it D = molar feed rate, F:

$$Fx_F - W\frac{dx}{dt} = Dy_D = Fy_D \qquad \text{Rearranging,} \quad \frac{dx}{dt} = \frac{F(x_F - y_D)}{W_0} \qquad (2)$$

Eq. (2) is integrated as follows, noting that $y_D = y$. Substituting Eq. (1) into Eq. (2) gives,

$$\frac{F}{W_0}dt = \frac{10}{20}dt = \frac{dx}{x_F - \dfrac{\alpha x}{1 + x(\alpha - 1)}} = \frac{dx}{0.30 - \dfrac{2.5x}{1 + 1.5x}} = \frac{(1 + 1.5x)dx}{0.30 - 2.05x}$$

$$0.5\int_0^t dt = 0.50t = \int_{0.305}^{0.2105} \frac{(1 + 1.5x)dx)}{0.305 - 2.05x} = 0.585 \qquad \text{Therefore, } t = 0.585/0.5 = 1.17 \text{ h}$$

Exercise 13.9

Subject: Batch distillation of a mixture of isopropyl alcohol (P) and water (W) in a column with 2 equilibrium stages and a reboiler, under conditions of a constant reflux ratio.

Given: Feed contains 40 mol% P and 60 mol% W. Distillation at 1 atm with a reflux of L/V = 0.9. Vapor-liquid equilibrium data in Exercise 13.2.

Assumptions: Perfect mixing in the still. No holdup on the stages or in the condenser.

Find: Compositions of the residue in the still and cumulative distillate when 70 mol% of the charge has been distilled ($W/W_0 = 0.30$).

Analysis: Make calculations in terms of P, the more volatile component. Eq. (13-2) applies, where y_D is the mole fraction of P in the vapor leaving the top stage, and x_W is the mole fraction of P in the liquid in the reboiler.

$$\ln\left(\frac{W_0}{W}\right) = \ln\left(\frac{1}{0.3}\right) = 1.204 = \int_{x_W}^{0.40} \frac{dx_W}{y_D - x_W} \qquad (1)$$

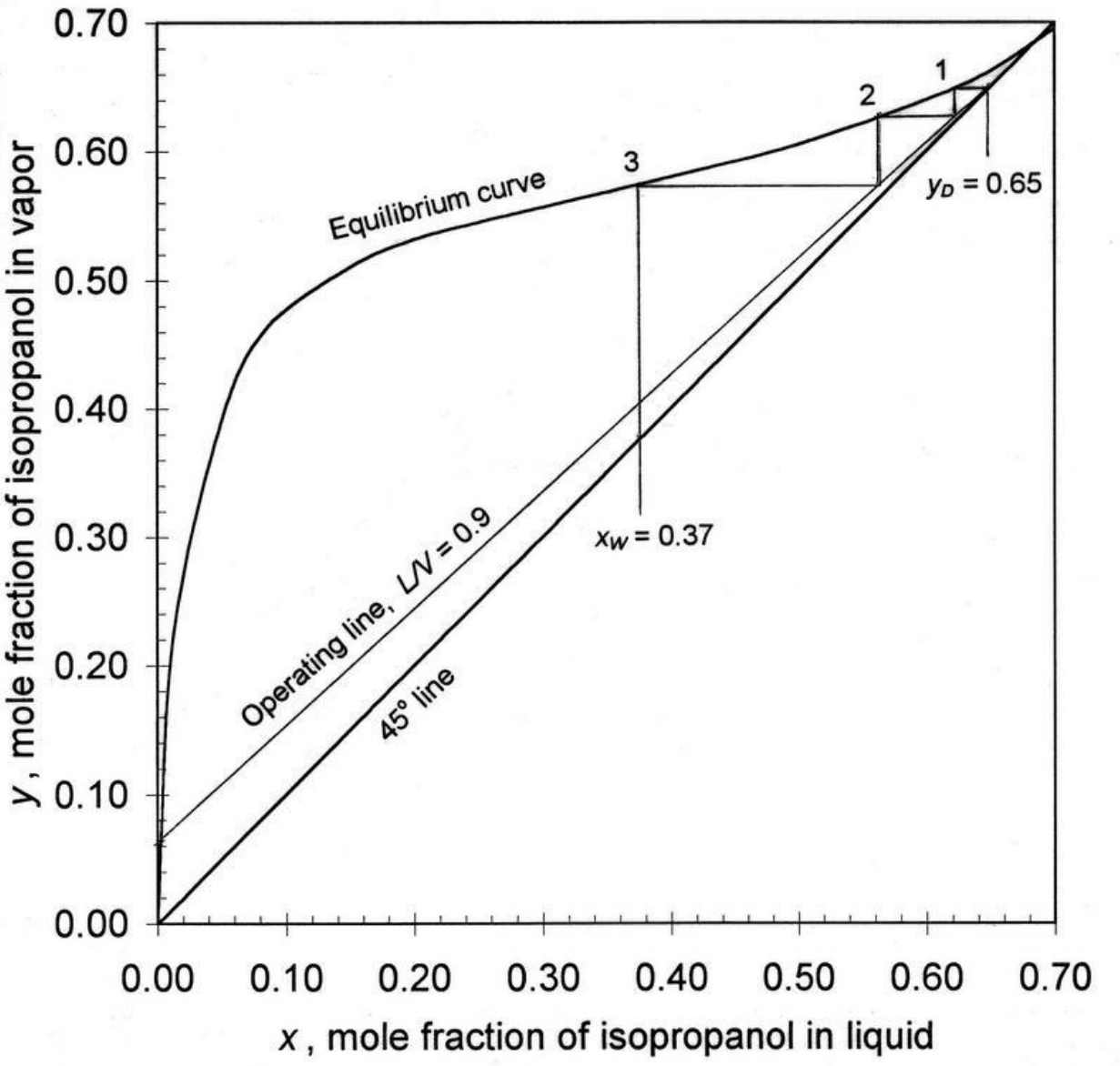
The relationship between y_D and x_W is obtained from a McCabe-Thiele diagram by drawing a series of operating lines of slope = L/V = 0.9. For each operating line, starting from the intersection with the 45° line, which is y_D, 3 stages are stepped off to determine the corresponding x_W. A typical construction that starts from $y_D = 0.65$ is shown on the next page, where the $x_W = 0.37$. Other sets of values are given in the following table, which also includes values of the integrand, $f = 1/(y_D - x_W)$, from which the integral is evaluated by the trapezoidal rule with variable increments of Δx_W. For example, the increment of the integral from x_1 to x_2 is $(x_1 - x_2)(f_1/2 + f_2/2)$.
The increments are summed over the region from $x_W = 0.40$ to the value corresponding to 70 mol% distilled.

x_W	y_D from McCabe-Thiele	$f = 1/(y_D - x_W)$	Increment of Integral	Cumulative $\ln(W_0/W)$
0.400	0.66	3.90		
0.370	0.65	3.61	0.113	0.113
0.260	0.645	2.60	0.342	0.455
0.170	0.64	2.13	0.213	0.668
0.080	0.63	1.82	0.178	0.846
0.015	0.60	1.71	0.115	0.961
0.008	0.55	1.85	0.013	0.974
0.002	0.50	2.01	0.012	0.986

Exercise 13.9

Analysis: (continued)

The results in the above table indicate that all of the isopropanol is evaporated, because at x_W = 0.002, the value of $\ln(W_0/W) = 0.986$, which corresponds to $W/W_0 = 0.565$ or only 43.5 mol% distilled. By the time, 70 mol% of the isopropanol is evaporated, the mole fraction of isopropanol in the residue will be essentially 0. The mole fraction of isopropanol in the cumulative distillate = 40/70 = 0.571.



Exercise 13.10

Subject: Batch distillation of a mixture of benzene (B) and toluene (T) in a column with 3 equilibrium stages and a reboiler (4 total stages), under conditions of a constant reflux ratio.

Given: Feed of 100 moles contains 30 mol% B and 70 mol% T. Distillation at 1 atm with a reflux of $L/V = 0.6$. Constant relative volatility of 2.5 for B with respect to T.

Assumptions: Perfect mixing in the still. No holdup on the stages or in the condenser.

Find: Moles of residue when the cumulative distillate is 45 mol% B.

Analysis: Make calculations in terms of B, the more volatile component. Eq. (13-2) applies, where y_D is the mole fraction of B in the instantaneous vapor leaving the top stage, and x_W is the mole fraction of B in the liquid in the reboiler.

$$\ln\left(\frac{W_0}{W}\right) = \ln\left(\frac{100}{W}\right) = \int_{x_W}^{0.30} \frac{dx_W}{y_D - x_W} \qquad (1)$$

From Eq. (13-6), the mole fraction of benzene in the cumulative distillate is given by:

$$\left(y_D\right)_{\text{avg}} = 0.45 = \frac{30 - Wx_W}{100 - W} \qquad (2)$$

or

$$x_W = 0.45 - \frac{15}{W} \qquad (3)$$

From Eq. (4-8), the vapor-liquid equilibrium curve is given by,

$$y = \frac{\alpha x}{1 + x(\alpha - 1)} = \frac{2.5x}{1 + 1.5x} \qquad (4)$$

This is the equilibrium curve for applying the McCabe-Thiele method. The relationship between y_D and x_W in Eq. (1) is obtained from a McCabe-Thiele diagram by drawing a series of operating lines of slope = $L/V = 0.6$. For each operating line, starting from the intersection with the 45° line, which is y_D, 4 stages are stepped off to determine the corresponding x_W. A typical construction that starts from $y_D = 0.74$ is shown on the next page, where the $x_W = 0.277$. Other sets of values are given in the following table.

y_D	x_W
0.78	0.307
0.74	0.277
0.70	0.245
0.60	0.185
0.50	0.145
0.40	0.107
0.30	0.077
0.20	0.050

Exercise 13.10 (continued)

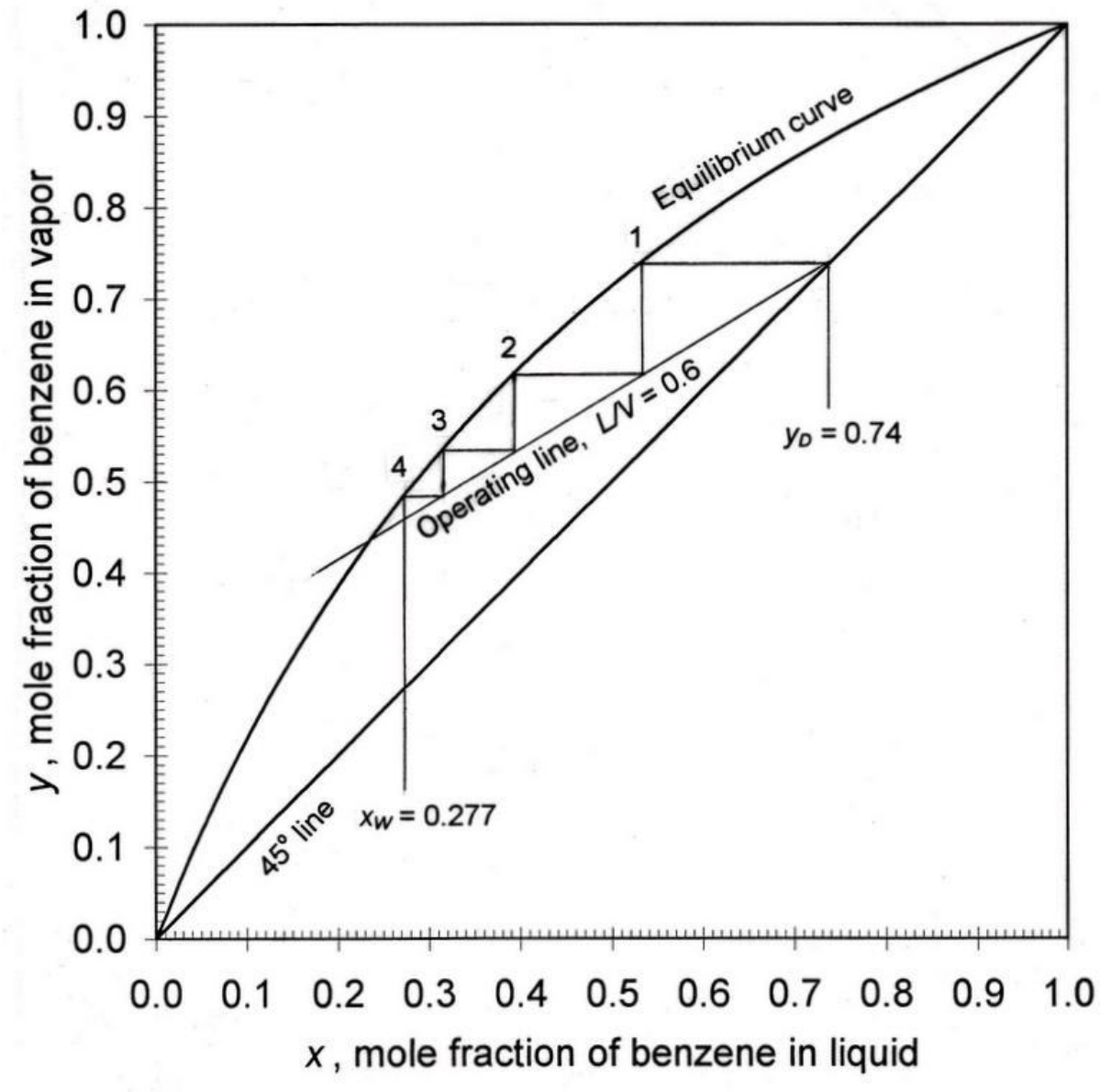
Analysis: (continued)

A curve fit of the above data gives:

$$y_D = 0.0059054 + 4.24118\, x_W - 5.66817\, x_W^2 \qquad (5)$$

Substituting Eq. (5) into Eq. (1) gives:

$$\ln\left(\frac{100}{W}\right) = \int_{x_W}^{0.30} \frac{dx_W}{0.0059054 + 4.24118\, x_W - 5.66817\, x_W^2} \qquad (6)$$



Exercise 13.10 (continued)

Analysis: (continued)

Eq. (6) can be solved analytically or numerically. A numerical solution is used here with a spreadsheet. The integral is evaluated by the trapezoidal rule. The following table starts at the upper limit of 0.30 and moves in increments downward. For each increment, the increment of the integral from x_1 to x_2 is $(x_1 - x_2)(f_1/2 + f_2/2)$, where f is the integrand. For the addition of each integral increment, W is computed, and then the benzene mole fraction in the cumulative distillate from Eq. (2), until the value of 0.45 is reached.

x_W	$y_D - x_W$	$1/(y_D - x_W)$	Increment of integral	ln(Wo/W)	W/Wo	Cum y_D
0.30	0.4681	2.1362				
0.28	0.4691	2.1320	0.0427	0.0427	0.9582	0.7587
0.26	0.4654	2.1485	0.0428	0.0855	0.9181	0.7482
0.24	0.4573	2.1867	0.0434	0.1288	0.8791	0.7363
0.22	0.4446	2.2491	0.0444	0.1732	0.8410	0.7231
0.20	0.4274	2.3396	0.0459	0.2191	0.8033	0.7083
0.18	0.4057	2.4651	0.0480	0.2671	0.7656	0.6919
0.16	0.3794	2.6358	0.0510	0.3181	0.7275	0.6738
0.14	0.3486	2.8688	0.0550	0.3732	0.6885	0.6537
0.12	0.3132	3.1926	0.0606	0.4338	0.6480	0.6314
0.10	0.2733	3.6584	0.0685	0.5023	0.6051	0.6065
0.09	0.2517	3.9730	0.0382	0.5405	0.5825	0.5930
0.08	0.2289	4.3683	0.0417	0.5822	0.5587	0.5785
0.07	0.2050	4.8777	0.0462	0.6284	0.5334	0.5630
0.06	0.1800	5.5565	0.0522	0.6806	0.5063	0.5462
0.05	0.1538	6.5022	0.0603	0.7409	0.4767	0.5277
0.04	0.1265	7.9062	0.0720	0.8129	0.4436	0.5073
0.03	0.0980	10.2000	0.0905	0.9034	0.4052	0.4839
0.02	0.0685	14.6067	0.1204	1.0275	0.3579	0.4561

From this table, the residue is 35 lbmol at a benzene mole fraction in the residue of about 0.02.

Exercise 13.11

Subject: Batch distillation of a mixture of benzene (B) and toluene (T) in a column with 2 equilibrium stages and a reboiler (3 total stages), under conditions of a constant reflux ratio.

Given: Feed of 1 kmole containing 50 mol% B and 50 mol% T. Distillation with a reflux of $L/D = R = 4$. Constant relative volatility of 2.5 for B with respect to T.

Assumptions: Perfect mixing in the still. No holdup on the stages or in the condenser.

Find: kmoles and composition of cumulative distillate when the instantaneous distillate is 55 mol% B.

Analysis: Make calculations in terms of B, the more volatile component. Eq. (13-2) applies, where y_D is the mole fraction of B in the instantaneous vapor leaving the top stage, and x_W is the mole fraction of B in the liquid in the reboiler.

$$\ln\left(\frac{W_0}{W}\right) = \ln\left(\frac{1}{W}\right) = \int_{x_W}^{0.50} \frac{dx_W}{y_D - x_W} \qquad (1)$$

From Eq. (4-8), the vapor-liquid equilibrium curve is given by,

$$y = \frac{\alpha x}{1 + x(\alpha - 1)} = \frac{2.5x}{1 + 1.5x} \qquad (4)$$

This is the equilibrium curve for applying the McCabe-Thiele method. The relationship between y_D and x_W in Eq. (1) is obtained from a McCabe-Thiele diagram by drawing a series of operating lines of slope = $L/V = R/(1+R) = 4/5 = 0.8$ For each operating line, starting from the intersection with the 45° line, which is y_D, 3 stages are stepped off to determine the corresponding x_W. A typical construction that starts from $y_D = 0.90$ is shown on the next page, where the $x_W = 0.465$. Other sets of values are given in the following table, which also includes values of the integrand, $f = 1/(y_D - x_W)$, from which the integral is evaluated by the trapezoidal rule with variable increments of Δx_W. For example, the increment of the integral from x_1 to x_2 is $(x_1 - x_2)(f_1/2 + f_2/2)$.

The increments are summed over the region from $x_W = 0.40$ to the value corresponding to 70 mol% distilled.

x_W	y_D from McCabe-Thiele	$f = 1/(y_D - x_W)$	Increment of Integral	Cumulative $\ln(W_0/W)$
0.500	0.91	2.439		
0.465	0.90	2.300	0.083	0.083
0.365	0.85	2.062	0.218	0.301
0.233	0.75	1.934	0.264	0.565
0.172	0.65	2.092	0.123	0.688
0.125	0.55	2.353	0.105	0.793

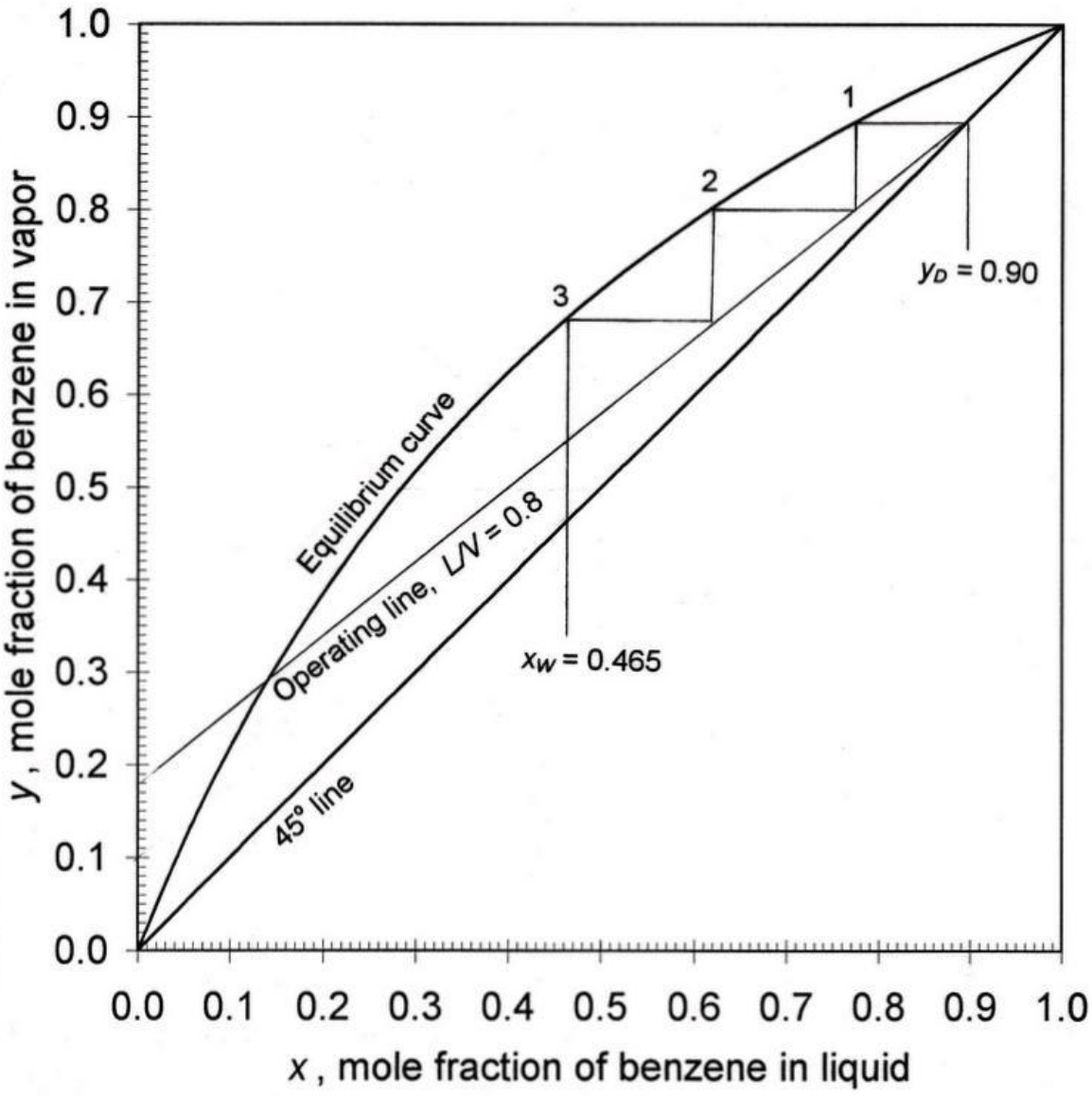
Exercise 13.11 (continued)

Analysis: (continued)

From the above table, $\ln(W_0/W) = 0.793$ when the instantaneous distillate reaches a mole fraction of 0.55 for benzene. Solving, $W = 0.452$ kmole.

The composition of the cumulative distillate is given by Eq. (13-6), which becomes:

$$(y_D)_{avg} = \frac{1(0.5) - Wx}{1 - W} = \frac{0.5 - 0.452(0.125)}{1 - 0.452} = 0.809$$



Exercise 13.12

Subject: Batch distillation of a mixture of ethanol (E) and water (W) by both simple differential (Rayleigh) distillation and in a column with 2 equilibrium stages and a reboiler (3 total stages), under conditions of a constant reflux ratio.

Given: Feed containing 3.3 mol% E and 96.7 mol% W. Vapor-liquid equilibrium data from Exercise 7.29. 20 mol% of charge is distilled.

Assumptions: Perfect mixing in the still. No holdup on the stages or in the condenser.

Find: Plot of instantaneous vapor composition as a function of mole percent distilled for Rayleigh distillation. Maximum ethanol purity that can be obtained when using the column with the equivalent of 3 stages.

Analysis:

Rayleigh distillation:

Because the vapor-liquid equilibrium data indicate that E is the more volatile component below 89 mol% E in the liquid, base the calculations on E. Use Eq. (13-3), with $x_0 = 0.033$ and $W/W_0 = 1 - 0.2 = 0.8$ (20 mol% vaporized). Thus, Eq. (13-3) becomes:

$$\int_{0.033}^{x} \frac{dx}{y-x} = \ln 0.8 = -0.223 \quad \text{or} \quad \int_{x}^{0.033} \frac{dx}{y-x} = 0.223 \qquad (1)$$

where x in the lower integration limit is the mole fraction of E in the residue at 20 mol% distilled and y is in equilibrium with x.

Equilibrium data from Exercise 7.29 that are in the lower mole fraction range are:

y	0.1700	0.3891	0.4375	0.4704
x	0.0190	0.0721	0.0966	0.1238

A fit of these data to a cubic equation that goes through the origin gives:

$$y = 10.4016\,x - 89.8114\,x^2 + 295.358\,x^3 \qquad (2)$$

Substitute Eq. (2) into Eq. (1) and, using a spreadsheet, integrate the resulting equation using the trapezoidal rule with a Δx increment of 0.001 starting from $x = 0.033$ with decreasing values of x until the integral equals 0.223 or $W/W_0 = 0.8$. As an example, using this method for the first four increments, the integral is equal to $\Delta x[\, 0.5f_{x=0.40} + f_{x=0.39} + f_{x=0.38} + f_{x=0.37} + 0.5f_{x=0.36}\,]$, where $f = 1/(y\text{-}x)$.

The complete spreadsheet is given on the following page. From it, the following result is obtained: Mole fraction of E in the residue at 20 mol% distilled = 0.0055. A plot of instantaneous vapor composition as a function of mole percent distilled is given on a following page. For $x = 0.0055$, Eq. (13-6) for the mole fraction of E in the cumulative distillate gives,

$$\left(y_D\right)_{\text{avg}} = \frac{W_0 x_0 - Wx}{W_0 - W} = \frac{x_0 - (W/W_0)x}{1-(W/W_0)} = \frac{0.033 - 0.8(0.0055)}{1-0.8} = 0.143 \qquad (3)$$

Exercise 13.12 (continued)

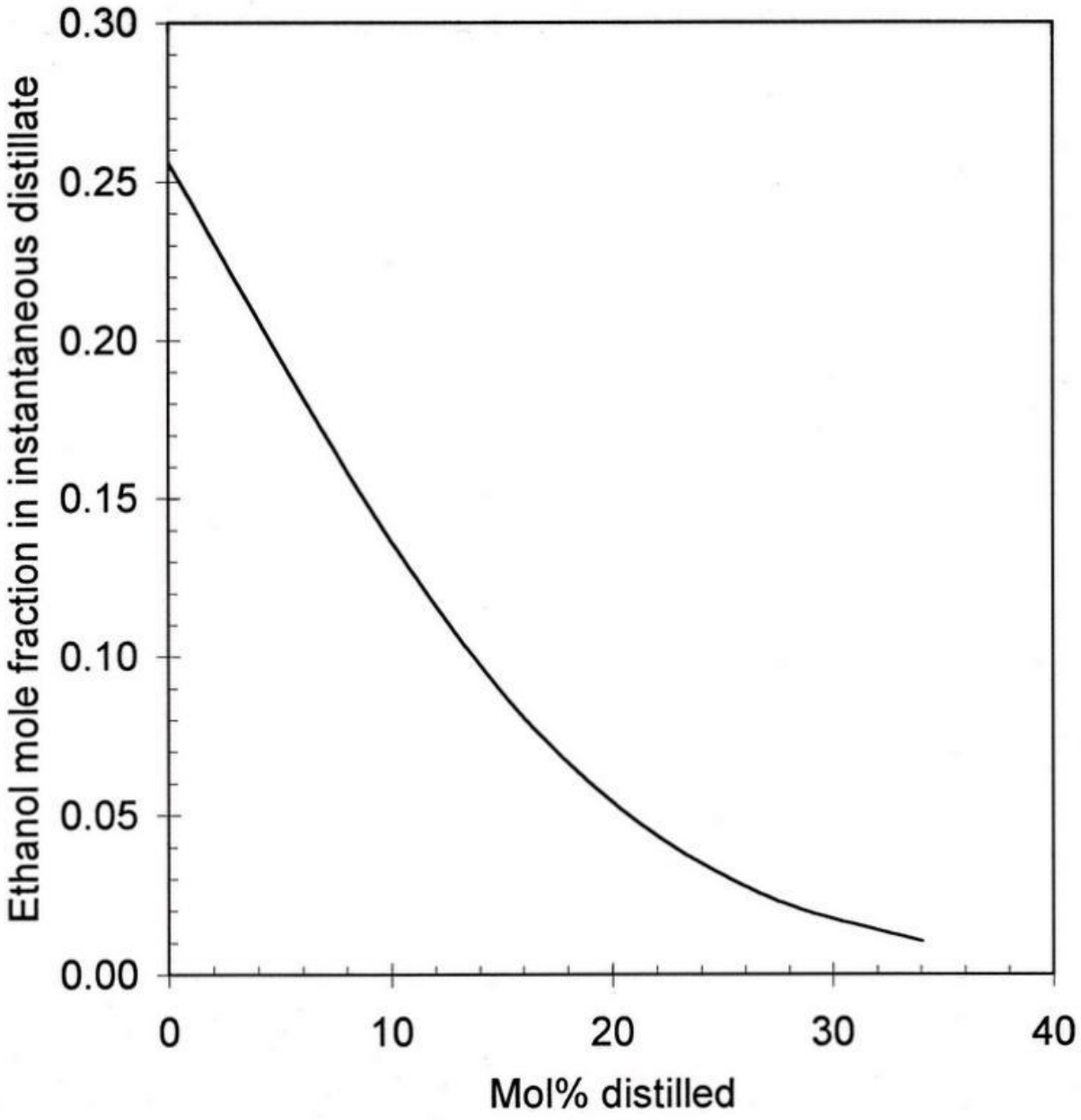
Analysis: Rayleigh Distillation (continued)

x	y	$f=1/(y-x)$	Increment of integral	Cumulative $\ln(W_0/W)$	W/W_0
0.033	0.2561	4.483			1.000
0.032	0.2506	4.575	0.00453	0.00453	0.995
0.031	0.2449	4.674	0.00462	0.00915	0.991
0.030	0.2392	4.780	0.00473	0.01388	0.986
0.029	0.2333	4.894	0.00484	0.01872	0.981
0.028	0.2273	5.017	0.00496	0.02367	0.977
0.027	0.2212	5.150	0.00508	0.02876	0.972
0.026	0.2149	5.293	0.00522	0.03398	0.967
0.025	0.2085	5.449	0.00537	0.03935	0.961
0.024	0.2020	5.618	0.00553	0.04488	0.956
0.023	0.1953	5.803	0.00571	0.05059	0.951
0.022	0.1885	6.006	0.00590	0.05650	0.945
0.021	0.1816	6.228	0.00612	0.06262	0.939
0.020	0.1745	6.474	0.00635	0.06897	0.933
0.019	0.1672	6.746	0.00661	0.07558	0.927
0.018	0.1599	7.050	0.00690	0.08247	0.921
0.017	0.1523	7.390	0.00722	0.08969	0.914
0.016	0.1446	7.773	0.00758	0.09728	0.907
0.015	0.1368	8.209	0.00799	0.10527	0.900
0.014	0.1288	8.709	0.00846	0.11373	0.893
0.013	0.1207	9.286	0.00900	0.12272	0.885
0.012	0.1124	9.960	0.00962	0.13235	0.876
0.011	0.1039	10.759	0.01036	0.14271	0.867
0.010	0.0953	11.719	0.01124	0.15395	0.857
0.009	0.0866	12.894	0.01231	0.16625	0.847
0.008	0.0776	14.364	0.01363	0.17988	0.835
0.007	0.0685	16.257	0.01531	0.19519	0.823
0.006	0.0592	18.783	0.01752	0.21271	0.808
0.005	0.0498	22.322	0.02055	0.23326	0.792

A plot of the ethanol mole fraction in the instantaneous distillate as a function of mol% distilled is given on the following page.

Exercise 13.12 (continued)

Analysis: Rayleigh distillation (continued)



Exercise 13.12 (continued)

Analysis: (continued)

Distillation with 2 stages plus a reboiler:

To obtain the maximum cumulative distillate purity for 20 mol% distilled, operate close to total reflux, $L/V = 1$. The relationship between y_D and x_W in Eq. (1), with $x = x_W$ and $y = y_D$, is obtained from a McCabe-Thiele diagram by drawing a series of operating lines of slope = L/V = 1 (45° line). For each operating line, starting from the intersection with the 45° line, which is y_D, 3 stages are stepped off to determine the corresponding x_W. A typical construction that starts from $y_D = 0.65$ is shown on the next page, where the $x_W = 0.02$. Other sets of values are given in the following table, which also includes values of the integrand, $f = 1/(y_D - x_W)$, from which the integral is evaluated by the trapezoidal rule with variable increments of Δx_W. For example, the increment of the integral from x_1 to x_2 is $(x_1 - x_2)(f_1/2 + f_2/2)$.

The increments are summed over the region from $x_W = 0.033$ to the value corresponding to 20 mol% distilled.

x_W	y_D from McCabe-Thiele	$f = 1/(y_D - x_W)$	Increment of Integral	Cumulative $\ln(W_0/W)$
0.033	0.663	1.587		
0.030	0.66	1.587	0.0048	0.0048
0.020	0.65	1.587	0.0159	0.0207
0.010	0.61	1.667	0.0163	0.0370
0.005	0.55	1.834	0.0088	0.0458
0.001	0.40	2.506	0.0087	0.0545

From the above table, at $x_W = 0.001$, a very low value, $\ln(W_0/W) = 0.0545$. Thus, $W/W_0 = 0.947$ or only 5.3% distilled. Thus, essentially all of the ethanol will be distilled when 20 mol% of the charge has been distilled.

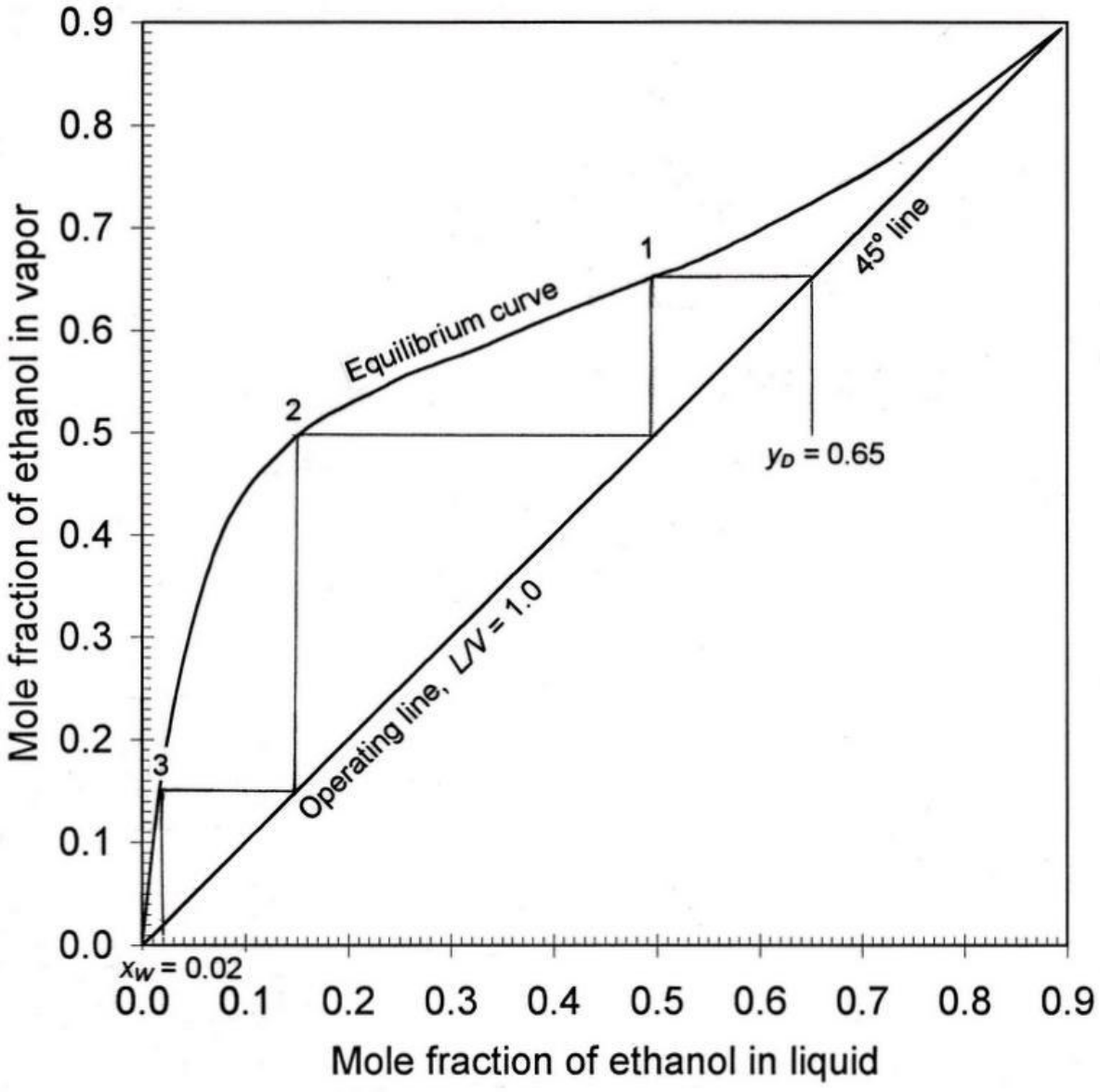
The composition of the cumulative distillate is given by Eq. (13-6), which becomes:

$$(y_D)_{avg} = \frac{W_0 x_0 - Wx}{W_0 - W} = \frac{x_0 - (W/W_0)x}{1 - (W/W_0)} = \frac{0.033 - 0.8(0.0)}{1 - 0.8} = 0.165$$

It should be noted from the above table that if only 5.3 mol% of the charge were distilled, the composition of the cumulative distillate would be 60.5 mol% ethanol.

Exercise 13.12 (continued)

Analysis: Distillation with 2 stages plus a reboiler (continued)



Exercise 13.13

Subject: Batch distillation of a mixture of acetone (A) and ethanol (E) at 101 kPa in a column with equilibrium stages and a reboiler.

Given: Feed of 50 mol% A and 50 mol% E. Vapor-liquid equilibrium data at 101 kPa.

Assumptions: Perfect mixing in the still. No holdup on the stages or in the condenser.

Find: (a) Number of equilibrium stages if the instantaneous distillate composition is 90 mol% acetone when the residue is 10 mol% acetone for a reflux ratio, L/D = 1.5 times the minimum value.

(b) Plot of reflux ratio versus the still pot composition and amount of residue left if the column has 8 stages (9 including the reboiler) and the reflux rate is varied to maintain the distillate composition constant at 90 mol% acetone.

(c) Total vapor generated for distillation with 8 stages (9 including the reboiler) at constant reflux ratio to obtain a residue of 10 mol% acetone and a cumulative distillate composition of 90 mol% acetone

Which method of operation requires more energy.

A more efficient operating policy to produce a distillate of 90 mol% acetone.

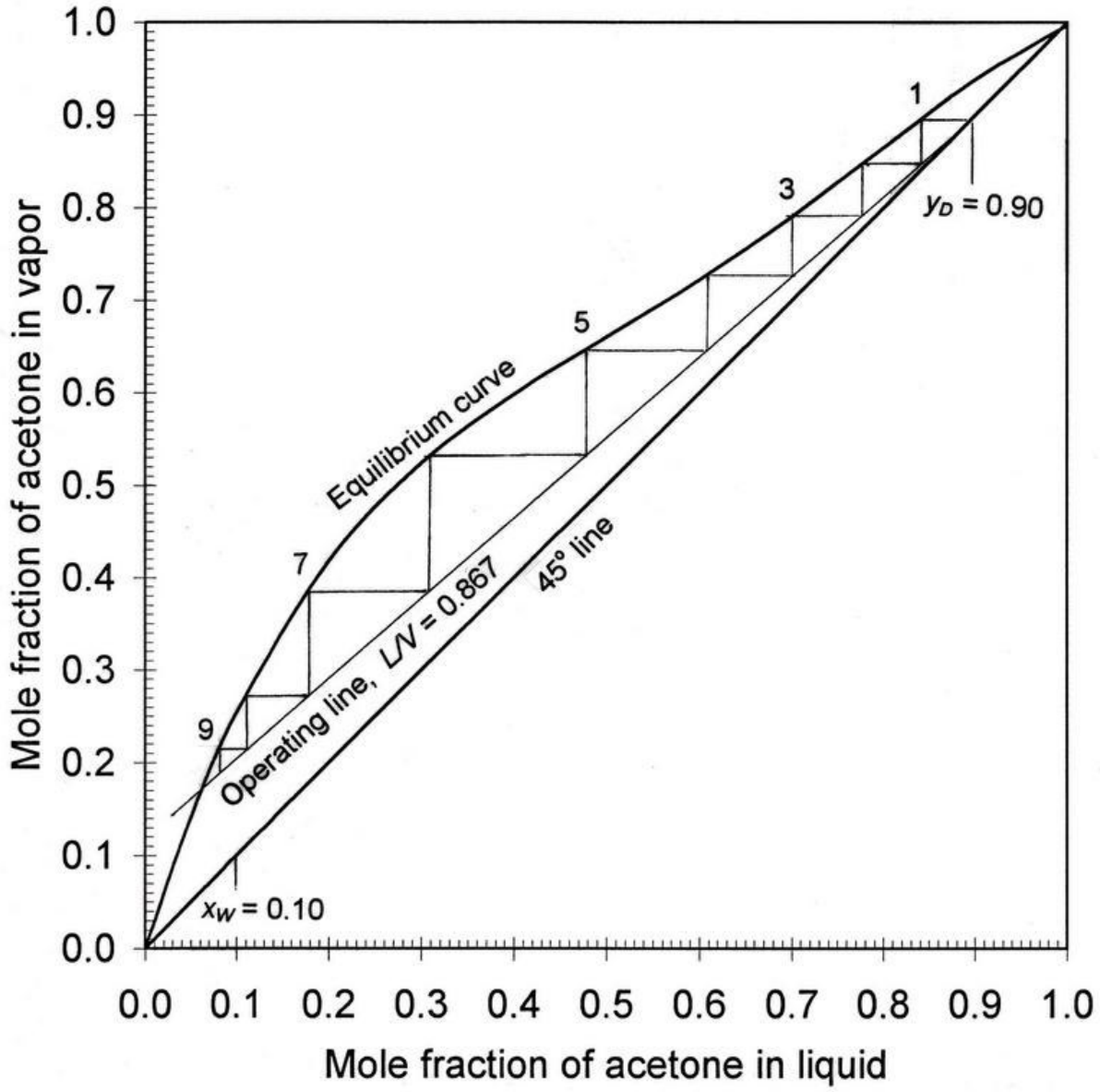
Analysis: (a) First compute the minimum L/V. The slope of the operating line for this condition is given by:

$$\left(\frac{L}{V}\right)_{\min} = \frac{(y \text{ at } 0.9) \text{ - } (y \text{ in equilibrium with } x \text{ at } 0.10)}{(x \text{ at } 0.9) \text{ - } (x \text{ at } 0.10)} = \frac{0.9 - 0.25}{0.9 - 0.1} = 0.8125$$

From Eq. (7-27), $R_{\min} = 0.8125/(1 - 0.8125) = 4.33$. Therefore, $R = 1.5R_{min} = 1.5(4.33) = 6.5$. Operating $L/V = R/(R+1) = 6.5/7.5 = 0.867$. On the next page, the number of equilibrium stages are stepped off by the McCabe-Thiele method, where the given vapor-liquid equilibrium data are plotted, operating line has a slope of 0.867, and the steps start at $x = 0.9$ and end at $x = 0.1$. Almost 9 equilibrium stages are stepped off.

Exercise 13.13 (continued)

Analysis: (continued)



Exercise 13.13 (continued)

Analysis: (continued)

(b) For constant acetone mole fraction in the distillate = 0.90, and 8 equilibrium stages plus a reboiler, the McCabe-Thiele diagram can be used to determine the residue composition and amount of residue as a function of reflux ratio. For example, as shown at the bottom of the following page, when $L/V = 0.90$, $R = 0.9/(1\text{-}0.9) = 9$, and $x_W = 0.065$. From Eq. (13-6),

$$(y_D)_{avg} = 0.90 = \frac{x_0 - (W/W_0)x_W}{1-(W/W_0)} \qquad \text{Solving, } \frac{W}{W_0} = \frac{0.4}{0.9 - x_W} \qquad \text{For } x_W = 0.065,\ W/W_0 = 0.48$$

For other reflux ratios, the following results are obtained and plotted on the next page.

$R=L/D$	2.33	3.0	4.0	5.67	9.0	19	∞
x_W	0.48	0.35	0.22	0.13	0.065	0.035	0.006
W/W_0	0.95	0.73	0.59	0.52	0.48	0.46	0.45

(c) The case of constant reflux ratio is a tedious trial and error problem. A guess of the reflux ratio is made and a series of McCabe-Thiele constructions is carried out as in Fig. 13.4 or 13.5 with 9 total stages, such that the initial $x_W = 0.5$ and the final $x_W = 0.1$. This gives a series of values of instantaneous y_D and x_W. Using these values, Eq. (13-2) is integrated to obtain W when the final $x_W = 0.1$is reached. Then, Eq. (13-6) is solved for $(y_D)_{avg}$. If the value is not 0.9, the procedure is repeated with different values of the reflux ratio until the value is close to 0.9. An easier approach is to use the batch distillation program in Chemcad, which follows the same procedure. If the Wilson equation is used, with the built-in Wilson binary interaction parameters of 151.089 for acetone-ethanol and 292.508 for ethanol-acetone, to predict the vapor-liquid equilibrium, the following results are obtained for a single operation step that is stopped when $x_W = 0.1$. As indicated, a reflux ratio of 2.2 gives the desired result.

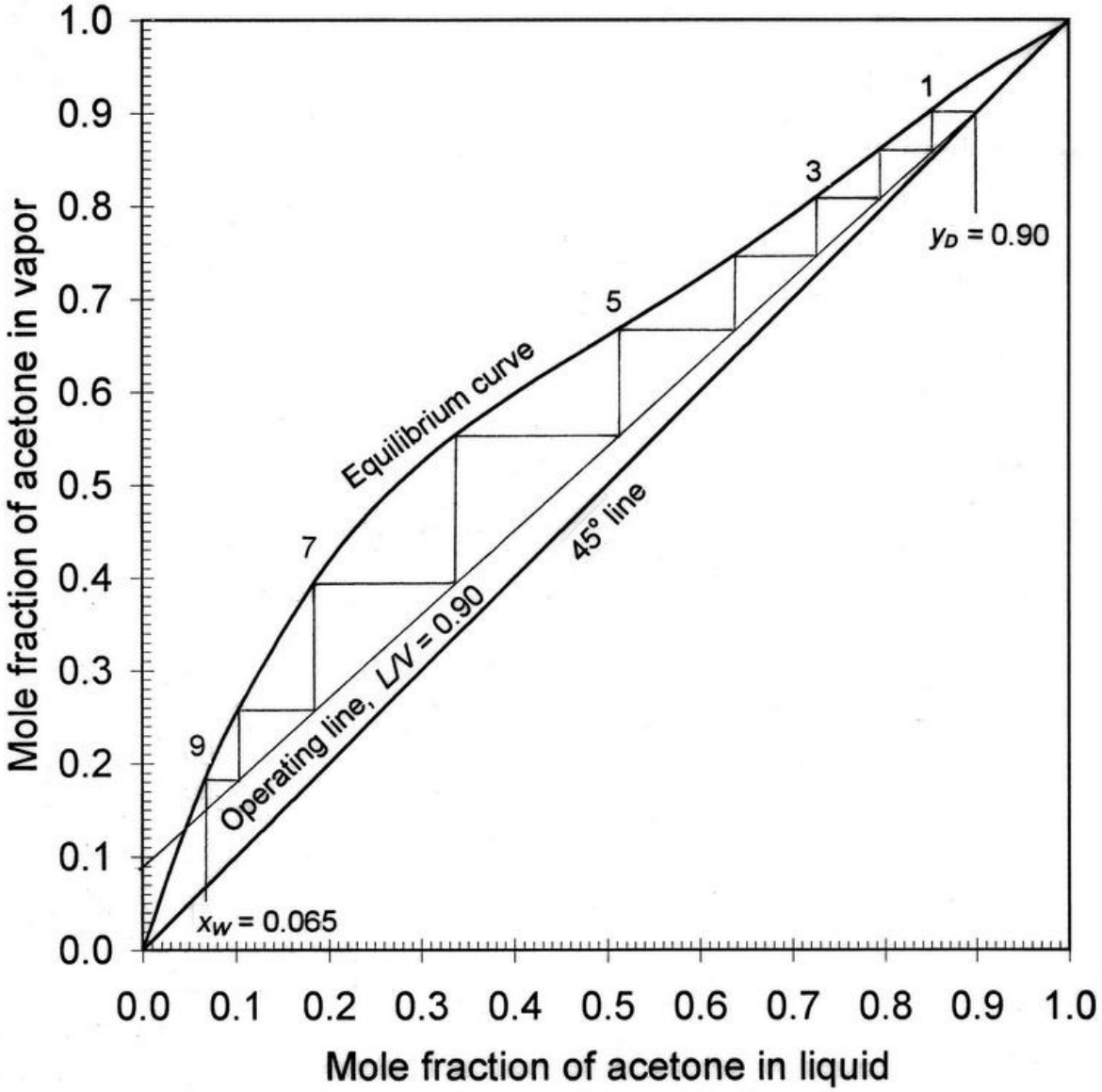
$R=L/D$	$(y_D)_{avg}$
6.5	0.971
4	0.955
3	0.930
2.5	0.911
2.35	0.905
2.2	0.90

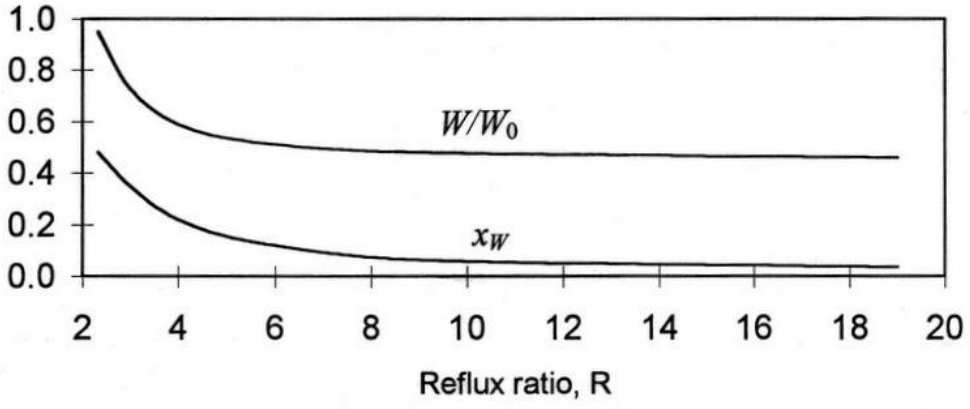
Assume the initial charge is 100 kmol. An acetone material balance gives a total distillate of 50 kmol. At $R = 2.2$, the total vapor generated in the still = 3.2(50) = 160 kmol/100 kmol of initial charge.

From the above table in Part (b) for the constant distillate composition case, it is seen that the reflux ratio starts at a value of about 2 and increases up to approximately 7 when the mole fraction of acetone in the residue has dropped to the desired value of 0.1. Therefore, the energy requirement for the constant distillate composition case is greater than for the constant reflux case because the reflux ratio is almost always greater than 2.2 and thus more vapor generation is needed. One possible operating policy that might be more efficient is to start with constant distillate composition, but switch to constant reflux ratio when the value becomes 2.2.

Exercise 13.13 (continued)

Analysis: (b) (continued)





Exercise 13.13 (continued)

Analysis: (c) (continued)

It is noted that the determination of the optimal operating policy for batch distillation has received considerable attention in the literature. An early article, "The time-optimal problem in binary batch distillation" by I. Coward, Chem. Eng. Sci., 22, 503-516 (1967), considers the case of batch rectification of a binary mixture at constant boilup rate. The optimal variation of reflux ratio is determined so as to minimize the operating time for achieving a distillate of a specified cumulative composition. The results are compared to the constant reflux ratio and constant distillate composition cases, with the finding for a few examples that only a few per cent of time is saved. A more recent article, Accurate Determination of Optimal Reflux Policies for the Maximum Distillate Problem in Batch Distillation", by J. S. Logsdon and L. T. Biegler, Ind. Eng. Chem. Res., 32, 692-700 (1993) considers the case of optimizing the reflux ratio policy to obtain the maximum amount of distillate of a desired composition for a specified distillation time.

Exercise 13.14

Subject: Batch rectification of a mixture of ethanol and water at constant distillate composition and constant molar vapor boilup rate.

Given: Initial charge of 2,000 gallons of 70 wt% ethanol and 30 wt% water having a specific gravity of 0.871. Operation at 1 atm to produce a distillate product of 85 mol% ethanol and a residual waste water of 3 wt% ethanol in 24 - 4 = 20 hours of rectification. Vapor-liquid equilibrium data from Exercise 7.29

Assumptions: Perfect mixing in the still. No holdup on the stages or in the condenser. No pressure drop.

Find: (a) Number of theoretical plates in the column.
(b) Reflux ratio when the residue contains 25 mol% ethanol.
(c) Instantaneous distillate rate in lbmol/h when the residue contains 15 mol% ethanol.
(d) Lbmol of distillate product.
(e) Lbmol of residual.

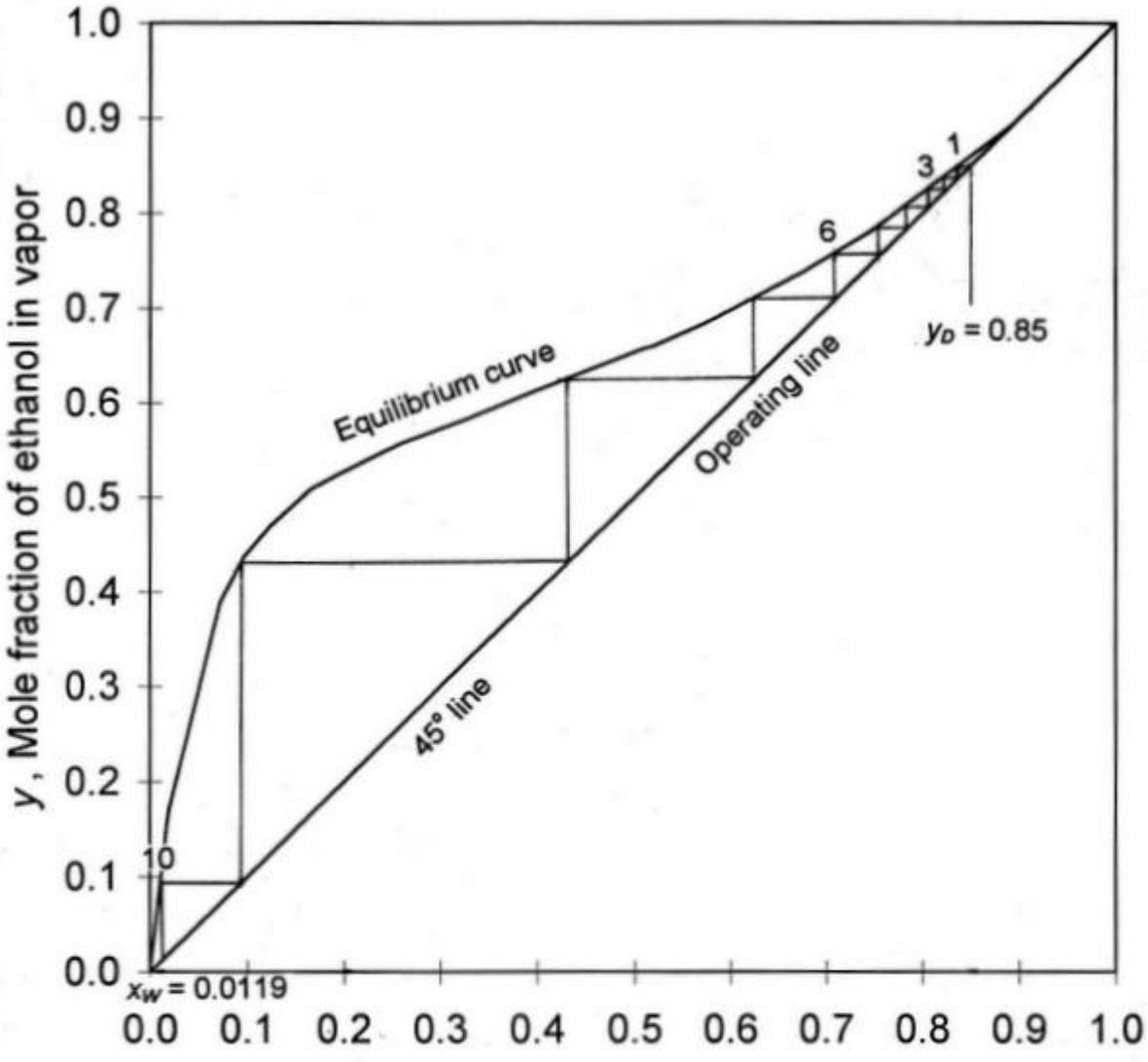
Analysis: First, compute compositions in moles. Density of charge = 8.33(0.871) = 7.26 lb/gal. Amount of charge = 7.26(2,000) = 14,500 lb. Molecular weights are 46.07 for ethanol and 18.02 for water. Lbmoles of ethanol in the charge = 14,500(0.70)/46.07 = 220 lbmoles. Lbmoles of water in the charge = 14,500(0.30)/18.02 = 241 lbmoles. Therefore, the total charge = 220 + 241 = 461 lbmoles. The mole fraction of ethanol in the charge = 220/461 = 0.477. Take a basis of 100 lb for the final residue. The lbmoles of ethanol in the final residue = 3/46.07 = 0.0651. The lbmoles of water in the final residue = 97/18.02 = 5.3829. The total lbmoles of final residue = (0.0651 + 5.3829) = 5.4480 lbmoles/100 lb. The ethanol mole fraction in the final residue = 0.0651/5.4480 = 0.0119.

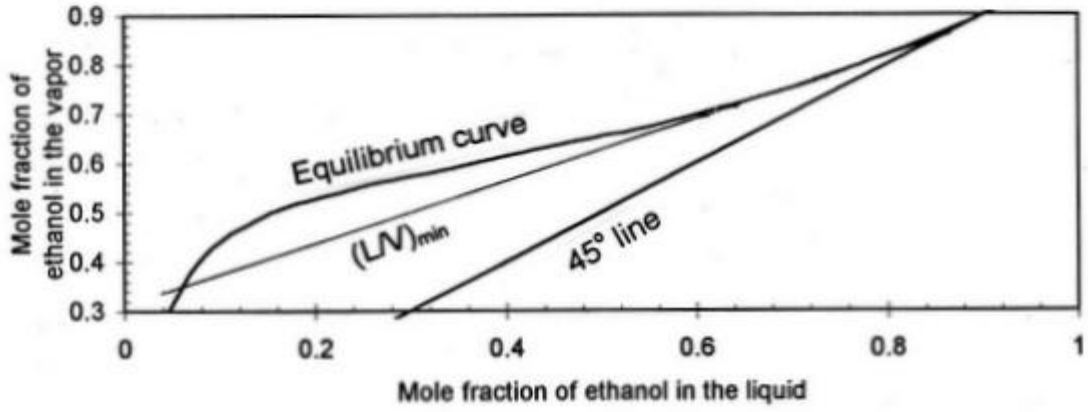
(a) One approach to determine a reasonable number of theoretical stages is to use the McCabe-Thiele method for estimating the minimum number of stages at total reflux and then multiplying that value by two to obtain the number of theoretical stages at actual reflux. The minimum number of stages can be stepped between the constant $x_D = 0.85$ and the final $x_W = 0.0119$. The construction is shown on the following page, where approximately 10 stages are stepped off. Therefore, the number of theoretical stages at actual reflux is estimated at 2(10) = 20 (19 plus a reboiler).

(b) To estimate the reflux ratio, use the McCabe-Thiele method for estimating the minimum reflux ratio, R_{min} and then assume the actual reflux ratio = $R = 1.2R_{min}$. The construction is shown on the following page, where the position of the operating line is controlled not by a line from the constant $x_D = 0.85$ to $x_W = 0.25$, but by the equilibrium line, as in Fig. 7.12b. The slope is 0.62 = $(L/V)_{min}$. From Eq. (7-27), $R_{min} = (L/V)_{min}/[1 - (L/V)_{min}]$ = 0.62/(1 - 0.62) = 1.63. Therefore, take the actual reflux ratio = $R = 1.2R_{min} = 1.2(1.63) = 1.98$.

Exercise 13.14 (continued)

Analysis: (a) and (b) (continued)





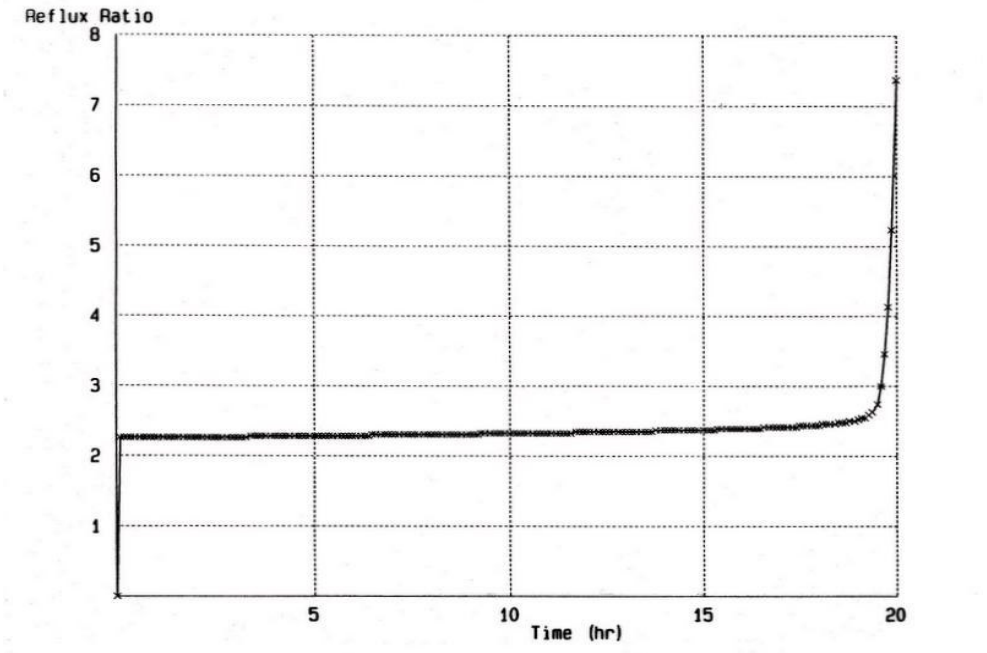
Exercise 13.14 (continued)

Analysis: (continued)

(d) and (e) Compute these before Part (c).
A total molar material balance is: $W_0 = 461 = W + D$. (1)
An ethanol molar material balance is: $220 = 0.0119W + 0.85D$ (2)
Solving Eqs. (1) and (2),
$D = 256$ lbmoles and $W = 205$ lbmoles

(c) When the residue contains 15 mol% ethanol, the minimum reflux is still controlled by the equilibrium curve. Therefore, take a reflux ratio of 1.98. Assume that the distillate rate is constant over the 20 hour period. Therefore, the distillate rate = 256/20 = 12.8 lbmol/h. For a reflux ratio of 1.98, the boilup (vapor rate) = $2.98D = 2.98(12.8) = 38.1$ lbmol/h

Alternatively, this exercise can be solved with the batch distillation model of Chemcad. To do this, the Wilson equation might be used to compute vapor-liquid equilibrium. Also, a decision must be made as to whether a constant distillate rate or a constant boilup rate should be specified. Based on the above findings, it is probable that a nearly constant reflux ratio can be used. Assuming this is so, either the distillate rate or boilup rate can be held constant. To verify this, a run was made with a constant distillate rate of 12.8 lbmol/h, as computed above in Part (c). The result shown below shows that the reflux ratio varies only slightly from approximately 2.3 to 2.5, except for the last hour, where it increases dramatically. The higher reflux ratios, compared to the value of 1.98 computed in Part (b) above are probably due to differences in the vapor-liquid equilibrium data used and the inaccuracy of the graphical determination in Part (b) of R_{min} and the use of an $R = 1.2R_{min}$.



Exercise 13.15

Subject: Batch rectification of an ethanol-water mixture under conditions of constant boilup rate and constant distillate composition.

Given: Charge of 1,000 kmol of 20 mol% ethanol and 80 mol% water. Operation in a column with 6 theoretical plates plus a partial reboiler (7 equilibrium stages) at 101.3 kPa with a boilup rate of 100 kmol/h to give a constant mole fraction of 0.80 for ethanol in the distillate. Vapor-liquid equilibrium data in Exercise 7.29.

Assumptions: Negligible liquid holdup on trays and in the condenser. No pressure drop. Perfect mixing in the reboiler.

Find: (a) Time in hours for the residue to reach an ethanol mole fraction of 0.05.
(b) Kmol of distillate produced at conditions of Part (a).
(c) Minimum and maximum reflux ratios during the rectification.
(d) Variation of the distillate rate during the rectification.

Analysis: This exercise can be solved by the procedure outlined in Section 13.3, with the McCabe-Thiele construction shown in Fig. 13.7, where here the calculations are made for ethanol with $x_D = 0.8$. From a series of operating lines through that point with slopes L/V, values of x_W are determined by stepping off 7 equilibrium stages. With $W_0 = 1{,}000$ kmol/h, $V = 100$ kmol/h, and $x_0 = 0.20$, Eq. (13-16) is numerically integrated to the final $x_W = 0.05$. This is a straightforward, but tedious procedure. Alternatively, this exercise is solved rapidly with the batch distillation model of Chemcad based on the following input:
Topology: BATC (the column with reboiler, condenser and reflux line) connected to TANK.
Components: Ethanol (1) and water (2)
Thermodynamics: Wilson equation with built in binary interaction parameters of:

$$\lambda_{12} - \lambda_{11} = 276.760 \text{ cal/gmol} \quad \text{and} \quad \lambda_{21} - \lambda_{22} = 975.490 \text{ cal/gmol}$$

Charge: 200 kmol of 1 and 800 kmol of 2 at 101.3 kPa and the bubble point.
Operation Step 1: Start from total reflux. 8 stages (includes total condenser). Simultaneous correction method with damping factor of 0.7 because nonideal system. Distillate sent to TANK.
First specification of 0.8 mole fraction of 1 in instantaneous distillate.
Second specification of 100 kmol/h of boilup
Stop operation when mole fraction of 1 in the bottoms (residue) = 0.05
Step size = 0.02 h recorded every 5 increments with stop tolerance of 0.001
Results are as follows:

(a) 7.28 h for operation step 1.
(b) kmol of cumulative distillate (from material balance) = 200 kmol at 78°C.
(c) Initial (minimum) reflux ratio = 2.35 Final (maximum) reflux ratio = 3.7
(d) The variation of the distillate rate, computed from the reflux ratios, is as follows:

Time, h	0	2	4	6	7.28
Distillate, kmol/hr	29.9	28.6	26.9	24.1	21.3

Exercise 13.16

Subject: Batch rectification with variable reflux ratio and constant distillation composition.

Given: 500 lbmol charge of 48.8 mol% A and 51.2 mol% B. $\alpha_{A,B} = 2.0$. Total condenser, 7 theoretical trays in column, and partial reboiler. Constant 95 mol% A in distillate. Boilup rate = 213.5 lbmol/h.

Assumptions: Negligible holdup on trays and in condensing system. Perfect mixing in reboiler. No pressure drop. Constant molar overflow.

Find: When mole fraction of A in boiler drops to 0.192:
(a) Time in h.
(b) Total amount of distillate, lbmol.

Analysis: (a) Using the procedure outlined in Section 13.3, a McCabe-Thiele construction is applied, as in Fig. 13.7, to obtain the relationship between the reflux ratio and the mole fraction of A in the residue for x_D = constant = 0.95 and 7 + 1 = 8 equilibrium stages. The construction for the initial residue composition of $x_W = x_0 = 0.488$ is shown on the following page, where the correct slope of the operating line was obtained by trial and error to be $L/V = 0.706$. From Eq. (7-7), the corresponding reflux ratio = $R = (L/V)/[1 - (L/V)] = 0.706/(1 - 0.706) = 2.40$. In the table below, other values of increasing L/V by the McCabe-Thiele construction give the values of x_W listed below until the final value of 0.192 is reached. These values are used to obtain time, t, for distillation starting from a bubble-point charge, with Eq. (13-16):

$$t = \frac{W_0(x_D - x_0)}{V}\int_{x_{W_f}}^{x_0}\frac{dx_W}{(1-L/V)((x_D - x_W)^2} = \frac{500(0.95-0.488)}{213.5}\int_{0.192}^{0.488}\frac{dx_W}{(1-L/V)(0.95-x_W)^2} \qquad (1)$$

L/V	x_W	R	$I = \frac{1}{(1-L/V)((x_D - x_W)^2}$	Δt, h
0.706	0.488	2.4	15.9	
0.744	0.425	2.9	14.2	1.03
0.783	0.365	3.6	13.5	0.90
0.828	0.290	4.8	13.4	1.09
0.870	0.230	6.7	14.8	0.92
0.898	0.192	8.8	17.1	0.66

The above table includes the numerical integration of Eq. (1) by the trapezoidal rule. For example, the Δt of 0.95 in the 3rd row is obtained from:

$$\Delta t = \frac{500(0.95-0.488)}{213.5} I_{avg}\,(\Delta x_W) = 1.08[(15.9 + 14.2)/2](0.488 - 0.425) = 1.03 \text{ h}$$

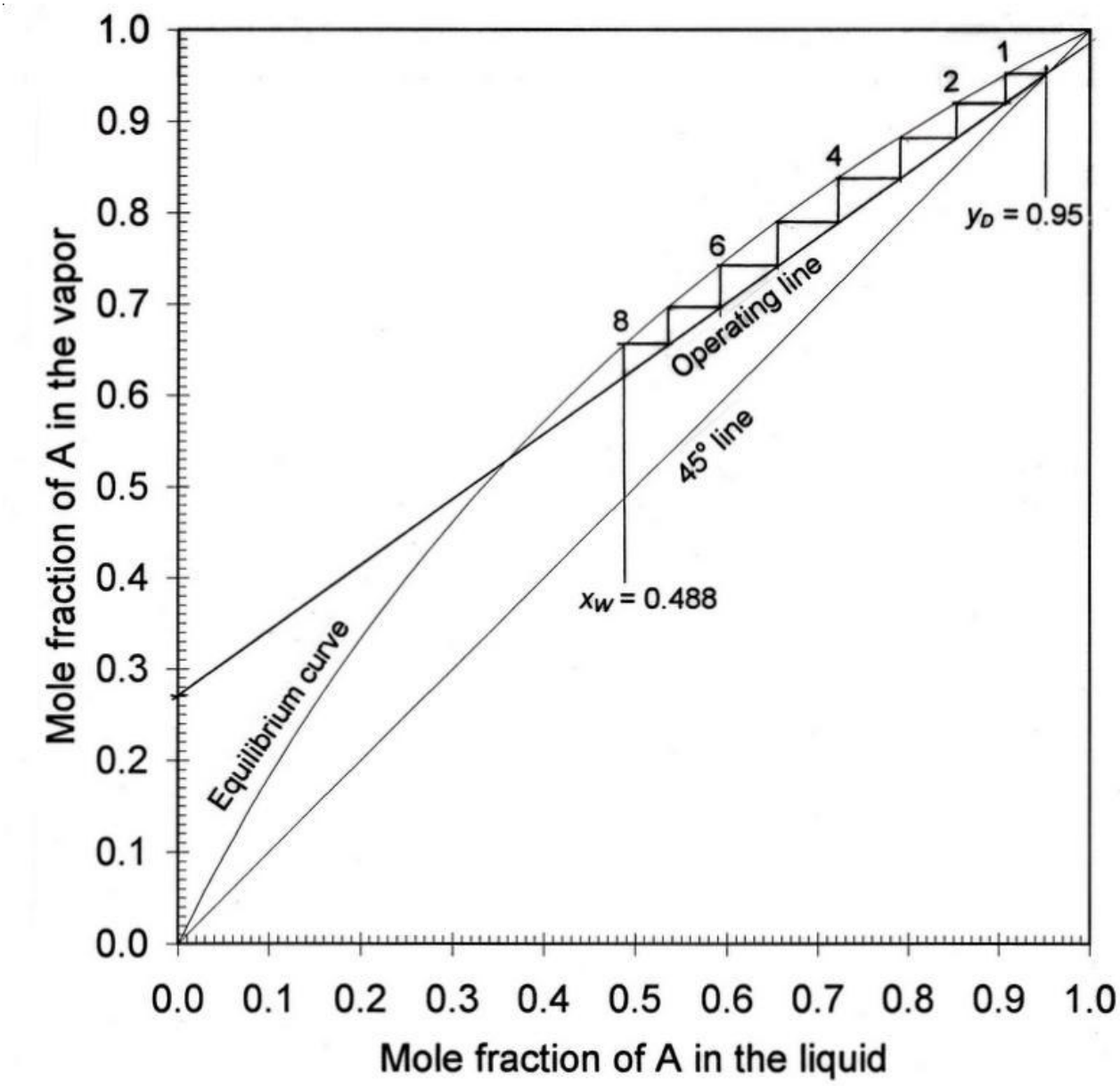
Exercise 13.16 (continued)

Analysis: (continued)

The total time is the sum of Δt values from the above table:

$t = 1.03 + 0.90 + 1.09 + 0.92 + 0.66 = 4.60$ h

This is close to the value of 4.75 h obtained using the batch distillation program of Chemcad.



(b) The total distillate is obtained by material balance on component A, giving an equation like

(13-13): $$D = W_0\left[1-\left(\frac{x_D - x_0}{x_D - x_W}\right)\right] = 500\left[1-\left(\frac{0.95-0.488}{0.95-0.192}\right)\right] = 195.3 \text{ lbmol}$$

Exercise 13.17

Subject: Calculation procedure for binary batch stripping with constant boilup ratio.

Given: Equipment arrangement of Fig. 13.8, where the initial charge is placed in the condenser accumulator.

Assumptions: No holdup on the trays or in the reboiler or condenser. No pressure drop. Equilibrium stages. Constant molar overflow.

Find: A calculation procedure like that developed in Section 13.2 for batch rectification with constant reflux ratio, but with constant boilup ratio, $V_B = V/B$ or from Eq. (7-12), $L/V = (1 + V_B)/V_B$.

Analysis: Refer to Fig. 13.4. Plot the *y-x* equilibrium curve for the more volatile component on a McCabe-Thiele diagram. Add the 45° line. From the specified boilup ratio, compute the slope of the operating line, *L/V*, from Eq. (7-12). Locate an arbitrary value of the instantaneous bottoms composition, x_B on the 45° line and draw an operating line from this point to an intersection with the equilibrium curve. Starting at the point x_B on the 45° line, step off a number of stages = number of equilibrium stages in the column plus one for the reboiler, as shown in the diagram on the next page. The point for the uppermost stage is the mole fraction for the vapor leaving the top stage, which, with the total condenser, is the composition in feed tank, x_C, (condenser accumulator). Locate several other operating lines, all of the same slope. Each x_C must be equal to or greater than the initial feed tank composition, x_0. The range of the corresponding x_B values depends on the operation step stop specification. With constant molar overflow, the following form of Eq. (13-2) applies, where W_0 is the initial moles of charge to the feed tank and W_t is the moles left in the feed tank at the end of the operation step:

$$\ln\left(\frac{W_0}{W_t}\right) = \int_{x_0}^{x_{C_t}} \frac{dx_C}{\left(x_C - x_B\right)}$$

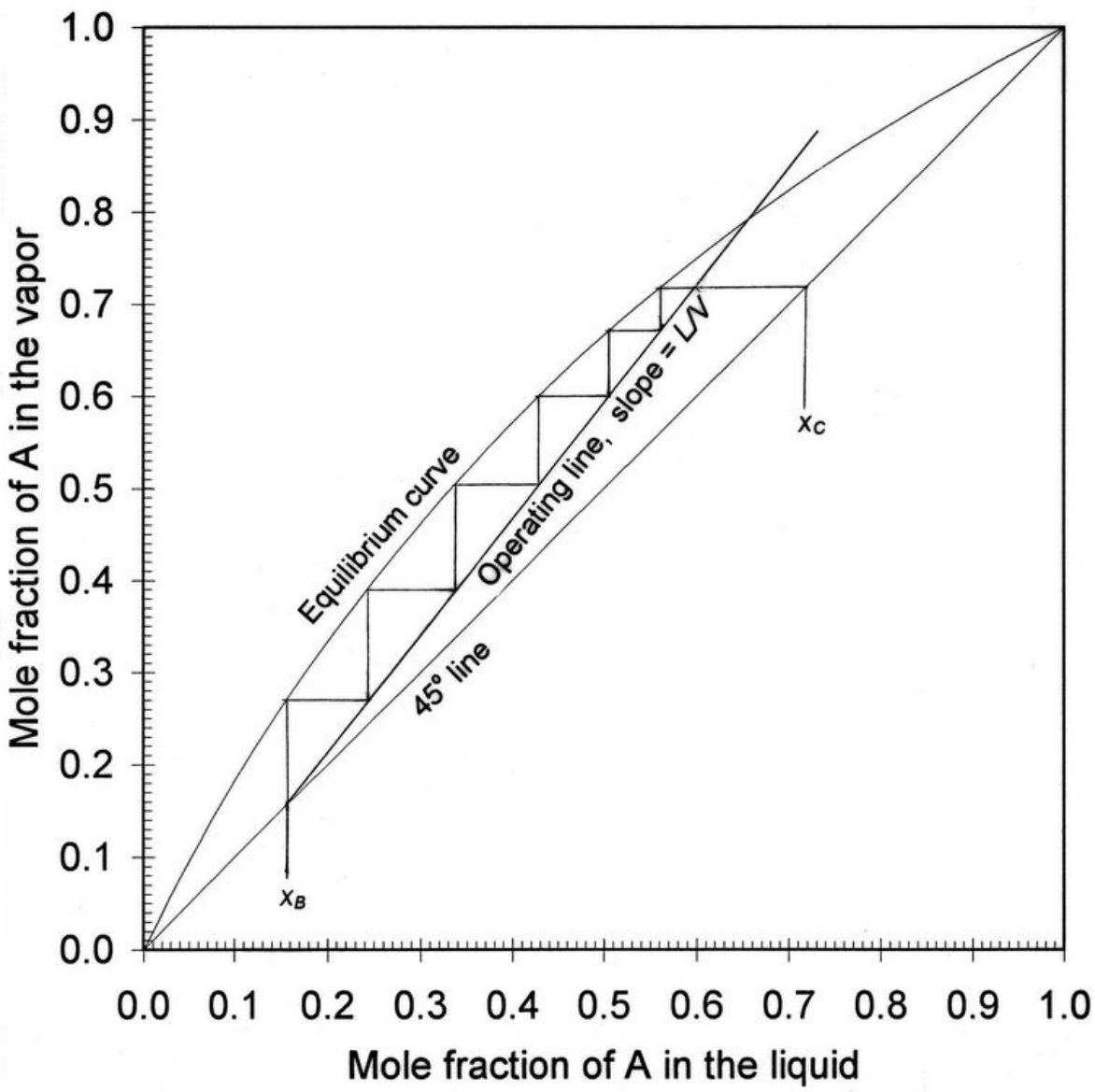
The cumulative bottoms composition is given by material balance in a manner used to develop Eq. (13-12):

$$x_{B_{\text{avg}}} = \frac{W_0 x_0 - W_t x_{C_t}}{W_0 - W_t}$$

This procedure is applied in Exercise 13.18.

Exercise 13.17 (continued)

Analysis: (continued)



Exercise 13.18

Subject: Batch stripping of a mixture of normal hexane (H) and normal octane (O).

Given: Charge of 100 kmol of 10 mol% H and 90 mol% O. Boilup up rate, V = 30 kmol/h. Boilup ratio, V/L = 0.5. Partial reboiler and column with 2 equilibrium stages (total of 3 stages).

Assumptions: No holdup except in feed tank. Perfect mixing in the feed tank. 1 atm pressure. No pressure drop. Configuration is in Fig. 13.8.

Find: Instantaneous bottoms and cumulative bottoms compositions at 2 h of operation.

Analysis: By the end of 2 hours of operation, the total amount of boilup = 2(30) = 60 kmol. The total liquid rate running down the column is 60/0.5 = 120 kmol. Therefore, the bottoms produced = 120 - 60 = 60 kmol. The liquid left in the feed tank will be 100 - 60 = 40 kmol. If a perfect separation took place, the bottoms would be pure O and the liquid left in the feed tank would be 25 mol% H. Therefore the mole fraction of H in the feed tank, call it x_C, is restricted to the range of 0.10 to 0.25. At time zero, it is 0.10 and then increases, but can not exceed 0.25. The instantaneous mole fraction of H in the bottoms, call it x_B, is restricted to the range of 0.0 to 0.10. It starts at a low value and increases, but probably falls far short of 0.1 because of the relatively large relative volatility, as indicated in the following. Vapor-liquid equilibrium data are given in Figs. 4.3 and 4.4, from which the following data are extracted for the range of interest:

***T*, °C**	125	120	115	110	106	102	98	95	92	90	87
***y* of H**	0.00	0.193	0.34	0.46	0.55	0.63	0.69	0.74	0.785	0.82	0.85
***x* of H**	0.0	0.05	0.1	0.15	0.2	0.25	0.3	0.35	0.4	0.45	0.5

These data are plotted in the McCabe-Thiele diagram on the next page, where it is seen that in the range of interest, the slope of the equilibrium curve is almost constant at approximately 3.9. A typical operating line is shown, with 3 stages stepped off. Because the slope of the operating line is also constant at a value of 2 and there are only 3 stages, an algebraic method is reasonable to obtain the relationship between x_B and x_C for use in the following form of Eq. (13-3):

$$\ln\left(\frac{W_0}{W_t}\right) = \ln\left(\frac{100}{40}\right) = 0.916 = \int_{x_0=0.10}^{x_{C_t}} \left(\frac{dx_C}{x_C - x_B}\right) \qquad (1)$$

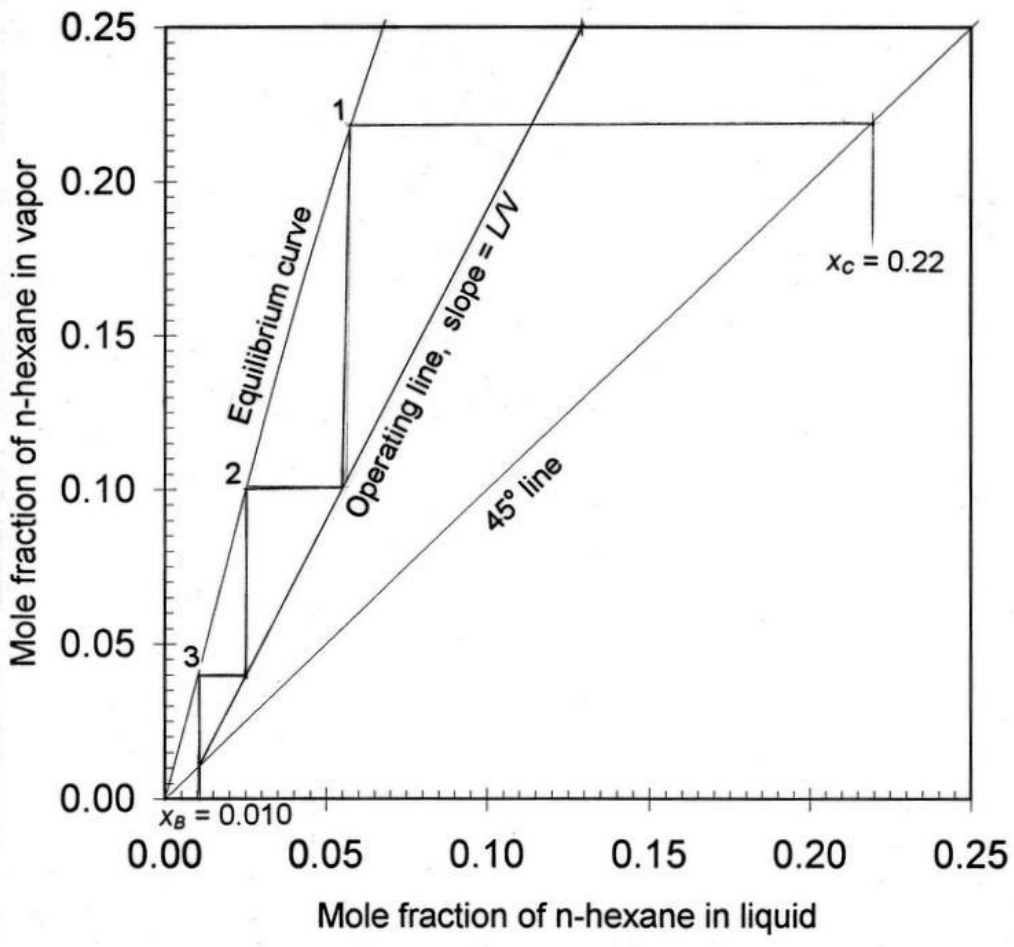
For 3 stages, the algebraic equation derived by combining the equilibrium equations, $y = 3.9x$, with the operating lines, $y = (L/V)x - x_B = 2x - x_B$ is: $x_C = 22x_B$. The value of x_{C_t} that satisfies Eq. (1) is derived by integrating Eq. (1) numerically with the trapezoidal rule as follows:

Exercise 13.18 (continued)

Analysis: (continued)

x_C	x_B	$I = 1/(x_C - x_B)$	Δx_C	$I_{avg}\Delta x_C$
0.100	0.00455	10.48		
0.110	0.005	9.52	0.010	0.100
0.132	0.006	7.94	0.022	0.192
0.154	0.007	6.80	0.022	0.162
0.176	0.008	5.95	0.022	0.140
0.198	0.009	5.29	0.022	0.124
0.220	0.010	4.76	0.022	0.111
0.242	0.011	4.33	0.022	0.100
0.250	0.0114	4.18	0.008	0.034

If the right-hand column is added from $x_C = 0.100$ to 0.242, the sum is 0.929, which is too large. From $x_C = 0.100$ to 0.220, the sum is 0.829, which is too small. For 0.916, $x_C = 0.249$ and the corresponding instantaneous bottoms H mole fraction = 0.0113. The cumulative bottoms mole fraction for H is approximately 0.008.



Exercise 13.19

Subject: Complex batch binary distillation with a middle feed vessel, a rectification section, and a stripping section.

Given: Equipment arrangement of Fig. 13.9.

Find: A calculation procedure of the McCabe-Thiele type.

Analysis: For a binary mixture, if the middle feed vessel is located in the optimal location, the composition of the charge will remain constant during the distillation. Thus, if the reflux ratio and distillate rate are kept constant, the batch distillation will behave like a continuous distillation, with constant compositions of the distillate and bottoms. Therefore, the standard McCabe-Thiele method presented in Chapter 7 applies. With a middle feed vessel, a binary mixture can be separated into nearly pure products.

The general case of multicomponent batch distillation in a column with a middle feed vessel is considered in detail by A. G. Davidyan, V. N. Kiva, G. A. Meski, and M. Morari, Chem. Eng. Sci., 49, 3033-3051 (1994). They find that for a ternary mixture, reflux and boilup ratios can be found that the composition of the middle vessel can tend to one of the three components. For a multicomponent mixture, both light and heavy impurities can be removed simultaneously.

Exercise 13.20

Subject: Effect of holdup on batch rectification.

Given: Appreciable column holdup.

Find: (a) After total reflux conditions are established, why is the composition of the charge to the still lower in the light component compared to the charge?

(b) Why is the separation more difficult than with zero holdup?

Analysis:

(a) When the holdups in the column (trays or packing) and condenser-reflux drum are appreciable compared to the original charge, the composition in the boiler will become higher in the heavier components because of the fractionation that occurs during the establishment of the total reflux condition. The average composition of the holdups above the boiler will be higher in the lighter components, and, thus, the average composition of the boiler holdup will be lower in the light components, compared to the original charge.

(b) When distillation with distillate accumulation begins, the mixture in the boiler is now less rich in the lighter component than it would be if the column and condenser-reflux drum holdups were zero. Thus, the separation into a nearly pure light component is more difficult.

Exercise 13.21

Subject: Effect of holdup on batch rectification.

Given: Appreciable column holdup.

Find: Why tray compositions change less rapidly when column holdup is appreciable compared to zero holdup.

Why is the degree of separation improved with appreciable column holdup?

Analysis:

Column (plate or packed) holdup causes a flywheel-like inertia effect, which decreases the rate of change of stage compositions. This can be observed in Eq. (13-36), where the rate of change in stage composition is inversely proportional to the stage holdup. Thus, the degree of separation is improved because the composition does not as rapidly as it would with zero holdup.

Exercise 13.22

Subject: Effect of holdup on batch rectification.

Given: Statements in Exercises 13.20 and 13.21.

Find: Reasons why it is difficult to predict the effect of column holdup.

Analysis:

When the holdups in the column (trays or packing) and condenser-reflux drum are not negligible compared to the original charge, the composition in the boiler will become higher in the heavier components because of the fractionation that occurs during the establishment of the total reflux condition. The average composition of the holdups above the boiler will be higher in the lighter components, and, thus, the average composition of the boiler holdup will be lower in the light components, compared to the original charge.

When distillation with distillate accumulation begins, the mixture in the boiler is now less rich in the lighter component than it would be if the column and condenser-reflux drum holdups were zero. Thus, the separation into a nearly pure light component is more difficult.

However, column (plate or packed) holdup causes a flywheel-like inertia effect, which decreases the rate of change of stage compositions. This can be observed in Eq. (13-36), where the rate of change in stage composition is inversely proportional to the stage holdup. Thus, the degree of separation is improved because the composition does not as rapidly as it would with zero holdup.

Thus, these two effects oppose each other and it is difficult to predict what the overall effect of holdup will be.

Exercise 13.23

Subject: Calculation of batch rectification of a binary mixture by the shortcut method of Sandaram and Evans.

Given: Conditions in Example 13.7. Charge of 100 kmol of an equimolar mixture of n-hexane (A) and n-heptane (B). Reflux rate of 10 kmol/h and a distillate rate of 10 kmol/h. Column has one equilibrium plate, a total condenser, and a partial reboiler. Rectification at 15 psia.

Assumptions: Zero condenser and column holdups. Constant molar overflow. Constant *K*-values for A of 1.212 at the plate and 1.420 in the reboiler, while for B, 0.4838 at the plate and 0.5810 in the reboiler. No pressure drop.

Find: Mole fractions of A and B for $t = 0.05$ h at the condenser and the reboiler.

Analysis: With a constant reflux rate of 10 kmol/h and a distillate rate of 10 kmol/h, the vapor rate is 20 kmol/h and the reflux ratio is 1. Assuming startup conditions of total reflux, use Eq. (13-27) to compute the distillate composition. For the relative volatility, use the arithmetic average value based on the above *K*-values.

$$\alpha_{A,B} = \frac{\frac{1.420}{0.5810} + \frac{1.212}{0.4838}}{2} = 2.47$$

From Eq. (13-27), with $N = 2$, $x_{D_B} = \dfrac{0.50}{0.5(2.47)^2 + 0.5(1)^2} = 0.141$ and $x_{D_A} = 1 - 0.141 = 0.859$

Take a time increment = $\Delta t = 0.05$ h. Note that $V = 20$ kmol/h and $R = 1$.

From Eq. (13-22), $W^{(1)} = 100 - \left(\dfrac{20}{2}\right)0.05 = 99.5$ kmol

From Eq. (13-23), $x_{W_A}^{(1)} = 0.5 + (0.859 - 0.5)\left[\dfrac{99.5 - 100}{100}\right] = 0.498$ and $x_{W_B}^{(1)} = 1 - 0.498 = 0.502$

From Eq. (13-28), $$\frac{2 - N_{min}}{3} = 0.75\left[1 - \left(\frac{1 - R_{min}}{2}\right)^{0.5668}\right] \qquad (1)$$

From Eq. (13-30), $$R_{min} = \frac{2.47^{N_{min}} - 2.47}{(2.47 - 1)[0.498(2.47)^{N_{min}} + 0.502(1)^{N_{min}}]} \qquad (2)$$

Unfortunately, when Eqs. (1) and (2) are solved simultaneously, the results are $R_{min} = -0.0714$, which is impossible, and $N_{min} = 0.92$. Ignoring the impossible R_{min} value and using the value of 0.92 for N_{min} in Eq. (13-27),

$$x_{D_B} = \frac{0.502}{0.498(2.47)^{0.92} + 0.502(1)^{0.92}} = 0.305 \quad \text{and} \quad x_{D_A} = 1 - 0.305 = 0.695$$

This result does not compare well with that of Example 13.7, where $x_{D_A} = 0.8116$.

It appears that the shortcut method may not work well for a very small number of stages.

Exercise 13.24

Subject: Calculation of batch rectification of a ternary mixture by the shortcut method of Sandaram and Evans.

Given: Charge of 100 kmol of an equimolar mixture of an equimolar mixture of A, B, and C. Reflux ratio, $R = 5$ and vapor rate, $V = 100$ kmol/h. Column has three equilibrium plates, a total condenser, and a partial reboiler. Thus, $N = 4$. $\alpha_{A,C} = 4$, $\alpha_{B,C} = 2$, and $\alpha_{C,C} = 1$.

Assumptions: No condenser and column holdups. Constant molar overflow. No pressure drop. Startup under total reflux.

Find: Variation of instantaneous residue and distillate compositions with time following startup.

Analysis: For startup conditions of total reflux, use Eq. (13-27) to compute the distillate composition using $N = 4$, $x_{D_C}^{(0)} = \dfrac{0.333}{0.333(4)^4 + 0.333(2)^4 + 0.333(1)^4} = 0.00366$

From Eq. (13-25), $x_{D_A}^{(0)} = 0.333\left(\dfrac{0.00366}{0.333}\right)4^4 = 0.9370$ and $x_{D_B}^{(0)} = 1 - 0.0037 - 0.9370 = 0.0593$

Take a time increment = $\Delta t = 0.25$ h.

From Eq. (13-22), $W^{(1)} = 100 - \left(\dfrac{100}{1+5}\right)0.25 = 95.83$ kmol

From Eq. (13-23), $x_{W_A}^{(1)} = 0.3333 + (0.9370 - 0.3333)\left[\dfrac{95.83 - 100}{100}\right] = 0.3081$

$$x_{W_B}^{(1)} = 0.3333 + (0.0593 - 0.3333)\left[\frac{95.83 - 100}{100}\right] = 0.3447$$

$$x_{W_C}^{(1)} = 1 - 0.3081 - 0.3448 = 0.3471$$

From Eq. (13-28), $$\frac{4 - N_{\min}}{4+1} = 0.75\left[1 - \left(\frac{5 - R_{\min}}{5+1}\right)^{0.5668}\right] \qquad (1)$$

From Eq. (13-30), $$R_{\min} = \frac{4^{N_{\min}} - 4}{(4-1)[0.3081(4)^{N_{\min}} + 0.3448(2)^{N_{\min}} + 0.3471(1)^{N_{\min}}]} \qquad (2)$$

When Eqs. (1) and (2) are solved simultaneously, the results are $R_{\min} = 0.917$ and $N_{\min} = 3.265$. Using the latter value in Eq. (13-27),

$$x_{D_C} = \frac{0.3471}{0.3081(4)^{3.265} + 0.3447(2)^{3.265} + 0.3471(1)^{3.265}} = 0.0108$$

From Eq. (13-25),

$$x_{D_A} = 0.3081\left(\frac{0.0108}{0.3471}\right)4^{3.265} = 0.8861 \text{ and } x_{D_B} = 0.3447\left(\frac{0.0108}{0.3471}\right)2^{3.265} = 0.1031$$

Exercise 13.24 (continued)

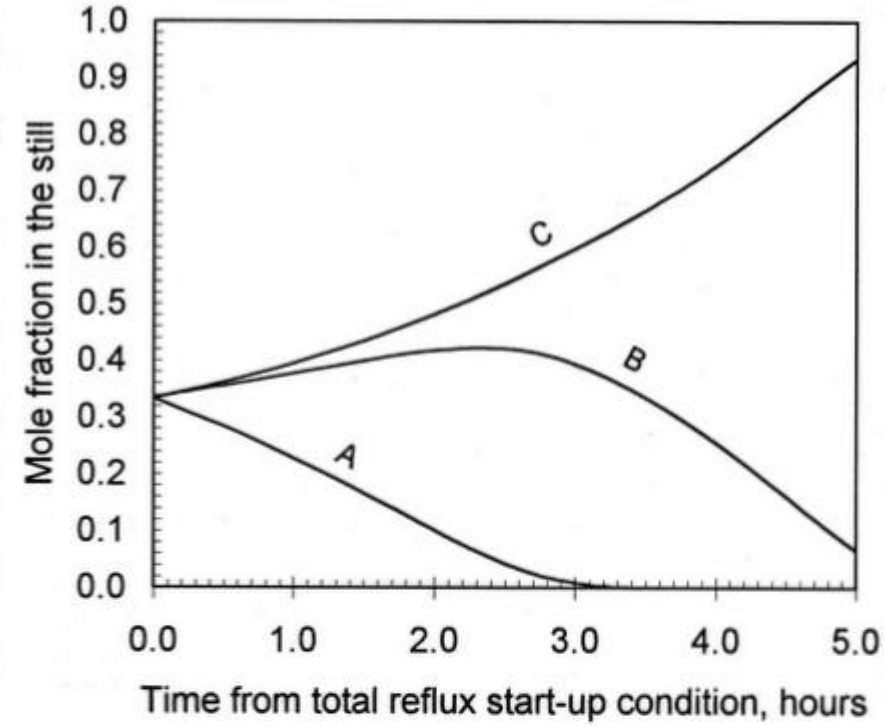
Analysis:

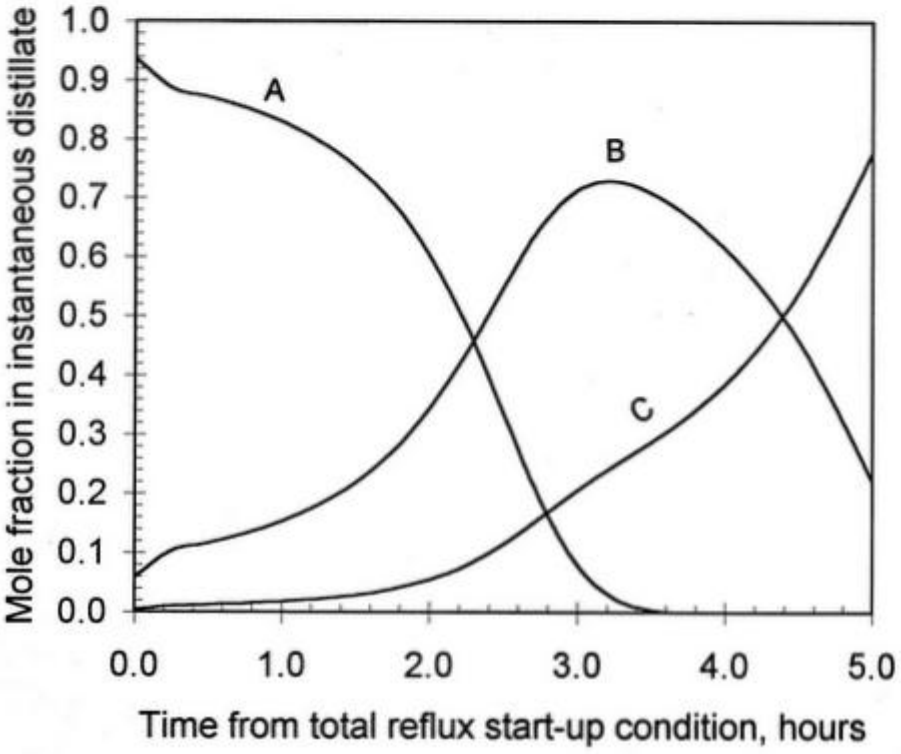
The calculations above for the first time increment are repeated for subsequent time increments, using a spread sheet, up to 5 hours. The results are as follows. On the next page, the mole fraction compositions are plotted as a function of time.

Time,		Mole fractions in residue:					Mole fractions in distillate:		
hours	*W*, kmol	A	B	C	*R* min	*N* min	A	B	C
0.00	100.00	0.3333	0.3333	0.3333			0.9370	0.0593	0.0037
0.25	95.83	0.3081	0.3447	0.3471	0.917	3.265	0.8861	0.1031	0.0108
0.50	91.67	0.2830	0.3552	0.3618	0.980	3.238	0.8716	0.1159	0.0125
0.75	87.50	0.2563	0.3661	0.3776	1.058	3.206	0.8531	0.1321	0.0148
1.00	83.33	0.2278	0.3772	0.3949	1.153	3.165	0.8291	0.1530	0.0179
1.25	79.17	0.1978	0.3885	0.4138	1.271	3.114	0.7969	0.1808	0.0223
1.50	75.00	0.1662	0.3994	0.4344	1.421	3.048	0.7526	0.2186	0.0287
1.75	70.83	0.1337	0.4094	0.4569	1.605	2.966	0.6905	0.2708	0.0387
2.00	66.67	0.1009	0.4176	0.4815	1.837	2.859	0.6020	0.3434	0.0546
2.25	62.50	0.0696	0.4222	0.5082	2.098	2.734	0.4816	0.4390	0.0794
2.50	58.33	0.0421	0.4211	0.5368	2.361	2.604	0.3346	0.5501	0.1153
2.75	54.17	0.0212	0.4119	0.5669	2.585	2.489	0.1886	0.6516	0.1598
3.00	50.00	0.0084	0.3934	0.5982	2.745	2.403	0.0803	0.7144	0.2053
3.25	45.83	0.0024	0.3667	0.6309	2.850	2.346	0.0239	0.7293	0.2468
3.50	41.67	0.0004	0.3337	0.6659	2.925	2.304	0.0043	0.7092	0.2865
3.75	37.50	0.0000	0.2962	0.7038	2.994	2.265	0.0002	0.6691	0.3307
4.00	33.33	0.0000	0.2547	0.7453	3.067	2.223	0.0000	0.6148	0.3852
4.25	29.17	0.0000	0.2097	0.7903	3.148	2.176	0.0000	0.5453	0.4547
4.50	25.00	0.0000	0.1618	0.8382	3.236	2.124	0.0000	0.4569	0.5431
4.75	20.83	0.0000	0.1126	0.8874	3.328	2.068	0.0000	0.3472	0.6527
5.00	16.67	0.0000	0.0657	0.9343	3.416	2.013	0.0000	0.2210	0.7790

Exercise 13.24 (continued)

Analysis: (continued)





Exercise 13.25

Subject: Calculation of batch rectification of a ternary mixture by the shortcut method of Sandaram and Evans.

Given: Charge of 200 kmol of 40 mol% A, 50 mol% B, and 10 mol% C. Reflux ratio, $R = 10$ and vapor rate, $V = 100$ kmol/h. Column has two equilibrium plates, a total condenser, and a partial reboiler. Thus, $N = 3$. $\alpha_{A,C} = 2$, $\alpha_{B,C} = 1.5$, and $\alpha_{C,C} = 1$.

Assumptions: No condenser and column holdups. Constant molar overflow. No pressure drop. Startup under total reflux.

Find: Variation of instantaneous residue and distillate compositions for 1hour following startup.

Analysis: For startup conditions of total reflux, use Eq. (13-27) to compute the distillate composition using $N = 3$, $x_{D_C}^{(0)} = \dfrac{0.100}{0.4(2)^3 + 0.5(1.5)^3 + 0.1333(1)^3} = 0.0199$

From Eq. (13-25), $x_{D_A}^{(0)} = 0.4\left(\dfrac{0.0199}{0.1}\right)2^3 = 0.6368$ and $x_{D_B}^{(0)} = 1 - 0.0199 - 0.6368 = 0.3433$

Take a time increment = $\Delta t = 0.10$ h.

From Eq. (13-22), $W^{(1)} = 200 - \left(\dfrac{100}{1+10}\right)0.10 = 199.09$ kmol

From Eq. (13-23), $x_{W_A}^{(1)} = 0.4 + (0.6368 - 0.4)\left[\dfrac{199.09 - 200}{200}\right] = 0.3989$

$$x_{W_B}^{(1)} = 0.5 + (0.3433 - 0.5)\left[\frac{199.09 - 200}{200}\right] = 0.5007$$

$$x_{W_C}^{(1)} = 1 - 0.3989 - 0.5007 = 0.1004$$

From Eq. (13-28), $$\frac{3 - N_{\min}}{3+1} = 0.75\left[1 - \left(\frac{10 - R_{\min}}{10+1}\right)^{0.5668}\right] \qquad (1)$$

From Eq. (13-30), $$R_{\min} = \frac{2^{N_{\min}} - 2}{(2-1)[0.3989(2)^{N_{\min}} + 0.5007(1.5)^{N_{\min}} + 0.1004(1)^{N_{\min}}]} \qquad (2)$$

When Eqs. (1) and (2) are solved simultaneously, the results are $R_{\min} = 1.058$ and $N_{\min} = 2.668$. Using the latter value in Eq. (13-27),

$$x_{D_C} = \frac{0.1004}{0.3989(2)^{2.668} + 0.5007(1.5)^{2.668} + 0.1004(1)^{2.668}} = 0.0244$$

From Eq. (13-25),

$$x_{D_A} = 0.3989\left(\frac{0.0244}{0.1004}\right)2^{2.668} = 0.6164 \text{ and } x_{D_B} = 0.5007\left(\frac{0.0244}{0.1004}\right)1.5^{2.668} = 0.3592$$

Exercise 13.25 (continued)

Analysis:

The calculations above for the first time increment are repeated for subsequent time increments, using a spread sheet, up to 1 hour. The results are as follows.

Time,		Mole fractions in residue:					Mole fractions in distillate:		
hours	W,kmol	A	B	C	R min	N min	A	B	C
0.00	200.00	0.4000	0.5000	0.1000			0.6368	0.3433	0.0199
0.10	199.09	0.3989	0.5007	0.1004	1.058	2.668	0.6164	0.3592	0.0244
0.20	198.18	0.3979	0.5014	0.1007	1.060	2.667	0.6155	0.3600	0.0245
0.30	197.27	0.3969	0.5020	0.1011	1.061	2.667	0.6145	0.3608	0.0246
0.40	196.36	0.3959	0.5027	0.1014	1.062	2.667	0.6136	0.3617	0.0247
0.50	195.45	0.3949	0.5033	0.1018	1.063	2.667	0.6126	0.3625	0.0249
0.60	194.55	0.3939	0.5040	0.1021	1.064	2.667	0.6117	0.3634	0.0250
0.70	193.64	0.3929	0.5046	0.1025	1.065	2.666	0.6107	0.3642	0.0251
0.80	192.73	0.3919	0.5053	0.1028	1.066	2.666	0.6097	0.3651	0.0252
0.90	191.82	0.3908	0.5059	0.1032	1.067	2.666	0.6087	0.3659	0.0253
1.00	190.91	0.3898	0.5066	0.1036	1.068	2.666	0.6077	0.3668	0.0254

Exercise 13.26

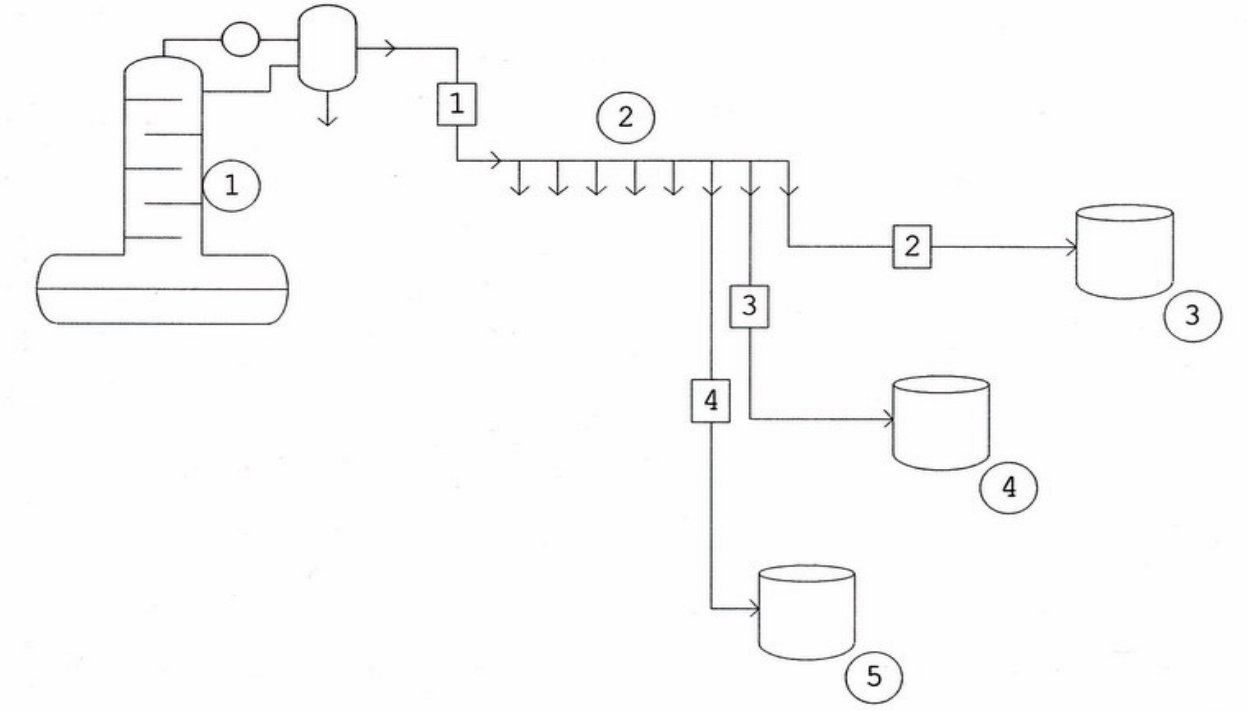
Subject: Calculation of batch rectification of a ternary mixture by a method that accounts for holdup.

Given: Charge of 100 lbmol of 35 mol% n-hexane (C6), 35 mol% n-heptane (C7), and 30 mol% n-octane (C8). Batch rectification at 1 atm. Column with the equivalent of 10 theoretical stages, plus a partial reboiler and a total condenser. Constant reflux ratio, $R = 5$ and vapor boilup rate, $V = 50$ lbmol/h. Total reflux condition is established by time zero. Ideal thermodynamics (Raoult's law K-values). Holdup of condenser-reflux drum = 1 lbmol. Three operation steps:
Step 1. Stop when accumulated distillate purity drops to 95 mol% C6.
Step 2. Empty the C6-rich cut and resume rectification until instantaneous distillate composition drops reaches 80 mol% C7.
Step 3. Empty the C6-rich cut and resume rectification until accumulated distillate composition reaches 4 mol% C8.

Assumptions: No pressure drop.

Find: Compositions and amounts of each of the 4 products for:
Column 1: Plate column with a total liquid holdup of 8 lbmol.
Column 2: Packed column with a total liquid holdup of 2 lbmol.
Effect of holdup for the two columns.

Analysis: Use the Batch distillation program of Chemcad to make the calculations. The flowsheet below includes a batch column (1), a time switch (2), and 3 tanks (3, 4, and 5).



Exercise 13.26 (continued)

Analysis (continued):

To determine the effect of holdup, make a run with no holdup in the column or the condenser-reflux drum. For all three runs, the initial charge is first brought to the bubble point temperature, which is computed to be 193.2°F at 1 atm.

Case 1: Column and condenser-reflux drup with no holdup:
The input data for Chemcad are as follows, where distillate rate = $D = V/(1+R) = 50/6 = 8.333$ lbmol/h.

Batch column:
No. of stages = 12 (10 in column + reboiler + condenser)
No. of operation steps = 3
Total condenser
Condenser pressure = 1 atm
Holdup units in moles (lbmoles in this case)
Condenser holdup = 0
Stage holdup = 0
Method of calculation = Inside-out

Operation parameters:

Step	**1**	**2**	**3**
Startup option	Total reflux	Column content	Column content
Tank no.	3	4	5
First specification	Reflux ratio = 5	Reflux ratio = 5	Reflux ratio = 5
Second specification	Distillate rate = 8.333 lbmol/h	Distillate rate = 8.333 lbmol/h	Distillate rate = 8.333 lbmol/h
Step size, hr	0.02	0.02	0.02
Record frequency	3	3	3
Stop criterion	Mole fraction of C6 in accumulator = 0.95	Mole fraction of C7 in instantaneous distillate = 0.80	Mole fraction of C8 in accumulator = 0.04
Stop tolerance	0.0001	0.0001	0.0001

Case 2: Plate column:
Chemcad input data same as for Case 1 except:
Condenser holdup = 1 lbmol
Stage holdup = 0.8 lbmol per stage (total of 8 lbmol for 10 stages)

Case 3: Packed column:
Chemcad input data same as for Case 1 except:
Condenser holdup = 1 lbmol
Stage holdup = 0.2 lbmol per stage (total of 2 lbmol for 10 stages)

Exercise 13.26 (continued)

Analysis:

All 3 cases converged. The results are as follows for the contents of tanks 3, 4, and 5 after Steps 1, 2, and 3, respectively, and the final residue:

Case 1: No holdups:

Vessel	Tank 3	Tank 4	Tank 5	Final residue
Amount, lbmol	32.9987	7.6664	27.1655	32.1696
Mole fractions:				
C6	0.9487	0.3537	0.0362	0.0000
C7	0.0513	0.6460	0.9231	0.1019
C8	0.0000	0.0003	0.0407	0.8981
Operation time, hr	3.96	0.92	3.26	8.14

Case 2: Plate column:

Vessel	Tank 3	Tank 4	Tank 5	Final residue
Amount, lbmol	34.9987	3.4999	30.9987	21.5030
Mole fractions:				
C6	0.9478	0.2859	0.0267	0.0000
C7	.0.0522	0.7136	0.9136	0.0244
C8	0.0000	0.0005	0.0417	0.9756
Operation time, hr	4.20	0.42	3.72	8.34

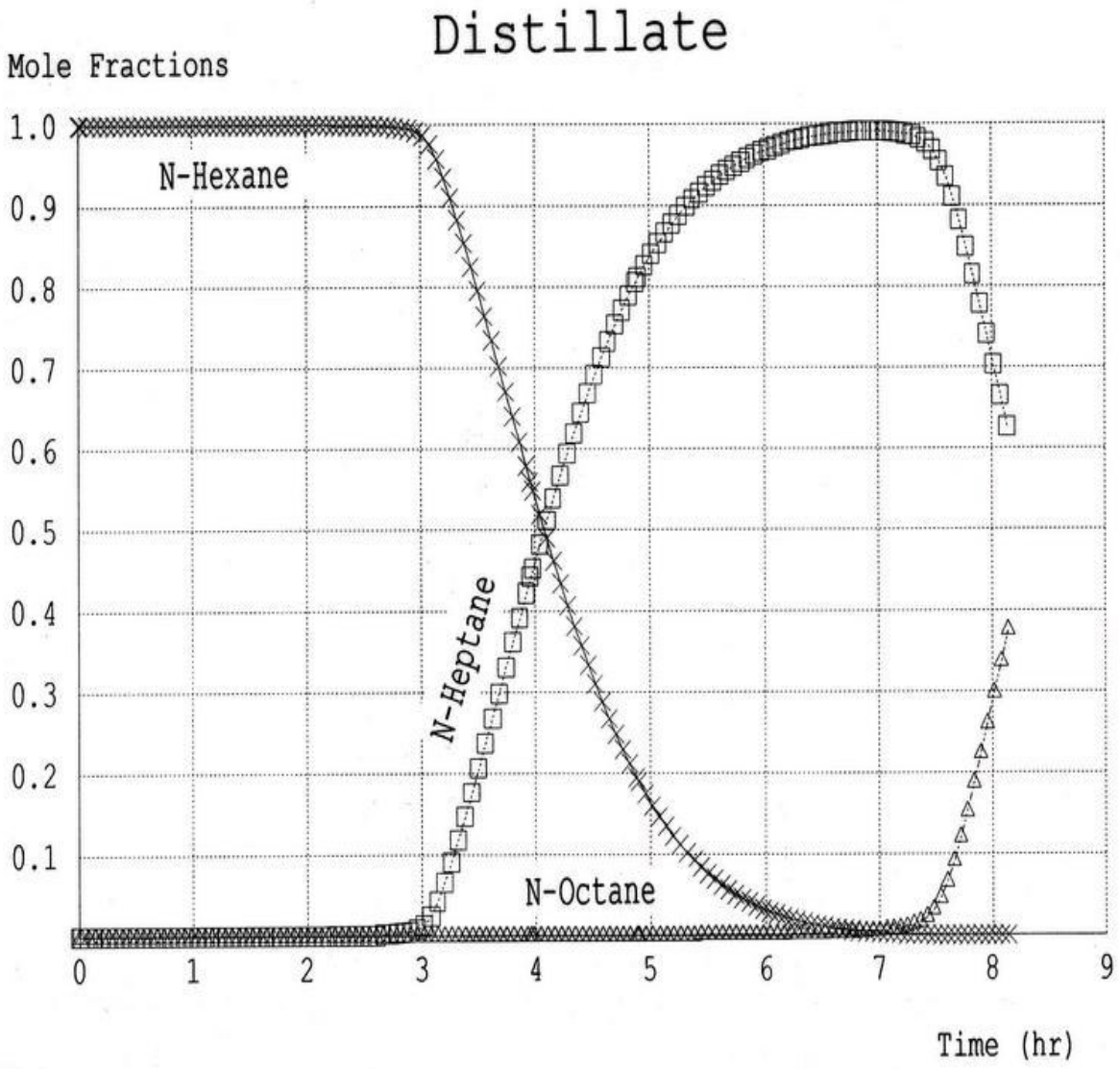
Case 3: Packed column:

Vessel	Tank 3	Tank 4	Tank 5	Final residue
Amount, lbmol	33.4988	6.6664	28.1655	28.6694
Mole fractions:				
C6	0.9497	0.3334	0.0342	0.0000
C7	.0.0503	0.6662	0.9255	0.0677
C8	0.0000	0.0004	0.0403	0.9323
Operation time, hr	4.02	0.80	3.38	8.20

The above results show a significant effect of holdup. If the 4 amounts are totaled, Case 1 gives 100.0002 lbmol (since no holdup), Case 2 gives 91.0003 lbmol (since 1+ 9 lbmol of holdup), and Case 3 gives 97.0001 lbmol (since 1+2 lbmol of holdup). The plate column gives the most product from Step 1, by far the least from Step 2, and the most from Step 3. The compositions for Tank 3 (Step 1) are all close. The compositions for Tank 4 (Step 2) are all different, with the best cumulative purity for C7 being the plate column. The compositions for Tank 5 (Step 3) are fairly close, while the compositions of the final residue are different, with the best purity for C8 given by the plate column. Total operation times are close, but the time for Step 2 is much lower for the plate column. This exercise shows the great difficulty in predicting the effect of holdup. Composition plots for the no holdup case are shown on the following pages.

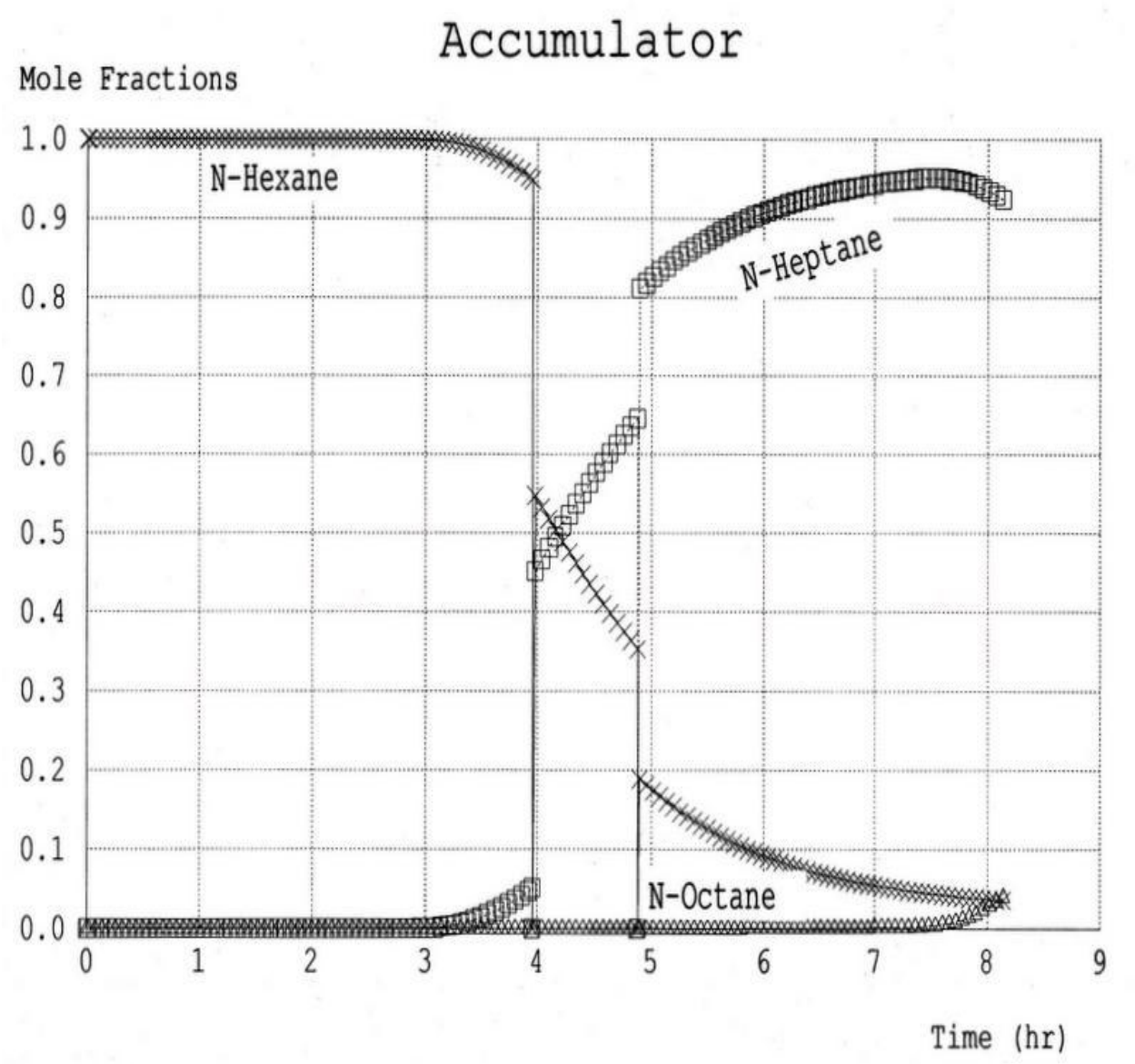
Exercise 13.26 (continued)

Analysis: (continued) No holdup case



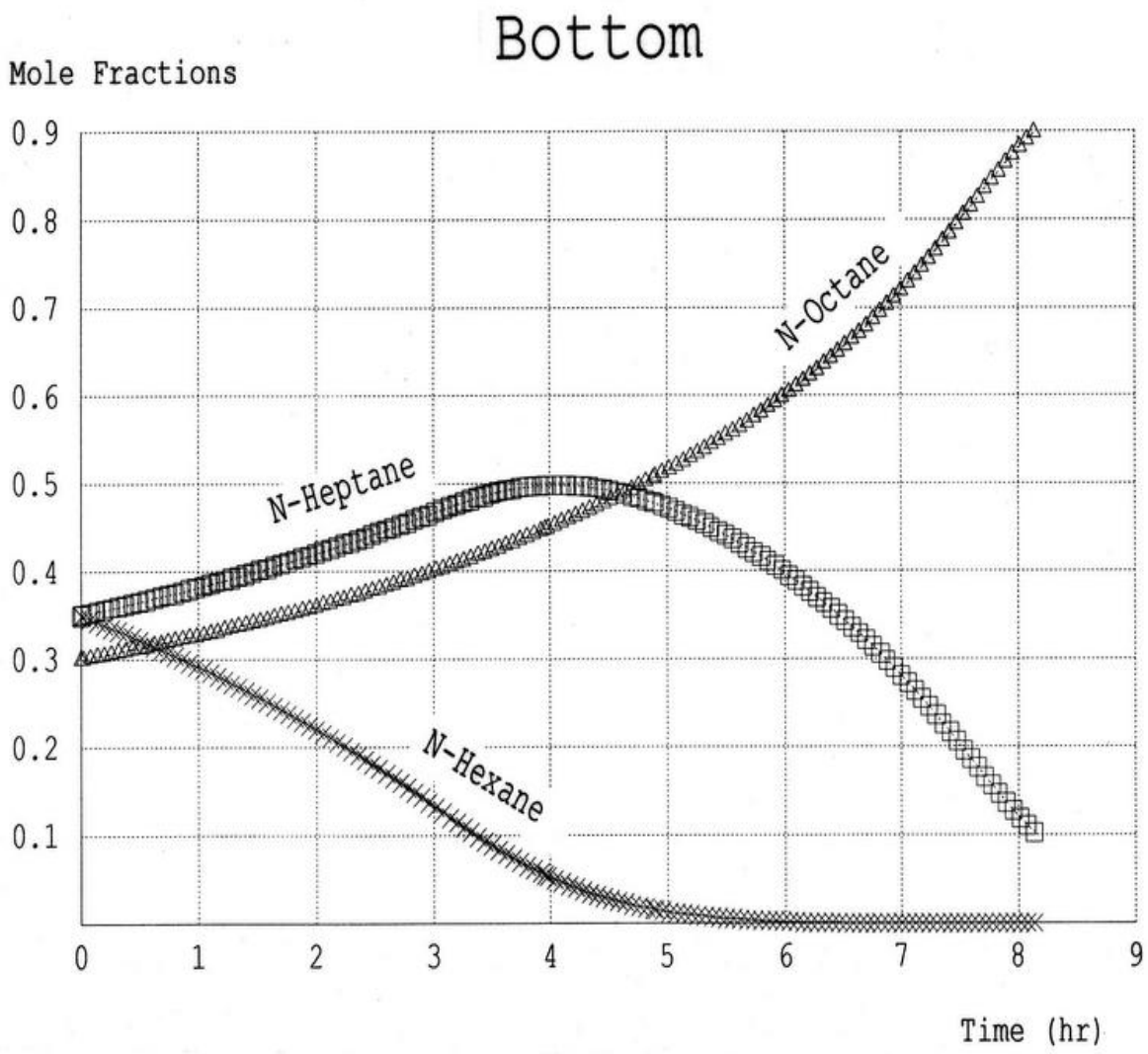
Exercise 13.26 (continued)

Analysis: (continued) No holdup case



Exercise 13.26 (continued)

Analysis: (continued) No holdup case



Exercise 13.27

Subject: Calculation of batch rectification of a four-component mixture by a method that accounts for holdup.

Given: Charge of 100 lbmol of 10 mol% propane (C3), 30 mol% n-butane (C4), 10 mol% n-pentane (C5), and 50 mol% n-hexane (C6). Batch rectification with 50 psia in condenser a column pressure drop of 2 psia. Column with the equivalent of 8 theoretical stages, plus a partial reboiler and a total condenser. Vapor boilup rate, $V = 40$ lbmol/h. Holdup of condenser-reflux drum = 1 ft^3. Holdup in the column is 0.10 ft^3 for each stage. Rectification campaign:

Step	Reflux ratio	Stop criterion
1	5	98 mol% C3 in accumulator
2	20	95 mol% C4 in instantaneous distillate
3	25	99.8 mol% C4 in accumulator
4	15	80 mol% C5 in instantaneous distillate
5	25	99 mol% C6 in final residue

Assumptions: SRK thermodynamics. Total reflux condition is established by time zero. Product compositions are in mol%.

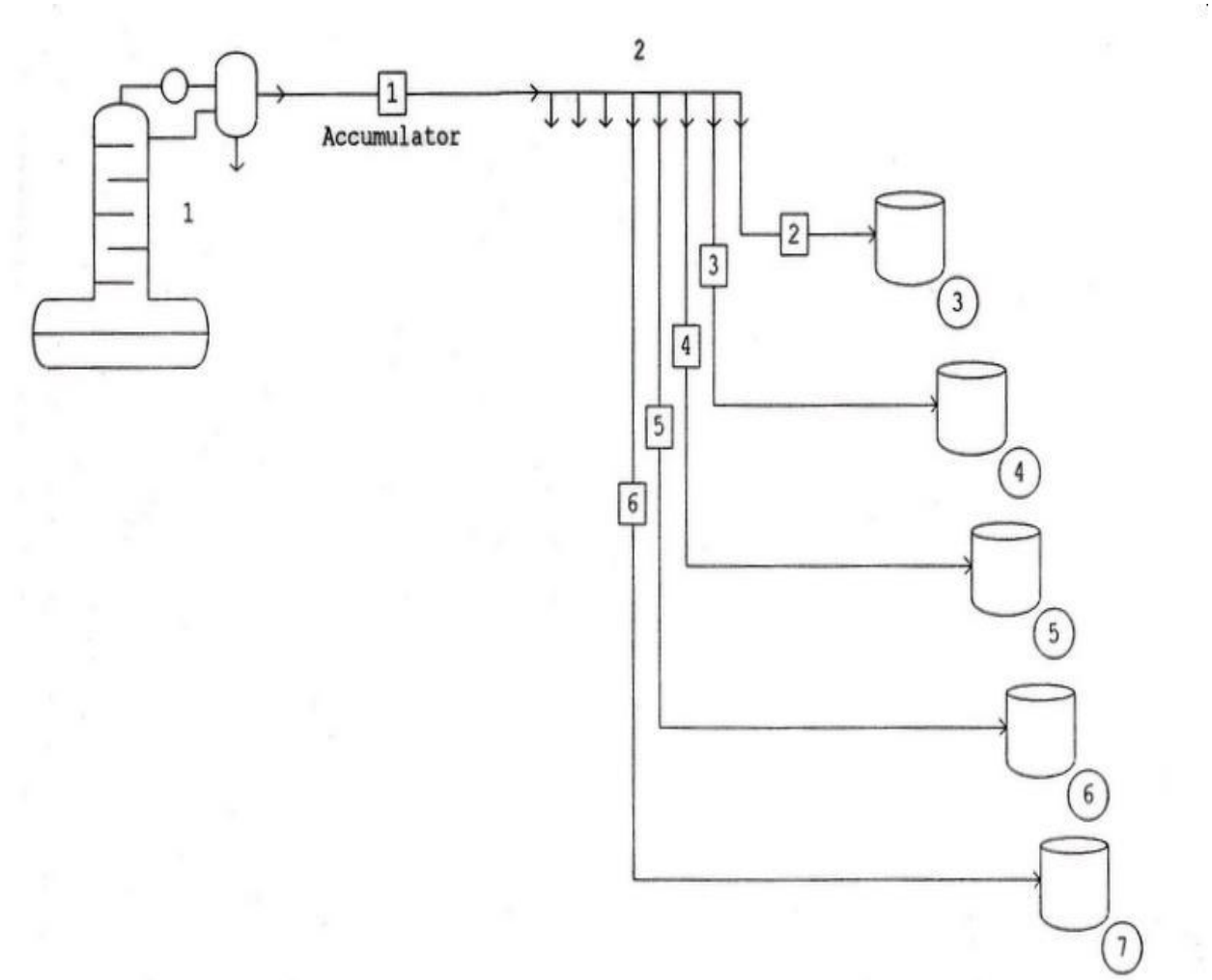
Find: (a) Time for rectification.
(b) Total amount of distillate produced.
A campaign that will get larger amounts of the main products (Cuts 1, 3, and final residue)

Analysis: Use the Batch distillation program of Chemcad to make the calculations. The flowsheet for Chemcad is shown below. Note that it includes the batch column (1), a time switch (2), and 5 tanks (3, 4, 5, 6, and 7).

The input data for Chemcad are as follows:
Batch column:
No. of stages = 10 (8 in column + reboiler + condenser)
No. of operation steps = 5
Total condenser
Condenser pressure =50 psia
Column pressure drop = 2 psia (52 psia in the boiler)
Holdup units in ft^3
Condenser holdup = 1 ft^3
Stage holdup = 0.1 ft^3 per stage (total of 0.8 ft^3)
Method of calculation = Inside-out

Exercise 13.27 (continued)

Analysis:



Exercise 13.27 (continued)

Analysis:

Operation parameters:

Step	**1**	**2**	**3**	**4**	**5**
Startup option	**Total reflux**	**Column content**	**Column content**	**Column content**	**Column content**
Tank no.	3	4	5	6	7
Reflux ratio	5	20	25	15	25
Boilup,lbmol/h	40	40	40	40	40
Step size, hr	0.02	0.02	0.05	0.02	0.02
Record frequency	3	3	3	3	3
Stop criterion	*x* of C3 in accum. = 0.98	*x* of C4 in instant. distillate = 0.95	*x* of C4 in accum. = 0.998	*x* of C5 in instant. distillate = 0.80	*x* of C6 in final residue = 0.99
Stop tolerance	0.0001	0.0001	0.0001	0.0001	0.0001

The results are as follows for the contents of tanks 3, 4, 5, 6, and 7 after Steps 1, 2, 3, 4, and 5, respectively, and the final residue:

Vessel	**Tank 3**	**Tank 4**	**Tank 5**	**Tank 6**	**Tank 7**	**Final residue**
Amount, lbmol	5.70	7.18	24.54	3.87	9.29	48.65
Mole fractions:						
C3	0.9766	0.6103	0.0022	0.0000	0.0000	0.0000
C4	0.0234	0.3897	0.9976	0.6031	0.0273	0.0000
C5	0.0000	0.0000	0.0002	0.3945	0.8399	0.0100
C6	0.0000	0.0000	0.0000	0.0024	0.1328	0.9900
Operation time, hr	0.62	2.88	12.3	1.34	5.65	22.79

(a) The total time for rectification = 22.79 hours.

(b) The total amount of distillates = 5.70+7.18+24.54+3.87+9.29 = 50.58 lbmol.

The above data indicate that the column and condenser holdup at the end of the campaign = 100 - 5.70 - 7.18 - 24.54 - 3.87 - 9.29 - 48.65 = 0.77 lbmol, which is relatively small.

The amount of C3 product (Step 1) is only 5.70/10.0 = 57% of the C3 in the feed.

The amount of C4 product (Step 3) is 24.54/30 = 81.8% of the C4 in the feed.

The amount of C6 (Step 5) in the final residue product = 48.65/50 = 97.3% of C6 in the feed.

Thus, there is room for improvement in the campaign, especially in the recovery of C3. The very high purity requirement for C4 probably makes it difficult to significantly increase the recovery of C4.

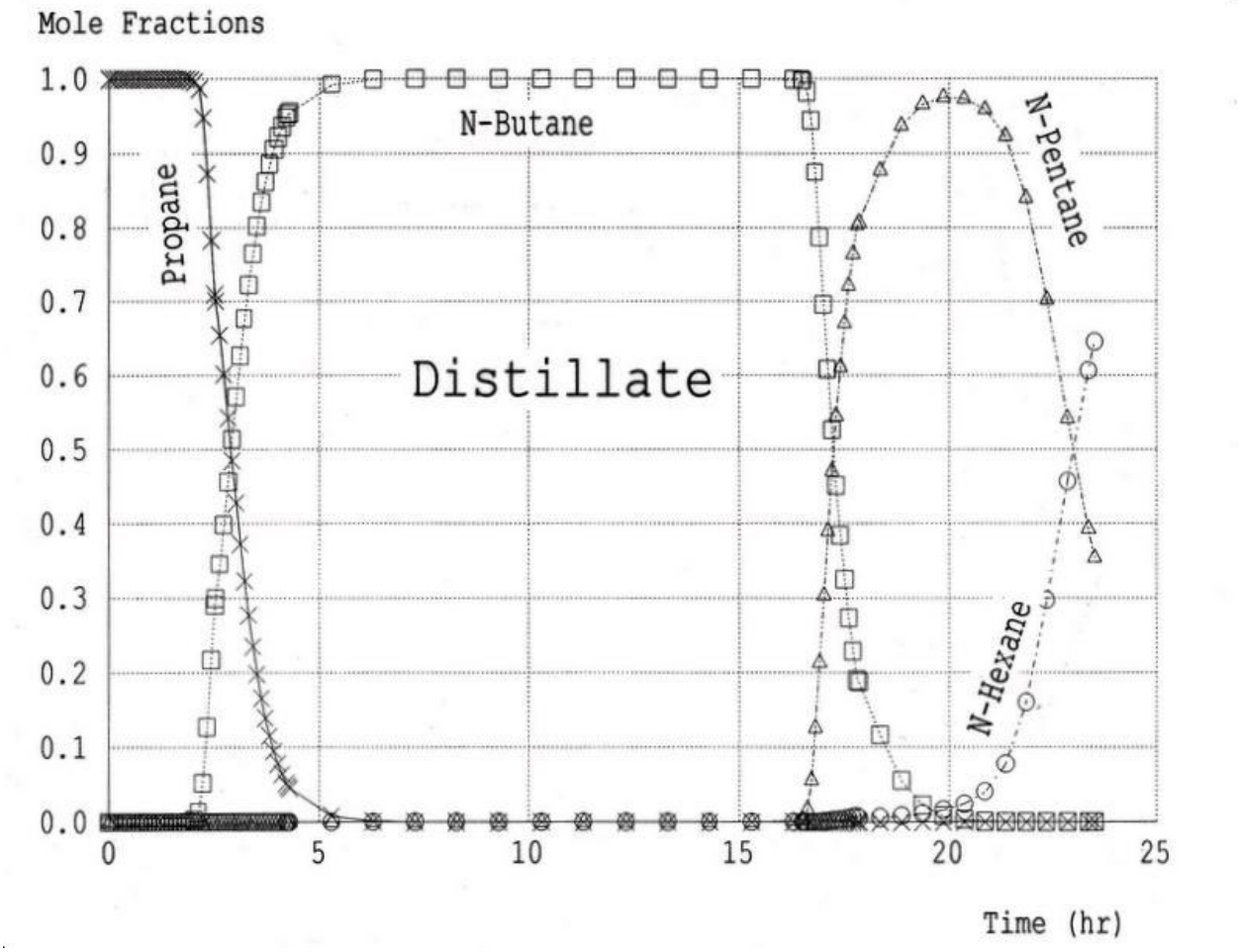
Exercise 13.27 (continued)

Analysis: (continued)

Try increasing the reflux ratio for Step 1 from 5 to 15, noting that although it will increase the time for rectification, the increase will be small because the time for Step 1 is small. The result for this change in reflux ratio is as follows:

(a) The total time for rectification = 2.50+1.76+12.25+1.32+5.70 = 23.53 hours, a small increase.

(b) The total amount of distillates = 8.89+4.10+24.45+3.81+9.37 = 50.62 lbmol. Of more importance is the amount of C3 cut (Step 1) is increased from 5.70 to 8.89 lbmol. The chart below shows the mole fractions in the instantaneous distillate with time.



Exercise 13.28

Subject: Stability and stiffness of batch rectification calculations

Given: Compositions, holdups, and total exiting flow rates for the top three equilibrium stages of a column separating a mixture of benzene (B), monochlorobenzene (MCB), and o-dichlorobenzene (DCB) at a time of 0.60 hour after total reflux conditions are established. Holdups in the reboiler and condenser-reflux drum.

Find: Using Eqs. (13-36) and (13-39) to estimate the liquid-phase mole fraction of benzene leaving Stage 2 from the top at 0.61 hour, using the explicit Euler method with a $\Delta t = 0.01$ h. If result is unreasonable, explain why using stability and stiffness considerations.

Analysis: Assume that over this small period of time (0.01 h) that the molar holdups on the stages do not change. Then, Eq. (13-36) becomes:

$$\frac{dx_{B,2}}{dt} = \left(\frac{L_1}{M_2}\right)x_{B,1} - \left[\frac{L_2 + K_{B,2}V_2}{M_2}\right]x_{B,2} + \left[\frac{K_{B,3}V_3}{M_2}\right]x_{B,3} \qquad (1)$$

From the given data, the K-values are: $K_{B,2} = 0.0449/0.0121 = 3.71$ and $K_{B,3} = 0.0331/0.00884 = 3.74$. Using other data in the given tables, with the explicit Euler discretization of Eq. (13-49),

$$\frac{dx_{B,2}}{dt} = \frac{\Delta x_{B,2}}{\Delta t} = \frac{\Delta x_{B,2}}{0.01} = \left(\frac{157.5}{0.01092}\right)(0.0276) - \left[\frac{158.0 + 3.71(209.0)}{0.01092}\right](0.0121) + \left[\frac{3.74(209.5)}{0.01092}\right](0.00884)$$

$$= 398.077 - 1034.251 + 634.286 = -1.8880$$

Therefore, $x_{B,2}$ at $t = 0.61$h = 0.0121 - 1.8880(0.01) = -0.00678

This negative value is unacceptable, so first determine stability. The criterion for stability is $\Delta t <$ or = 2 divided by the maximum eigenvalue. A rough estimate of the maximum eigenvalue is given by Eq. (13-52), where in this case, taking benzene, which has the highest K-value and using Stage 3 data where the holdup is the smallest,

$$|\lambda|_{max} = 2\left[\frac{L_3 + K_{B,3}V_3}{M_3}\right] = 2\left[\frac{158.1 + 3.74(209.5)}{0.01087}\right] = 173{,}300$$

Therefore, max. $\Delta t = 2/173{,}300 = 0.0000115$ h, which is much smaller than the value of 0.01 h. Therefore, we have instability.

Now check the stiffness ratio. Use Eq. (13-54), which requires estimations of $|\lambda|_{min}$ and $|\lambda|_{max}$.

From Eq. (13-53), where N+1 refers to the boiler and other quantities are estimated,

$$|\lambda|_{min} = \left[\frac{L_N + K_{DCB,N}V_{N+1}}{M_{N+1}}\right] = \left[\frac{158 + 1(210)}{66.4}\right] = 5.54$$

From Eq. (13-54), SR = $|\lambda|_{max} / |\lambda|_{min} = 173{,}300/5.54 = 31{,}300$, which is quite stiff.

Thus, in this case the explicit Euler method gives an unreasonable answer because we have instability and stiffness. It is probably best to switch to an implicit Euler method or a Gear method.

Exercise 13.29

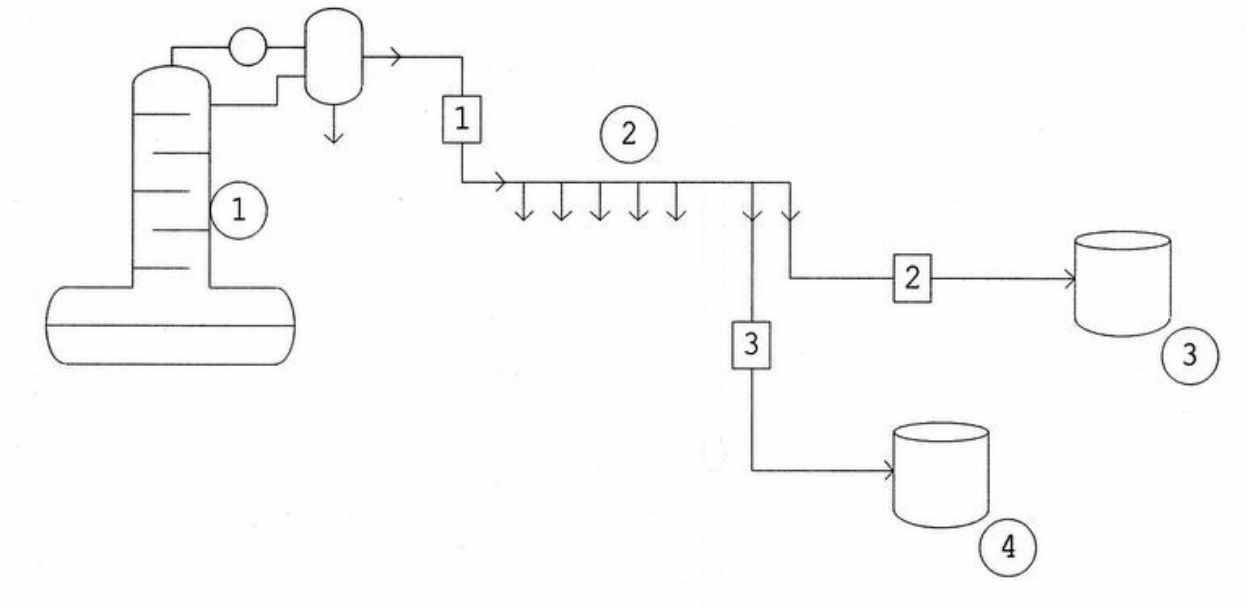
Subject: Calculation of batch rectification of a ternary mixture with a process-simulation program.

Given: Charge of 100 kmol of 30 mol% methanol, 30 mol% ethanol, and 40 mol% n-propanol at 120 kPa. Column with the equivalent of 10 theoretical stages, plus a still and a total condenser. Total reflux condition is established by time zero. UNIFAC method for liquid-phase activity coefficients. Column pressure drop is 8 kPa. Condenser pressure drop is 2 kPa. Two operation steps, each of:
15 hours duration at a distillate flow rate of 2 kmol/h and a reflux ratio of 10.

Assumptions: Negligible holdup in the column and the condenser system.

Find: Mole-fraction compositions and amounts of each of the 3 products.

Analysis: Use the Batch distillation program of Chemcad to make the calculations. The flowsheet below includes a batch column (1), a time switch (2), and 2 tanks (3 and 4).



The following pages are printouts of the input data and the results of the calculations by the Chemcad program. This is followed by a summary of the results for the three products.

Exercise 13.29 (continued)

Analysis: (continued)

Process Simulator Input Data:

Batch Distillation

Equip. No.	1
Name	
No. of stages	12
Operation steps	2
Cond pressure kPa	110.0000
Cond pres drop kPa	2.0000
Colm pres drop kPa	8.0000
Method	1
Top stage	1.0000
Last stage	1.0000
Current time h	29.9998

Batch column # 1

Batch Operation Parameters:

Step no.	1	2
Startup option:	1	0
Overhead tank #	3.0000	4.0000
First spec value	10.0000	10.0000
Second spec value	2.0000	2.0000
Step size (hr)	0.0500	0.0500
Record frequency	3.0000	3.0000
Stop value	15.0000	15.0000
Stop tolerance	0.0010	0.0010
Elapsed time hr	15.0000	15.0000
Condenser duty MJ	-11692.9570	-12721.7559
Reboiler duty MJ	11759.8145	12750.8223

Exercise 13.29 (continued)

Analysis: (continued)

Process-Simulator Results:

BATCH DISTILLATION 1 CALCULATION RESULTS

Operation Step 1:

Stream Name	Pot Charge	Accumulator	Pot Residue	Distillate
Temp C	0.0000	67.1626	90.8203	71.3872
Pres kPa	120.0000	110.0000	120.0000	110.0000
Enth MJ	0.00000	-7145.6	-19657.	-25.308
Vapor mole fraction	0.00000	0.00027257	0.00000	0.00000
Total kmol	100.0000	30.0000	70.0001	0.1000
Total kg	4747.1702	993.8202	3753.3550	3.8951
Total std L m3	5.9031	1.2423	4.6609	0.0049
Component mole fractions				
Methanol	0.300000	0.922668	0.033142	0.507786
Ethanol	0.300000	0.077292	0.395447	0.491842
N-Propanol	0.400000	0.000041	0.571411	0.000372

Operation Step 2:

Stream Name	Accumulator	Pot Residue	Distillate
Temp C	79.3095	100.7203	89.4478
Pres kPa	110.0000	120.0000	110.0000
Enth MJ	-8070.0	-11558.	-28.207
Vapor mole fraction	0.0019183	0.00000	0.00000
Total kmol	30.0000	40.0001	0.1000
Total kg	1371.3886	2381.9692	5.3989
Total std L m3	1.7199	2.9410	0.0067
Component mole fractions			
Methanol	0.077331	0.000000	0.000012
Ethanol	0.870718	0.038994	0.435241
N-Propanol	0.051951	0.961005	0.564747

Exercise 13.29 (continued)

Analysis: (continued)

Summary of Results:

Cut	Methanol-Rich	Ethanol-Rich	Propanol-Rich
Amount, kmol	30	30	40
Mole fractions:			
Methanol	0.923	0.077	0.000
Ethanol	0.077	0.871	0.039
n-Propanol	0.000	0.052	0.961

Exercise 13.30

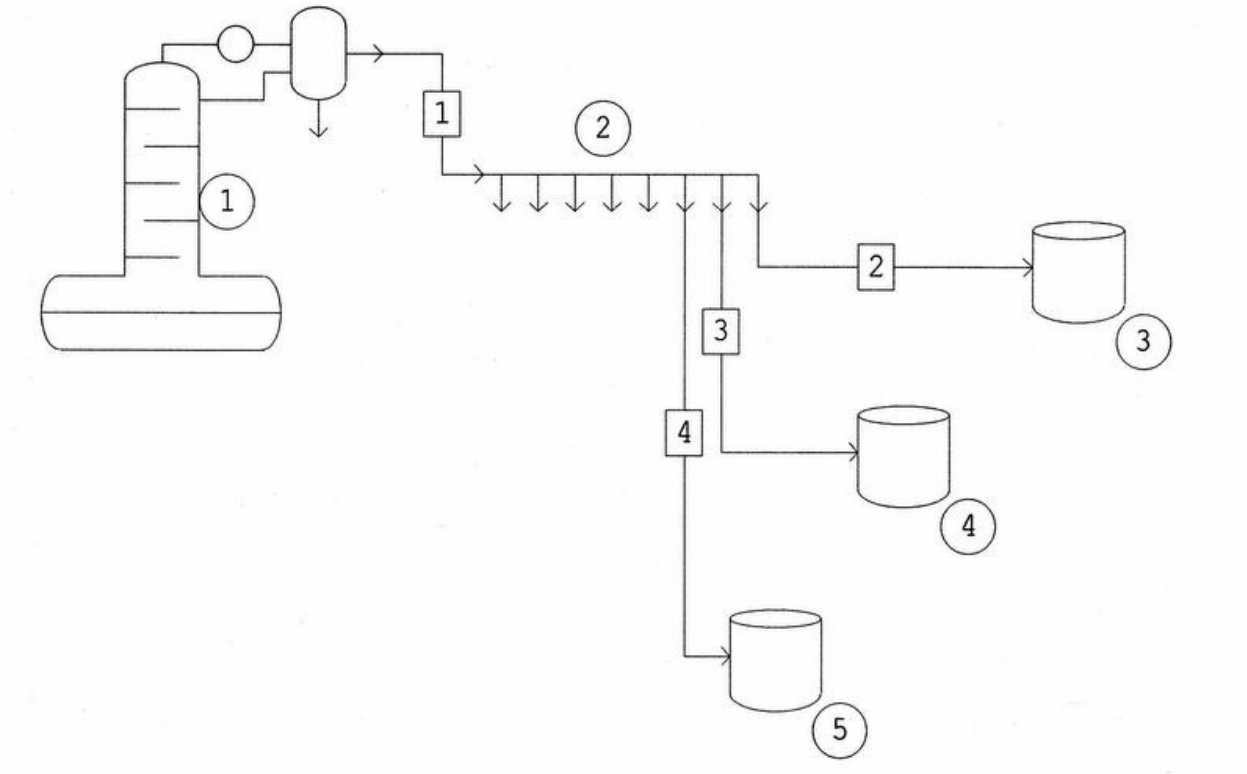
Subject: Calculation of batch rectification of a ternary mixture with a simulation program.

Given: Charge of 100 kmol of 30 mol% methanol, 30 mol% ethanol, and 40 mol% n-propanol at 120 kPa. Column with the equivalent of 10 theoretical stages, plus a still and a total condenser. Total reflux condition is established by time zero. UNIFAC method for liquid-phase activity coefficients. Column pressure drop is 8 kPa. Condenser pressure drop is 2 kPa. Three operation steps, each of:
at a distillate flow rate of 2 kmol/h and a reflux ratio of 10.
Duration of the operation steps: Step 1: 13 hours, Step 2: 4 hours, Step 3: 13 hours

Assumptions: Negligible holdup in the column and the condenser system.

Find: Mole-fraction compositions and amounts of each of the 4 products.

Analysis: Use the Batch distillation program of Chemcad to make the calculations. The flowsheet below includes a batch column (1), a time switch (2), and 2 tanks (3, 4, and 5).



The following pages are printouts of the input data and the results of the calculations by the Chemcad program. This is followed by a summary of the results for the three products.

Exercise 13.30 (continued)

Analysis: (continued)

Process Simulator Input Data:

Batch Distillation

Equip. No.	1
Name	
No. of stages	12
Operation steps	3
Cond pressure kPa	110.0000
Cond pres drop kPa	2.0000
Colm pres drop kPa	8.0000
Method	1
Top stage	1.0000
Last stage	1.0000
Current time h	29.9998

Batch column # 1

Batch Operation Parameters:

Step no.	1	2	3
Startup option:	1	0	0
Overhead tank #	3.0000	4.0000	5.0000
First spec value	10.0000	10.0000	10.0000
Second spec value	2.0000	2.0000	2.0000
Step size (hr)	0.0500	0.0500	0.0500
Record frequency	3.0000	3.0000	3.0000
Stop value	13.0000	4.0000	13.0000
Stop tolerance	0.0010	0.0010	0.0010
Elapsed time hr	13.0000	4.0000	13.0000
Condenser duty MJ	-10090.9746	-3256.7014	-11067.0410
Reboiler duty MJ	10147.2510	3273.3464	11090.0430

Exercise 13.30 (continued)

Analysis: (continued)

Process Simulator Results:

BATCH DISTILLATION 1 CALCULATION RESULTS

Operation Step 1:

Stream Name	Pot Charge	Accumulator	Pot Residue	Distillate
Temp C	0.0000	66.8739	89.1927	67.7634
Pres kPa	120.0000	110.0000	120.0000	110.0000
Enth MJ	0.00000	-6158.1	-20655.	-24.083
Vapor mole fraction	0.00000	0.00000	0.00000	0.00000
Total kmol	100.0000	26.0000	74.0001	0.1000
Total kg	4747.1702	847.7917	3899.3834	3.4150
Total std L m3	5.9031	1.0594	4.8437	0.0043
Component mole fractions				
Methanol	0.300000	0.959711	0.068210	0.849842
Ethanol	0.300000	0.040273	0.391256	0.150087
N-Propanol	0.400000	0.000016	0.540535	0.000071

Operation Step 2:

Stream Name	Accumulator	Pot Residue	Distillate
Temp C	71.2548	92.1130	75.5861
Pres kPa	110.0000	120.0000	110.0000
Enth MJ	-2021.3	-18617.	-26.271
Vapor mole fraction	0.0013507	0.00000	0.00000
Total kmol	8.0000	66.0001	0.1000
Total kg	310.4307	3588.9537	4.2821
Total std L m3	0.3890	4.4547	0.0054
Component mole fractions			
Methanol	0.518362	0.013645	0.232421
Ethanol	0.481228	0.380350	0.766707
N-Propanol	0.000410	0.606005	0.000872

Exercise 13.30 (continued)

Analysis: (continued)

Process Simulator Results:

Operation Step 3:

Stream Name	Accumulator	Pot Residue	Distillate
Temp C	80.3932	100.7203	89.4478
Pres kPa	110.0000	120.0000	110.0000
Enth MJ	-7036.2	-11558.	-28.207
Vapor mole fraction	0.0010347	0.00000	0.00000
Total kmol	26.0000	40.0001	0.1000
Total kg	1206.9864	2381.9692	5.3989
Total std L m3	1.5137	2.9410	0.0067
Component mole fractions			
Methanol	0.034638	0.000000	0.000012
Ethanol	0.905514	0.038994	0.435241
N-Propanol	0.059848	0.961005	0.564747

Summary of Results:

Product	Methanol-Rich	Slop Cut	Ethanol-Rich	Propanol-Rich
Amount, kmol	26	8	26	40
Mole fractions:				
Methanol	0.960	0.518	0.035	0.000
Ethanol	0.040	0.481	0.906	0.039
n-Propanol	0.000	0.001	0.059	0.961

Exercise 13.31

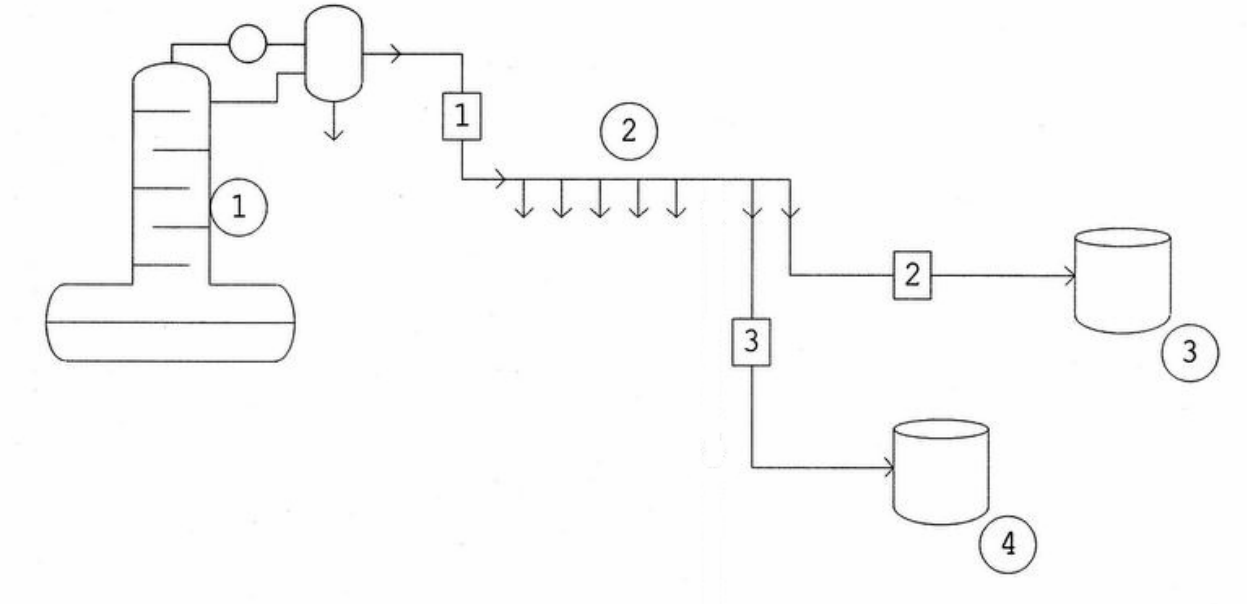
Subject: Calculation of batch rectification of a ternary mixture with a process simulator

Given: Charge of 100 kmol of 45 mol% acetone, 30 mol% chloroform, and 25 mol% benzene. Batch rectification at 101.3 kPa. Column with the equivalent of 10 theoretical stages, plus a boiler and a total condenser. Total reflux condition is established by time zero. Use UNIFAC for liquid-phase activity coefficients. Two operation steps, each at a distillate flow rate of 2 kmol/h and a reflux ratio of 10, as follows:
Step 1: 13.3 h
Step 2: 24.2 h

Assumptions: No pressure drop and no holdup

Find: Mole-fraction compositions and amounts of each of the 3 products.

Analysis: Use the Batch distillation program of Chemcad to make the calculations. The flowsheet below includes a batch column (1), a time switch (2), and 2 tanks (3 and 4).



The following pages are printouts of the input data and the results of the calculations by the Chemcad program. This is followed by a summary of the results for the three products.

Exercise 13.31 (continued)

Analysis: (continued)

Process Simulator Input Data:

Batch Distillation

Equip. No.	1
Name	
No. of stages	12
Operation steps	2
Cond pressure kPa	101.3000
Method	1
Top stage	1.0000
Last stage	1.0000
Current time h	37.4997

Batch column # 1

Batch Operation Parameters:

Step no.	1	2
Startup option:	1	0
Overhead tank #	3.0000	4.0000
First spec value	10.0000	10.0000
Second spec value	2.0000	2.0000
Step size (hr)	0.0500	0.0500
Record frequency	3.0000	3.0000
Stop value	13.3000	24.2000
Stop tolerance	0.0010	0.0010
Elapsed time hr	13.3000	24.2000
Condenser duty MJ	-8730.8174	-15727.4492
Reboiler duty MJ	8729.7100	15745.1777

Exercise 13.31 (continued)

Analysis: (continued)

Process Simulator Results:

BATCH DISTILLATION 1 CALCULATION RESULTS

Operation Step 1:

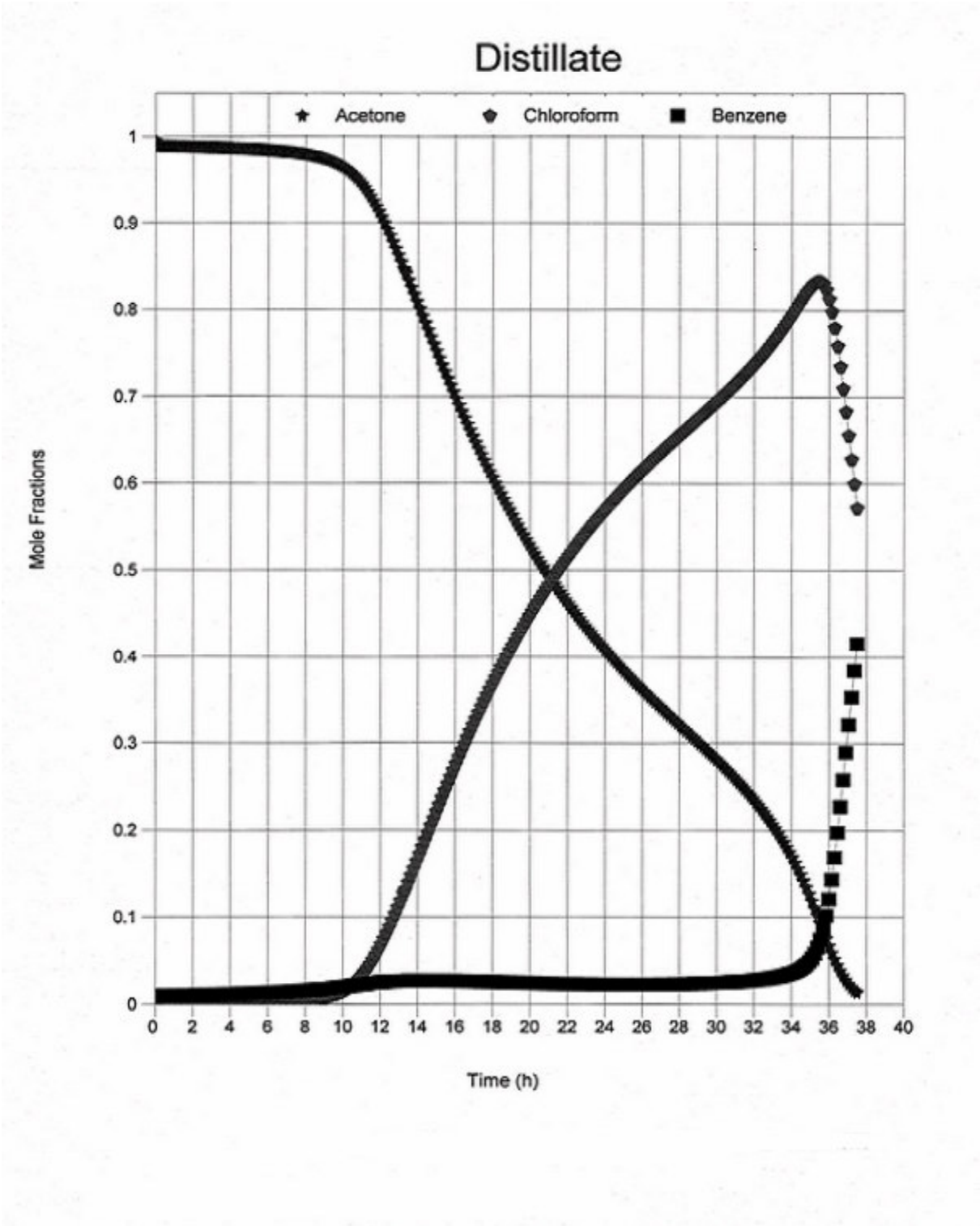
Stream Name	Pot Charge	Accumulator	Pot Residue	Distillate
Temp C	0.0000	56.5945	67.3558	58.6955
Pres kPa	101.3000	101.3000	101.3000	101.3000
Enth MJ	0.00000	-6325.0	-7149.3	-22.152
Vapor mole fraction	0.00000	2.1319E-005	0.00000	0.00000
Total kmol	100.0000	26.6000	73.4001	0.1000
Total kg	8147.7601	1581.7404	6566.0277	6.6544
Total std L m3	7.8634	1.9445	5.9188	0.0074
Component mole fractions				
Methanol	0.000000	0.000000	0.000000	0.000000
Ethanol	0.000000	0.000000	0.000000	0.000000
N-Propanol	0.000000	0.000000	0.000000	0.000000
Acetone	0.450000	0.966853	0.262693	0.844038
Benzene	0.250000	0.015701	0.334909	0.026563
Chloroform	0.300000	0.017446	0.402397	0.129399

Operation Step 2:

Stream Name	Accumulator	Pot Residue	Distillate
Temp C	63.6598	78.4298	69.3538
Pres kPa	101.3000	101.3000	101.3000
Enth MJ	-8089.8	958.23	-5.4025
Vapor mole fraction	0.00000	0.00000	0.00000
Total kmol	48.4000	25.0001	0.1000
Total kg	4511.8293	2054.2038	10.1428
Total std L m3	3.7327	2.1861	0.0083
Component mole fractions			
Methanol	0.000000	0.000000	0.000000
Ethanol	0.000000	0.000000	0.000000
N-Propanol	0.000000	0.000000	0.000000
Acetone	0.398006	0.000729	0.013459
Benzene	0.042674	0.900675	0.415034
Chloroform	0.559321	0.098596	0.571507

Exercise 13.31 (continued)

Analysis: (continued)



Exercise 13.31 (continued)

Analysis: (continued)

Summary of Results:

Cut	Acetone-Rich	Slop Cut	Benzene-Rich
Amount, kmol	26.6	48.4	25
Mole fractions:			
Acetone	0.967	0.398	0.001
Benzene	0.016	0.043	0.901
Chloroform	0.017	0.559	0.098

Note, that a chloroform-rich cut is not obtained.

Exercise 13.32

Subject: Improving a batch distillation campaign to eliminate or reduce slop cuts.

Given: Conditions of Example 13.11. A charge of 150 kmol of equimolar n-hexane (C6), n-heptane (C7), and n-octane (C8). Batch rectification at 1 atm. Column with the equivalent of 5 theoretical stages, plus a partial reboiler and a total condenser. Vapor boilup rate, $V = 100$ kmol/h. Initial campaign consists of four operation steps, all at a reflux ratio of 8, to produce five products:

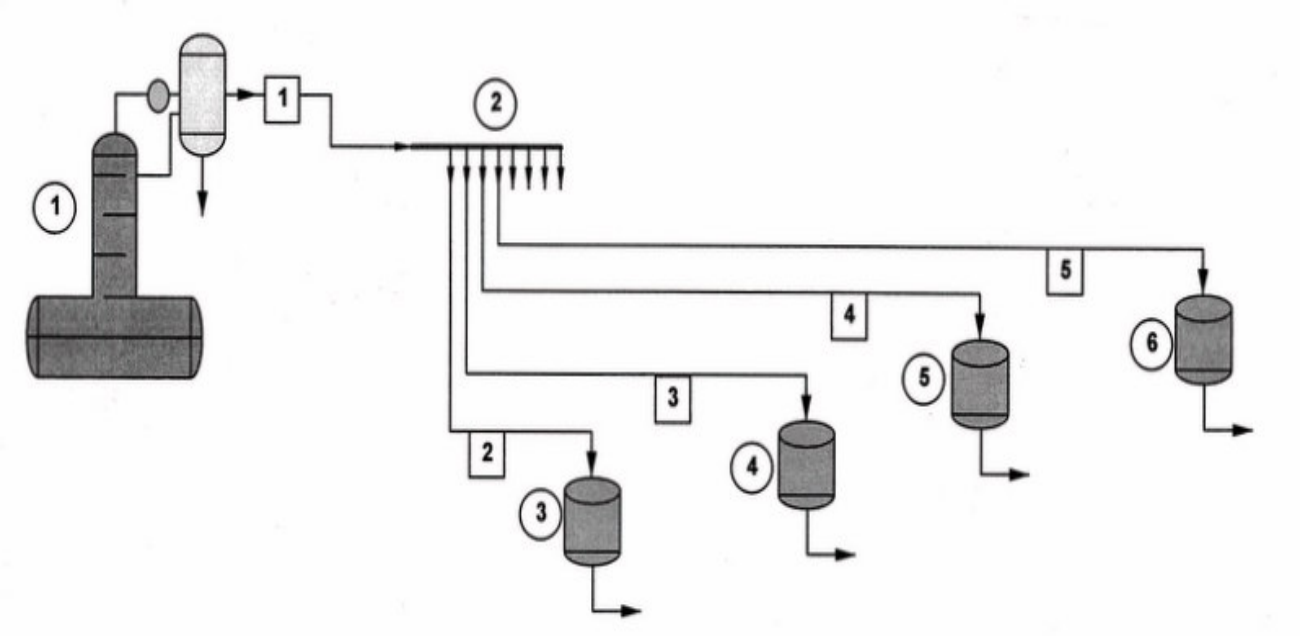
1. 95 mol% C6, 2. Slop cut one, 3. 90 mol% C7, 4. Slop cut two, 5. 95 mol% C8

Assumptions: No holdup and no pressure drop. Total reflux condition is established by time zero. Reflux ratio is held constant during each operation step.

Find: (a) A reflux ratio above 8 that will eliminate the second slop cut.

(b) A revised termination specification for the second step that will reduce the amount of the first slop cut, without failing to meet all three product specifications.

Analysis: Use the Batch distillation program of Chemcad to make the calculations. The flowsheet for Chemcad is shown below. Note that it includes the batch column (1), a time switch (2), and 4 tanks (3, 4, 5, and 6).



Exercise 13.32 (continued)

Analysis (continued):

(a) A number of reflux ratios can accomplish the goal of eliminating the second slop cut, which, from Example 13.11 for a reflux ratio of 8 for all 4 steps, is a total of only 4.38 kmols out of the 150 kmol charge. For only three steps, each with a reflux ratio of 12, the Chemcad input data and results are as follows:

Batch column:
No. of stages = 7 (5 in column + reboiler + condenser)
No. of operation steps = 3 (no second slop cut)
Total condenser
Condenser pressure = 1 atm
Condenser holdup = 0
Stage holdup = 0
Method of calculation = Inside-out

Operation parameters:

Step	1	2	3
Startup option	Total reflux	Column content	Column content
Tank no.	3	4	5
First specification	Reflux ratio = 12	Reflux ratio = 12	Reflux ratio = 12
Second specification	Boilup rate = 100 kmol/h	Boilup rate = 100 kmol/h	Boilup rate = 100 kmol/h
Step size, hr	0.01	0.01	0.01
Record frequency	10	5	5
Stop criterion	Mole fraction of C6 in accumulator = 0.95	Amount in the accumulator = 6 kmol	Mole fraction of C8 in residue = 0.95
Stop tolerance	0.001	0.001	0.001

Results:

C6 product: 49.15 kmols of 95 mol% C6 and 5 mol% C7
Slop cut 1: 6.05 kmols of 38.6 mol% C6, 60.6 mol% of C7, and 0.8 mol% C8.
C7 product: 46.1 kmols of 90 mol% C7, 2 mol% C6, and 8 mol% C8.
C8 product: 48.7 kmols of 95 mol% C8 and 5 mol% C7.

Exercise 13.32 (continued)

Analysis (continued):

(b) A number of changes can accomplish the goal of reducing the amount of the first slop cut, which, from Example 13.11 for a reflux ratio of 8 for all 4 steps, is a total of 16.67 kmols out of the 150 kmol charge. For three steps, each with a reflux ratio of 12, the Chemcad input data and results are as follows, where the amount of the first slop cut is reduced from an amount of 6 kmols in part (a) to 5 kmols.

Batch column:
No. of stages = 7 (5 in column + reboiler + condenser)
No. of operation steps = 3 (no second slop cut)
Total condenser
Condenser pressure = 1 atm
Condenser holdup = 0
Stage holdup = 0
Method of calculation = Inside-out

Operation parameters:

Step	1	2	3
Startup option	Total reflux	Column content	Column content
Tank no.	3	4	5
First specification	Reflux ratio = 12	Reflux ratio = 12	Reflux ratio = 12
Second specification	Boilup rate = 100 kmol/h	Boilup rate = 100 kmol/h	Boilup rate = 100 kmol/h
Step size, hr	0.01	0.01	0.01
Record frequency	10	5	5
Stop criterion	Mole fraction of C6 in accumulator = 0.95	Amount in the accumulator = 5 kmol	Mole fraction of C8 in residue = 0.95
Stop tolerance	0.001	0.001	0.001

Results:

C6 product: 49.15 kmols of 95 mol% C6 and 5 mol% C7
Slop cut 1: 5.00 kmols of 41.7 mol% C6, 57.6 mol% of C7, and 0.7 mol% C8.
C7 product: 47.2 kmols of 89.6 mol% C7, 2.6 mol% C6, and 7.8 mol% C8.
C8 product: 48.7 kmols of 94.9 mol% C8 and 5.1 mol% C7.

Exercise 14.1

Subject: Differences of membrane separations from some other separation operations.

Find: How membrane separations differ from:
(a) Absorption and stripping
(b) Distillation
(c) Liquid-liquid extraction
(d) Extractive distillation

Analysis: In general, membrane separations differ from absorption, stripping, distillation, liquid-liquid extraction, and extractive distillation in the following respects:

1. The separating agent for membrane separations is a semi-permeable membrane.
2. Rate-based modeling must be used for membrane separations because an equilibrium model does not apply.

Compared to distillation and extractive distillation, membranes usually can not achieve sharp separations

Compared to liquid-liquid extraction, absorption, and stripping, membranes produce products that are usually miscible, rather than immiscible.

Exercise 14.2

Subject: Calculation of permeabilities of hydrogen and methane in barrer units.

Given: Feed gas at 450 psia and 200°F, with the following component flow rates in lbmol/h: H_2 1,872.3, CH_4 193.1, C_2 11.4, Benzene 4.8, Toluene 4.2, and p-Xylene 0.6. Membrane system has a total area of 16,000 ft^2, with a thickness of 0.3 microns. The permeate exits at 50 psia with 1,685.1 lbmol/h of H_2 and 98.8 lbmol/h of CH_4. The retentate exits at 450 psia.

Assumptions: Mass transfer driving force based on the difference between the average partial pressure of the feed and retentate, minus the partial pressure of the permeate.

Find: The permeabilities of H_2 and CH_4 in barrer units.

Analysis: Use Eq. (14-1) and the definition of the barrer,
1 barrer = 10^{-10} cm^3 gas (STP of 0°C and 1 atm)-cm/(cm^2-s-cm^2 Hg pressure head)
The total feed flow rate = 2086.3 lbmol/h. The permeate rate = 1783.9 lbmol/h.
The retentate flow rate = 2086.3 - 1783.9 = 302.4 lbmol/h.
Hydrogen: Flux through the membrane = N_{H2} = 1,685.1/16,000 = 0.1053 lbmol/h-ft^2
Partial pressure driving force =

$$\left(\Delta p_{H_2}\right)_{avg} = 450\left(\frac{\frac{1872.3}{2086.3}+\frac{187.2}{302.4}}{2}\right) - 50\left(\frac{1685.1}{1783.9}\right) = 341.2 - 47.2 = 294 \text{ psi}$$

From Eq. (14-1), permeability = $P_{M_{H_2}} = \frac{N_{H_2} l_M}{\left(\Delta p_{H_2}\right)_{avg}} = \frac{0.1053(0.3)}{294} = 1.075\times10^{-4} \frac{\text{lbmol - µm}}{\text{h - ft}^2 - \text{psi}}$

To convert to barrer, use: 0.4536 kmol/lbmol, 22.42 x 10^6 cm^3 (STP)/kmol, 10^{-4} cm/µm, 3600 s/h, 9.29 x 10^2 cm^2/ft^2, and 5.17 cm Hg/psi. Thus,

$$P_{M_{H_2}} = 1.075\times10^{-4}\left[\frac{(0.4536)(22.42\times10^6)(10^{-4})}{(9.29\times10^2)(3600)(5.17)}\right] = 1.075\times10^{-4}\left[5.882\times10^{-5}\right] =$$

$$6.32\times10^{-9} \frac{\text{cm}^3\text{(STP)-cm}}{\text{cm}^2\text{-s-cm Hg}} = 63.2 \text{ barrer}$$

Methane: Flux through the membrane = N_{CH4} = 98.8/16,000 = 0.00618 lbmol/h-ft^2

$$\left(\Delta p_{CH_4}\right)_{avg} = 450\left(\frac{\frac{193.1}{2086.3}+\frac{94.3}{302.4}}{2}\right) - 50\left(\frac{98.8}{1783.9}\right) = 91.0 - 2.8 = 88.2 \text{ psi}$$

$$P_{M_{CH_4}} = \frac{N_{CH_4} l_M}{\left(\Delta p_{CH_4}\right)_{avg}} = \frac{0.00618(0.3)}{88.2}\left[\frac{5.882\times10^{-5}}{10^{-10}}\right] = 12.4 \text{ barrer}$$

Exercise 14.3

Subject: Separation of N_2 from CH_4 by an asymmetric polyimide polymer membrane.

Given: Feed gas of 200 kmol/h of N_2 and 800 kmol/h of CH_4 at 5500 kPa and 30°C. Permeances are 50,000 barrer/cm for N_2 and 10,000 barrer/cm for CH_4. Retentate leaves at 5,450 kPa and 30°C, containing 20 kmol/h of N_2, while permeate leaves at 100 kPa and 30°C, containing 180 kmol/h of N_2.

Assumptions: Diffusion driving force based on arithmetic average partial pressures of the feed and retentate on the feed side, and based on the permeate product on the permeate side.

Find: Membrane surface are in m_2. CH_4 flow rate in the permeate in kmol/h.

Analysis: From Eq. (14-1),

$$n_{N_2} = 180 \text{ kmol/h} = A_M \left(\overline{P_M}\right)_{N_2} \left(\Delta P_{N_2}\right)_{avg} \quad \text{and} \quad n_{CH_4} = A_M \left(\overline{P_M}\right)_{CH_4} \left(\Delta P_{CH_4}\right)_{avg}$$

Convert permeances in barrer/cm to kmol/m^2-h-kPa:
From Section 14.1, 1 barrer/cm = 10^{-10} cm^3(STP)/cm^2-s-cmHg
Conversion factors: 22.42 x 10^6 cm^3(STP)/kmol, 10^{-4} m^2/cm^2, 3600 s/h, and 1.333 kPa/cmHg

$$\text{Therefore, 1 barrer/cm} = \frac{1\times10^{-10}(3600)}{(22.42\times10^6)(10^{-4})(1.333)} = 1.205\times10^{-10}\ \frac{\text{kmol}}{\text{m}^2\text{-h-kPa}}$$

$$\left(\overline{P_M}\right)_{N_2} = 50{,}000(1.205\times10^{-10}) = 6.03\times10^{-6}\ \frac{\text{kmol}}{\text{m}^2\text{-h-kPa}}$$

$$\left(\overline{P_M}\right)_{CH_4} = 10{,}000(1.205\times10^{-10}) = 1.21\times10^{-6}\ \frac{\text{kmol}}{\text{m}^2\text{-h-kPa}}$$

Let x = kmol/h of CH_4 in permeate. Then 800 - x = kmol/h of CH_4 in retentate.

$$N_{N_2} = \frac{n_{N_2}}{A_M} = \frac{180}{A_M} = 6.03\times10^{-6}\left(\Delta P_{N_2}\right)_{avg} \qquad (1)$$

$$N_{CH_4} = \frac{n_{CH_4}}{A_M} = \frac{x}{A_M} = 1.21\times10^{-6}\left(\Delta P_{CH_4}\right)_{avg} \qquad (2)$$

$$\left(\Delta P_{N_2}\right)_{avg} = \frac{0.2(5500) + 5450\left(\frac{20}{820-x}\right)}{2} - 100\left(\frac{180}{180+x}\right) \qquad (3)$$

$$\left(\Delta P_{CH_4}\right)_{avg} = \frac{0.8(5500) + 5450\left(\frac{800-x}{820-x}\right)}{2} - 100\left(\frac{x}{180+x}\right) \qquad (4)$$

Combining Eqs. (1) and (3), and (2) and (4) and solving the resulting two nonlinear equations, x = 281 kmol/h of CH_4 in the permeate and the membrane area = 48,800 m^2.

$$\left(\Delta P_{N_2}\right)_{avg} = 612 \text{ kPa} \quad \text{and} \quad \left(\Delta P_{CH_4}\right)_{avg} = 4760 \text{ kPa}$$

Exercise 14.4

Subject: Hollow-fiber module

Given: Hollow fibers, each 42 microns i.d., 85 microns o.d., and 1.2 m long in a membrane module with 4,000 ft^2 of membrane surface area based on the i.d.

Assumptions: Module is a right circular cylinder in shape.

Find: (a) Number of hollow fibers in the module.
(b) Diameter of the module if fibers on a square spacing of 120 microns center to center.
(c) Membrane surface area per unit volume of module (packing density) in m^2/m^3.
Compare results to Table 14.4.

Analysis:

(a) For one fiber, the inside surface area = $A_i = \pi D_i L = 3.14(42/10^6)(1.2) = 0.000158$ m^2 or $0.000158/(9.29 \times 10^{-2}) = 0.001704$ ft^2. Therefore, number of fibers = $N = 4000/0.001704 =$ 2,350,000 fibers.

(b) For square spacing of 120 microns center to center, each fiber occupies a cross-sectional area of 120 by 120 microns or $120(120)/10^{12} = 14.4 \times 10^{-9}$ m^2. For 2,350,000 fibers, cross-sectional area of the membrane module = $2{,}350{,}000(14.4 \times 10^{-9}) = 0.0338$ $m^2 = 338$ cm^2. If the area is circular, the diameter of the module = $[4(338)/3.14]^{1/2} = 20.8$ cm.

(c) The volume of the module for a length of 1.2 m = $0.0338(1.2) = 0.0406$ m^3.
The packing density = membrane surface area based on the inside diameter/unit module volume. Thus, the packing density = $0.000158(2{,}350{,}000)/0.0406 = 9{,}150$ m^2/m^3. Table 14.4 gives a range of 500 to 9,000 m^2/m^3 for a hollow-fiber module.

Exercise 14.5

Subject: Geometry of a spiral-wound membrane module.

Given: Module of 0.3 m diameter (D) and 3 m length (L). Packing density = 500 m^2/m^3.

Assumptions: Collection tube of 1 cm in diameter.

Find: Center to center spacing of membrane in the spiral.

Analysis: Membrane volume = $V = \pi D^2 L/4 = 3.14(0.3)^2 3/4 = 0.212$ m^3.
Membrane area = membrane volume x packing density = 0.212(500) = 106 m^2.
Length around the spiral = 106/3 = 35.3 m
Circumference of outer circle = πD = 3.14(0.3) = 0.943 m
Circumference of inner circle = 3.14(0.01) = 0.0314 m
Average circumference = (0.943 + 0.0314)/2 = 0.487 m
Number of turns of the spiral = length around spiral/aver. circumference = 35.3/0.487 = 72.5
Call it 72 turns Radial distance of the turns = (0.3 - 0.01)/2 = 0.145 m
Center to center distance between turns = 0.145/72 = 0.002 m or 2 mm.

Exercise 14.6

Subject: Module volume and packing density of a monolithic membrane element.

Given: Element of 0.85 m length, with 19 flow channels (see Fig. 14.4d) of 0.5 cm inside diameter each. 9 elements per module.

Assumptions: Center to center triangular spacing of holes = l = 0.5 cm.

Find: (a) Module volume in m^3.
(b) Packing density in m^2/m^3, with comparison to Table 14.4.

Analysis: Each equilateral triangle of 0.5 cm includes one-sixth of a hole at each apex or 50% of the area of one hole. The area of each triangle = 0.433 l^2 = 0.433$(0.5)^2$ = 0.1083 cm^2. The number of triangles within the area covered by the holes (that is, excluding the borders) = 24. For the borders we might assume that the triangular spacing extends to the edges of the monolith. If so, we add 30 more triangles, giving a total of 54. Then, the total cross-sectional area of one element = 54(0.1083) = 5.85 cm^2.
(a) Module volume for 9 elements = $9(5.85)(0.85)/(10^4)$ = 0.00448 m^2
(b) Membrane area of one element = $3.14(0.5)(19)(0.85)/(10^2)$ = 0.253 m^2
Module membrane area for 9 elements = 9(0.253) = 2.28 m^2
Packing density = 2.28/0.00448 = 508 m^2/m^3. This is higher than given in Table 14.4.

Exercise 14.7

Subject: Passage of water at 70°C through a porous polyethylene membrane by a pressure differential

Given: Membrane of 25% porosity, with 0.3 μm diameter pores and a tortuosity of 1.3. Pressures on either side of the membrane are 500 kPa and 125 kPa.

Assumptions: Assume membrane is 1 micron thick and flow is fully developed laminar flow.

Find: Flow rate of water in m^3/m^2-day = Q/A_M

Analysis: Provided that the flow is laminar and fully developed, Eq. (14-) applies, with a correction for the tortuosity:

$$\frac{Q}{A_M} = \frac{N}{\rho} = \frac{\varepsilon D^2 (P_0 - P_L)}{32 \mu l_M \tau} \qquad (1)$$

At 70°C, μ of water = 0.42 cP or (0.42)(0.001) = 0.00042 Pa-s and ρ = 1000 kg/m^3
P_0 = 500 kPa = 500,000 Pa and P_L = 125 kPa = 125,000 Pa
ε = 0.25, D = 0.3 μm = 3 x 10^{-7} m, l_M = 1 x 10^{-6} m, and τ = 1.3.

Substitution into Eq. (1) gives:

$$\frac{Q}{A_M} = \frac{N}{\rho} = \frac{(0.25)(3\times10^{-7})^2 (500{,}000 - 125{,}000)}{32(0.42\times10^{-3})(1\times10^{-6})(1.3)}(3600)(24) = 41{,}700 \text{ m}^3/\text{m}^2\text{-day}$$

Now check the Reynolds number.
Velocity in the pore from Eq. (14.2) =

$$v = \frac{D^2}{32\mu l_M}(P_0 - P_L) = \frac{(3\times10^{-7})^2 (500{,}000 - 125{,}000)}{32(0.42\times10^{-3})(1\times10^{-6})} = 2.51 \text{ m/s}$$

$$N_{\text{Re}} = \frac{D v \rho}{\mu} = \frac{(3\times10^{-7})(2.51)(1000)}{0.42\times10^{-3}} = 1.78$$

Since the Reynolds number is < 2100, the flow is laminar, but it probably is not fully developed.

Exercise 14.8

Subject: Knudsen flow through a porous glass membrane

Given: Porous glass membrane with an average pore diameter of 40 Angstroms. Pressures are not more than 120 psia upstream and 15 psia downstream. At 25°C and this pressure range, permeability of helium = 117,000 barrer. Experimental permeability of CO_2 = 68,000 barrer.

Assumptions: Knudsen flow is dominant.

Find: Theoretical value of permeability for CO_2 based on the value for helium.

Analysis: For Knudsen flow, Eq. (14-22) applies. Therefore,

$$P_{M_{CO_2}} = P_{M_{He}}\left(\frac{M_{CO_2}}{M_{He}}\right)^{1/2} = 117{,}000\left(\frac{4.00}{44.01}\right)^{1/2} = 35{,}300 \text{ barrer}$$

This is substantially lower than the experimental value. Therefore, check to see if Knudsen flow is dominant by computing combined Knudsen and molecular diffusivities for He and CO_2.

Helium:

From Eq. (14-21), $D_{K_{He}} = 4850 d_p\left(\frac{T}{M}\right)^{1/2} = 4850(40\times10^{-8})\left(\frac{298}{4.0}\right)^{1/2} = 0.0167 \text{ cm}^2/\text{s}$

For molecular diffusivity, use Eq. (3-36) with Table 3.1 at the highest pressure (8.16 atm),

$$D_{He,CO_2} = \frac{0.00143(298)^{1.75}}{8.16\left[\frac{2}{(1/4.0)+(1/44.01)}\right]^{1/2}\left(2.67^{1/3}+26.7^{1/3}\right)^2} = 0.0722 \text{ cm}^2/\text{s}$$

From a modification of Eq. (14-18), the combined diffusivity is

$$D_{He} = \frac{1}{(1/0.0167)+(1/0.0722)} = 0.0136 \text{ cm}^2/\text{s}$$

Carbon Dioxide:

From Eq. (14-21), $D_{K_{CO_2}} = 4850 d_p\left(\frac{T}{M}\right)^{1/2} = 4850(40\times10^{-8})\left(\frac{298}{44.01}\right)^{1/2} = 0.00505 \text{ cm}^2/\text{s}$

The combined diffusivity is $D_{He} = \frac{1}{(1/0.00505)+(1/0.0722)} = 0.00472 \text{ cm}^2/\text{s}$

For both helium and carbon dioxide, the combined diffusivities are within 20% of the Knudsen values. One explanation for the larger value of the CO_2 permeability is the possibility that CO_2 is partly adsorbed in the pores causing an increase in the permeability over that caused by Knudsen diffusion alone.

Exercise 14.9

Subject: Effect of partial condensation and surface diffusion on the permeability of components of a gas mixture.

Given: Porous carbon membrane of not more than 5 microns thickness, with pores of 4 to 15 Angstroms in diameter. Feed gas mixture of hydrogen and the first four normal paraffins with component mol% values given below in terms of partial pressures using Dalton's law. Permeabilities of the components in the mixture are much different than for the pure components. Pressure of 1.2 atm on feed side. Sweep gas on the permeate side such that the partial pressures of the permeating components are negligible.

Assumptions: Mixture permeabilities are constant through the membrane.

Find: Permeate composition on a sweep-gas-free basis.

Analysis: From Eq. (14-1),

$$\text{Flux}_i = \frac{P_{M_i}}{l_M}\Delta p_i \quad \text{with} \quad \Delta p_i = p_{i_{\text{feed}}} - p_{i_{\text{permeate}}} = p_{i_{\text{feed}}} - 0$$

Therefore, the flux is proportional to $P_{M_i}\, p_{i_{\text{feed}}}$ and $y_{i_{\text{permeate}}} = \dfrac{P_{M_i}\, p_{i_{\text{feed}}}}{\sum P_{M_i}\, p_{i_{\text{feed}}}}$

The permeate composition in mole fractions is developed with the above equations:

Component	p, atm in feed	P_M, barrer in mixture	$P_M p$, barrer-atm	y in permeate
H_2	0.492	1.2	0.590	0.019
CH_4	0.242	1.3	0.315	0.010
C_2H_6	0.114	7.7	0.878	0.028
C_3H_8	0.113	25.4	2.870	0.091
nC_4H_{10}	0.239	112.3	26.840	0.852
Total	1.200		31.493	1.000

Exercise 14.10

Subject: Effect of module flow pattern on the material balance and membrane area for the separation of propylene and propane by gas permeation.

Given: Gas feed of 100 lbmol/h of 60 mol% propylene (C3=) and 40 mol% propane (C3) at 25°C and 300 psia. Polyvinyltrimethylsilane polymer membrane with a 0.1μm skin in spiral-wound modules. From Table 14.9, P_M for C3= is 9 barrer, and 2.8 barrer for C3. Pressure on the permeate side = 15 psia.

Assumptions: No pressure drop on feed side or on the permeate side. Negligible film resistances on either side of the membrane.

Find: Material balance and membrane area in m^2 as a function of the cut, θ, for:
(a) Perfect mixing on both sides of the membrane.
(b) Crossflow

Analysis: Ideal separation factor from Eq. (14-40) = $\alpha^*_{C3=,C3} = \dfrac{P_{M_{C3=}}}{P_{M_{C3}}} = \dfrac{9}{2.8} = 3.21$

Pressure ratio = $P_P iP_F$ = 15/300 = 0.05.
From the bottom of Eq. (14-1) and the definition of a barrer in Section 14.1,

$$\overline{P}_{M_{C3=}} = \frac{P_{M_{C3=}}}{l_M} = \frac{9\left(1\times10^{-10}\right)}{0.1\times10^{-4}} = 9\times10^{-5}\,\text{cm}^3\text{(STP)}/\text{cm}^2-\text{s}-\text{cmHg}$$

Rearranging Eq. (14-36), $$y = \frac{\alpha x}{1+(\alpha-1)x} \qquad (1),$$

where, y and x refer to C3= and $\alpha = \alpha_{C3=,C3}$.

From Eq. (14-43), $$\alpha = \alpha^*_{C3=,C3}\left[\frac{x(\alpha-1)+1-r\alpha}{x(\alpha-1)+1-r}\right] = 3.21\left[\frac{x(\alpha-1)+1-0.05\alpha}{x(\alpha-1)+1-0.05}\right] \qquad (2)$$

For a given value of x, Eq. (2) is solved for α. Substituting this α into Eq. (1), y is obtained.

(a) Perfect mixing:
On the feed side, $x_R = x$. On the permeate side, $y_P = y$.
From a rearrangements of Eqs. (3) and (5) in Example 14.5,

for C3=, $$\theta = \frac{x_F - x}{y - x} = \frac{0.6 - x}{y - x} \qquad (3)$$

and the membrane area, $$A_M = \frac{y\theta n_F}{\overline{P}_{M_{C3=}}\left(xP_F - yP_P\right)} \qquad (4)$$

where, n_F = 100 lbmol/h or 100(453.6)(22,400)/3600 = 282,000 cm^3 (STP)/s
Pressures are P_F = 300(76/14.7) = 1,551 cmHg, and P_P = 15(76/14.7) = 77.6 cmHg

Exercise 14.10 (continued)

Analysis: (a) (continued)

Therefore, A_M in $m^2 = \dfrac{y\theta(282{,}000)}{9.0\times10^{-5}\left[x(1{,}551) - y(76.6)\right](10{,}000)}$

The calculations are carried out in a spreadsheet, with the following results:

x of C3= in R	α	y of C3= in P	θ	nP, lbmol/h	Area, m2
0.6000	3.0588	0.8211	0.0000	0.00	0.00
0.5800	3.0560	0.8084	0.0876	8.76	26.48
0.5600	3.0531	0.7953	0.1700	17.00	52.45
0.5400	3.0500	0.7817	0.2483	24.83	78.19
0.5200	3.0469	0.7675	0.3233	32.33	103.96
0.5000	3.0437	0.7527	0.3957	39.57	130.02
0.4800	3.0403	0.7373	0.4664	46.64	156.61
0.4600	3.0368	0.7212	0.5360	53.60	184.01
0.4400	3.0331	0.7044	0.6051	60.51	212.51
0.4200	3.0293	0.6869	0.6745	67.45	242.42
0.4000	3.0253	0.6685	0.7448	74.48	274.10
0.3800	3.0212	0.6493	0.8168	81.68	307.97
0.3600	3.0169	0.6292	0.8915	89.15	344.52
0.3400	3.0124	0.6081	0.9697	96.97	384.34
0.3326	3.0106	0.6000	1.0000	100.00	400.15

(b) Crossflow:

We have the following relationships between C3= mole fractions in the permeate and retentate as a function of the cut, $\theta = n_P/n_F$.

From material balance Eq. (1), Example 14.6, $y_P = \dfrac{x_F - x_R(1-\theta)}{\theta} = \dfrac{0.60 - x_R(1-\theta)}{\theta}$ (5)

From Eq. (14-49), where the *y* and *x* pertain to C3=,

$$y_P = x_R^{\left(\frac{1}{1-\alpha}\right)}\left(\frac{1-\theta}{\theta}\right)\left[(1-x_R)^{\left(\frac{\alpha}{\alpha-1}\right)}\left(\frac{x_F}{1-x_F}\right)^{\left(\frac{\alpha}{\alpha-1}\right)} - x_R^{\left(\frac{\alpha}{\alpha-1}\right)}\right] = x_R^{\left(\frac{1}{1-\alpha}\right)}\left(\frac{1-\theta}{\theta}\right)\left[(1-x_R)^{\left(\frac{\alpha}{\alpha-1}\right)}\left(\frac{0.60}{1-0.60}\right)^{\left(\frac{\alpha}{\alpha-1}\right)} - x_R^{\left(\frac{\alpha}{\alpha-1}\right)}\right]$$

Exercise 14.10 (continued)

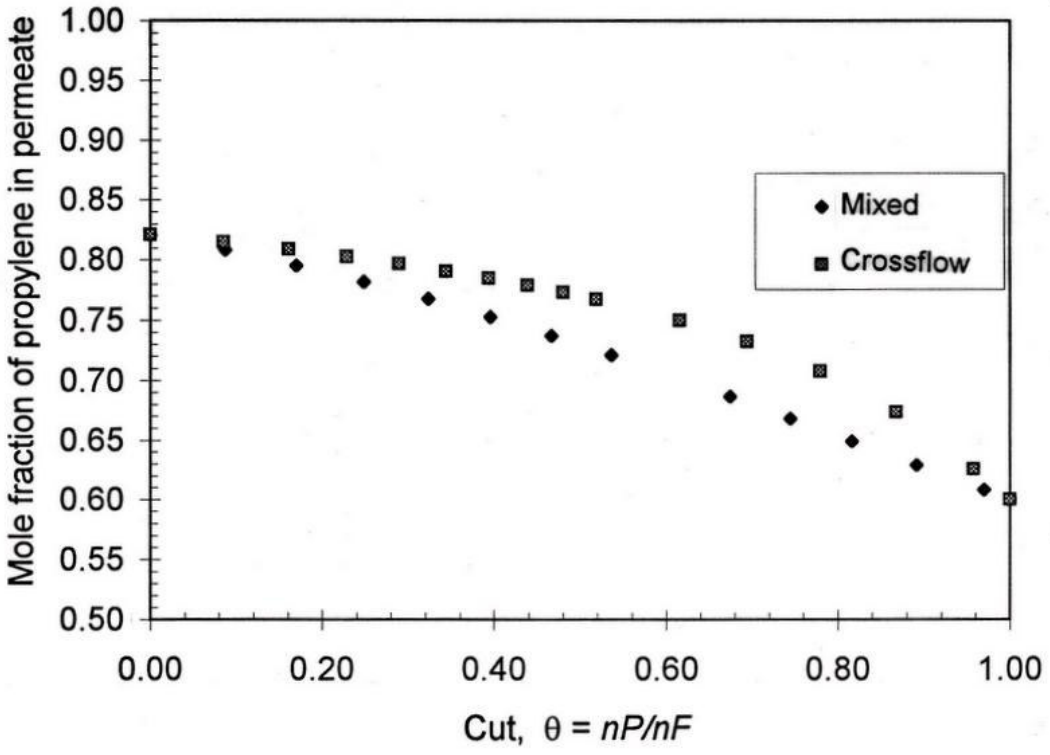
Analysis: (b) (continued)
Combine this equation with Eq. (5) to obtain:

$$1-\theta = \frac{0.60}{x_R + x_R^{\left(\frac{1}{1-\alpha}\right)}\left[(1-x_R)^{\left(\frac{\alpha}{\alpha-1}\right)}\left(\frac{0.60}{0.40}\right)^{\left(\frac{\alpha}{\alpha-1}\right)} - x_R^{\left(\frac{\alpha}{\alpha-1}\right)}\right]} \qquad (6)$$

For C3=, x_R begins at 0.60 at the feed end and decreases toward the retentate end. For each step in x, Eq. (2) is used to calculate α. Use Eq. (6) to compute values of θ as x_R decreases. Use Eq. (5) to compute the corresponding value of y_P. Eq. (1) is used to compute the local value of y. For a differential molar transfer rate, dn, the differential membrane area required is given by Eq. (14-50), which is also given in incremental form for numerical calculation. If we base this calculation on C3=,

$$dA_M = \frac{y\,dn}{\overline{P}_{M_{O_2}}\left(xP_F - yP_P\right)}, \qquad \Delta A_M,\ \text{m}^2 = \frac{y\theta(282{,}000)}{9.0\times10^{-5}\left[x(1{,}551) - y(76.6)\right](10{,}000)} \qquad (7)$$

where y is the local value given by Eq. (3) and Δn is the incremental decrease in the feed flow. Using the equations, the calculations are carried out on a spreadsheet with the results shown in the table on the next page. The perfectly mixed case is compared to the crossflow case in the following plot of the mole fraction of propylene in the permeate as a function of the cut. The results are similar to those shown in Fig. 14.10. For example at a cut of 60%, the mole fraction of propylene in the permeate is 0.75 for crossflow, while only 0.70 for perfect mixing.



Exercise 14.10 (continued)

Analysis: (b) (continued)

Results of crossflow:

x of C3= in R	α	$\alpha/(\alpha-1)$	1-θ	θ	y of A in P	Δn, lbmol/hr	local y	Δ Area, m^2	Cumulative Area, m^2
0.6000	3.0588	1.48572	1.0000	0.0000	0.8211		0.8211	0	
0.5800	3.0560	1.48639	0.9148	0.0852	0.8148	8.5164	0.8084	25.75	25.75
0.5600	3.0531	1.48708	0.8392	0.1608	0.8087	7.5663	0.7953	23.35	49.10
0.5400	3.0500	1.48779	0.7716	0.2284	0.8027	6.7606	0.7817	21.29	70.39
0.5200	3.0469	1.48854	0.7108	0.2892	0.7967	6.0725	0.7675	19.53	89.92
0.5000	3.0437	1.48932	0.6560	0.3440	0.7907	5.4811	0.7527	18.01	107.93
0.4800	3.0403	1.49013	0.6063	0.3937	0.7848	4.9700	0.7373	16.69	124.62
0.4600	3.0368	1.49098	0.5611	0.4389	0.7790	4.5259	0.7212	15.54	140.16
0.4400	3.0331	1.49186	0.5197	0.4803	0.7731	4.1384	0.7044	14.53	154.69
0.4200	3.0293	1.49278	0.4817	0.5183	0.7673	3.7987	0.6869	13.65	168.34
0.4000	3.0253	1.49375	0.4467	0.5533	0.7615	3.5000	0.6685	12.88	181.22
0.3800	3.0212	1.49476	0.4143	0.5857	0.7556	3.2364	0.6493	12.20	193.43
0.3600	3.0169	1.49582	0.3843	0.6157	0.7498	3.0033	0.6292	11.61	205.03
0.3400	3.0124	1.49693	0.3563	0.6437	0.7439	2.7967	0.6081	11.08	216.12
0.3200	3.0077	1.49809	0.3302	0.6698	0.7380	2.6133	0.5860	10.63	226.75
0.3000	3.0027	1.49932	0.3057	0.6943	0.7321	2.4504	0.5627	10.23	236.98
0.2800	2.9976	1.50061	0.2826	0.7174	0.7261	2.3059	0.5383	9.89	246.87
0.2600	2.9922	1.50196	0.2609	0.7391	0.7200	2.1778	0.5125	9.61	256.48
0.2400	2.9865	1.50339	0.2402	0.7598	0.7138	2.0648	0.4854	9.37	265.85
0.2200	2.9806	1.50490	0.2206	0.7794	0.7075	1.9657	0.4567	9.19	275.04
0.2000	2.9744	1.50649	0.2018	0.7982	0.7011	1.8797	0.4265	9.05	284.09
0.1800	2.9678	1.50817	0.1837	0.8163	0.6945	1.8065	0.3945	8.97	293.06
0.1600	2.9610	1.50996	0.1662	0.8338	0.6877	1.7461	0.3606	8.95	302.00
0.1400	2.9537	1.51185	0.1492	0.8508	0.6807	1.6992	0.3247	8.99	311.00
0.1200	2.9461	1.51385	0.1326	0.8674	0.6734	1.6674	0.2866	9.12	320.12
0.1000	2.9381	1.51598	0.1160	0.8840	0.6656	1.6539	0.2461	9.36	329.48
0.0800	2.9296	1.51825	0.0994	0.9006	0.6574	1.6652	0.2030	9.76	339.24
0.0600	2.9206	1.52067	0.0822	0.9178	0.6484	1.7145	0.1571	10.42	349.66
0.0400	2.9112	1.52324	0.0639	0.9361	0.6382	1.8342	0.1082	11.57	361.22
0.0200	2.9012	1.52599	0.0426	0.9574	0.6258	2.1317	0.0559	13.96	375.19
0.0001	2.8906	1.52892	0.0025	0.9975	0.6015	4.0104	0.0003	27.31	402.50

Exercise 14.11

Subject: Material balance and membrane area for the separation of propylene and propane by gas permeation using two-stage membrane systems.

Given: Gas feed of 100 lbmol/h of 60 mol% propylene (C3=) and 40 mol% propane (C3) at 25°C and 300 psia. Polyvinyltrimethylsilane polymer membrane with a 0.1μm skin in spiral-wound modules. From Table 14.9, P_M for C3= is 9 barrer, and 2.8 barrer for C3. Pressure on the permeate side = 15 psia.

Assumptions: Perfect mixing on both sides of the membrane. No pressure drop on feed side or on the permeate side. Negligible film resistances on either side of the membrane. Equal membrane areas for the two stages.

Find: Material balances and membrane areas in m^2 for 40 lbmol/h of final retentate for:
Case 1: Two-stage stripping cascade, as shown in Fig. 14.12a.
Case 2: Two-stage enriching cascade, as shown in Fig. 14.12b.

Analysis: Assume that the permeate-side pressure is 15 psia for each stage for each case.

Ideal separation factor from Eq. (14-40) = $\alpha^*_{C3=,C3} = \dfrac{P_{M_{C3=}}}{P_{M_{C3}}} = \dfrac{9}{2.8} = 3.21$

Pressure ratio = $P_P i P_F$ = 15/300 = 0.05.
From Eq. (14-1) and the definition of a barrer in Section 14.1,,

$$\overline{P}_{M_{C3=}} = \frac{P_{M_{C3=}}}{l_M} = \frac{9\left(1\times10^{-10}\right)}{0.1\times10^{-4}} = 9\times10^{-5}\,\text{cm}^3(\text{STP})/\text{cm}^2-\text{s}-\text{cmHg}$$

Rearranging Eq. (14-36), $\qquad y = \dfrac{\alpha x}{1+(\alpha-1)x} \qquad (1)$,

where, y and x refer to C3= and $\alpha = \alpha_{C3=,C3}$.

From Eq. (14-43), $\alpha = \alpha^*_{C3=,C3}\left[\dfrac{x(\alpha-1)+1-r\alpha}{x(\alpha-1)+1-r}\right] = 3.21\left[\dfrac{x(\alpha-1)+1-0.05\alpha}{x(\alpha-1)+1-0.05}\right] \qquad (2)$

For a given value of x, Eq. (2) is solved for α. Substituting this α into Eq. (1), y is obtained.

Case 1:
On the feed side, $x_R = x$. On the permeate side, $y_P = y$.
From rearrangements of Eqs. (3) and (5) of Example 14.5, for each stage,

for C3=, $\theta = \dfrac{x_F - x}{y - x} \qquad (3)$

and the membrane area for each stage is given by, $A_M = \dfrac{y\theta n_F}{\overline{P}_{M_{C3=}}\left(xP_F - yP_P\right)}$

where, n_F = combined feed, F, is in lbmol/h times (453.6)(22,400)/3600 to give cm^3 (STP)/s

Exercise 14.11 (continued)

Analysis: Case 1 (continued)

Pressures are P_F = 300(76/14.7) = 1,551 cmHg, and P_P = 15(76/14.7) = 77.6 cmHg

Therefore, $$A_M \text{ in m}^2 = \frac{y\theta n_F(2820)}{9.0\times10^{-5}\left[x(1{,}551) - y(76.6)\right](10{,}000)} \qquad (4)$$

Assume that the membrane areas for Stages 1 and 2 are equal. Let 1 refer to Stage 1 (Memb 1) and 2 refer to Stage 2 (Memb 2) in Fig. 14.12a. Let F = feed rate, R = retentate rate, and P = permeate rate, all in lbmol/h, for a stage. Let T = θ and xF1 refer to the combined feed for Stage 1. For $x = x_F$ = 0.60, Eq. (2) gives α = 3.05. Assume this value is constant for both stages. The governing equations then are as follows where R2 = 40 lbmol/h and by overall total balance, P1 = 60 lbmol/h:

Total balance around the mixing point:	0 = 100 + P2 - F1	(5)
Total balance around Stage 1:	0 = 60 + R1 - F1	(6)
Eq. (1) for Stage 1:	0 = 3.05*x1 - y1 - 2.05*y1*x1	(7)
Eq. (1) for Stage 2:	0 = 3.05*x2 - y2 - 2.05*y2*x2	(8)
Eq. (3) for Stage 1:	0 = xF1 - x1 - T1*y1 + T1*x1	(9)
Eq. (3) for Stage 2:	0 = x1 - x2 - T2*y2 + T2*x2	(10)
Eq. (4) for equal A_M:	y1*T1*F1*(1551*x2 - 76.6* y2) = y2*T2*R1*(1551*x1 - 76.6*y1)	(11)
C3= balance around the mixing point:	0 = xF1*F1-60-y2*P2	(12)
C3= balance around Stage 1:	0 = 60*y1 + x1*R1 - xF1*F1	(13)
C3= balance around Stage 2:	0 = y2*P2 + 40*x2 -x1*R1	(14)

Eqs. (5) to (14) are a set of 10 equations (8 of which are nonlinear) in 10 unknowns. Solving with a nonlinear solver, such as Polymath, the following results are obtained, based on the following guesses to start the iterative process:

	F1	R1	P2	T1	T2	xF1	x1	y1	x2	y2
Guess	133	73	33	0.45	0.45	0.55	0.5	0.8	0.4	0.7
Result	150.2	90.2	50.2	0.399	0.556	0.610	0.510	0.761	0.359	0.631

Thus, the product obtained is a permeate, P1, of 60 lbmol/h with a propylene mole fraction of 0.761. The membrane area for each stage is computed from Eq. (4), which for Stage 1 is:

$$A_{M_1} \text{ in m}^2 = \frac{0.761(0.399)(150.2)(2820)}{9.0\times10^{-5}\left[0.510(1{,}551) - 0.761(76.6)\right](10{,}000)} = A_{M_2} = 195 \text{ m}^2$$

Exercise 14.11 (continued)

Analysis: (continued)

Case 2: Configuration of Fig. 14.12b

Again take $\alpha = 3.05$. Assume this value is constant for both stages. Again assume that the membrane areas for Stages 1 and 2 are equal. The governing equations then are as follows where R1 = 40 lbmol/h and by overall total balance, P2 = 60 lbmol/h:

Total balance around the mixing point:	0 = 100 + R2 - F1	(15)
Total balance around Stage 1:	0 = 40 + P1 - F1	(16)
Eq. (1) for Stage 1:	0 = 3.05*x1 - y1 - 2.05*y1*x1	(17)
Eq. (1) for Stage 2:	0 = 3.05*x2 - y2 - 2.05*y2*x2	(18)
Eq. (3) for Stage 1:	0 = xF1 - x1 - T1*y1 + T1*x1	(19)
Eq. (3) for Stage 2:	0 = x1 - x2 - T2*y2 + T2*x2	(20)
Eq. (4) for equal A_M:	y1*T1*F1*(1551*x2 - 76.6* y2) = y2*T2*P1*(1551*x1 - 76.6*y1)	(21)
C3= balance around the mixing point:	0 = xF1*F1-60-x2*R2	(22)
C3= balance around Stage 1:	0 = P1*y1 + x1*40 - xF1*F1	(23)
C3= balance around Stage 2:	0 = y2*60 + R2*x2 -y1*P1	(24)

Eqs. (15) to (24) are a set of 10 equations (8 of which are nonlinear) in 10 unknowns. Solving with a nonlinear solver, such as Polymath, the following results are obtained, based on the following guesses to start the iterative process:

	F1	R2	P1	T1	T2	xF1	x1	y1	x2	y2
Guess	160	60	120	0.75	0.50	0.60	0.3	0.7	0.6	0.8
Result	100	0	60	0.60	1.00	0.60	0.4407	0.7062	0.4407	0.7062

Unfortunately, this is not a useful solution because all of the feed to Stage 2 passes through the membrane. Thus, nothing is achieved by Stage 2. Therefore, other solutions were sought in an attempt to achieve a higher mole fraction of propylene in the final permeate. This was achieved by eliminating the equal area condition of Eq. (21) and replacing it by a specification on y2. The following results were obtained for Cases 2a, 2b, and 2c:

	y2	F1	R2	P1	T1	T2	xF1	x1	y1	x2
a	0.74	126.58	26.58	86.58	0.684	0.693	0.5754	0.3900	0.6610	0.4827
b	0.761	164.64	64.64	124.64	0.757	0.481	0.5648	0.3590	0.6308	0.5103
c	0.78	271.64	171.64	231.64	0.853	0.259	0.5605	0.3300	0.6004	0.5376

For Case 2b, which corresponds to the same y2 as for Case 1, the membrane areas are as follows:

$$A_{M_1} \text{ in m}^2 = \frac{0.6308(0.757)(124.64)(2820)}{9.0\times10^{-5}\left[0.510(1{,}551)-0.761(76.6)\right](10{,}000)} = 254.5 \text{ m}^2$$

$$A_{M_2} \text{ in m}^2 = \frac{0.76064(0.481)(60)(2820)}{9.0\times10^{-5}\left[0.510(1{,}551)-0.761(76.6)\right](10{,}000)} = 93.9 \text{ m}^2$$

The total membrane area for Case 2b is 348.4 m^2, compared to a total of 390 m^2 for Case 1.

Exercise 14.12

Subject: Importance of concentration polarization in dialysis.

Given: From Example 14.7: At a certain location in a tubular membrane separator, for the dialysis of solute A from solvent B, concentrations for A of 5 x 10^{-2} kmol/m^3 on the feed side and 1.5 x 10^{-2} kmol/m^3 on the permeate side. Permeance for A = 7.3 x 10^{-5} m/s and feed passes through the tube of inside diameter = D = 0.4 cm. Permeate-side mass-transfer coefficient = 0.06 cm/s or 6 x 10^{-4} m/s For the feed side mass-transfer coefficient, Reynolds number = 25,000 and Schmidt number for solute A = 500, with a molecular diffusivity for A of 6.5 x 10^{-5} cm^2/s.

Find: Importance of concentration polarization.

Analysis: The flux of A through the membrane, in terms of the three resistances is given by a modification of Eq. (14-53), with :

$$N_A = \frac{c_{A_F} - c_{A_P}}{\frac{1}{k_{A_F}} + \frac{1}{\overline{P}_{M_A}} + \frac{1}{k_{A_P}}} = \frac{5.0\times10^{-2} - 1.5\times10^{-2}}{\frac{1}{k_{A_F}} + \frac{1}{7.3\times10^{-5}} + \frac{1}{6\times10^{-4}}} \qquad (1)$$

Since the Reynolds number is greater than 10,000, turbulent flow exists inside the tube and if fully developed flow is assumed, the mass-transfer coefficient is given by a modification of Eq. (14-54), where, if the analogy to heat transfer is applied with Eqs. (3-165) and (3-166) for a circular tube, a = 0.023, $d_H = D$, and the $(d_H/L)^d$ correction for the entry effect is not necessary. In Example 14.7, the feed-side mass-transfer coefficient for N_{Re} = 15,000 and D = 0.5 cm is computed to be 5.1 x 10^{-4} m/s. Therefore, for this exercise, by ratios, using Eq. (14-54),

$$k_{A_F} = 5.1\times10^{-4}\left(\frac{0.5}{0.4}\right)\left(\frac{25{,}000}{15{,}000}\right)^{0.8} = 9.6\times10^{-4}\ \text{m/s}$$

Substituting into Eq. (1),

$$N_A = \frac{5.0\times10^{-2} - 1.5\times10^{-2}}{\frac{1}{9.6\times10^{-4}} + \frac{1}{7.3\times10^{-5}} + \frac{1}{6\times10^{-4}}} = \frac{2.5\times10^{-2}}{1{,}042 + 13{,}700 + 1{,}667} = \frac{2.5\times10^{-2}}{16{,}409} = 2.1\times10^{-6}\ \text{kmol/s-m}^2$$

The sum of the feed-side and permeate-side mass-transfer resistances is 2,709 of a total of 16,409. Therefore 2,709/16,409 or 16.5% of the total resistance is due to the two external resistances. Therefore, concentration polarization is important, but not to a major extent.

Exercise 14.13

Subject: Dialysis of an aqueous stream to separate Na_2SO_4 from a high-molecular-weight substance (A).

Given: Aqueous feed of 100 gal/h at 20°C, containing 8 wt% Na_2SO_4 and 6 wt% A. Continuous countercurrent-flow dialyzer, using a pure water sweep of 100 gal/h. Membrane of microporous cellophane with $\varepsilon = 0.5$, wet thickness, $l_M = 0.0051$ cm, $\tau = 4.1$, and pore diameter = $d_p = 31$ Angstroms. Properties of Na_2SO_4 and A:

Component	Na_2SO_4	A
Molecular weight	142	1000
Molecular diameter, Angstroms	5.5	15.0
Molecular diffusivity, cm^2/s	0.77×10^{-5}	0.25×10^{-5}

Assumptions: Log-mean driving forces. Mass-transfer resistances on each side of the membrane are each 25% of the total mass-transfer resistance for each component. No transfer of water through the membrane.

Find: Membrane area in m^2 for a 10% transfer of A through the membrane. Corresponding percent transfer of Na_2SO_4.

Analysis: For a concentration driving force, using Eqs. (14-13), (14-14), and (14-15) and taking into account restrictive diffusion because of the small pore size,

the permeances are given by: $$\overline{P}_{M_i} = \frac{\varepsilon D_i}{l_M \tau}\left(1 - \frac{d_M}{d_p}\right)^4 \qquad (1)$$

For Na_2SO_4, $$\overline{P}_{M_{Na_2SO_4}} = \frac{0.5\left(0.77\times10^{-5}\right)}{0.0051(4.1)}\left(1-\frac{5.5}{31}\right)^4 = 8.43\times10^{-5} \text{ cm/s}$$

For A, $$\overline{P}_{M_A} = \frac{0.5(0.25\times10^{-5})}{0.0051(4.1)}\left(1-\frac{15.0}{31.0}\right)^4 = 0.424\times10^{-5} \text{ cm/s}$$

Using Eq. (14-56), with the two film resistances together being equal to half the total resistance, the overall mass transfer coefficients are one-half of the permeances. Therefore,

$$K_{Na_2SO_4} = 4.22\times10^{-5} \text{ cm/s} \quad \text{or} \quad 1.52\times10^{-3} \text{ m/h}$$

$$K_A = 0.212\times10^{-5} \text{ cm/s} \quad \text{or} \quad 7.63\times10^{-5} \text{ m/h}$$

Assume that the density of the feed is that of 14 wt% aqueous Na_2SO_4 at 20°C. From Perry's Handbook, the density = 1.13 g/cm^3 or 1130 kg/m^3 or 9.41 lb/gal.
Therefore, the mass flowrate of the feed = 100(9.41) = 941 lb/h, comprised of 0.08(941) = 75.3 lb/h of Na_2SO_4, 56.5 lb/h of A, and 941 - 75.3 - 56.5 = 809.2 lb/h of water.
The density of the sweep is 8.33 lb/gal.

Exercise 14.13 (continued)

Analysis: (continued)

The sweep liquid enters at a flow rate of 100(8.33) = 833 lb/h of water.
The permeate contains 10% of A in the feed or 0.10(56.5) = 5.7 lb/h.
To obtain the concentrations, assume that 75% of the Na_2SO_4 in the feed is transferred through the membrane. Thus, the permeate contains 0.75(75.3) = 56.5 lb/h of Na_2SO_4. The retentate contains 56.5 - 5.7 = 50.8 lb/h of A and 75.3 - 56.5 = 18.8 lb/h of Na_2SO_4. Compute the concentrations in kg/m^3. For example, the feed is 941 lb/h or 427 kg/h. Its volume is 427/1130 = 0.378 m^3/h. Therefore, the concentration of Na_2SO_4 in the feed = 0.08(427)/0.378 = 90.4 kg/m^3.
Assume the density of the permeate is 1.07 g/cm^3 or 1070 kg/m^3.
Assume the density of the retentate is 1.07 g/cm^3 or 1070 kg/m^3.
The total permeate = 895.2 lb/h or 406.1 kg/h with a volume of 0.394 m^3/h.
The total retentate = 878.8 lb/h or 398.6 kg/h with a volume of 0.373 m^3/h.
The results of the concentration calculations are:

	Concentrations in kg/m^3:			
Component	Feed	Sweep	Retentate	Permeate
Na_2SO_4	90.4	0.0	22.9	65.0
A	67.8	0.0	61.8	6.6

The log-mean driving force for A is $\Delta c_A = \dfrac{(67.8-6.6)-(61.8-0.0)}{\ln\left(\dfrac{67.8-6.6}{61.8-0.0}\right)} = 61.5 \text{ kg/m}^3$

From a modification of Eq. (14-55), $A_M = \dfrac{m_A}{K_A \Delta c_A} = \dfrac{5.7(0.4536)}{7.63\times10^{-5}(61.5)} = 551 \text{ m}^2$

The log-mean driving force for Na_2SO_4 is $\Delta c_A = \dfrac{(90.4-65.0)-(22.9-0.0)}{\ln\left(\dfrac{90.4-65.0}{22.9-0.0}\right)} = 24.2 \text{ kg/m}^3$

From a modification of Eq. (14-55), $A_M = \dfrac{m_{Na_2SO_4}}{K_{Na_2SO_4} \Delta c_{Na_2SO_4}} = \dfrac{56.5(0.4536)}{1.53\times10^{-3}(24.2)} = 692 \text{ m}^2$

Because the membrane area for Na_2SO_4 is larger than for A, the % transfer of Na_2SO_4 is less than the assumed 75%. Repeat the calculations assuming 70% transfer of Na_2SO_4, but use the same liquid densities. Now the permeate contains 0.7(75.3) = 52.7 lb/h Na_2SO_4 and the retentate contains 22.6 lb/h Na_2SO_4. The new concentrations are:

	Concentrations in kg/m^3:			
Component	Feed	Sweep	Retentate	Permeate
Na_2SO_4	90.4	0.0	28.1	65.0
A	67.8	0.0	63.1	7.0

Δc of Na_2SO_4 = 26.8 kg/m^3 and membrane area = 52.7(0.4536)/[1.53x10^{-3} (26.8)] = 583 m^2
Δc of Na_2SO_4 = 62.0 kg/m^3 and membrane area = 5.7(0.4536)/[7.63x10^{-5} (62.0)] = 547 m^2
By extrapolation, membrane area = 545 m^2 and the % transfer of Na_2SO_4 = 65%.

Exercise 14.14

Subject: Removal of HCl from an aqueous solution by dialysis.

Given: 300 L/h of an aqueous solution of 0.1 M NaCl and 0.1 M HCl. Sweep of 300 L/h of H_2O. Microporous membrane for which lab experiments give the following overall mass-transfer coefficients:

Component	*K*, cm/min
H_2O	0.0025
NaCl	0.021
HCl	0.055

Assumptions: Log mean concentration driving force. Negligible change in volume flow rate of feed and sweep with permeation.

Find: Membrane area in m^2 and material balance for 90, 95, and 98% transfer of HCl.

Analysis: Determine feed conditions, noting that it is very dilute in NaCl and HCl. Therefore, assume that it contains 55.5 mol of H_2O per liter. For 300 L/h,

$$\left(n_{\mathrm{NaCl}}\right)_F = 0.1(300) = 30 \text{ mol/h}$$

$$\left(n_{\mathrm{HCl}}\right)_F = 0.2(300) = 60 \text{ mol/h}$$

$$\left(n_{\mathrm{H_2O}}\right)_F = 55.5(300) = 16{,}700 \text{ mol/h}$$

The feed concentrations are:

$$\left(c_{\mathrm{NaCl}}\right)_F = 0.1/1000 = 0.0001 \text{ mol/cm}^3$$

$$\left(c_{\mathrm{HCl}}\right)_F = 0.2/1000 = 0.0002 \text{ mol/cm}^3$$

$$\left(c_{\mathrm{H_2O}}\right)_F = 55.5/1000 = 0.0555 \text{ mol/cm}^3$$

The sweep flow rate = 55.5(300) = 16,700 mol/h of pure water.

Case 1 (90% transfer of HCl:

Transfer of HCl to the permeate = 0.9(60) = 54 mol/h

Neglect any transfer of water. Then the concentrations of HCl are:

$$\left(c_{\mathrm{HCl}}\right)_P = 54/300{,}000 = 0.00018 \text{ mol/cm}^3$$

$$\left(c_{\mathrm{HCl}}\right)_R = 6/300{,}000 = 0.00002 \text{ mol/cm}^3$$

$$\left(c_{\mathrm{HCl}}\right)_{Sweep} = 0.0 \text{ mol/cm}^3$$

Note that because the volumetric flow rates of feed and sweep are equal to each other and to the permeate and retentate, by material balance, the concentration driving forces for HCl and NaCl are equal at both ends and equal to $\left(c_i\right)_F - \left(c_i\right)_P$

Therefore, $\left(\Delta c_{\mathrm{HCl}}\right)_{\mathrm{LM}} = \left(c_{\mathrm{HCl}}\right)_F - \left(c_{\mathrm{HCl}}\right)_P = 0.0002 - 0.00018 = 0.00002 \text{ mol/cm}^3$

Exercise 14.14 (continued)

Analysis: Case 1 (continued)

From Eq. (14-57), $A_M = \dfrac{n_{HCl}}{K_{HCl}(\Delta c_{HCl})_{LM}} = \dfrac{(54/60)}{0.055(0.00002)} = 818{,}000 \text{ cm}^2$ or 81.8 m^2

Now determine the rate of permeation of NaCl.

From Eq. (14.57,

$$n_{NaCl} = K_{NaCl} A_M (\Delta c_{NaCl})_{LM} = 0.021(818{,}000)(\Delta c_{NaCl})_{LM} = 17{,}200(\Delta c_{NaCl})_{LM} \quad (1)$$

But, $n_{NaCl} = (c_{NaCl})_P \left(\dfrac{300{,}000}{60}\right) = 5{,}000(c_{NaCl})_P$ (2)

$$(\Delta c_{NaCl})_{LM} = (c_{NaCl})_F - (c_{NaCl})_P = 0.0001 - (c_{NaCl})_P \quad (3)$$

Substituting Eqs. (2) and (3) into (1),

$$5{,}000(c_{NaCl})_P = 17{,}200\left[0.0001 - (c_{NaCl})_P\right]$$

Solving, $(c_{NaCl})_P = 0.0000775$ and the transfer of NaCl = $30(0.0000775/0.0001) = 23.3$ mol/h

Therefore, the material balance in kmol/h is:

Component	Feed	Sweep	Retentate	Permeate
HCl	60	0	6.0	54.0
NaCl	30	0	6.7	23.3
H_2O	16,650	16,650	16,650.0	16,650.0
Total	16,740	16,650	16,662.7	16,727.3

Case 2 (95% transfer of HCl:

Transfer of HCl to the permeate = 0.95(60) = 57 mol/h

Neglect any transfer of water. Then the concentrations of HCl are:

$$(c_{HCl})_P = 57/300{,}000 = 0.00019 \text{ mol/cm}^3$$

$$(c_{HCl})_R = 3/300{,}000 = 0.00001 \text{ mol/cm}^3$$

$$(c_{HCl})_{Sweep} = 0.0 \text{ mol/cm}^3$$

Note that because the volumetric flow rates of feed and sweep are equal to each other and to the permeate and retentate, by material balance, the concentration driving forces for HCl and NaCl are equal at both ends and equal to $(c_i)_F - (c_i)_P$

Therefore, $(\Delta c_{HCl})_{LM} = (c_{HCl})_F - (c_{HCl})_P = 0.0002 - 0.00019 = 0.00001 \text{ mol/cm}^3$

From Eq. (14-57), $A_M = \dfrac{n_{HCl}}{K_{HCl}(\Delta c_{HCl})_{LM}} = \dfrac{(57/60)}{0.055(0.00001)} = 1{,}730{,}000 \text{ cm}^2$ or 173.0 m^2

Now determine the rate of permeation of NaCl.

From Eq. (14.57,

$$n_{NaCl} = K_{NaCl} A_M (\Delta c_{NaCl})_{LM} = 0.021(1{,}730{,}000)(\Delta c_{NaCl})_{LM} = 36{,}300(\Delta c_{NaCl})_{LM} \quad (1)$$

But, $n_{NaCl} = (c_{NaCl})_P \left(\dfrac{300{,}000}{60}\right) = 5{,}000(c_{NaCl})_P$ (2)

$$(\Delta c_{NaCl})_{LM} = (c_{NaCl})_F - (c_{NaCl})_P = 0.0001 - (c_{NaCl})_P \quad (3)$$

Exercise 14.14 (continued)

Analysis: Case 2 (continued)

Substituting Eqs. (2) and (3) into (1),

$$5{,}000\left(c_{\text{NaCl}}\right)_P = 36{,}300\left[0.0001 - \left(c_{\text{NaCl}}\right)_P\right]$$

Solving, $\left(c_{\text{NaCl}}\right)_P = 0.0000879$ and the transfer of NaCl = $30(0.0000879/0.0001) = 26.4$ mol/h

Therefore, the material balance in kmol/h is:

Component	Feed	Sweep	Retentate	Permeate
HCl	60	0	3.0	57.0
NaCl	30	0	3.6	26.4
H_2O	16,650	16,650	16,650.0	16,650.0
Total	16,740	16,650	16,656.6	16,733.4

Case 3 (98% transfer of HCl:

Transfer of HCl to the permeate = 0.98(60) = 58.8 mol/h

Neglect any transfer of water. Then the concentrations of HCl are:

$$\left(c_{\text{HCl}}\right)_P = 58.8/300{,}000 = 0.000196 \text{ mol/cm}^3$$

$$\left(c_{\text{HCl}}\right)_R = 1.2/300{,}000 = 0.000004 \text{ mol/cm}^3$$

$$\left(c_{\text{HCl}}\right)_{Sweep} = 0.0 \text{ mol/cm}^3$$

Note that because the volumetric flow rates of feed and sweep are equal to each other and to the permeate and retentate, by material balance, the concentration driving forces for HCl and NaCl are equal at both ends and equal to $\left(c_i\right)_F - \left(c_i\right)_P$

Therefore, $\left(\Delta c_{\text{HCl}}\right)_{\text{LM}} = \left(c_{\text{HCl}}\right)_F - \left(c_{\text{HCl}}\right)_P = 0.0002 - 0.000196 = 0.000004$ mol/cm^3

From Eq. (14-57), $A_M = \dfrac{n_{\text{HCl}}}{K_{\text{HCl}}\left(\Delta c_{\text{HCl}}\right)_{\text{LM}}} = \dfrac{(58.8/60)}{0.055(0.000004)} = 4{,}450{,}000 \text{ cm}^2$ or 445.0 m^2

Now determine the rate of permeation of NaCl. From Eq. (14.57),

$$n_{\text{NaCl}} = K_{\text{NaCl}} A_M \left(\Delta c_{\text{NaCl}}\right)_{\text{LM}} = 0.021(4{,}450{,}000)\left(\Delta c_{\text{NaCl}}\right)_{\text{LM}} = 93{,}500\left(\Delta c_{\text{NaCl}}\right)_{\text{LM}} \qquad (1)$$

But, $n_{\text{NaCl}} = \left(c_{\text{NaCl}}\right)_P \left(\dfrac{300{,}000}{60}\right) = 5{,}000\left(c_{\text{NaCl}}\right)_P$ (2)

$$\left(\Delta c_{\text{NaCl}}\right)_{\text{LM}} = \left(c_{\text{NaCl}}\right)_F - \left(c_{\text{NaCl}}\right)_P = 0.0001 - \left(c_{\text{NaCl}}\right)_P \qquad (3)$$

Substituting Eqs. (2) and (3) into (1),

$$5{,}000\left(c_{\text{NaCl}}\right)_P = 93{,}500\left[0.0001 - \left(c_{\text{NaCl}}\right)_P\right]$$

Solving, $\left(c_{\text{NaCl}}\right)_P = 0.0000949$ and the transfer of NaCl = $30(0.0000949/0.0001) = 28.5$ mol/h

Therefore, the material balance in kmol/h is:

Component	Feed	Sweep	Retentate	Permeate
HCl	60	0	1.2	58.8
NaCl	30	0	1.5	28.5
H_2O	16,650	16,650	16,650.0	16,650.0
Total	16,740	16,650	16,652.7	16,737.3

Exercise 14.15

Subject: Desalinization of an aqueous solution by electrodialysis.

Given: 86,000 gal/day of an aqueous solution of 3,000 ppm of NaCl. Desalinization to 400 ppm by electrodialysis with a 40% conversion. 4 stages with 3 stacks of 150 cell pairs in each stage. Fractional desalinization is the same in each stage. Expected current efficiency = 90%. Applied voltage for first stage = 220 v. Each cell pair has an area = 1160 cm^2.

Find: Current density in mA/cm^2, current in amperes, and power in kW for the first stage.

Analysis: For the four stages, the overall fractional demineralization is:

$f = (3{,}000 - 400)/3{,}000 = 0.8667$

For equal fractional demineralization in each stage, $(1-f) = (1-f_s)^4$

Therefore, $(1 - 0.8667) = (1-f_s)^4$. Solving, $(1-f_s) = 0.6043$

Thus, the salt concentration changes from stage to stage as follows:

Stage	NaCl concentration, ppm
Feed	3,000
leaving 1	1,813
leaving 2	1,096
leaving 3	662
leaving 4	400

For a 50% conversion, the volumetric feed flow rate = Q = 80,000 (0.5)/[24(3,600)] = 0.463 gal/s or 0.00175 m^3/s.

Take the solution density = 1,000,000 g/m^3. Then for Stage 1, the NaCl concentrations are:

Feed: 3,000 ppm (assume by weight) or $c = 3{,}000(1{,}000{,}000)/1{,}000{,}000 = 3{,}000\ g/m^3$

Leaving Stage 1: 1,813 ppm or $c = 1{,}813(1{,}000{,}000)/1{,}000{,}000 = 1{,}813\ g/cm^3$

MW of NaCl = 58.5. Therefore, in mol, $\Delta c = (3{,}000 - 1{,}813)/58.5 = 20.3\ mol/m^3$ or $equiv/m^3$

Membrane area for Stage 1 = A_M = (1,160 cm^2/cell pair)(150 cell pairs/stack)(3 stacks/stage) = 522,000 cm^2 or 52.2 m^2

Use a rearrangement of Eq. (14-58) to compute the current density:

$$i = \frac{zFQ(\Delta c)}{A_M \xi} = \frac{(1)(96{,}520)(0.00175)(20.3)}{(52.2)(0.9)} = 73\ amp/m^2$$

Therefore, the current flow through a cell pair = $I = iA_M/n$ = (73)(52.5)/150 = 25.6 amp

From Eq. (14-59), for a voltage of 220 volts across all cell pairs,

the power = $P = IE$ = 25.6(220) = 5,630 W = 5.6 kW

Exercise 14.16

Subject: Reverse osmosis of sea water.

Given: 30,000,000 gal/day of sea water at 20°C, containing 3.5 wt% dissolved solids. Permeate is 10,000,000 gal/day of water containing 500 ppm of dissolved solids. Retentate contains 5.25 wt% dissolved solids. Feed-side pressure = 2000 psia constant, and permeate pressure = 50 psia constant. One stage of spiral-wound membranes with total membrane area of 2,000,000 ft^2.

Assumptions: Crossflow.

Find: Permeance for water, and salt passage for the dissolved solids.

Analysis: First make an approximate calculation assuming perfect mixing on the permeate side and an arithmetic average of feed and retentate on the feed side. Rearranging Eq. (14-69),

$$\overline{P}_{M_{H_2O}} = \frac{n_{H_2O}}{A_M(\Delta P - \Delta\pi)_{avg}} = \frac{10{,}000{,}000}{2{,}000{,}000(\Delta P - \Delta\pi)_{avg}} \qquad (1)$$

ΔP = 2,000 - 50 = 1,950 psi

To estimate osmotic pressure, assume dissolved solids are NaCl (M = 58.5).

Salt concentrations are approximately:

Feed: 3.5(1,000)/[58.5(96.5)] = 0.620 mol/L

Retentate: 5.25(1,000)/[58.5(94.75)] = 0.947 mol/L

Permeate: $\frac{500}{1{,}000{,}000}(100)\left[\frac{(1{,}000z0}{58.5(99.95)}\right] = 0.00855$ mol / L

From Eq. (14-68), for T = 293 K and $\sum \overline{m}_i = 2\sum \overline{m}_{NaCl}$

Feed: π = 1.12(293)(2)(0.620) = 407 psia

Retentate: π = 1.12(293)(2)(0.947) = 622 psia

Permeate: π = 1.12(293)(2)(0.00855) = 5.6 psia

$$\Delta\pi_{\alpha\varpi\gamma} = \left[\frac{407 + 622}{2} - 5.6\right] = 514.5 - 5.6 = 508.9 \text{ psi}$$

$(\Delta P - \Delta\pi)_{avg}$ = 1,950 - 508.9 = 1,441 psi

From Eq. (1), $\overline{P}_{M_{H_2O}} = \frac{n_{H_2O}}{A_M(\Delta P - \Delta\pi)_{avg}} = \frac{10{,}000{,}000}{2{,}000{,}000(1{,}441)} = 3.47\times10^{-3}$ $\frac{\text{gal}}{\text{day-ft}^2 - \text{psi}}$

Now consider the actual crossflow case. The (P - π) on the permeate side is very small (less than 4% of that on the feed-permeate side). Therefore, the change in (ΔP - $\Delta\pi$) along the length of the membrane is little affected by conditions on the permeate side. Therefore, the case computed above well approximates crossflow.

From Eq. (14-70), $SP = (c_{salt})_{Permeate} / (c_{salt})_{Feed} = 0.00855 / 0.620 = 0.0138$

Exercise 14.17

Subject: Reverse osmosis with multiple stages.

Given: 100 gal/min of feed.

Assumptions: All units of same size.

Find:

Design 1 - Drawing for single stage of 4 units in parallel to obtain 50% recovery.

Design 2 - Drawing and % recovery for 2 stages in series with respect to retentate (4 units in parallel followed by 2 units in parallel).

Design 3 - Drawing and % recovery for 3 stages in series with respect to retentate (4 units in parallel, then 2 units in parallel, then 1 unit).

Analysis:

Design 1: The design is shown in a sketch below. Consider the following conditions for the single stage of 4 units in parallel. To simplify calculations and comparison of designs, assume:

1. Water feed dilute in dissolved salts. Take the 100 gal/min of feed = F, containing 1 lb salt/100 lb of water = XF1.
2. Density of all streams = 8.33 lb water/gal = ρ.
3. Driving force for water transfer across membrane = ΔP - $\Delta\pi$ = 1,000 psi for all units.
4. Water flux across all membrane units = 4.5 gal/day-ft^2.
5. Salt concentration in permeate from the stage = 0.01 lb salt/100 lb of water = Y1.

Therefore for the single stage of 4 units in parallel, the water transfer rate for 50% recovery of potable water = 0.5(100) = 50 gal/min. Therefore, the total membrane area is,

A_M = (50)(60)(24)/4.5 = 16,000 ft^2 or 4,000 ft^2 per unit.

Compute the permeance for water transport from a modification of Eq. (14-69):

$$\overline{P}_{M_{\text{water}}} = \frac{m_{\text{water}}}{A_M(\Delta P - \Delta\pi)} = \frac{8.33(50)}{16{,}000(1{,}000)} = 1.666\times10^{-5}\ \text{lb/min-ft}^2\text{-psi}$$

Compute the permeance for salt transport from a modification of Eq. (14-52), where the transport of salt across the membrane = 50(8.33)(0.0001) = 0.0416 lb/min, and a concentration difference in terms of mass ratios is used, based on an arithmetic average on the feed side and perfect mixing on the permeate side. Therefore,

$$\overline{P}_{M_{\text{salt}}} = \frac{m_{\text{salt}}}{A_M\left[\frac{(X_F + X_R)}{2} - Y_P\right]} = \frac{0.0416}{16{,}000\left[\frac{(0.01+0.0199)}{2} - 0.0001\right]} = 1.75\times10^{-4}\ \text{lb/min-ft}^2\text{-}(\Delta\ \text{mass ratio})$$

Exercise 14.17 (continued)

Analysis: (continued)

Design 2: The design is shown in a sketch below. Retentate, R1 from Stage 1 is feed to the Stage 2. Stage 1 consists of 4 membrane modules in parallel, each with 4,000 ft^2 for a total of 16,000 ft^2, and Stage 2 consists of 2 membrane modules in parallel, each with 4,000 ft^2 for a total of 8,000 ft^2. Permeates from Stage 1 and 2 are combined. As is Design 1, P1 = 50 gal/min. With only 50% of the membrane area of Stage 1, P2 = 25 gal/min and R2 = 25 gal/min. Thus, the total permeate is 75 gal/min, giving a recovery of 75%.

Design 3: The design is shown in a sketch below. Retentates R1 and R2 are feeds to Stages 2 and 3, respectively. Permeates from the 3 stages are combined to give the final permeate. Stage 1 consists of 4 membrane modules in parallel, each with 4,000 ft^2 for a total of 16,000 ft^2; Stage 2 consists of 2 membrane modules in parallel, each with 4,000 ft^2 for a total of 8,000 ft^2; and Stage 3 consists of a single unit of 4,000 ft^2. The permeate from Stage 3 is only 12.5 gal/min because of the single unit. The total permeate = 50 + 25 + 12.5 = 87.5 gal/min for an 87.5% recovery.

It is also of interest to compute the purity of the potable water produced. For example, for Design 2, the permeate from Stage 1 is 50 gal/min with 0.0001 lb salt/lb water. The feed to Stage 2 is 50 gal/min with 0.0199 lb salt/lb water. Using the results above from Design 1,
Salt mass balance around Stage 2:

$$0 = \rho(R1*X1 - P2*Y2 - R2*X2 \quad \text{or} \quad 0 = 50(0.0199) - 25*X2 - 25*Y2 \qquad (1)$$

Salt mass transfer rate in Stage 2:

$$0 = \rho*P2*Y2 - \overline{P}_{M_{salt}} A_M \left[\frac{(X1+X2)}{2} - Y2\right] \quad \text{or}$$

$$8.33(25)*Y2 - 1.75 \times 10^{-4}(8{,}000)\left[\frac{(0.0199+X2)}{2} - Y2\right] \qquad (2)$$

Solving these 2 equations with a nonlinear solver such as POLYMATH, the following results are obtained: X2 = 0.0396 and Y2 = 0.000199.
Therefore, the final combined permeate contains a salt mass ratio of

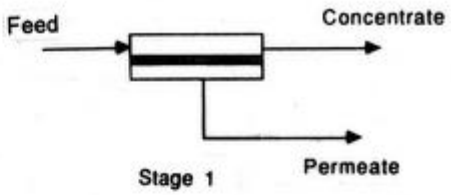
$$[50(0.0001) + 25(0.0001987)]/75 = 0.0001329$$

which is higher than the mass ratio of 0.0001 for Design 1. Thus, a higher recovery is counterbalanced by a less pure potable water.

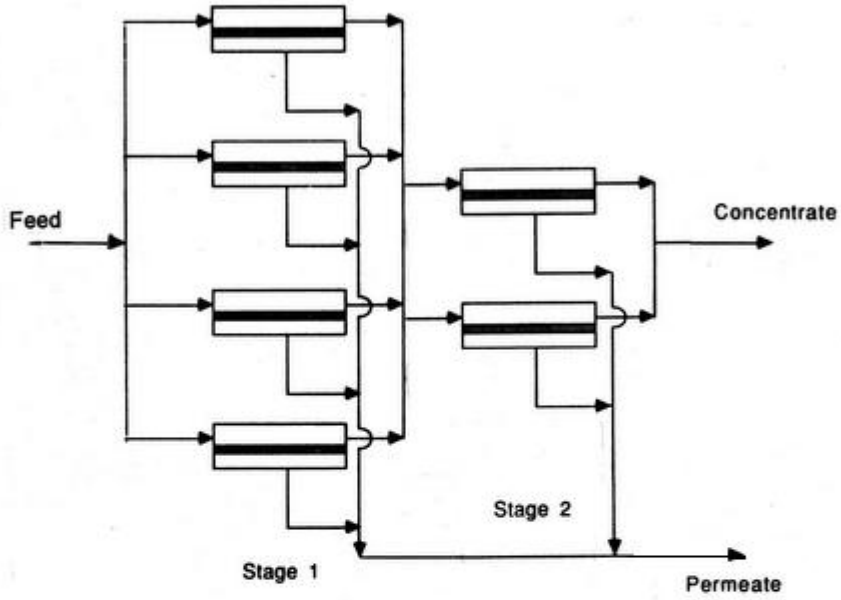
Exercise 14.17 (continued)

Analysis: (continued)

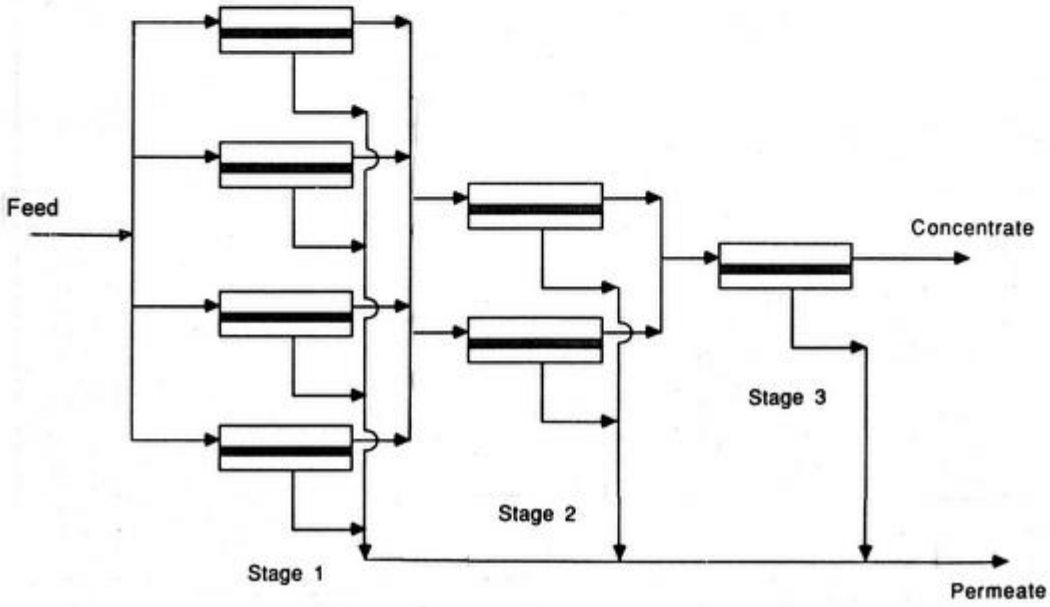
Design 1 (single stage):



Design 2 (two stages):



Design 3 (three stages):



Exercise 14.18

Subject: Concentration of Kraft black liquor by a two-stage reverse osmosis process.

Given: Fresh feed of 1,000 lb/h at 180°F and containing 15 wt% dissolved solids. Two-stage arrangement shown in Fig. 14.36, with recycle of retentate from Stage 2 to Stage 1. Combined feed to Stage 1 at 1,756 psia. Permeate from Stage 1 contains 0.4 wt% dissolved solids at a pressure of 15 psia. It is pumped to 518 psia to become feed to Stage 2. Permeate from Stage 2 contains 300 ppm dissolved solids at 15 psia. Retentate from Stage 2 contains 2.6 wt% dissolved solids and is recycled to Stage 1. Permeance for water = 0.0134 lb/ft^2-h-psi. Osmotic pressure for 25 wt% dissolved solids is 1,700 psia. Other osmotic pressures are proportional to wt% dissolved solids.

Assumptions: Arithmetic-mean osmotic pressure for plug flow on feed side of both stages. Perfect mixing on permeate side. No pressure drop on feed side.

Find: Material balance and membrane areas.

Analysis: Compute overall material balance:
Let R_1 = retentate flow rate from Stage 1, and P_2 = permeate flow rate from Stage 2.
Fresh feed in is 850 lb/h of H_2O and 150 lb/h of dissolved solids.
Total material balance: $1{,}000 = R_1 + P_2$ (1)
Dissolved solids material balance: $150 = 0.25\ R_1 + [300/(1{,}000{,}000+300)]\ P_2$ (2)
Solving Eqs. (1) and (2) simultaneously gives, R_1 = 599.5 lb/h and P_2 = 400.5 lb/h
Dissolved solids in purified water, P_2, equals [300/(1,000,000 + 300)](400.5) = 0.12 lb/h
Dissolved solids in the concentrate (retentate from Stage 1) = 150 - 0.12 = 149.88 lb/h

Compute material balance for Stage 2:
Let P_1 = permeate flow rate from Stage 1 = feed flow rate to Stage 2.
Dissolved solids material balance: $0.004\ P_1 = 0.12 + 0.026\ (P_1 - 400.5)$ (3)
Solving Eq. (3), P_1 = 467.9 lb/h, containing 0.004(467.9) = 1.87 lb/h dissolved solids
Retentate flow rate from Stage 2 = 467.9 - 400.5 = 67.4 lb/h,
containing 1.87 - 0.12 = 1.75 lb/h dissolved solids
The complete material balance is as follows:

	Flow rate, lb/h:					
Component	**Fresh feed**	**Combined feed to Stage 1**	**Retentate from Stage 1**	**Permeate from Stage 1**	**Retentate from Stage 2**	**Permeate from Stage 2**
Dissolved solids	150	151.75	149.88	1.87	1.75	0.12
Water	850	915.65	449.62	466.03	65.65	400.38
Total	1,000	1,067.40	599.50	467.90	67.40	400.50

Exercise 14.18 (continued)

Analysis: (continued)

Now calculate the membrane area of each stage using Eq. (14-69).

Assume osmotic pressure = $\pi = C$ (wt% solids), with π = 1,700 psia for 25 wt% solids.

Therefore, C = 1,700/25 = 68.

For the feed, π = 68(151.75/1,067.40)100 = 967 psia

For the retentate from Stage 1, π = 68(25) = 1,700 psia

For the permeate from Stage 1, π = 68(0.4) = 27.2 psia

For the retentate from Stage 2, π = 68(2.6) = 176.8 psia

For the permeate from Stage 2, π = 68(0.12/400.50)100 = 2.0 psia

From Eq. (14-69), $A_M = \dfrac{n_{H_2O}}{\overline{P}_{M_{H_2O}}(\Delta P - \Delta\pi)_{avg}} = \dfrac{n_{H_2O}}{0.0134(\Delta P - \Delta\pi)_{avg}}$

Stage 1:

$(\Delta P - \Delta\pi)_{avg}$ = (1,756 - 15) - [(967 + 1,700)/2 - 27.2] = 1,741 - 1,306 = 435 psi

$$A_M = \frac{466.03}{0.0134(435)} = 80 \text{ ft}^2$$

Stage 2:

$(\Delta P - \Delta\pi)_{avg}$ = (518 - 15) - [(27.2 + 176.8)/2 - 2.0] = 503 - 100 = 403 psi

$$A_M = \frac{400.38}{0.0134(403)} = 74 \text{ ft}^2$$

Exercise 14.19

Subject: Recovery of VOCs from air by gas permeation.

Given: Feed gas of 1500 scfm (0°C, 1 atm) of air at 40°C and 1.2 atm, containing 0.5 mol% acetone (A). Pressure of permeate side = 5 cmHg. Membrane of thin-composite with 2μm-thick silicone rubber skin gives 4 barrer for air and 20,000 barrer for acetone.

Assumptions: Crossflow.

Find: Membrane area for retentate containing 0.05 mol% acetone and permeate containing 5 mol% acetone.

Analysis: First complete the overall material balance.
Feed flow rate = 1,500(60)/359 = 250.7 lbmol/h
Acetone in the feed = 0.005(250.7) = 1.25 lbmol/h
Air in the feed = 250.7 - 1.25 = 249.45 lbmol/h
Overall total molar balance: $F = 250.7 = R + P$ (1)
Overall acetone molar balance: $1.25 = 0.0005\,R + 0.05\,P$ (2)
Solving Eqs. (1) and (2) simultaneously, $R = 228.0$ lbmol/h and $P = 22.7$ lbmol/h
The resulting component material balance is as follows:

lbmol/hr:

Component:	Feed	Retentate	Permeate
Acetone	1.25	0.11	1.14
Air	249.45	227.89	21.56
Total	250.70	228.00	22.70

Convert the given permeabilities in barrer to permeances in American Engineering units.

$$\overline{P}_{M_A} = \frac{20{,}000}{2\times10^{-4}} = 1.0\times10^{8} \text{ barrer/cm}$$

$$= 1.0\times10^{-2} \text{ cm}^3\text{(STP)/cm}^2\text{-s-cmHg}$$

Convert permeance to American Engineering units of lbmol/ft^2-h-psi:
1 barrer/cm = 1 x 10^{-10} (30.48 cm/ft)^2 (76 cmHg/14.696 psi) / (22,400 x 454 cm^3 (STP)/lbmol)
= 1.70 x 10^{-10} lbmol/ft^2-h-psi
Therefore, the permeances are:

$$\overline{P}_{M_A} = 1.0\times10^{8}\left(1.70\times10^{-10}\right) = 1.70\times10^{-2} \text{ lbmol/ft}^2\text{-h-psi}$$

$$\overline{P}_{M_{Air}} = \frac{4}{2\times10^{-4}}\left(1.70\times10^{-10}\right) = 3.40\times10^{-6} \text{ lbmol/ft}^2\text{-h-psi}$$

Compute entering and exiting partial pressures.
Feed: $p_A = (1.2)(14.7)(1.25)/250.70 = 0.088$ psia
$p_{Air} = (1.2)(14.7)(249.45)/250.70 = 17.552$ psia

Exercise 14.19 (continued)

Analysis: (continued)

Retentate: $p_A = (1.2)(14.7)(0.11)/228.00 = 0.0085$ psia
$p_{Air} = (1.2)(14.7)(227.89)/228.00 = 17.6315$ psia
Permeate: $p_A = (5/76)(14.7)(1.14)/22.7 = 0.0486$ psia
$p_{Air} = (5/76)(14.7)(21.56)/22.7 = 0.9185$ psia

Now check to see if it is even possible to obtain a permeate of 5 mol% acetone (A).
For crossflow, the initial acetone content of the local permeate at the feed end must be greater than 5 mol% because the mol% will decrease as the feed moves to the other end.
$P_F = P_R = 1.2$ atm $= 17.64$ psia, $P_P = 5$ cmHg $= 0.9671$ psia, $r = P_P/P_F = 0.9671/17.64 = 0.0548$

Rearranging Eq. (14-36), $y = \dfrac{\alpha x}{1+(\alpha-1)x}$ (3) ,where, y and x refer to A and α is for A to air.

From Eq. (14-43), $\alpha = \alpha^*_{A\text{-air}}\left[\dfrac{x(\alpha-1)+1-r\alpha}{x(\alpha-1)+1-r}\right] = 5000\left[\dfrac{x(\alpha-1)+1-0.0548\alpha}{x(\alpha-1)+1-0.0548}\right]$ (4)

Solving Eq. (4), for $x = x_F = 0.005$, $\alpha = 19.8872$. Substituting this α into Eq. (3), $y = 0..0909$.
Therefore, it is possible to obtain a permeate with a 5 mol% acetone.
For this exercise, it is found that α for all values of x can not be assumed constant because the mole fraction of A in the cumulative permeate is very sensitive to the value of α. Therefore, Eq. (4) is used to compute a new α at each step with a new value of x. For crossflow with a binary mixture, we have the following relationships between acetone mole fractions in the permeate and retentate as a function of the cut, $\theta = n_P/n_F$.

From material balance Eq. (1), Example 14.6, $y_P = \dfrac{x_F - x_R(1-\theta)}{\theta} = \dfrac{0.005 - x_R(1-\theta)}{\theta}$ (5)

From Eq. (14-49), where the y and x pertain to A,

$$y_P = x_R^{\left(\frac{1}{1-\alpha}\right)}\left(\frac{1-\theta}{\theta}\right)\left[(1-x_R)^{\left(\frac{\alpha}{\alpha-1}\right)}\left(\frac{x_F}{1-x_F}\right)^{\left(\frac{\alpha}{\alpha-1}\right)} - x_R^{\left(\frac{\alpha}{\alpha-1}\right)}\right] = x_R^{\left(\frac{1}{1-\alpha}\right)}\left(\frac{1-\theta}{\theta}\right)\left[(1-x_R)^{\left(\frac{\alpha}{\alpha-1}\right)}\left(\frac{0.005}{1-0.005}\right)^{\left(\frac{\alpha}{\alpha-1}\right)} - x_R^{\left(\frac{\alpha}{\alpha-1}\right)}\right]$$

Combine this equation with Eq. (5) to obtain:

$$1-\theta = \frac{0.005}{x_R + x_R^{\left(\frac{1}{1-\alpha}\right)}\left[(1-x_R)^{\left(\frac{\alpha}{\alpha-1}\right)}\left(\frac{0.005}{0.995}\right)^{\left(\frac{\alpha}{\alpha-1}\right)} - x_R^{\left(\frac{\alpha}{\alpha-1}\right)}\right]} \qquad (6)$$

For A, x_R begins at 0.005 at the feed end and decreases toward the retentate end. For each step in x, Eq. (4) is used to calculate α. Use Eq. (6) to compute values of θ as x_R decreases. Use Eq. (5) to compute the corresponding value of y_P. Eq. (3) is used to compute the local value of y.
For a differential molar transfer rate, dn, the differential membrane area required is given by Eq. (14-50), which is also given in incremental form for numerical calculation. If we base this calculation on A,

Exercise 14.19 (continued)

Analysis: (continued)

$$dA_M = \frac{y\,dn}{\overline{P}_{M_{O_2}}\left(xP_F - yP_P\right)}, \qquad \Delta A_M = \frac{y\,\Delta n}{1.70\times10^{-2}\left[x(17.64) - y(0.9671)\right]} \tag{9}$$

where y is the local value given by Eq. (3) and Δn is the incremental decrease in the feed flow. Using the equations, the calculations are carried out on a spreadsheet with the results below.

From the spreadsheet results, the membrane area is, by interpolation, 314,500 ft^2 when the acetone mole fraction in the permeate = 0.05. However, at that condition, the calculations show a retentate with an acetone mole fraction of 0.00136, where 0.0005 is desired. At that value, the permeate acetone content drops to 3.55 mol% and the membrane area increases to 548,400 ft^2.

Exercise 14.19 (continued)

Analysis: (continued)

x of A in R	alpha	α/(α−1)	1-θ	θ	*y* of A in P	Δ*n*, lbmol/hr	local *y*	Δ Area, sq. ft.	Cumulative Area, sq. ft.
0.0050	19.8872	1.05295	1.0000	0.0000	0.0909		0.0909	0	
0.0049	19.8497	1.05305	0.9988	0.0012	0.0899	0.2951	0.0890	4742	4742
0.0048	19.8123	1.05316	0.9976	0.0024	0.0889	0.3013	0.0872	4852	9593
0.0047	19.7751	1.05326	0.9964	0.0036	0.0879	0.3078	0.0854	4966	14560
0.0046	19.7380	1.05337	0.9951	0.0049	0.0869	0.3146	0.0836	5085	19645
0.0045	19.7011	1.05347	0.9939	0.0061	0.0859	0.3216	0.0818	5209	24854
0.0044	19.6643	1.05358	0.9925	0.0075	0.0849	0.3289	0.0800	5339	30193
0.0043	19.6277	1.05368	0.9912	0.0088	0.0839	0.3366	0.0781	5473	35666
0.0042	19.5912	1.05379	0.9898	0.0102	0.0828	0.3445	0.0763	5614	41281
0.0041	19.5549	1.05389	0.9884	0.0116	0.0818	0.3529	0.0745	5761	47042
0.0040	19.5187	1.05400	0.9870	0.0130	0.0808	0.3616	0.0727	5915	52956
0.0039	19.4826	1.05410	0.9855	0.0145	0.0798	0.3707	0.0709	6076	59032
0.0038	19.4467	1.05421	0.9840	0.0160	0.0787	0.3803	0.0691	6245	65277
0.0037	19.4109	1.05432	0.9824	0.0176	0.0777	0.3903	0.0672	6422	71699
0.0036	19.3752	1.05442	0.9808	0.0192	0.0766	0.4008	0.0654	6608	78307
0.0035	19.3397	1.05453	0.9792	0.0208	0.0756	0.4119	0.0636	6805	85112
0.0034	19.3043	1.05463	0.9775	0.0225	0.0745	0.4236	0.0618	7011	92123
0.0033	19.2691	1.05474	0.9758	0.0242	0.0734	0.4360	0.0600	7230	99353
0.0032	19.2340	1.05484	0.9740	0.0260	0.0723	0.4491	0.0582	7461	106814
0.0031	19.1990	1.05495	0.9721	0.0279	0.0712	0.4629	0.0563	7706	114520
0.0030	19.1642	1.05505	0.9702	0.0298	0.0701	0.4776	0.0545	7966	122486
0.0029	19.1295	1.05516	0.9682	0.0318	0.0690	0.4932	0.0527	8242	130728
0.0028	19.0949	1.05526	0.9662	0.0338	0.0679	0.5099	0.0509	8537	139265
0.0027	19.0604	1.05537	0.9641	0.0359	0.0668	0.5277	0.0491	8852	148117
0.0026	19.0261	1.05548	0.9619	0.0381	0.0656	0.5468	0.0473	9189	157306
0.0025	18.9919	1.05558	0.9597	0.0403	0.0645	0.5672	0.0454	9552	166858
0.0024	18.9579	1.05569	0.9573	0.0427	0.0633	0.5893	0.0436	9942	176800
0.0023	18.9240	1.05579	0.9549	0.0451	0.0621	0.6131	0.0418	10364	187163
0.0022	18.8902	1.05590	0.9523	0.0477	0.0609	0.6389	0.0400	10821	197984
0.0021	18.8565	1.05600	0.9497	0.0503	0.0597	0.6670	0.0382	11318	209302
0.0020	18.8229	1.05611	0.9469	0.0531	0.0585	0.6978	0.0364	11861	221163
0.0019	18.7895	1.05621	0.9440	0.0560	0.0572	0.7314	0.0345	12458	233621
0.0018	18.7562	1.05632	0.9409	0.0591	0.0559	0.7686	0.0327	13115	246736
0.0017	18.7230	1.05642	0.9377	0.0623	0.0546	0.8098	0.0309	13844	260579
0.0016	18.6900	1.05653	0.9342	0.0658	0.0533	0.8557	0.0291	14657	275236
0.0015	18.6571	1.05663	0.9306	0.0694	0.0520	0.9073	0.0273	15569	290805
0.0014	18.6243	1.05674	0.9268	0.0732	0.0506	0.9657	0.0254	16602	307408
0.0013	18.5916	1.05685	0.9227	0.0773	0.0491	1.0323	0.0236	17781	325188
0.0012	18.5590	1.05695	0.9182	0.0818	0.0477	1.1092	0.0218	19140	344328
0.0011	18.5266	1.05706	0.9135	0.0865	0.0462	1.1988	0.0200	20725	365053
0.0010	18.4942	1.05716	0.9082	0.0918	0.0446	1.3048	0.0182	22599	387651
0.0009	18.4620	1.05727	0.9025	0.0975	0.0430	1.4322	0.0164	24851	412502
0.0008	18.4300	1.05737	0.8962	0.1038	0.0413	1.5883	0.0145	27612	440114
0.0007	18.3980	1.05748	0.8891	0.1109	0.0395	1.7846	0.0127	31080	471194
0.0006	18.3661	1.05758	0.8809	0.1191	0.0376	2.0390	0.0109	35577	506771
0.0005	18.3344	1.05769	0.8714	0.1286	0.0355	2.3828	0.0091	41652	548423
0.0004	18.3028	1.05779	0.8600	0.1400	0.0333	2.8747	0.0073	50342	598765

Exercise 14.20

Subject: Separation of air by gas permeation.

Given: Permeate of 5 ton/day (2,000 lb/ton) of 40 mol% O_2 and retentate of 90 mol% N_2 from a feed of air. 500 psia on feed side and 20 psia on permeate side.

Assumptions: Crossflow. No pressure drop on feed side.

Find: Membrane area in m^2 for the following membranes:

Company	**A**	**B**
Module type	Hollow-fiber	Spiral-wound
Permeance for O_2, barrer/μm	15	35
Ratio of O_2 to N_2 permeances	3.5	1.9

Analysis: First calculate the overall material balance. $P = 5(2{,}000) = 10{,}000$ lb/day
The average molecular weight of the permeate = [0.4(32) + 0.6(28)] = 29.6
Therefore, $P = 10{,}000/29.6 = 337.8$ lbmol/day.
Total molar balance: $F = R + 337.8$ (1)
O_2 molar balance: $0.21F = 0.1R + 0.4(337.8) = 0.1R + 135.1$ (2)
Solving Eqs. (1) and (2), $F = 921.2$ lbmol/h and $R = 583.4$ lbmol/h
On a component basis, the overall material balance is:

lbmol/day:

Component:	**Feed**	**Retentate**	**Permeate**
O_2	193.5	58.3	135.2
N_2	727.7	525.1	202.6
Total	921.2	583.4	337.8

Now check each module type to see if it is even possible to obtain a permeate of 40 mol% O_2. For crossflow, the initial oxygen content of the local permeate at the feed end must be greater than 40 mol% because the mol% will decrease as the feed moves to the other end.
$P_F = P_R = 500$ psia, $P_P = 20$ psia, $r = P_P/P_F = 20/500 = 0.04$

Rearranging Eq. (14-36), $y = \dfrac{\alpha x}{1+(\alpha-1)x}$ (3) ,where, y and x refer to O_2 and α is for O_2 to N_2.

From Eq. (14-43), $\alpha = \alpha^*_{O_2\text{-}N_2}\left[\dfrac{x(\alpha-1)+1-r\alpha}{x(\alpha-1)+1-r}\right] = \alpha^*_{O_2\text{-}N_2}\left[\dfrac{0.21(\alpha-1)+1-0.04\alpha}{0.21(\alpha-1)+1-0.04}\right]$ (4)

For Company A, $\alpha^*_{O_2\text{-}N_2} = 3.5$. Substituting this into Eq. (4) and solving, $\alpha = 3.28$.

Substituting this α into Eq. (3), $y = 0.4658$. Therefore, consider Company A.
For Company B, $\alpha^*_{O_2\text{-}N_2} = 1.9$. Substituting this into Eq. (4) and solving, $\alpha = 1.84$.

Substituting this α into Eq. (3), $y = 0.3285$. Therefore, Company B is dropped.

Exercise 14.20 (continued)

Analysis: Company A (continued)

$$\overline{P}_{M_{O_2}} = \frac{15}{10^{-4}} = 150{,}000 \text{ barrer / cm}$$

$$= 1.50\times10^{-5} \text{ cm}^3\text{(STP)} / \text{cm}^2 \text{ - s - cmHg}$$

Convert permeance to American Engineering units of lbmol/ft^2-h-psi:

1 barrer/cm = 1 x 10^{-10} (30.48 cm/ft)^2 (76 cmHg/14.696 psi) / (22,400 x 454 cm^3 (STP)/lbmol)

= 1.70 x 10^{-10} lbmol/ft^2-h-psi

Therefore, the permeances are:

$$\overline{P}_{M_{O_2}} = 150{,}000\left(1.70\times10^{-10}\right) = 2.55\times10^{-5} \text{ lbmol / ft}^2 \text{ - h - psi}$$

Using the given selectivity,

$$\overline{P}_{M_{N_2}} = 7.29\times10^{-6} \text{ lbmol / ft}^2 \text{ - h - psi}$$

Assume that $\alpha = \alpha_{O2\text{-}N2}$ = a constant = 3.28 from above. Then, for crossflow with a binary mixture, we have the following relationships between oxygen mole fractions in the permeate and retentate as a function of the cut, $\theta = n_P/n_F$.

From material balance Eq. (1), Example 14.6, $y_P = \dfrac{x_F - x_R(1-\theta)}{\theta} = \dfrac{0.21 - x_R(1-\theta)}{\theta}$ (5)

From Eq. (14-49), where the *y* and *x* pertain to O_2,

$$y_P = x_R^{\left(\frac{1}{1-\alpha}\right)}\left(\frac{1-\theta}{\theta}\right)\left[(1-x_R)^{\left(\frac{\alpha}{\alpha-1}\right)}\left(\frac{x_F}{1-x_F}\right)^{\left(\frac{\alpha}{\alpha-1}\right)} - x_R^{\left(\frac{\alpha}{\alpha-1}\right)}\right] = x_R^{-0.4386}\left(\frac{1-\theta}{\theta}\right)\left[0.1486(1-x_R)^{1.439} - x_R^{1.439}\right]$$

Combine this equation with Eq. (5) to obtain:

$$1-\theta = \frac{0.21}{x_R + x_R^{-0.4386}\left[0.1486(1-x_R)^{1.439} - x_R^{1.439}\right]} \qquad (6)$$

For O_2, x_R begins at 0.21 at the feed end and decreases toward the retentate end. Use Eq. (6) to compute values of θ as x_R is stepped toward 0. Use Eq. (5) to compute the corresponding value of y_P.

For a differential molar transfer rate, *dn*, the differential membrane area required is given by Eq. (14-50), which is also given in incremental form for numerical calculation. If we base this calculation on O_2,

$$dA_M = \frac{y\,dn}{\overline{P}_{M_{O_2}}\left(xP_F - yP_P\right)}, \qquad \Delta A_M = \frac{y\Delta n}{2.55\times10^{-5}\left[x(500) - y(20)\right]} \qquad (9)$$

where *y* is the local value given by Eq. (3) and Δn is the incremental decrease in the feed flow.

Exercise 14.20 (continued)

Analysis: Company A (continued)

Using the above equations, the calculations are carried out on a spreadsheet with results below. From the spreadsheet results, the membrane area is, by interpolation, 2,388 ft^2 when the oxygen mole fraction in the permeate = 0.40. However, at that condition, the calculations show a retentate with an oxygen mole fraction of 0.128 and, therefore, a nitrogen mole fraction of 0.872. Thus, the ideal of 90 mol% N_2 is not quite achieved. At that value, the oxygen content of the permeate drops to 37.4 mol% and the membrane area increases to 3,262 ft^2.

x of O2 in R	1-θ	θ	*y* of O2 in P	Δ*n*, lbmol/hr	local *y*	Δ Area, sq. ft.	Cumulative Area, sq. ft.
0.210	1.000	0.000	0.466		0.466	0	
0.205	0.980	0.020	0.461	0.749	0.458	144	144
0.200	0.961	0.039	0.458	0.739	0.451	144	288
0.195	0.942	0.058	0.454	0.732	0.443	143	431
0.190	0.923	0.077	0.451	0.726	0.435	143	575
0.185	0.904	0.096	0.447	0.720	0.427	144	718
0.180	0.886	0.114	0.443	0.715	0.419	144	862
0.175	0.867	0.133	0.439	0.709	0.410	144	1006
0.170	0.849	0.151	0.435	0.705	0.402	144	1150
0.165	0.831	0.169	0.431	0.700	0.393	145	1295
0.160	0.813	0.187	0.427	0.696	0.385	145	1440
0.155	0.795	0.205	0.423	0.692	0.376	146	1586
0.150	0.777	0.223	0.419	0.689	0.367	146	1732
0.145	0.759	0.241	0.414	0.686	0.357	147	1879
0.140	0.741	0.259	0.410	0.684	0.348	148	2028
0.135	0.723	0.277	0.406	0.682	0.339	149	2177
0.130	0.705	0.295	0.402	0.681	0.329	150	2327
0.125	0.688	0.312	0.397	0.680	0.319	152	2479
0.120	0.670	0.330	0.393	0.680	0.309	153	2632
0.115	0.652	0.348	0.388	0.680	0.299	155	2786
0.110	0.635	0.365	0.384	0.681	0.288	157	2943
0.105	0.617	0.383	0.379	0.683	0.278	159	3101
0.100	0.599	0.401	0.374	0.686	0.267	161	3262

Exercise 14.21

Subject: Removal of CO_2 and H_2S from high-pressure sour natural gas by gas permeation to produce a pipeline gas.

Given: Feed and product conditions:

Stream	Feed gas	Pipeline gas
Pressure, psia	1000	980
Composition, mol%:		
CH_4	70	97.96
H_2S	10	0.04
CO_2	20	2.00

Hollow-fiber membrane of 0.5 μm skin thickness with a permeability for CO_2 of 13.3 barrer, and selectivities of CO_2 to CH_4 and of H_2S to CH_4, both of 50.

Assumptions: $T = 60^oF$ and permeate-side pressure = 20 psia. Crossflow.

Find: Membrane area for feed flow rate of 10,000 scfm (0^oC, and 1 atm).

Analysis: The feed molar flow rate = 10,000 scfm/[(379 scf/lbmol)(60 s/min)] = 0.44 lbmol/s
The membrane thickness = l_M = 0.5 microns = 0.5 x 10^{-4} cm From Eq. (14-1),

$$\overline{P}_{M_{CO_2}} = \frac{P_{M_{CO_2}}}{l_M} = \frac{13.3}{0.5\times10^{-4}} = 266{,}000 \text{ barrer / cm}$$

$$= 2.66\times10^{-5} \text{ cm}^3\text{(STP)} / \text{cm}^2 \text{ - s - cmHg}$$

Convert permeance to American Engineering units of lbmol/ft^2-s-psi:
1 barrer/cm = 1 x 10^{-10} (30.48 cm/ft)^2 (76 cmHg/14.696 psi) / (22,400 x 454 cm^3 (STP)/lbmol)
= 4.724 x 10^{-14} lbmol/ft^2-s-psi
Therefore, the permeances are:

$$\overline{P}_{M_{CO_2}} = 266{,}000\left(4.724\times10^{-14}\right) = 1.26\times10^{-8} \text{ lbmol / ft}^2 \text{ - s - psi}$$

Using the given selectivities,

$$\overline{P}_{M_{H_2S}} = 1.26\times10^{-8} \text{ lbmol / ft}^2 \text{ - s - psi}$$

$$\overline{P}_{M_{CH_4}} = 2.52\times10^{-10} \text{ lbmol / ft}^2 \text{ - s - psi}$$

Now make the crossflow calculations, letting A = H_2S, B = CO_2, C = CH_4, and n = local molar flow rate on the feed-retentate side. Local mole fractions are x on the feed-retentate side and y on the permeate side. From a rearrangement of Eq. (14-45), the differential component material balances are as follows, including the incremental Euler form for making the numerical calculations,

Exercise 14.21 (continued)

Analysis: (continued)

$$\frac{dx_A}{dn} = \frac{y_A - x_A}{n}, \qquad \frac{x_A^{(k+1)} - x_A^{(k)}}{\Delta n} = \frac{y_A^{(k)} - x_A^{(k)}}{n_{avg}} \tag{1}$$

$$\frac{dx_B}{dn} = \frac{y_B - x_B}{n}, \qquad \frac{x_B^{(k+1)} - x_B^{(k)}}{\Delta n} = \frac{y_B^{(k)} - x_B^{(k)}}{n_{avg}} \tag{2}$$

$$\text{with} \quad x_C^{(k+1)} = 1 - x_A^{(k+1)} - x_B^{(k+1)} \tag{3}$$

In the absence of film mass-transfer resistances on either side of the membrane, the ratios of mass transfer rates through the membrane are given by Eq. (14-39) combined with Eq. (14-40), which are as follows, including the Euler form for making the numerical calculations,

$$\frac{y_A}{y_C} = \alpha^*_{AC}\left(\frac{x_A P_F - y_A P_P}{x_C P_F - y_C P_P}\right), \quad \left(\frac{y_A}{y_C}\right)^{(k+1)} = \alpha^*_{AC}\left(\frac{x_A^{(k+1)} P_F - y_A^{(k)} P_P}{x_C^{(k+1)} P_F - y_C^{(k)} P_P}\right) \tag{4}$$

$$\frac{y_B}{y_C} = \alpha^*_{BC}\left(\frac{x_B P_F - y_B P_P}{x_C P_F - y_C P_P}\right), \quad \left(\frac{y_B}{y_C}\right)^{(k+1)} = \alpha^*_{BC}\left(\frac{x_B^{(k+1)} P_F - y_B^{(k)} P_P}{x_C^{(k+1)} P_F - y_C^{(k)} P_P}\right) \tag{5}$$

Since, $y_A + y_B + y_C = 1$, $\frac{y_A}{y_C} + \frac{y_B}{y_C} + 1 = \frac{1}{y_C}$ and, therefore,

$$y_C^{(k+1)} = \frac{1}{1 + \left(\frac{y_A}{y_C}\right)^{(k+1)} + \left(\frac{y_B}{y_C}\right)^{(k+1)}} \tag{6}$$

$$\text{with} \quad y_A^{(k+1)} = y_C^{(k+1)}\left(\frac{y_A}{y_C}\right)^{(k+1)} \tag{7}$$

$$\text{and} \quad y_B^{(k+1)} = y_C^{(k+1)}\left(\frac{y_B}{y_C}\right)^{(k+1)} \tag{8}$$

For a differential molar transfer rate, *dn*, the differential membrane area required is given by Eq. (14-50), which is also given in Euler incremental form for numerical calculation. If we base this calculation on H_2S,

$$dA_M = \frac{y_A dn}{\overline{P}_{M_A}\left(x_A P_F - y_A P_P\right)}, \qquad \Delta A_M = \frac{y_A^{(k+1)} \Delta n}{\overline{P}_{M_A}\left(x_A^{(k+1)} P_F - y_A^{(k+1)} P_P\right)} \tag{9}$$

The calculations are made with spreadsheet, using Eqs. (1) to (9), with the following values that remain constant: $P_P = 20$ psia, $\alpha^*_{AC} = 50$, $\alpha^*_{BC} = 50$, $\overline{P}_{M_A} = 1.26 \times 10^{-8}$ lbmol / ft^2 - s - psi .

Exercise 14.21 (continued)

Analysis: (continued)

The pressure on the feed-retentate side, P_F, decreases from 1,000 to 980 psia. The incremental change in this pressure will have to be adjusted by trial and error so that when the pipeline gas composition is reached on the feed-retentate side, the pressure will have decreased to 980 psia. It is not possible to obtain the exact specified pipeline gas composition with respect to H_2S and CO_2. So the specification (retentate) is changed to a mol% for H_2S of not more than 0.04 and a mol% for CO_2 of not more than 2.0. Either H_2S or CO_2 will control.

The initial value of n is 0.44 lbmol/s. Choose an increment, Δn = -0.005 lbmol/s. The initial values of $x^{(0)}$ are 0.1 for A, 0.2 for B, and 0.7 for C. The following is a set of calculations for the first increment of n, which takes n to 0.44 - 0.005 = 0.435, with an n_{avg} = (0.44 + 0.435)/2 =0.4375

Because the permeate side pressure is very low compared to the feed-side pressure, the initial composition of the permeate is given by simplifications of Eqs. (4) and (5):

$y_A/y_C = 50(x_A/x_C) = 50(0.1/0.7) = 7.14$ and $y_B/y_C = 50(x_B/x_C) = 50(0.2/0.7) = 14.29$

Substitution into Eqs. (6) to (8) gives $y_A^{(0)} = 0.3183$, $y_B^{(0)} = 0.6372$, $y_C^{(0)} = 0.0445$

From Eqs. (1), (2), and (3),

$$x_A^{(1)} = x_A^{(0)} + \frac{y_A^{(0)} - x_A^{(0)}}{n_{avg}}\Delta n = 0.10 + \frac{0.3183 - 0.10}{0.4375}(-0.005) = 0.0975$$

$$x_B^{(1)} = x_B^{(0)} + \frac{y_B^{(0)} - x_B^{(0)}}{n_{avg}}\Delta n = 0.20 + \frac{0.6372 - 0.20}{0.4375}(-0.005) = 0.1950$$

$$x_C^{(1)} = 1 - x_A^{(1)} - x_B^{(1)} = 1 - 0.0975 - 0.1950 = 0.7075$$

Substitution into Eqs. (4) and (5) gives:

$$\left(\frac{y_A}{y_C}\right)^{(1)} = \alpha_{AC}^{*}\left(\frac{x_A^{(1)}P_F - y_A^{(0)}P_P}{x_C^{(1)}P_F - y_C^{(0)}P_P}\right) = 50\left[\frac{0.0975(1000) - 0.3183(20)}{0.7075(1000) - 0.0445(20)}\right] = 6.449$$

$$\left(\frac{y_B}{y_C}\right)^{(1)} = \alpha_{BC}^{*}\left(\frac{x_B^{(1)}P_F - y_B^{(0)}P_P}{x_C^{(1)}P_F - y_C^{(0)}P_P}\right) = 50\left[\frac{0.1950(1000) - 0.6372(20)}{0.7075(1000) - 0.0445(20)}\right] = 12.897$$

Using Eqs. (6) to (8),

$$y_C^{(1)} = \frac{1}{1 + 6.449 + 12.897} = 0.0491$$

$$y_A^{(1)} = 0.04915(6.449) = 0.3170$$

$$y_B^{(1)} = 0.04915(12.897) = 0.6339$$

Exercise 14.21 (continued)

Analysis: (continued)

From Eq. (9), $\Delta A_M = \dfrac{y_A^{(1)} \Delta n}{\overline{P}_{M_A}\left(x_A^{(1)} P_F - y_A^{(1)} P_P\right)} = \dfrac{0.3170(0.005)}{1.26\times10^{-8}[0.0975(1000) - 0.3170(20)]} = 1{,}380 \text{ ft}^2$

Calculations for succeeding increments of n are given below from spreadsheet calculations.

From the spreadsheet results, it is seen that when the mole fraction of H_2S in the retentate reaches 0.0004, the mole fraction of CO_2 is well below the specified 0.02. Thus, H_2S controls. The mole fractions of the permeate in the spreadsheet table are the local values. The average composition of the final combined permeate is obtained by material balance from the feed gas and calculated pipeline gas (final retentate from the spreadsheet) with the following results:

Component mol%:	**Feed gas**	**Pipeline gas**	**Permeate**
CH_4	70	99.89	28.80
H_2S	10	0.04	23.73
CO_2	20	0.07	47.47
Total flow,lbmol/s	0.440	0.255	0.185

From 10,000 scfm of feed gas, 1,000(0.255/0.44) = 580 scfm of pipeline gas is obtained.
From the spreadsheet table, the final retentate pressure is very close to the required 980 psia.
The required membrane area = 197,000 ft^2. If each module contained 4,000 ft^2, as mentioned for one case in the industrial example at the beginning of this chapter, then the number of modules in parallel = 197,000/4,000 = say 50 modules.

This is not unreasonable.

Exercise 14.21 (continued)

Analysis: (continued)

n, lbmol/s	x H2S	x CO2	x CH4	y H2S/ y CH4	y CO2/ y CH4	y H2S	y CO2	y CH4	Based on H2S: dAM ft2	Cum AM ft2	PF, psi
0.440	0.1000	0.2000	0.7000			0.3183	0.6372	0.0445	0	0	1000
0.435	0.0975	0.1950	0.7075	6.449	12.897	0.3170	0.6339	0.0491	1380	1380	999.5
0.430	0.0950	0.1899	0.7151	6.205	12.411	0.3163	0.6327	0.0510	1416	2796	998.9
0.425	0.0924	0.1848	0.7229	5.961	11.921	0.3157	0.6314	0.0530	1456	4251	998.4
0.420	0.0897	0.1795	0.7308	5.716	11.431	0.3150	0.6299	0.0551	1498	5749	997.8
0.415	0.0870	0.1741	0.7389	5.472	10.943	0.3142	0.6284	0.0574	1544	7293	997.3
0.410	0.0843	0.1686	0.7472	5.228	10.456	0.3134	0.6267	0.0599	1594	8887	996.7
0.405	0.0815	0.1629	0.7556	4.985	9.969	0.3124	0.6249	0.0627	1648	10536	996.2
0.400	0.0786	0.1572	0.7642	4.742	9.484	0.3114	0.6229	0.0657	1708	12243	995.6
0.395	0.0757	0.1513	0.7730	4.500	8.999	0.3104	0.6207	0.0690	1773	14016	995.1
0.390	0.0727	0.1454	0.7819	4.258	8.517	0.3091	0.6183	0.0726	1845	15861	994.5
0.385	0.0696	0.1393	0.7911	4.018	8.035	0.3078	0.6156	0.0766	1924	17785	994.0
0.380	0.0665	0.1330	0.8004	3.778	7.556	0.3063	0.6126	0.0811	2013	19797	993.4
0.375	0.0633	0.1267	0.8100	3.539	7.078	0.3046	0.6093	0.0861	2112	21909	992.9
0.370	0.0601	0.1202	0.8197	3.302	6.603	0.3028	0.6055	0.0917	2223	24132	992.3
0.365	0.0568	0.1136	0.8296	3.066	6.131	0.3006	0.6013	0.0981	2349	26480	991.8
0.360	0.0534	0.1069	0.8397	2.831	5.662	0.2982	0.5964	0.1053	2493	28973	991.2
0.355	0.0500	0.1000	0.8499	2.598	5.196	0.2954	0.5909	0.1137	2658	31631	990.7
0.350	0.0465	0.0931	0.8604	2.367	4.735	0.2922	0.5844	0.1234	2849	34480	990.1
0.345	0.0430	0.0860	0.8710	2.139	4.278	0.2884	0.5768	0.1348	3074	37554	989.6
0.340	0.0394	0.0788	0.8817	1.914	3.828	0.2839	0.5678	0.1483	3339	40892	989.0
0.335	0.0358	0.0716	0.8926	1.693	3.386	0.2785	0.5570	0.1645	3656	44548	988.5
0.330	0.0321	0.0643	0.9036	1.476	2.952	0.2719	0.5439	0.1842	4040	48588	987.9
0.325	0.0285	0.0570	0.9145	1.265	2.530	0.2638	0.5276	0.2085	4510	53099	987.4
0.320	0.0248	0.0497	0.9255	1.062	2.123	0.2537	0.5074	0.2390	5093	58192	986.8
0.315	0.0212	0.0425	0.9363	0.867	1.735	0.2408	0.4816	0.2776	5820	64012	986.3
0.310	0.0177	0.0354	0.9468	0.686	1.371	0.2243	0.4486	0.3272	6724	70736	985.7
0.305	0.0144	0.0287	0.9569	0.520	1.039	0.2031	0.4061	0.3908	7822	78558	985.2
0.300	0.0112	0.0225	0.9663	0.375	0.749	0.1764	0.3528	0.4708	9072	87630	984.6
0.295	0.0085	0.0169	0.9746	0.256	0.512	0.1448	0.2895	0.5657	10308	97938	984.1
0.290	0.0061	0.0123	0.9816	0.167	0.334	0.1113	0.2226	0.6661	11290	109228	983.5
0.285	0.0043	0.0086	0.9871	0.107	0.214	0.0810	0.1620	0.7571	11946	121174	983.0
0.280	0.0030	0.0059	0.9911	0.068	0.137	0.0567	0.1133	0.8300	12362	133536	982.4
0.275	0.0020	0.0040	0.9940	0.044	0.087	0.0385	0.0770	0.8845	12582	146118	981.9
0.270	0.0013	0.0026	0.9961	0.028	0.056	0.0257	0.0513	0.9230	12718	158836	981.3
0.265	0.0009	0.0017	0.9974	0.018	0.035	0.0168	0.0335	0.9497	12703	171539	980.8
0.260	0.0006	0.0011	0.9983	0.011	0.023	0.0109	0.0218	0.9673	12795	184334	980.2
→ 0.255	0.0004	0.0007	0.9989	0.007	0.014	0.0069	0.0137	0.9794	12480	196814	979.7
0.250	0.0002	0.0005	0.9993	0.005	0.009	0.0045	0.0090	0.9865	13062	209876	979.1

Exercise 14.22

Subject: Separation of ethyl acetate (EA) from water by pervaporation.

Given: 100,000 gal/day of water containing 2.0 wt% EA at 30°C and 20 psia. Dense polydimethylsiloxane with a 1 μm-thick skin in a spiral-wound module. Permeate pressure = 3 cmHg. Membrane flux = 1.0 L/m^2-h with a separation factor of 100 for EA with respect to H_2O.

Assumptions: Crossflow.

Find: Membrane area in m^2 and temperature drop of feed for a retentate of 0.2 wt% EA and a permeate of 45.7 wt% EA as a vapor at 3 cmHg pressure.

Analysis: Use the Chemcad process simulator with the Wilson equation to determine thermodynamic properties of the liquid phases. The liquid density of the feed = 8.319 lb/gal
Feed rate = 100,000(8.319)/24 = 34,664 lb/h. The permeate and retentate flow rates are obtained by material balance:

Total material balance: $34{,}664 = R + P$ (1)

Ethyl acetate material balance: $0.02(34{,}664) = 0.002\,R + 0.457\,P$ (2)

Solving Eqs. (1) and (2), R = 33,293 lb/h and P = 1,371 lb/h
Using a MW of 80.10 for ethyl acetate, the following component material balance is obtained:

	lb/h:			lbmol/h:		
Component	**Feed**	**Retentate**	**Permeate**	**Feed**	**Retentate**	**Permeate**
Ethyl acetate	693	66.5	626.5	7.87	0.76	7.11
Water	33,971	33,226.5	744.5	1,885.73	1,844.40	41.33
Total	34,664	33,293.0	1,371.0	1,893.60	1,845.16	48.44

Assume that the membrane flux is based on a liquid phase of permeate at 30°C. From the Chemcad program, the liquid density at 30°C is 58.82 lb/ft^3 or 2.077 lb/L. Therefore, the volume flow of the permeate is 1,371/2.077 = 660 L/h. Therefore, since the flux is 1.0 L/m^2-h,
the membrane area = 660/1.0 = 660 m^2.
As discussed in Section 14.7, assume the permeate vapor leaves at the dew-point temperature at the permeate pressure of 3 cmHg. From the Chemcad program the permeate temperature = 26.2°C.
As discussed in Section 14.7, compute the exit temperature of the liquid retentate by an adiabatic enthalpy balance. Using Chemcad, the retentate temperature = 15.5°C. Therefore, temperature drop of the feed = 30 – 15.5 = 14.5°C.

Exercise 14.23

Subject: Calculation of permeances from laboratory data on pervaporation.

Given: Permeation flux of 1.6 kg/m^2-h for a 17 wt% ethanol in water feed, giving a permeate of 12 wt% ethanol at 60^{o}C and a permeate pressure of 15.2 mmHg. Other conditions in Example 14.12.

Find: Permeances for ethyl alcohol (1) and water (2). Selectivity for water.

Analysis: Molecular weights for ethyl alcohol and water are 46.07 and 18.02, respectively. From Example 14.12, the vapor pressure of ethyl alcohol = 352 mmHg, and that of water = 149 mmHg. The mole fractions in the feed are:

$$x_1 = \frac{0.17/46.07}{\dfrac{0.17}{46.07}+\dfrac{(1.0-0.17)}{18.02}} = 0.0742 \quad \text{and} \quad x_2 = 1-0.0742 = 0.9258$$

The mole fractions in the permeate are:

$$y_1 = \frac{0.12/46.07}{\dfrac{0.12}{46.07}+\dfrac{(1.0-0.12)}{18.02}} = 0.0506 \quad \text{and} \quad y_2 = 1-0.0506 = 0.9494$$

From Eq. (14-39), with no sweep, the component fluxes are proportional to the weight fractions in the permeate. Therefore,

$$N_1 = \frac{1.6(0.12)}{46.07} = 0.00417 \text{ kmol/h-m}^2 \quad \text{and} \quad N_2 = \frac{1.6(0.88)}{18.02} = 0.07814 \text{ kmol/h-m}^2$$

For Eq. (14-80), we need the activity coefficients in the feed mixture. Obtain these from the van Laar equations given in Example 14.12:

$$\gamma_1 = \exp\left\{1.6276\left[\frac{0.9232(0.9258)}{1.6276(0.0742)+0.9232(0.9258)}\right]^2\right\} = 3.488$$

$$\gamma_2 = \exp\left\{0.9232\left[\frac{1.6276(0.0742)}{1.6276(0.0742)+0.9232(0.9258)}\right]^2\right\} = 1.014$$

Exercise 14.23 (continued)

Analysis (continued)

From Eq. (14-80),

$$\bar{P}_{M_1} = \frac{N_1}{\gamma_1 x_1 P_1^s - y_1 p_1} = \frac{0.00417}{3.488(0.0742)(352) - 0.0506(15.2)} = 4.62\times10^{-5} \text{ kmol/h-m}^2 - \text{mmHg}$$

$$\bar{P}_{M_2} = \frac{N_2}{\gamma_2 x_2 P_2^s - y_2 p_2} = \frac{0.07814}{1.014(0.9258)(149) - 0.9496(15.2)} = 6.23\times10^{-4} \text{ kmol/h-m}^2 - \text{mmHg}$$

The selectivity is defined in Example 14.12. For water (2) in the permeate, the selectivity is given by:

$$\alpha_{2,1} = \frac{(100 - w_1)_P (w_1)_P}{(100 - w_1)_F (w_1)_F} \quad \text{with } w \text{ in wt\%}$$

In this exercise, w_1 = 12 wt% in the permeate and 17 wt% in the feed.

Therefore, the selectivity for water = $\alpha_{2,1} = \frac{(100-12)_P (12)_P}{(100-17)_F (17)_F} = 1.50$

Exercise 14.24

Subject: Laboratory data for separation of benzene (B) from cyclohexane (C) by a pervaporation process. Consideration of Stage 2 in a 3-stage process.

Given: Feed of 9,905 kg/h of 57.5 wt% B at 75°C to Stage 2. Retentate is 16.4 wt% B at 67.5°C. Permeate is 88.2 wt% B at 27.5°C. Total permeate flux = 1.43 kg/m^2-h. Selectivity for B = 8.

Find: Flow rates of retentate and permeate in kg/h. Membrane area in m^2.

Analysis: First, make a material balance to obtain the component flow rates in the feed, retentate, and permeate. Let R = retentate flow rate in kg/h and P = permeate flow rate in kg/h.

By total overall material balance, $R + P = 9905$ (1)

By an overall benzene material balance, $0.164R + 0.882P = 0.575(9905) = 5{,}695$ (2)

Solving Eqs. (1) and (2), P = 5,670 kg/h and R = 4,235 kg/h

Calculate the component flow rates in kg/h.

Stream	Feed	Retentate	Permeate
Component:	kg/h	kg/h	kg/h
B	5,695	694	5,001
C	4,210	3,541	669
Total	9,905	4,235	5,670

Membrane area = A_M = total permeate flow rate/permeate flux = 5,670/1.43 = 3,965 m^2

Exercise 14.25

Subject: Section 1 of a cheese whey ultrafiltration process to obtain a dry powder of combined TP and NPN as in Example 14.13

Given: Conditions of Example 14.13, including a whey feed of 1,000,000 lb/.day with the same composition and solute retention factors. Section 1 only with just two stages of continuous bleed-and-feed ultrafiltration to reach 55 wt% (dry basis) of combined TP and NPN.

Find: The component material balance in lb/day of operation, the % recovery (yield) from the whey of the TP and NPN in the final concentrate, and the number of cartridges required.

Analysis: Section 1 is shown in Figure 14.31. The calculations are similar to those of Example 14.13 where two cases are considered for Section 1, a single stage and four stages. As is the case in Example 14.13, the calculations assume equal membrane area for the two stages, and are carried out by a double "trial and error" procedure using a spreadsheet with a Solver function.

First assume a membrane area per stage. In Example 14.13, the computed area was 12,500 ft^2 for a single stage and 1,617 ft^2 per stage in a four-stage system, giving a total of 6,468 total ft^2. Assume a total area for two stages of 9,000 ft^2 or 4,500 ft^2 per stage.

Next, find by iteration, the overall concentration factor, $R_1 = P_2 + R_2$, that gives the fresh feed rate, F_1, to the first stage, which is computed in Example 14.13 at 5,882 gal/h for 20 hr/day operation. Use a spreadsheet, working backward from stage 2 to stage 1, using Equation (1) in Example 14.13, where J_n = hourly membrane flux at 1/24 of that equation, with $CF_2 = \overline{CF}$, Raffinate, $R_2 = F_1/CF_2$, $P_2 = AJ_2$, $R_1 = P_2 + R_2$, and $CF_1 = F_1/R_1$, $P_1 = AJ_1$, and back-calculated $F_1 = P_1 + R_1$. If the back-calculated F_1 is not equal to the actual value of 5,882 gal/h, then a new value of $\overline{CF}$ is assumed. The following values are calculated with the assumptions of A = 4,500 ft^2 and $\overline{CF} = 30$:

$CF_2 = \overline{CF} = 30$, $R_2 = 5{,}882/30 = 196$ gal/h, $P_2 = 4{,}500(0.411) = 1{,}851$gal/h, $R_1 = 1{,}851 + 196 =$ 2,047 gal/h, and $CF_1 = 5{,}882/2{,}047 = 2.873$, $P_1 = 4{,}500(0.929) = 4{,}182$ gal/h, and back-calculated $F_1 = 4{,}182 + 2{,}047 = 6{,}229$ gal/h. Since this is not the required value of 5,882, the Solver function, used with a spreadsheet gives $\overline{CF} = 36.487$. However, the assumed area of 4,500 ft^2 for each stage is not correct if it does not achieve the required value of 55 wt% (dry basis) for TP + NPN in the retentate from stage 2. To check this, the following calculations are made using the given values of the rejection factor, defined by (14-81), with the following form of (14-92):

$$\left(\text{wt\% } i\right)_{R_n} = \frac{\left(\text{wt\% } i\right)_{F_n} CF_n}{\left[CF_n\left(1-\sigma_i\right)+\sigma_i\right]} \qquad (1)$$

For example, for TP in stage 1, with a wt% of 0.6 in the feed, $\sigma = 0.97$, and for A = 4,500 ft^2 and $CF_1 = 2.873$,

Exercise 14.25 (continued)

Analysis: (continued)

$$\left(\text{wt\% } i\right)_{R_n} = \frac{0.6\left(2.873\right)}{\left[2.873\left(1-0.97\right)+0.97\right]} = 1.63$$

The resulting wt% TP + NPN (dry basis) is not 55 wt%, even for $\overline{CF}$ = 36.487. Therefore, the assumed area is not correct.

From the double trial and error, the following results are obtained in an effort to obtain the required value of 55 wt%:

Assumed A, ft^2	$\overline{CF}$ from Solver	Wt% TP+NPN (dry basis)
4,500	36.487	65.79
3,800	18.847	56.22
3,750	17.878	55.35
3,730	17.502	55.00

The last result in the table gives the following material balance in lb/day, and % overall yield:

Component	Feed	Stage 1 Concentrate	Stage 2 Concentrate	% Overall Yield
TP	6,000	5,733	4,874	81.2
NPN	3,000	1,464	293	9.8
Lactose	49,000	20,327	3,183	6.5
Ash	8,000	3,384	545	6.8
B Fat	500	500	500	100.0
Water	933,500	362,064	47,741	
Total	1,000,000	393,472	57,136	

The area per stage = 3,730 ft^2 or a total of 7,460 ft^2. The number of cartridges per stage = 141 or a total of 282 cartridges.

Exercise 14.26

Subject: Section 2, involving diafiltration, of a cheese whey filtration process to obtain a dry powder of combined TP and NPN as in Example 14.13, wherein section 3 is eliminated.

Given: Conditions of Example 14.13, including a whey feed of 1,000,000 lb/.day with the same composition and solute retention factors. Feed to the diafiltration section 2 is the 55 wt% concentrate from the 4-stage ultrafiltration section 1 of Example 14.13. The diafiltration section is to achieve 85 wt% concentrate (dry basis) of combined TP and NPN.

Assumption: Assume 4 stages of diafiltration, as in Example 14.13.

Find: A suitable set of operating conditions for section 2.

Analysis: From the results of Example 14.13, the component flow rates in the concentrate leaving section 1 and feeding the diafiltration section is as follows in lb/day:

Component	Feed rate to Diafiltration	Rejection, σ
TP	5,245	0.970
NPN	353	0.320
Lactose	3,476	0.085
Ash	603	0.115
BF	500	1.000
Water	49,897	
Total	60,074	

As in Example 14.13, assume the same membrane area for each of the 4 stages. Also, assume the same flow rate of dilution water, W_n, to each stage, and set the permeate rate for each stage equal to W_n. Therefore, the concentrate rate leaving each stage equals the feed rate above of 60,074 lb/day. This simplification leads to Eq. (2) of Example 14.13, which here for each stage is:

$$\overline{CF} = \frac{W + 60,074}{60,074} \tag{1}$$

Equation (3) of Example 14.13 then gives the flow rate of each component in the concentrate leaving stage *n*:

$$(m_i)_{R_n} = (m_i)_F \left[\frac{1}{\overline{CF}(1-\sigma_i)+\sigma_i} \right]^n \tag{2}$$

where, here, $n = 4$, and values of $(m_i)_F$ and σ_i are given in the above table.

Exercise 14.26 (continued)

Analysis: (continued)

This exercise is solved by assuming a dilution water flow rate, W, for each stage, calculating $\overline{CF}$ from (**1**), and calculating the flow rates of the components in the concentrate from the fourth diafiltration stage using (**2**). If the resulting wt% (dry basis) of NP + NPN is not 85 wt%, the procedure is repeated with a new assumed value of W. The procedure is carried out with a spreadsheet using the Solver function.

The result is a dilution water flow rate of 57,240 lb/day for each of the four diafiltration stages. The corresponding value of $\overline{CF}$ = 1.953. The component flow rates in the retentate leaving the fourth stage are:

Component	Final concentrate from Diafiltration, Lb/day
TP	4,686
NPN	48
Lactose	283
Ash	52
BF	500
Water	54,505
Total	60,074

This water flow rate per diafiltration stage is 2.45 times that in Example 14.13. The yield from the feed to diafiltration is (4,686 + 48)/(5,245 + 353) x 100% = 84.6%, which is less than the 91.9% in Exercise 14.13. The membrane flux is the same as in Example 14.13, namely 0.5415 gal/h-ft^2, but the volumetric permeate flow rate per stage is 57,240/[(20)(8.5)] = 337 gal/h. The membrane area per stage is, therefore, 337/0.5415 = 622 ft^2 and the number of cartridges per stage is 622/26.5 = 24.

Exercise 14.27

Subject: Dead-end microfiltration of diluted skim milk using a combined operation of constant permeate rate followed by constant pressure drop.

Given: Diluted skim milk with a protein concentration of 4.3 g/L. A constant permeate rate of 10 mL/min in stage 1 to a pressure drop of 25 psi, followed by stage 2 at this pressure drop until the permeate rate drops to 5 mL/min. Membrane area of 0.00173 m^2. Viscosity of 1 cP.

Assumption: Values of R_m = 1.43 x 10^{10} m^{-1} and K_2 = 3.78 x 10^{12} m/kg from Example 14.14.

Find: Permeate flux and cumulative permeate volume as a function of time.

Analysis: In stage 1, the permeate rate in m^3/s for a given rate of 10 mL/min is,

$$\frac{dV}{dt} = \frac{10\left(10^{-6}\right)}{60} = 0.167\times10^{-6} \text{ m}^3/\text{s}$$

The permeate flux in stage 1 is,

$$J = \frac{1}{A_M}\frac{dV}{dt} = \frac{0.167\times10^{-6}}{0.00173} = 9.63\times10^{-5} \text{ m/s}$$

c_F = solid matter/unit volume of feed = 4.3 g/L = 4.3 kg/m^3

From Example 14.14, viscosity = μ = 1 cP = 0.001 Pa-s

Pressure drop at the end of stage 1 = 25 psia = 172,400 Pa

Rearrange (14-103) to compute the time, t, in seconds to reach the pressure drop of 25 psia, using SI units.

$$t = \frac{\Delta P}{J^2\mu K_2 c_F} - \frac{R_m}{K_2 J c_F} = \frac{172,400}{\left(9.63\times10^{-5}\right)^2\left(0.001\right)\left(3.78\times10^{12}\right)\left(4.3\right)} - \frac{1.43\times10^{10}}{\left(3.78\times10^{12}\right)\left(9.63\times10^{-5}\right)\left(4.3\right)}$$

= 1,138 – 9 = 1,129 s = 18.82 min

During stage 1, the cumulative volume, mL, as a function of time in minutes is given by,

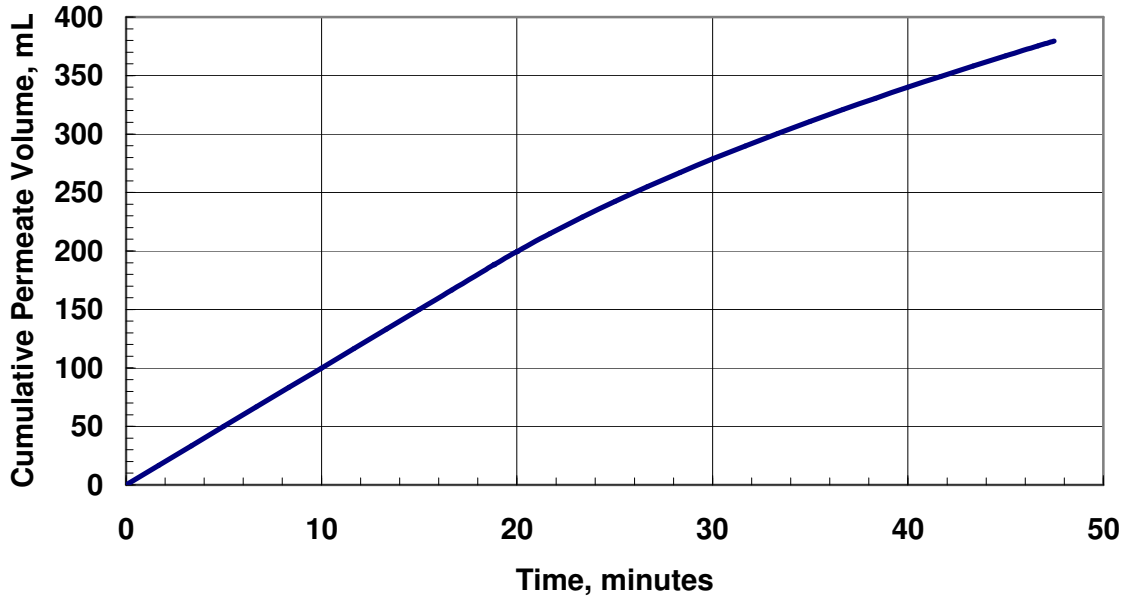
V (in mL) = 10 t (in minutes) up to 18.82 minutes

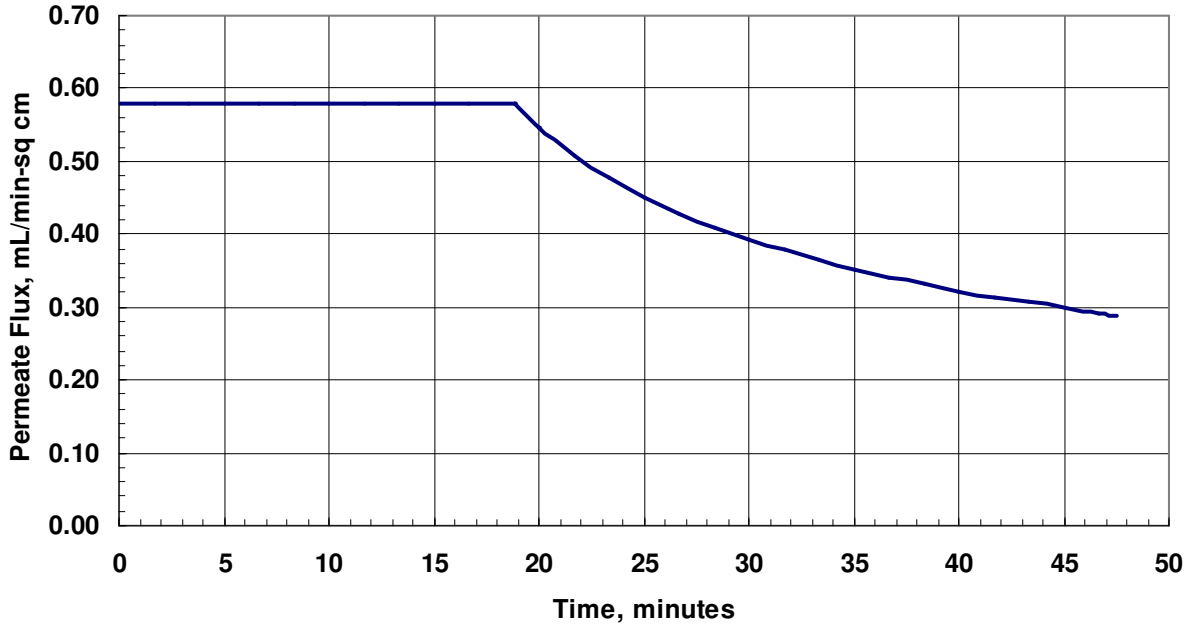
Exercise 14.27 (continued)

Analysis: (continued)

For the stage 2 with operation at constant pressure drop of 25 psia, (14-110) is used to compute the cumulative permeate volume V, starting from V_{CF} = volume at the end of stage 1 = 10(18.82) = 188.2 mL and t_{CF} = 18.82 minutes = 1,129 s. The decrease in permeate flux, J, in stage 2 is obtained from (14-111). The calculations are best carried out with a spreadsheet.

The results shown in the following two plots show that stage 2 ends at 2,850 seconds or 47.5 minutes.





Exercise 15.1

Subject: Estimation of adsorbent characteristics.

Given: Porous particles of activated alumina. BET area = 310 $m^2/g = S_g$. Particle porosity = 0.48 = ε_p. Particle density = 1.30 $g/cm^3 = \rho_p$.

Assumptions: Straight pores of circular cross-section with uniform diameter.

Find: (a) V_p = specific pore volume in cm^3/g.
(b) ρ_s = true solid density, g/cm^3.
(c) d_p = average pore diameter, angstoms.

Analysis:

(a) From Eq. (15-3), $V_p = \varepsilon_p/\rho_p = 0.48/1.30 = 0.369\ cm^3/g$

(b) From a rearrangement of Eq. (15-5), $\rho_s = \rho_p/(1 - \varepsilon_p) = 1.30/(1 - 0.48) = 2.50\ g/cm^3$

(c) From a rearrangement of Eq. (15-2), $d_p = 4\ \varepsilon_p/S_g\rho_g = 4(0.48)/[310 \times 10^4(1.30)]$
$= 4.76 \times 10^{-7}$ cm or 47.6 angstroms.

Exercise 15.2

Subject: Estimation of surface area of two forms of molecular sieves.

Given: Form A with $V_p = 0.18\ cm^3/g$ and average d_p = 5 angstroms.
Form B with $V_p = 0.38\ cm^3/g$ and average d_p = 2.0 microns.

Assumptions: Straight pores of circular cross-section with uniform diameter.

Find: Surface area, S_g, of each form.

Analysis: By substitution of Eq. (15-3) into (15-2), $S_g = 4\ V_g/d_p$ (1)

Form A: From Eq. (1), $S_g = 4(0.18)/(5 \times 10^{-8}) = 14.4 \times 10^6\ cm^2/g$ or $1{,}440\ m^2/g$

Form B: From Eq. (1), $S_g = 4(0.38)/(2 \times 10^{-4}) = 7{,}600\ cm^2/g$ or $0.760\ m^2/g$

This is a very large difference in surface area.

Exercise 15.3

Subject: Consistency of the characteristics of a small-pore silica gel.

Given: Small-pore silica gel. Pore diameter = 24 angstroms = d_p. Particle porosity = 0.47 = ε_p. Particle density = 1.09 g/cm^3 = ρ_p. Specific surface area = 800 m^2/g = S_g.

Assumption: Straight pores of circular cross-section with uniform diameter.

Find: (a) Reasonableness of the above values.
(b) Fraction of a monolayer adsorbed if the adsorption capacity for water vapor at 25°C and 6 mmHg partial pressure is 18% by weight.

Analysis: (a) From Eq. (15-2), based on the above assumption,

$S_g = 4\,\varepsilon_p/d_p\rho_g = 4(0.47)/[(1.09 \times 10^6)(24 \times 10^{-10})] = 719$ m^2/g

This is reasonable compared to the given value of 800 m^2/g.

The true density of silica gel, assuming it is SiO_2, depends on its crystalline form. From a handbook, the density is from 2.20 to 2.65 g/cm^3, with 3 of 4 forms from 2.20 to 2.26 g/cm^3. Therefore, using a value of ρ_s = 2.20 g/cm^3 with Eq. (15-5), $\varepsilon_p = 1 - \rho_p/\rho_s = 1 - 1.09/2.20 = 0.505$.

This is reasonable compared to the given value of 0.47.

(b) From the problem statement, it is not clear whether the 18 wt% refers to a dry basis or a wet basis, so consider both possibilities.

Dry basis: Adsorb 0.18 grams water per 1.0 gram of water-free silica gel. Therefore, for 1.0 gram of dry silica gel, the surface area for adsorption = 800 m^2.

From Eq. (15-8) and Example 15.1, the projected surface area per molecule = $\alpha = 10.51 \times 10^{-16}$ cm^2/molecule.

The number of water molecules adsorbed = $0.18(6.023 \times 10^{23})/18.02 = 6.02 \times 10^{21}$.

The number of molecules that could be adsorbed to cover 800 m^2 = $800(10^4)/10.51 \times 10^{-16} = 7.61 \times 10^{21}$.

Therefore, the fraction of the area covered = 6.02/7.61 = 0.79

Wet basis: Adsorb 0.18 grams water per 0.82 gram of water-free silica gel (1.00 gram total). Therefore, for 0.82 gram of dry silica gel, the surface area for adsorption = (0.82)800 = 656 m^2.

From Eq. (15-8) and Example 15.1, the projected surface area per molecule = $\alpha = 10.51 \times 10^{-16}$ cm^2/molecule.

The number of water molecules adsorbed = $0.18(6.023 \times 10^{23})/18.02 = 6.02 \times 10^{21}$.

The number of molecules that could be adsorbed to cover 656 m^2 = $656(10^4)/10.51 \times 10^{-16} = 6.89 \times 10^{21}$.

Therefore, the fraction of the area covered = 6.02/6.89 = 0.87

Exercise 15.4

Subject: Estimation of the specific surface area from BET data.

Given: Data for adsorption equilibrium of nitrogen on silica gel (SG) at -195.8°C:

P, N_2 partial pressure, torr	υ, Volume of N_2 adsorbed, cm^3 (0°C, 1 atm) per gram SG
6.0	6.1
24.8	12.7
14.3	17.0
230.3	19.7
285.1	21.5
320.3	23.0
430	27.7
505	33.5

Find: Specific surface area in m^2/g of SG. Compare to Table 15.2.

Analysis: From Eq. (15-6), $$\frac{P}{\upsilon(P_0 - P)} = \frac{1}{\upsilon_m c} + \frac{(c-1)}{\upsilon_m c}\left(\frac{P}{P_0}\right) \qquad (1)$$

where: P = total pressure = partial pressure of N_2 in the above table in mmHg
P_0 = vapor pressure of N_2 at -195.8°C = 760 mmHg
υ = volume of gas adsorbed at STP
υ_m = volume of monomolecular layer of gas adsorbed at STP
c = constant

Eq. (1) is of the form of a straight line, $y = mx + b$, where,

$$y = \frac{P}{\upsilon(P_0 - P)}, \quad x = \left(\frac{P}{P_0}\right), \quad m = \frac{(c-1)}{\upsilon_m c} \qquad (2) \qquad \text{and} \qquad b = \frac{1}{\upsilon_m c} \qquad (3)$$

If a least-squares fit of the data is made, using a spreadsheet or POLYMATH,
$m = 0.08557$ and $b = -0.0016905$

Combining Eqs. (2) and (3) to eliminate c,
$\upsilon_m = 1/(m + b) = 1/(0.08557 - 0.0016905) = 11.92\ cm^3/g$
$c = -49.62$

From Eq. (15-7), $$S_g = \frac{\alpha \upsilon_m N_A}{V} = \frac{\alpha(11.92)(6.023\times10^{23})}{22{,}400} = 3.205\times10^{20}\,\alpha$$

From Eq. (15-8), $$\alpha = 1.091\left(\frac{M}{N_A \rho_L}\right)^{2/3} = 1.091\left(\frac{28}{6.023\times10^{23}(0.808)}\right)^{2/3} = 1.626\times10^{-15}\ cm^2$$

Therefore, S_g = 3.205 x 10^{20} (1.626 x 10^{-15}) = 5.21 x 10^5 cm^2/g or 52.1 m^2/g
This is much smaller than the values given for silica gel in Table 15.2.

Exercise 15.5

Subject: Maximum ion-exchange capacity of a resin.

Given: Ion-exchange resin made from 8 wt% divinylbenzene and 92 wt% styrene.

Find: Maximum ion-exchange capacity in meq/g resin.

Analysis: Compute the moles of each aromatic component per 100 grams of resin:

	MW	grams	gmol
Styrene	104.14	92	0.8834
Divinylbenzene	130.18	8	0.0615
Total		100	0.9449

Therefore, need 0.9449 mol H_2SO_4 or 0.9449(81.07) = 76.6 g.
Total resin weight after sulfonation = 100 + 76.6 = 176.6 g.
Maximum ion-exchange capacity = 0.9449(1000)/176.6 = 5.35 meq/g of resin.

Exercise 15.6

Subject: Fitting adsorption data to linear, Freundlich, and Langmuir isotherms and computing the heat of adsorption.

Given: Silica gel adsorbent with: surface area = S_g = 832 m^2/g, pore volume = V_p = 0.43 cm^3/g, particle density = ρ_p = 1.13 g/cm^3, and average pore diameter = d_p = 22 angstroms. Equilibrium adsorption data for pure benzene vapor at 4 different temperatures as follows:

q, moles adsorbed /g gel x 10^5:

p, partial pressure, atm	70°C	90°C	110°C	130°C
0.0005	14.0	6.7	2.6	1.13
0.0010	22.0	11.2	4.5	2.0
0.0020	34.0	18.0	7.8	3.9
0.0050	68.0	33.0	17.0	8.6
0.0100	88.0	51.0	27.0	16.0
0.0200		78.0	42.0	26.0

Find: (a) For each temperature, best fits of the data to (1) linear, (2) Freundlich, and (3) Langmuir isotherms. Which give a reasonable fit?

(b) Do data represent less than a monolayer?

(c) Heat of adsorption, with comparison to heat of vaporization of benzene.

Analysis: The regression program of POLYMATH can be used to do nonlinear curve fits or a spreadsheet program can be used to do least squares curve fits on the linearized isotherms. For the former, the following results are obtained for fitting Eqs. (15-16), (15-19), and (15-24). Somewhat different results would be obtained with the linearized equations (15-20) and (15-25).

(1) $q = kp$ Linear

(2) $q = kp^{1/n}$ Freundlich

(3) $q = Kq_m p/(1 + Kp)$ Langmuir

Temperature, °C	Linear:	Freundlich:		Langmuir:	
	k	k	n	K	q_m
70	0.1011	0.0132915	1.71882	188.18	0.0013584
90	0.0431033	0.00944163	1.57209	67.55	0.0013337
110	0.0229401	0.00653397	1.43190	50.0327	0.00083383
130	0.0138306	0.00595422	1.25461	27.4455	0.00073471

The linear equation is a poor fit for all 4 temperatures.
The Freundlich equation a reasonably good fit for all 4 temperatures.
The Langmuir equation gives the best fit for all 4 temperatures.

Exercise 15.6 (continued)

Analysis: (continued)

(b) The surface area covered by one adsorbed molecule is given by Eq. (15-8), where for benzene, M = 78.11 and the liquid density, from Fig. 2.3, ranges from 0.82 cm^3/g at 90°C to 0.76 cm^3/g at 130°C. At 90°C,

$$\alpha = 1.091\left(\frac{M}{N_A \rho_L}\right)^{2/3} = 1.091\left(\frac{78.11}{6.023\times10^{23}(0.82)}\right)^{2/3} = 3.19\times10^{-15}\ cm^2$$

From the data, the maximum experimental adsorption is 0.00088 moles benzene/g silica gel. This is a coverage of 0.00088(6.023 x 10^{23})(3.19 x 10^{-15}) = 1.69 x 10^6 cm^2/g or 169 m^2/g. This is far less than the given S_g = 832 m^2/g. At higher temperatures, the experimental values for adsorption are even less, with just a slight increase in α. Therefore, the measured values of adsorption are equivalent to far less than a monolayer.

(c) The heat of adsorption is related to adsorption isotherm data by a rearrangement of Eq. (15-17), which is a form of the Clausius-Clapeyron equation. For a constant amount adsorbed,

$$-\Delta H_{ads} = RT^2 \frac{d\ln p}{dT} \qquad (1) \qquad \text{where, } R = 1.987 \text{ cal/mol-K}$$

Take an arbitrary value of 0.00025 mols of benzene adsorbed per gram of silica gel. For each temperature, calculate the partial pressure of benzene from the above fits of the Freundlich equation (the Langmuir equation could also be used). Evaluate $d\ln p/dT$ numerically and apply Eq. (1). The results are as follows.

Temperature, °C	Temperature, T, K	Benzene pressure, p, atm	ln p	$d\ln p/dT$	T_{avg}, K	- ΔH_{ads}, cal/mol
70	343	0.00108	-6.831			
				0.05615	353	13,900
90	363	0.00332	-5.708			
				0.05180	373	14,300
110	383	0.00935	-4.672			
				0.0347	393	10,650
130	403	0.01873	-3.978			

The average heat of adsorption = - 13,000 cal/mol.

From the ChemCad simulation program, the heat of condensation for benzene varies from -7,500 cal/mol at 70°C to -6,620 cal/mol at 130°C. Thus, the heat of adsorption is almost twice as great as the heat of condensation.

Exercise 15.7

Subject: Use of adsorption equilibria data to select the best adsorbent.

Given: Langmuir adsorption equilibrium constants, K and q_m in Eq. (15-24), for 3 zeolite molecular sieves and activated carbon for propylene (C3) and propane (C3=) at 25°C:

Adsorbent	Sorbate	q_m	K
ZMS 4A	C3	0.226	9.770
	C3=	2.092	95.096
ZMS 5A	C3	1.919	100.223
	C3=	2.436	147.260
ZMS 13X	C3	2.130	55.412
	C3=	2.680	100.000
Activated carbon	C3	4.239	58.458
	C3=	4.889	34.915

Find: (a) Most strongly adsorbed component for each adsorbent.
(b) Adsorbent with greatest adsorption capacity.
(c) Adsorbent with greatest selectivity.
(d) Best adsorbent for the separation of propylene from propane.

Analysis: (a) The Langmuir equation is: $q = Kq_m p/(1 + Kp)$
At high pressure, q approaches q_m. Thus, q_m is a measure of capacity. Because of the high values of K, the value of q_m is reached at about 1 bar. Thus, we can make the comparisons on the basis of q_m. Therefore, propylene is the most strongly adsorbed for all 4 adsorbents.

(b) The activated carbon has the highest values of q_m and, therefore, has the highest capacity.

(c) The selectivity is measured by the ratio of q_m for propylene to that of propane. With a value of 2.092/0.226 = 9.26, zeolite ZMS 4A is by far the best.

(d) Because of its very high selectivity of ZMS 4A, where the second best is only 1.27, and the high capacity of ZMS 4A, although only about 40% of that of activated carbon, ZMS 4A is the best adsorbent for the separation of propylene and propane.

Exercise 15.8

Subject: Fitting zeolite adsorption data to linear, Freundlich, and Langmuir isotherms.

Given: NaX zeolite adsorbent. Adsorption equilibrium data at 547 K for 1,2,3,5-tetramethylbenzene (TMB) as follows:

q, wt%	7.0	9.1	10.3	10.8	11.1	11.5
p, torr	0.012	0.027	0.043	0.070	0.094	0.147

Find: Best fit of the data to linear, Freundlich, and Langmuir isotherms, with q in mol/g and p in atm. Which isotherm fits best?

Analysis: First convert the given adsorption data to the desired units:

q in mols TMB/gram NaX = (wt% q/MW of TMB)/(100 - wt% q) (1)

MW of TMB = 134.1

Substitution of the data into Eq. (1) plus converting pressure from torr to atm gives:

q, mol/g	0.000562	0.000747	0.000856	0.000903	0.000931	0.000969
p, atm	0.0000158	0.0000355	0.0000566	0.0000921	0.0001237	0.0001934

The regression program of POLYMATH can be used to do nonlinear curve fits or a spreadsheet program can be used to do least squares curve fits on the linearized isotherms. For the former, the following results are obtained for fitting Eqs. (15-16), (15-19), and (15-24). Somewhat different results would be obtained with the linearized equations (15-20) and (15-25).

Linear: $q = kp = 7.12557\ p$

Freundlich: $q = kp^{1/n} = 0.00532\ p^{1/5.15605}$

Langmuir: $q = Kq_m p/(1 + Kp) = (75410)(0.001036)\ p/(1 + 75410\ p)$

The fits are shown on the next page, where it is clear that:

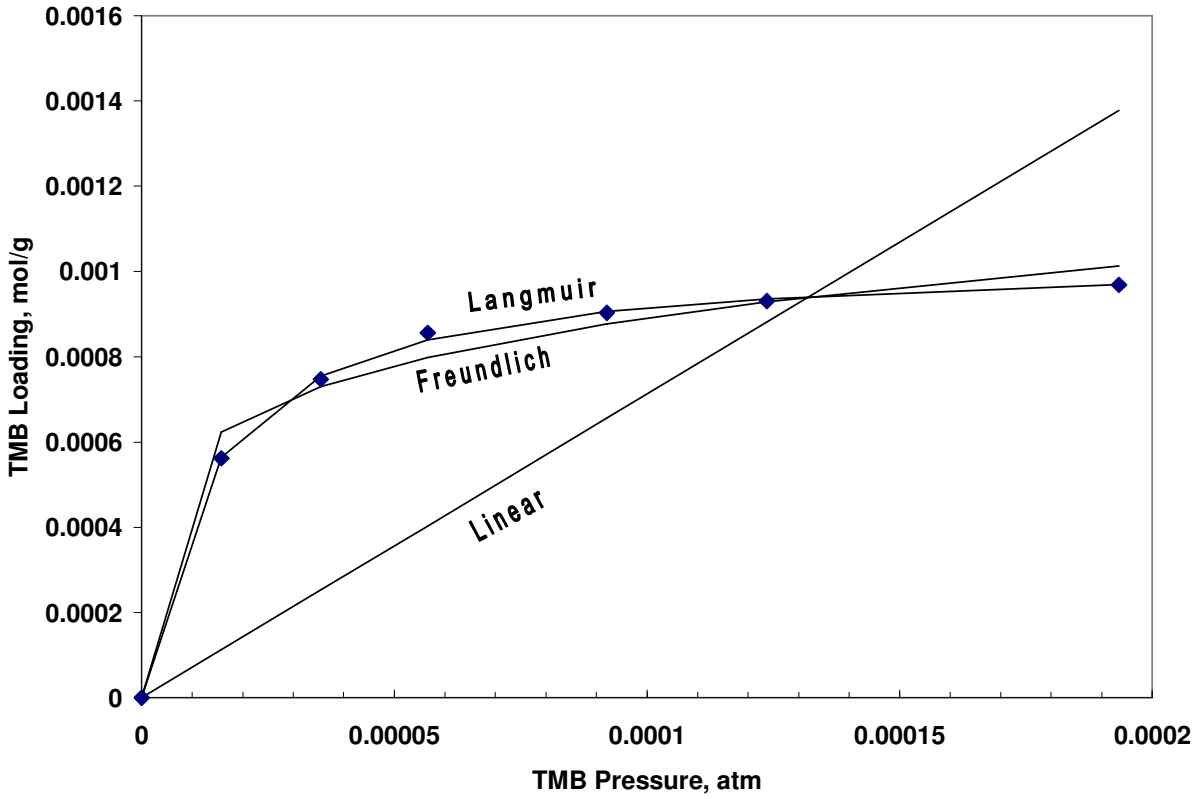
Linear model is a very poor fit.

Freundlich model is a fairly good fit.

Langmuir model is a very good fit and is the best fit.

Exercise 15.8 (continued)

Analysis: (continued)



Exercise 15.9

Subject: Fitting pure component and mixture adsorption data for gaseous propane (C3) and propylene (C3=) on silica gel (SG) at 25°C to Freundlich and Langmuir isotherms.

Given: Pure component adsorption equilibrium data for C3 and C3= on SG in the exercise statement. Adsorption equilibrium data for mixtures of C3 and C3= on SG in the exercise statement. Surface area of SG = 832 m^2/g, pore volume = 0.43 cm^3/g, particle density = 1.13 g/cm^3, and average pore diameter = 22 angstroms.

Find: (a) Fit of the data to Freundlich and Langmuir isotherms. Which isotherm is best? Which component is most strongly adsorbed?

(b) Prediction of mixture adsorption from the extended Langmuir isotherm based on the pure component fits.

(c) Fit of the mixture data to the extended Langmuir isotherm. Comparison to Part (b).

(d) Fit of the mixture data to the extended Langmuir-Freundlich isotherm. Comparison to Part (c).

(e) Relative selectivity from the mixture data. Does it vary widely?

Analysis: (a) The regression program of POLYMATH can be used to do nonlinear curve fits or a spreadsheet program, such as Excel, can be used to do least squares curve fits on the linearized isotherms. For the latter, the following results are obtained for fitting Eqs. (15-20) and (15-25). Somewhat different results would be obtained with the nonlinear Eqs. (15-19) and (15-24).

Component	Freundlich:		Langmuir:	
	k	n	K	q_m
Propane	0.01062	1.311	0.001853	2.5213
Propylene	0.06242	1.8306	0.003916	2.8201

For C3, the Freundlich equation, with $R^2 = 0.995$, is a slightly better fit than the Langmuir equation with $R^2 = 0.972$.

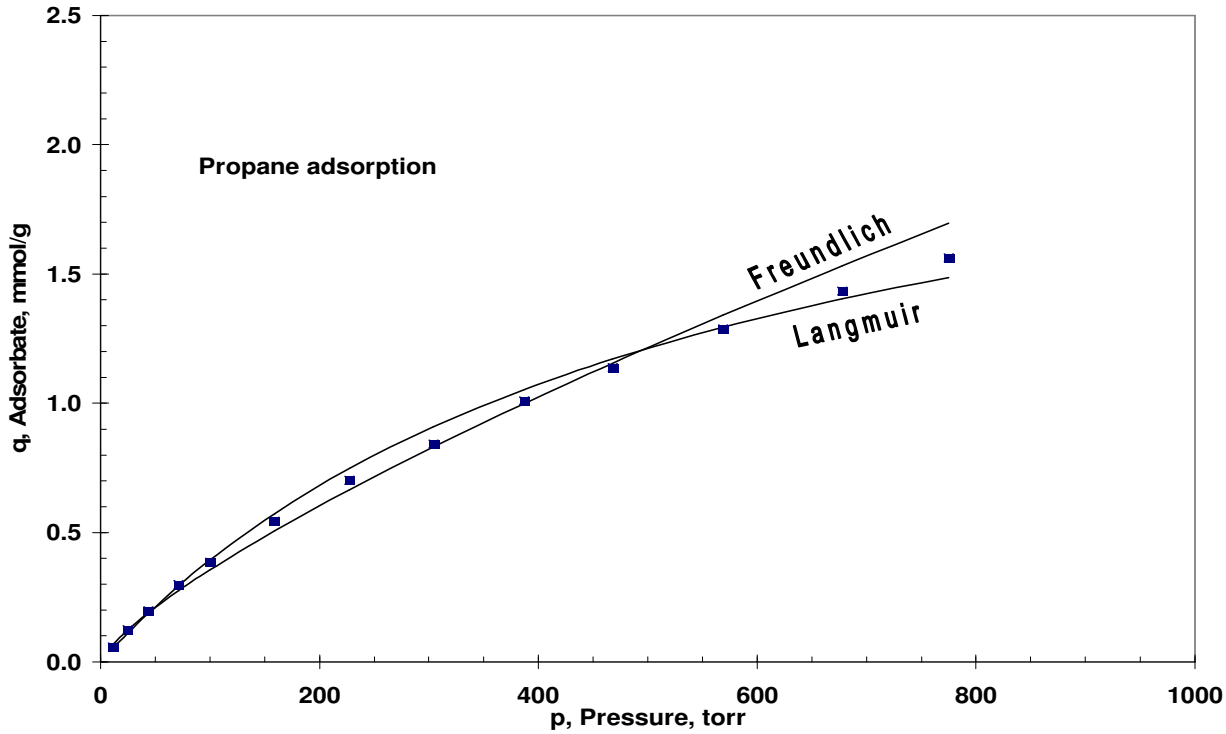
For C3=, the Langmuir equation, with $R^2 = 0.986$, is about the same goodness of fit as the Freundlich equation with $R^2 = 0.984$.

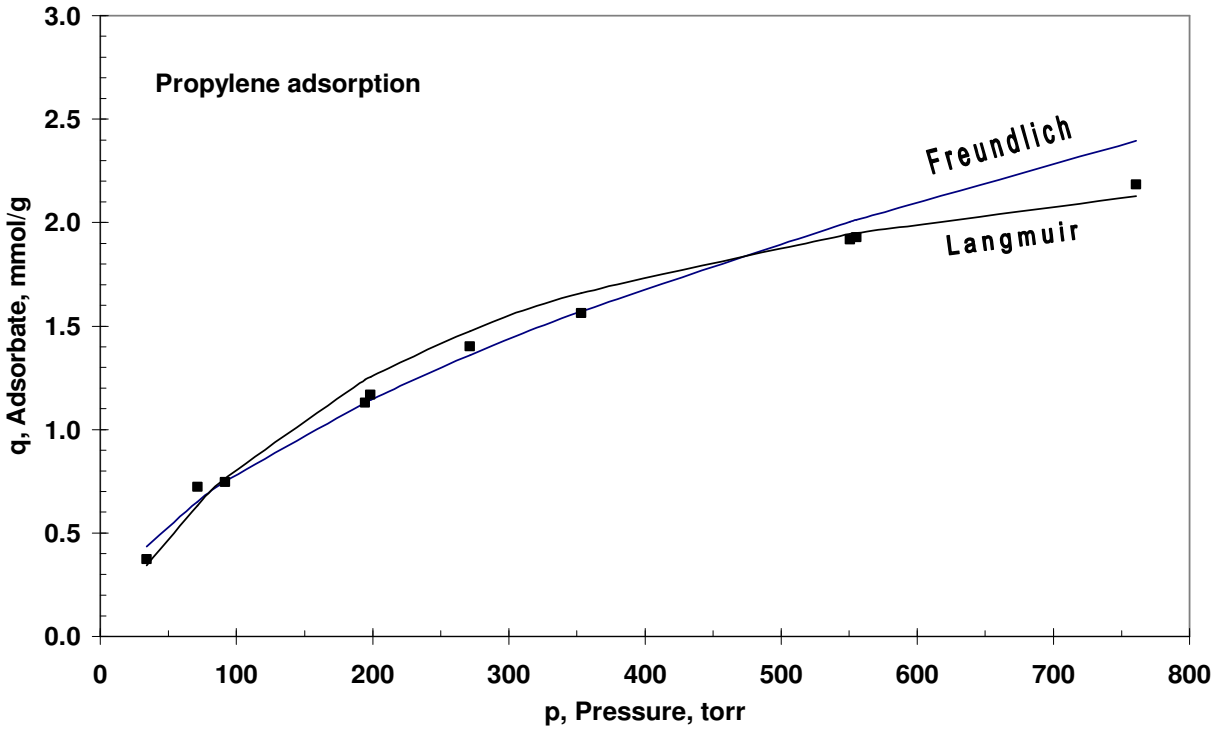
Considering both components, the Freundlich isotherm appears to be the best. However, as shown in the comparisons of the fits to the data (shown as markers) on the next page, the data, at the higher pressures, seems to be more in agreement with the asymptotic nature of the Langmuir isotherm. Probably, the Langmuir isotherm is best.

For a given pressure, the amount adsorbed is greater for C3=, so it is more strongly adsorbed.

Exercise 15.9 (continued)

Analysis: (a) (continued)





Exercise 15.9 (continued)

Analysis: (continued)

(b) Using the above pure component data fits, Eq. (15-32), the extended Langmuir isotherm becomes:

For C3:
$$q_{C3} = \frac{(q_{C3})_m K_{C3} p_{C3}}{1 + K_{C3} p_{C3} + K_{C3=} p_{C3=}} = \frac{2.5213(0.001853)\, p_{C3}}{1 + 0.001853 p_{C3} + 0.003916 p_{C3=}} \qquad (1)$$

For C3=:
$$q_{C3=} = \frac{(q_{C3=})_m K_{C3=} p_{C3=}}{1 + K_{C3} p_{C3} + K_{C3=} p_{C3=}} = \frac{2.8201(0.003916)\, p_{C3=}}{1 + 0.001853 p_{C3} + 0.003916 p_{C3=}} \qquad (2)$$

Using a spreadsheet, Eqs. (1) and (2) are used to predict the millimoles of components adsorbed from the given mixture data at 25°C, where the partial pressures are computed from the given total pressure and vapor mole fractions by Dalton's law, $p_i = P y_i$, and component adsorbate loadings are compared to the data using, $q_i = q_{\text{total}}\, x_i$.

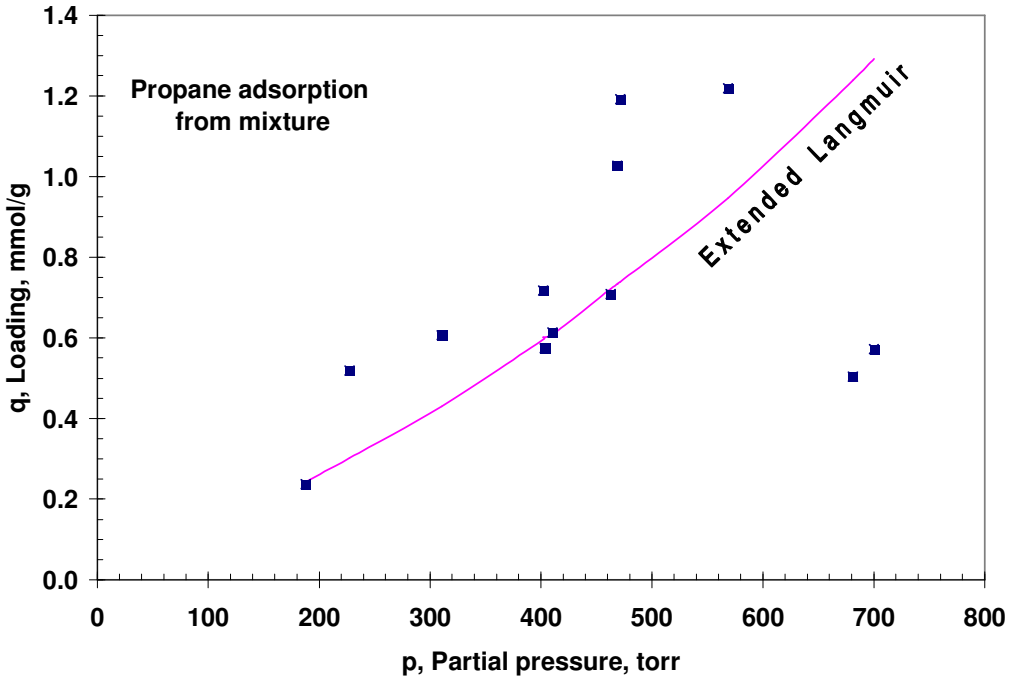
The results are as follows, where for measured partial pressures, the measured loadings are compared to those predicted by the extended Langmuir isotherm using constants fitted from pure component adsorption data. Plots are shown on the following page, where the points are the experimental data.

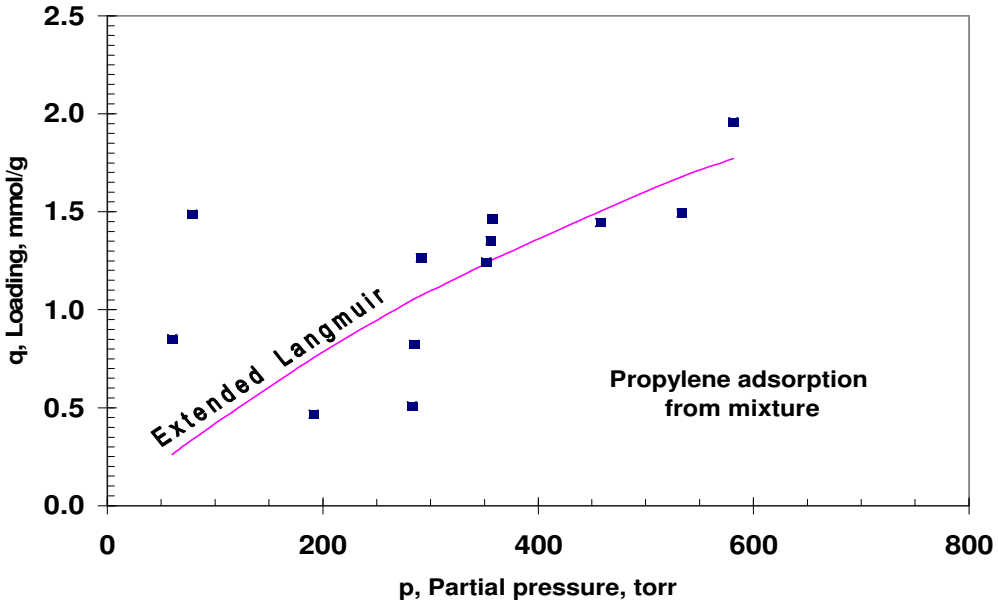
			Experimental data:		Predicted:	
Total pressure, torr	p of C3, torr	p of C3=, torr	q of C3, mmole/g	q of C3=, mmole/g	q of C3, mmole/g	q of C3=, mmole/g
769.20	188.07	581.13	0.237	1.960	0.242	1.771
760.90	227.51	533.39	0.519	1.494	0.303	1.678
767.80	310.19	457.61	0.607	1.445	0.430	1.501
761.00	403.33	357.67	0.575	1.466	0.599	1.255
753.60	401.89	351.71	0.717	1.246	0.601	1.244
766.30	410.43	355.87	0.614	1.353	0.608	1.246
754.00	462.96	291.04	0.709	1.265	0.722	1.072
753.60	468.74	284.86	1.027	0.824	0.734	1.054
754.00	471.40	282.60	1.192	0.509	0.739	1.047
760.00	568.48	191.52	1.219	0.467	0.947	0.754
760.00	681.26	78.74	0.504	1.489	1.238	0.338
760.00	699.96	60.04	0.572	0.854	1.291	0.262

From the above table and the plots on the following page, it is seen that the agreement is mostly poor.

Exercise 15.9 (continued)

Analysis: (b) (continued)





Exercise 15.9 (continued)

Analysis: (continued)

(c) To fit the mixture data to the extended Langmuir equation, to determine the best values of the four coefficients $(q_{C3})_m$, $(q_{C3=})_m$, K_{C3}, and $K_{C3=}$, Eqs. (1) and (2) above must be used simultaneously. Polymath does not permit more than one equation to be fitted at a time. Alternatively, the two equations can be added together to give one equation in the total loading, $q_t = q_{C3} + q_{C3=}$. However, this does not insure a good fit to the data for the individual loadings. Nevertheless, this technique was applied with Polymath. It was found that the minimum sum of squares of the deviations of the fit from the experimental data was not very sensitive to the values of the four coefficients. One reasonable set that was close to the set determined from the pure component data was:

$(q_{C3})_m = 2.5213$, $(q_{C3=})_m = 2.8201$, $K_{C3} = 0.002116$, and $K_{C3=} = 0.004752$

Unfortunately, this set showed little improvement in the fit of the mixture data as compared to the fit of the set determined in Part (b) from the pure component data. The plots are not much different from those on the previous page.

Another procedure that can be applied is to use the program MathCAD with the Minerr function. The MathCAD program and result is shown on the next page. Minerr searches for the values of the four constants that provide the best fit to the data. The objective function is the sum of the squares of the deviations of the data from the predictions (SSE) by the Eqs. (1) and (2). $$\text{SSE} = \sum_i \left\{ \left[(q_{C3})_i - \frac{(q_{C3})_m K_{C3} (p_{C3})_i}{1 + K_{C3}(p_{C3})_i + K_{C3=}(p_{C3=})_i} \right]^2 + \left[(q_{C3=})_i - \frac{(q_{C3=})_m K_{C3=} (p_{C3=})_i}{1 + K_{C3}(p_{C3})_i + K_{C3=}(p_{C3=})_i} \right]^2 \right\} \quad (3)$$

where the four constants are varied to find the smallest value of SSE. Initial quesses for the four constants must be provided, which, as shown on the next page for the MathCAD program were:

$(q_{C3})_m = 2.5$, $(q_{C3=})_m = 2.8$, $K_{C3} = 0.002$, and $K_{C3=} = 0.002$

The values computed are seen to be:

$(q_{C3})_m = 2.153$, $(q_{C3=})_m = 4.042$, $K_{C3} = 0.001642$, and $K_{C3=} = 0.001997$, with SSE = 3.501, which does not indicate a very good fit.

Unfortunately, different initial guesses give other results, none of which gives much, if any improvement to the fit.

(d) The procedure outlined in Part (c), although not very satisfactory, was applied to the extended Langmuir-Freundlich isotherm, Eq. (15-33), which for the total loading is:

$$q_t = \frac{(q_{C3})_0 k_{C3} (Py_{C3})^{1/n_{C3}}}{1 + k_{C3}(Py_{C3})^{1/n_{C3}} + k_{C3=}(Py_{C3=})^{1/n_{C3=}}} + \frac{(q_{C3=})_0 k_{C3=} (Py_{C3=})^{1/n_{C3=}}}{1 + k_{C3}(Py_{C3})^{1/n_{C3}} + k_{C3=}(Py_{C3=})^{1/n_{C3=}}} \quad (4)$$

When used with the nonlinear regression program of Polymath, the results obtained were not satisfactory because some coefficients were negative for the best fit.

When MathCAD was used with the Minerr function according to the program and result is shown on a following page, the following values were obtained for the six constants: $(q_{C3})_m = 1.706$, $(q_{C3=})_m = 4.507$, $K_{C3} = 0.0270$, $K_{C3=} = 0.03773$, $n_{C3} = 1.59$, and $n_{C3=} = 1.90$, with SSE = 2.583, which is a better fit than for the extended Langmuir equation. However, other initial guesses for the six constants gave other results, because of the the great sensitivity.

Exercise 15.9 (continued)

Analysis: (c) (continued)

MathCAD Program

$$p1 := \begin{pmatrix} 188.07 \\ 227.51 \\ 310.19 \\ 403.33 \\ 401.89 \\ 410.43 \\ 462.96 \\ 468.74 \\ 471.40 \\ 568.48 \\ 681.26 \\ 699.96 \end{pmatrix} \quad p2 := \begin{pmatrix} 581.13 \\ 533.39 \\ 457.61 \\ 357.67 \\ 351.71 \\ 355.87 \\ 291.04 \\ 284.86 \\ 282.60 \\ 191.52 \\ 78.74 \\ 60.04 \end{pmatrix} \quad q1 := \begin{pmatrix} 0.237 \\ 0.519 \\ 0.607 \\ 0.575 \\ 0.717 \\ 0.614 \\ 0.709 \\ 1.027 \\ 1.192 \\ 1.219 \\ 0.504 \\ 0.572 \end{pmatrix} \quad q2 := \begin{pmatrix} 1.960 \\ 1.494 \\ 1.445 \\ 1.466 \\ 1.246 \\ 1.353 \\ 1.265 \\ 0.824 \\ 0.509 \\ 0.467 \\ 1.489 \\ 0.854 \end{pmatrix}$$

$$SSE(Q1, Q2, K1, K2) := \sum_{i=1}^{12} \left[\left[q1_i - Q1 \cdot K1 \cdot \frac{p1_i}{\left(1 + K1 \cdot p1_i + K2 \cdot p2_i\right)} \right]^2 + \left[\left(q2_i - Q2 \cdot K2 \cdot \frac{p2_i}{1 + K1 \cdot p1_i + K2 \cdot p2_i} \right)^2 \right] \right]$$

$$Q1 := 2.5 \qquad Q2 := 2.8 \qquad K1 := 0.002 \qquad K2 := 0.004$$

Given

$$SSE(Q1, Q2, K1, K2) = 0 \quad 1 = 1 \quad 1 = 1 \quad 1 = 1$$

$$\begin{pmatrix} Q1 \\ Q2 \\ K1 \\ K2 \end{pmatrix} := Minerr(Q1, Q2, K1, K2)$$

$$Q1 = 2.153 \qquad Q2 = 4.042 \qquad K1 = 0.001642 \qquad K2 = 0.001997$$

$$SSE\left(Q1, Q2, K1, K2\right) = 3.501$$

Exercise 15.9 (continued)

Analysis: (d) (continued)

MathCAD Program

$$p1 := \begin{pmatrix} 188.07 \\ 227.51 \\ 310.19 \\ 403.33 \\ 401.89 \\ 410.43 \\ 462.96 \\ 468.74 \\ 471.40 \\ 568.48 \\ 681.26 \\ 699.96 \end{pmatrix} \quad p2 := \begin{pmatrix} 581.13 \\ 533.39 \\ 457.61 \\ 357.67 \\ 351.71 \\ 355.87 \\ 291.04 \\ 284.86 \\ 282.60 \\ 191.52 \\ 78.74 \\ 60.04 \end{pmatrix} \quad q1 := \begin{pmatrix} 0.237 \\ 0.519 \\ 0.607 \\ 0.575 \\ 0.717 \\ 0.614 \\ 0.709 \\ 1.027 \\ 1.192 \\ 1.219 \\ 0.504 \\ 0.572 \end{pmatrix} \quad q2 := \begin{pmatrix} 1.960 \\ 1.494 \\ 1.445 \\ 1.466 \\ 1.246 \\ 1.353 \\ 1.265 \\ 0.824 \\ 0.509 \\ 0.467 \\ 1.489 \\ 0.854 \end{pmatrix}$$

$$SSE(Q1, Q2, K1, K2, N1, N2) := \sum_{i=1}^{12} \left[\left[q1_i - Q1 \cdot K1 \cdot \frac{\left(p1_i\right)^{N1}}{\left[1 + K1 \cdot \left(p1_i\right)^{N1} + K2 \left(p2_i\right)^{N2}\right]} \right]^2 + \left[q2_i - Q2 K2 \frac{\left(p2_i\right)^{N2}}{\left[1 + K1 \cdot \left(p1_i\right)^{N1} + K2 \left(p2_i\right)^{N2}\right]} \right]^2 \right]$$

$Q1 := 1$ $Q2 := 4$ $K1 := 0.001$ $K2 := 0.001$ $N1 := 0.5$ $N2 := 0.5$

Given

$SSE(Q1, Q2, K1, K2, N1, N2) = 0$ $1 = 1$ $1 = 1$ $1 = 1$ $1 = 1$ $1 = 1$

$$\begin{pmatrix} Q1 \\ Q2 \\ K1 \\ K2 \\ N1 \\ N2 \end{pmatrix} := Minerr(Q1, Q2, K1, K2, N1, N2)$$

$Q1 = 1.706$ $Q2 = 4.507$ $K1 = 0.027$ $K2 = 0.037734$ $N1 = 0.628$ $N2 = 0.527$

$$SSE(Q1, Q2, K1, K2, N1, N2) = 2.583$$

Exercise 15.9 (continued)

Analysis: (continued)

(e) The relative selectivity is given by $\alpha_{C3,C3=} = y_{C3}(1 - x_{C3})/[x_{C3}(1 - y_{C3})]$ (4)

Using the mixture data with Eq. (4), the following results are obtained:

Pressure, torr	*y*, C3	*x*, C3	α C3 to C3=
769.2	0.2445	0.1078	2.678
760.9	0.2990	0.2576	1.229
767.8	0.4040	0.2956	1.615
761.0	0.5300	0.2816	2.877
753.6	0.5333	0.3655	1.984
766.3	0.5356	0.3120	2.543
754.0	0.6140	0.3591	2.839
753.6	0.6220	0.5550	1.319
754.0	0.6252	0.7007	0.713
760.0	0.7480	0.7230	1.137
760.0	0.8964	0.2530	25.547
760.0	0.9210	0.4010	17.415

For the mixture, propane adsorption is favored over propylene adsorption and α varies widely.

Exercise 15.10

Subject: Use of the extended Langmuir-Freundlich isotherm to fit mixture data for the system acetone (1), propionitrile (2) on activated carbon at 25°C.

Given: Mixture adsorption data in terms of solution concentrations in mol/L and loadings on the adsorbent in mmol/g.

Find: Coefficients in the extended Langmuir-Freundlich isotherm

Analysis: From Eq. (6) in Example 15.6, the extended Langmuir-Freundlich equations are:

$$q_1 = \frac{(q_0)_1 k_1 c_1^{1/n_1}}{1 + k_1 c_1^{1/n_1} + k_2 c_2^{1/n_2}} \qquad (1)$$

$$q_2 = \frac{(q_0)_2 k_2 c_2^{1/n_1}}{1 + k_1 c_1^{1/n_1} + k_2 c_2^{1/n_2}} \qquad (2)$$

Fit mixture adsorption equilibrium data for c_1, c_2, q_1, and q_2 to obtain the coefficients $(q_0)_1$, $(q_0)_2$, k_1, k_2, n_1, and n_2. Rather than fitting both Eqs. (1) and (2) simultaneously, the following procedure was used. First, fit Eq. (1) with the nonlinear regression program of Polymath. Then fit Eq. (2). The following results are obtained, with both equations giving good fits:

Coefficient	Eq. (1)	Eq. (2)	Refit of Eq. (2)	Refit of Eq. (1)
$(q_0)_1$	3.456			1.855
$(q_0)_2$		37.4	2.492	
k_1	14.92	13.65	14.92	14.92
k_2	14.95	2.14	20.48	20.48
n_1	1.295	3.906	1.295	1.295
n_2	2.469	1.290	1.136	1.136

Next, Eq. (2) is refitted, holding k_1 and n_1 at the values above that were obtained from fitting Eq. (1). The refit gives the above values. Eq. (1) is refitted to determine only $(q_0)_1$. The results are also given above. The final fits of Eqs. (1) and (2) are as follows with sum of squares of deviations of 0.0144 and 0.0163, respectively. A simultaneous fit would give better values.

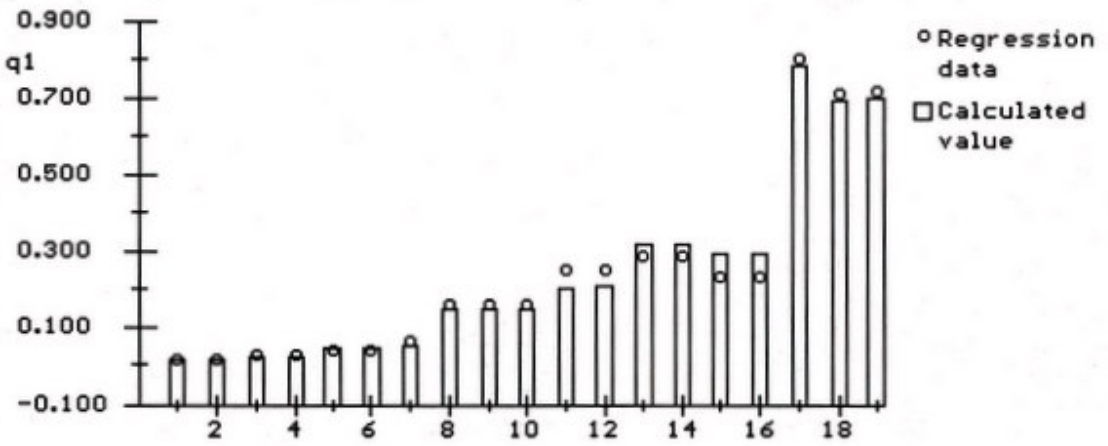
$$q_1 = \frac{1.855(14.92)c_1^{1/1.295}}{1 + 14.92c_1^{1/1.295} + 20.48c_2^{1/1.136}}$$

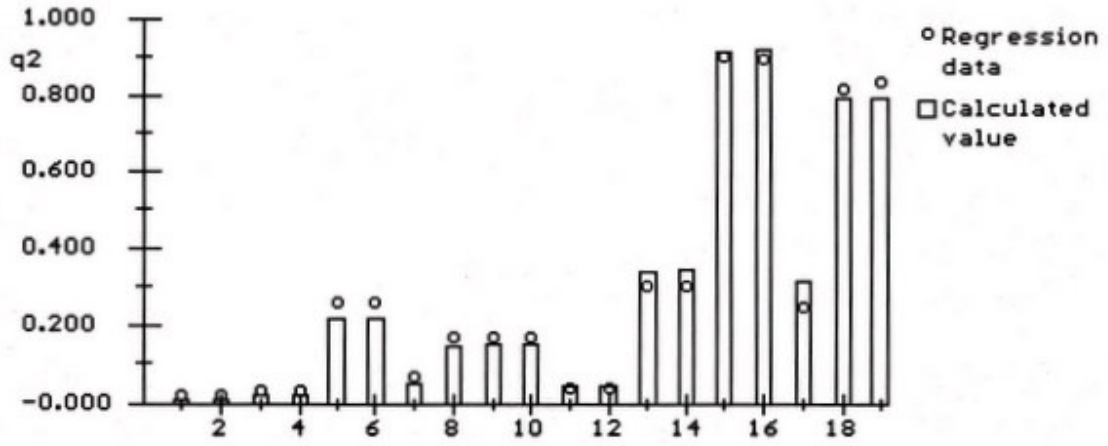
$$q_2 = \frac{2.492(20.48)c_2^{1/1.136}}{1 + 14.92c_1^{1/1.295} + 20.48c_2^{1/1.136}}$$

The fits of the data are shown in the bar charts on the following page.

Exercise 15.10 (continued)

Analysis: (continued)





Exercise 15.11

Subject: Analysis of liquid adsorption data for a mixture of cyclohexane (1) and ethyl alcohol (2) on activated carbon at 30°C.

Given: Data table for loading of (1) as a function of its mole fraction.

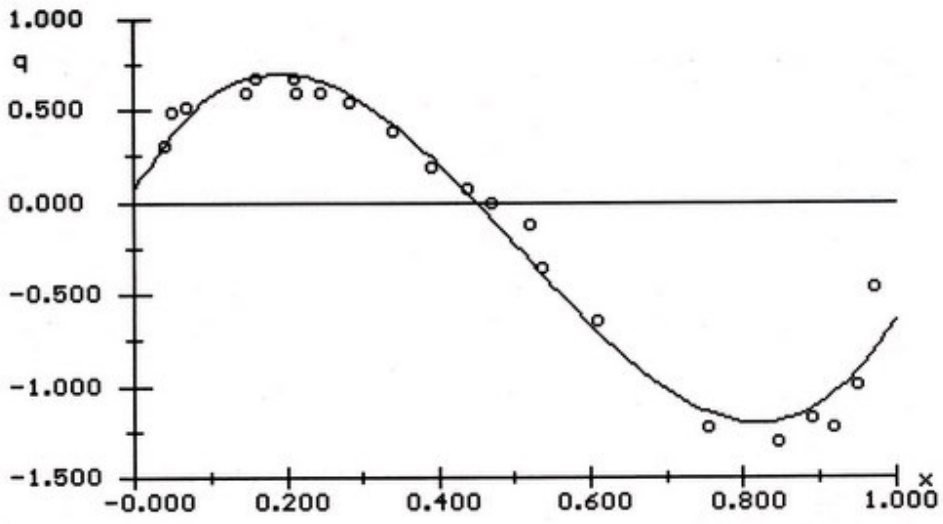
Assumption: No adsorption of (2).

Find: (a) Plot of loading as a function of mole fraction. Explain shape of curve.
(b) Fit of Freundlich equation over the low mole fraction region.

Analysis: (a) Using Polymath, the data for cyclohexane liquid adsorption are shown below for the entire composition region, with fitting to a cubic equation. The curve is of the type of Fig. 15.12c. The explanation for the shape of the curve is obtained from Fig. 15.13d. At low concentrations of (1), it begins to adsorb, with increasing adsorption for increasing mole fraction of (1), much like a Freundlich isotherm. The solvent, (2), contrary to the assumption of no adsorption is highly adsorbed at low concentrations of (1), but its adsorption gradually diminishes as the concentration of (2) decreases.

(b) For the cyclohexane mole fraction region from 0 to 0.250, the data are fitted with the Regress program of Polymath to a modification of the Freundlich Eq. (15-35), using mole fraction instead of concentration, with a plot on the following page.

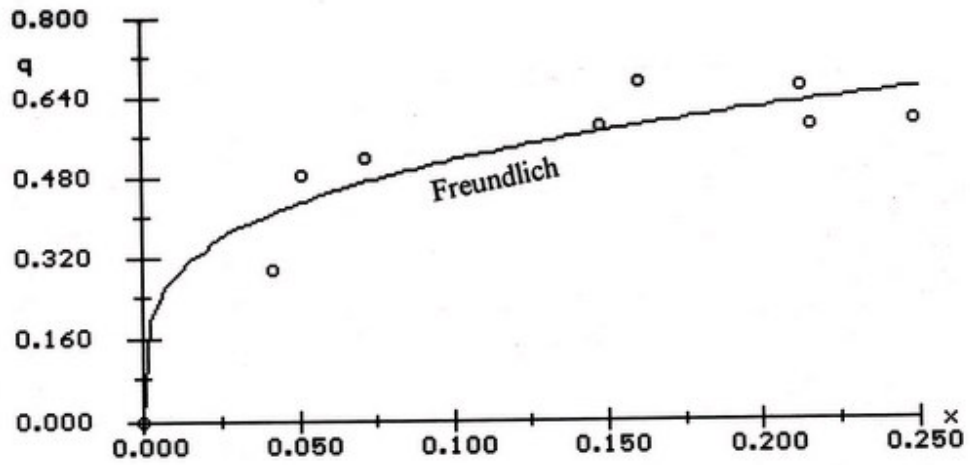
$$q = 0.94511\, x^{\frac{1}{3.813}}$$



$q(x) = 0.0598157 + 7.16146\,x - 23.1024\,x^2 + 15.232\,x^3$

Exercise 15.11 (continued)

Analysis: (b) (continued)



Exercise 15.12

Subject: Fitting adsorption equilibria data for small concentrations of toluene in water with activated carbon, and small concentrations of water in toluene with activated alumina, to Langmuir and Feundlich isotherms.

Given: Table of adsorption equilibrium data for toluene in water with activated carbon at 25°C. Table of adsorption equilibrium data for water in toluene with activated alumina at 25°C.

Assumptions: Negligible adsorption of water on activated carbon. Negligible adsorption of toluene on activated alumna.

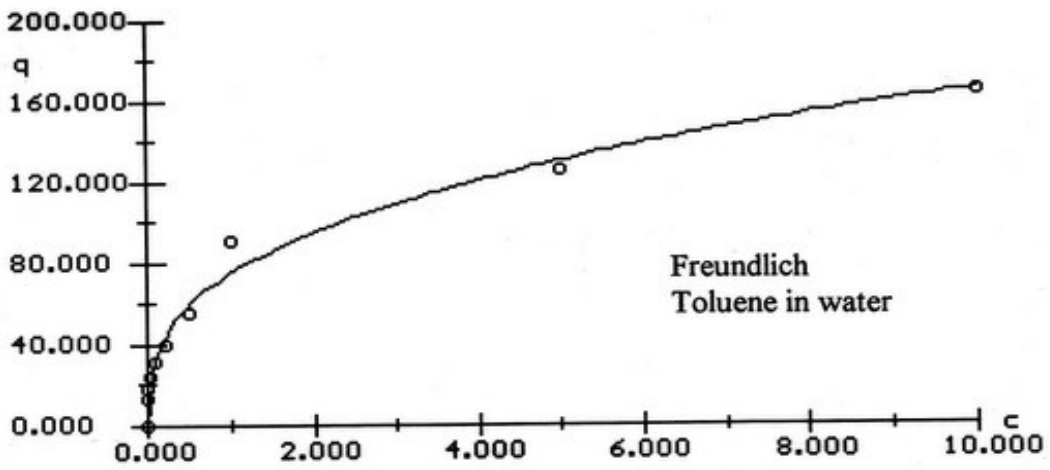
Find: Best fitting isotherms from Langmuir, Freundlich, and linear.

Analysis: Use the nonlinear regression program of Polymath. However, for toluene in water, the data point at $c = 2$ for $q = 70.2$ appears to be suspect, so discard it. The following results are obtained using Eq. (15-35) for the Freundlich isotherm: $q = k\,c^{1/n}$

and (15-36) for the Langmuir isotherm: $q = q_m Kc/(1 + Kc)$

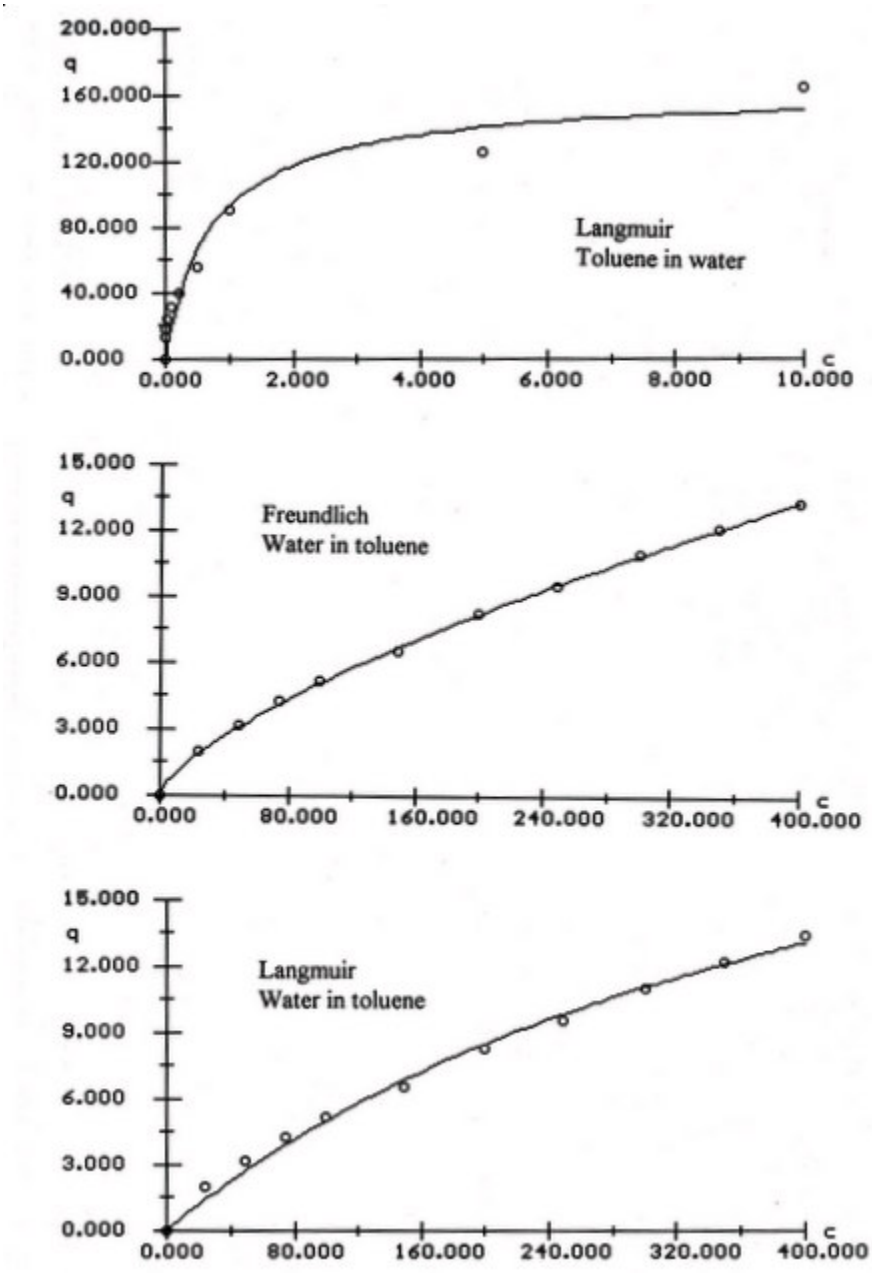
Component	Freundlich:		Langmuir:	
	k	n	K	q_m
Toluene in water	74.0218	2.86424	1.30434	161.863
Water in toluene	0.199624	1.42732	0.00214855	28.0673

The plots of the fits are shown below and on the next page.
For toluene in water, the Freundlich isotherm gives the best fit.
For water in toluene, the Freundlich isotherm gives a very good fit.
The linear isotherm gives a poor fit for both cases.


200.000
q
160.000
120.000
80.000
40.000
0.000
0.000
2.000
4.000
6.000
8.000
10.000
c
Freundlich
Toluene in water

Exercise 15.12 (continued)

Analysis: (continued)



Exercise 15.13

Subject: Ion exchange of sulfate ions with chloride ions, and regeneration of the resin.

Given: 60 L of water with sulfate ion and chloride ion concentrations of 0.018 eq/L and 0.002 eq/L, respectively. Remove sulfate ion by chloride ion exchange on 1 L of a strong-base resin. Regeneration of the resin with 30 L of 10 wt% aq. NaCl. Resin ion-exchange capacity of 1.2 eq/L. From Table 15.6, molar selectivities are: 1.0 for Cl- and 0.15 for SO_4=.

Find: Derivation of Eq. (15-44).

(a) Ion-exchange reaction.

(b) Value of chemical equilibrium constant for $K_{SO4=,Cl-}$.

(c) Equilibrium concentrations of SO_4= and Cl- ions in solution and in resin in eq/L for the ion-exchange step.

(d) Concentration of Cl- in eq/L for the regenerating solution.

(e) Equilibrium concentrations of SO_4= and Cl- ions in solution and in resin in eq/L for the regeneration step.

(f) Whether the steps are sufficiently selective.

Analysis: Let $A=SO_4^{=}$ and $B=Cl^{-}$

Eq. (15-44) is $$K_{A,B} = \left(\frac{C}{Q}\right)^{n-1}\left[\frac{y_A(1-x_A)^n}{x_A(1-y_A)^n}\right] \qquad (1)$$

This a case of unequal charges, so use Eq. (15-37) for the reaction:

(a) $$SO_{4(l)}^{2-} + 2Cl\,R_{(s)} \leftrightarrow SO_4R_{2(s)} + 2Cl^{-}{}_{(l)}$$

Thus, $n = 2$ and by the law of mass action:

$$K_{A,B} = \frac{q_{SO_4R}\, c_{Cl^-}^2}{q_{ClR}^2\, c_{SO_4^{2-}}} \qquad (2)$$

The counterion valences are: $z_A = 2$ and $z_B = 1$

From Eq. (15-39), $c_A = Cx_A/2$ and $c_B = Cx_B/1$ (3)

From Eq. (15-40), $q_{AR} = Qy_A/2$ and $q_{BR} = Qy_B/1$ (4)

Substitution of Eqs. (2) and (3) into (1), gives:

$$K_{A,B} = \frac{\left(\frac{Q}{2}\right)y_A C^2 x_B^2}{Q^2 y_B^2\left(\frac{C}{2}\right)x_A} = \left(\frac{C}{Q}\right)\left[\frac{y_A(1-x_A)^2}{x_A(1-y_A)^2}\right] = K_{A,B} = \left(\frac{C}{Q}\right)^{n-1}\left[\frac{y_A(1-x_A)^n}{x_A(1-y_A)^n}\right]$$

since, n =2. This is Eq. (15-44).

Exercise 15.13 (continued)

Analysis: (continued)

(b) From Eq. (15-45), using values of K_i from Table 15.6, $K_{A,B} = K_A/K_B = 0.15/1.0 = 0.15$ (5)

(c) For the initial ion-exchange step, $Q = 1.2$ eq/L and $C = c_A + c_B = 0.018 + 0.002 = 0.02$ eq/L

Let: a = eq of $SO_4^=$ exchanged. The equivalent fractions of the ions for 1.0 L of resin, 60 L of aq. solution, and $n = 2$ are:

$$x_{SO_4^=} = \frac{0.018 - \frac{a}{60}}{0.02} = 0.9 - 0.833a \qquad (6)$$

$$y_{SO_4^=} = \frac{a/1}{1.2} = \frac{a}{1.2} \qquad (7)$$

Combining Eqs (1), (5), (6), and (7),

$$K_{A,B} = \left(\frac{C}{Q}\right)^{n-1}\left[\frac{y_{SO_4^=}\left(x_{Cl^-}\right)^n}{x_{SO_4^=}\left(y_{Cl^-}\right)^n}\right] = 0.15 = \left(\frac{0.02}{1.2}\right)^{2-1}\left[\frac{\left(\frac{a}{1.2}\right)(1-0.9+0.833a)^2}{(0.9-0.833a)\left(1-\frac{a}{1.2}\right)^2}\right] \qquad (8)$$

Solving Eq. (8) with a nonlinear solver, $a = 0.755$ eq.

From Eqs. (6) and (7),

$$x_{SO_4^=} = 0.9 - 0.833(0.755) = 0.271$$

$$y_{SO_4^=} = \frac{0.755}{1.2} = 0.629$$

From Eq. (15-39),

$$c_{SO_4^=} = \frac{Cx_{SO_4^=}}{z_{SO_4^=}} = \frac{0.02(0.271)}{2} = 0.00271 \text{ mol/L} \quad \text{or} \quad 0.00542 \text{ eq/L}$$

$$c_{Cl^-} = \frac{Cx_{Cl^-}}{z_{Cl^-}} = \frac{0.02(1-0.271)}{1} = 0.01458 \text{ mol/L} \quad \text{or} \quad 0.01458 \text{ eq/L}$$

From Eq. (15-40),

$$q_{SO_4^=} = \frac{Qy_{SO_4^=}}{z_{SO_4^=}} = \frac{1.2(0.629)}{2} = 0.377 \text{ mol/L} \quad \text{or} \quad 0.754 \text{ eq/L}$$

$$q_{Cl^-} = \frac{Qy_{Cl^-}}{z_{Cl^-}} = \frac{1.2(1-0.629)}{1} = 0.445 \text{ mol/L} \quad \text{or} \quad 0.445 \text{ eq/L}$$

Exercise 15.13 (continued)

Analysis: (continued)

(d) The regenerating solution is 30 L of 10 wt% aq. NaCl. From Perry's Handbook, assuming a temperature of 25°C, the density is 1.0689 g/cm^3 or 1068.9 g/L. The MW of NaCl = 58.45. Therefore, the concentration of chloride ion = c_{Cl^-} = 0.10(1068.9)/58.45 = 1.829 eq/L.

(e) From Part (c), 1 L of resin includes: 0.445 eq of Cl^- and 0.754 eq
From Part (d), 30 L of regenerating solution includes: 30(1.829) = 54.870 eq. Cl^-
Thus, we have a total of 30 L of solution and 1 L of resin containing a total of:
0.754 eq. of $SO_4^=$ and 54.870 + 0.445 = 55.315 eq. of Cl^-

Let: a = eq of SO_4= on the resin at equilibrium. The equivalent fractions of the ions for 1.0 L of resin, 30 L of aq. solution, and n = 2 are:

$$x_{SO_4^=} = \frac{0.574 - a}{54.870} = 0.01046 - 0.01822a \qquad (9)$$

$$y_{SO_4^=} = \frac{a/1}{1.2} = \frac{a}{1.2} = 0.833a \qquad (10)$$

Combining Eqs (1), (5), (9), and (10), with C = 1.829 eq/L and
Q = 1.2 eq/L, with n = 2,

$$K_{A,B} = \left(\frac{C}{Q}\right)^{n-1}\left[\frac{y_{SO_4^=}\left(x_{Cl^-}\right)^n}{x_{SO_4^=}\left(y_{Cl^-}\right)^n}\right] = 0.15 = \left(\frac{1.829}{1.2}\right)^{2-1}\left[\frac{0.833a\left(1-0.01046+0.01822a\right)^2}{\left(0.01046-0.01822a\right)\left(1-0.833a\right)^2}\right] \qquad (11)$$

Solving Eq. (11) with a nonlinear solver, a = 0.00123 eq.
From Eqs. (9) and (10),

$$x_{SO_4^=} = 0.01046 - 0.01822(0.00123) = 0.01044$$

$$y_{SO_4^=} = 0.833(0.00123) = 0.001025$$

From Eq. (15-39),

$$c_{SO_4^=} = \frac{Cx_{SO_4^=}}{z_{SO_4^=}} = \frac{1.829(0.01044)}{2} = 0.00955 \text{ mol/L} \quad \text{or} \quad 0.0191 \text{ eq/L}$$

$$c_{Cl^-} = \frac{Cx_{Cl^-}}{z_{Cl^-}} = \frac{1.829(1-0.01044)}{1} = 1.810 \text{ mol/L} \quad \text{or} \quad 1.810 \text{ eq/L}$$

Exercise 15.13 (continued)

Analysis: (e) (continued)

From Eq. (15-40),

$$q_{SO_4^{=}} = \frac{Qy_{SO_4^{=}}}{z_{SO_4^{=}}} = \frac{1.2(0.001025)}{2} = 0.000615 \text{ mol/L} \quad \text{or} \quad 0.00123 \text{ eq/L}$$

$$q_{Cl^-} = \frac{Qy_{Cl^-}}{z_{Cl^-}} = \frac{1.2(1-0.001025)}{1} = 1.199 \text{ mol/L} \quad \text{or} \quad 1.199 \text{ eq/L}$$

(f) For the ion-exchange step, (0.755/1.080) x 100% = 70% of the sulfate ion is transferred from the solution to the resin. This is reasonably high considering the low and unfavorable chemical equilibrium constant of 0.15.

The regeneration step is very effective, with (0.754 - 0.00123)/0.754 x 100% = 99.84% of the sulfate ion removed from the resin.

Exercise 15.14

Subject: Equivalent fractions at equilibrium for the ion exchange of silver ion with sodium ion.

Given: Ion-exchange resin of Dowex 50 cross-linked with 8% divinylbenzene. Exchange of silver ion in methanol with sodium ion in the resin. Wet capacity of the resin = 2.5 eq/L. Resin is initially saturated with sodium ion. Experimental data for the molar selectivity coefficient as a function of equivalent fraction of sodium ion in the resin:

x_{Na+}	0.1	0.3	0.5	0.7	0.9
$K_{ag+,\ Na+}$	11.2	11.9	12.3	14.1	17.0

Find: Equivalent fractions if 50 L of 0.05 M Ag^+ in methanol is treated with 1 L of wet resin.

Analysis: 1 L of resin contains 2.5 eq of Na^+.
50 L of solution contains 0.05(5) = 2.5 eq Ag^+
Because both ions have a charge of one, Eq. (15-38) applies at equilibrium, with $n = 1$.
Let x = eq of Ag in resin at equilibrium. Since we begin with 2.5 eq of each ion, then, also, x = eq of Na^+ in the solution at equilibrium. Therefore,

$$K = \frac{q_{Ag} c_{Na^+}}{q_{Na} c_{Ag^+}} = \frac{\left(\frac{x}{1}\right)\left(\frac{x}{50}\right)}{\left(\frac{2.5-x}{1}\right)\left(\frac{2.5-x}{50}\right)} = \frac{x^2}{\left(6.25-5x+x^2\right)} \qquad (1)$$

To solve Eq. (1), the need the molar selectivity coefficient, which depends on x_{Na+} in the table above. Assume a value of 12. Eq. (1), which is a quadratic equation in x becomes: $11\ x^2 - 60\ x + 75 = 0$. Solving, x = 1.94 eq of Na^+ in solution. Therefore, the equivalent fraction of Na^+ in solution = 1.94/2.5 = 0.776. So we need to assume a higher value of K.
Using the above table of data, assume a value of 15.2 for the molar selectivity coefficient.
Then Eq. (1) becomes: $14.2\ x^2 - 76\ x + 95 = 0$. Solving, x = 2.0 and the equivalent fraction of Na^+ in solution = 2/2.5 = 0.80. From the above table, K = 15.6. Then Eq. (1) becomes: $14.6\ x^2 - 78\ x + 97.5 = 0$. Solving x = 1.995. The value of K = 15.6 is close enough.
Therefore, the equivalent fractions at equilibrium are:
In the resin, y_{Na} = 0.202 and y_{Ag} = 0.798
In the methanol solution, x_{Na+} = 0.798 and x_{Ag+} = 0.202

Exercise 15.15

Subject: Recovery of glycerol from an aqueous solution of NaCl by ion exclusion.

Given: Feed solution of 1,000 kg containing 6 wt% NaCl, 35 wt% glycerol, and 47 wt% water. Dowex 50 ion-exchange resin in the sodium form, prewetted to contain 40 wt% water. The equilibrium distribution coefficient for glycerol is given by:

$$K_d = \frac{\text{mass fraction glycerol in solution inside the resin}}{\text{mass fraction glycerol in solution outside the resin}}$$

Values of K_d depend on the mass fraction of glycerol in the solution outside the resin and on the wt% NaCl in the solution outside the resin, as given in a table in the problem statement.

Assumptions: The remainder of the feed solution (12 wt%) is inert material. During ion exclusion, no additional water or NaCl will transfer to the solution inside the resin.

Find: The kg of resin on a dry basis needed to transfer 75% of the glycerol to the solution inside the resin.

Analysis: Let R = kg of dry resin needed. Then the water in the prewetted resin = (40/60) R. The original solution contains 0.35(1000) = 350 kg of glycerol. For a transfer of 75%, the equilibrium solution inside the resin will contain 0.75(350) = 262.5 kg of glycerol, leaving 87.5 kg of glycerol in the equilibrium solution outside the resin. Therefore, we can write K_d as:

$$K_d = \frac{\dfrac{262.5}{(40/60)R + 262.5}}{\dfrac{87.5}{100}} = \frac{3000}{0.6667R + 262.5}$$

$$\text{Solving,} \quad R = \frac{3000 - 262.5K_d}{0.6667} = 4500 - 393.75K_d \qquad (1)$$

At equilbrium, the mass fraction of glycerine in the solution outside the resin is:
87.5/(1000-262.5) = 0.1186
The wt% NaCl in the solution outside the resin is: 0.06(1000)/(1000-262.5) x 100% = 8.13 wt%
Interpolate the given table for K_d to obtain: (0.759)(0.467) + (0.914)(0.533) = 0.842 = K_d
Therefore, from Eq. (1), R = 4500 - 393.75(0.842) = 4,170 kg dry resin.

Exercise 15.16

Subject: Estimation of external gas-to-particle mass-transfer and heat-transfer coefficients in a fixed-bed adsorption column.

Given: Fixed bed of 2-foot diameter packed with 4 x 6 mesh silica gel with an external void fraction of 0.5. Gas is benzene vapor in air, which flows through the bed at a benzene-free flow rate of 25 lb/min.

Find: External gas-to-particle mass-transfer and heat-transfer coefficients at a location in the bed where the pressure is 1 atm, temperature is 70°F, and benzene bulk mole fraction = 0.005.

Analysis: From Perry's Handbook, 4-mesh and 6-mesh screens have openings of 0.476 cm and 0.336 cm, respectively, with an average of (0.476 + 0.336)/2 = 0.406 cm. Aasssuming the silica gel is crushed particles, the sphericity = $\psi = 0.65$. Therefore, the effective particle diameter = 0.65(0.406) = 0.264 cm = 0.00264 m = D_p. Provided that the dimensionless groups are in the specified ranges of the correlations, Eqs. (15-65) and (15-66) can be used to estimate the coefficients:

$$k_c = \frac{D_i}{D_p}\left[2 + 1.1\left(\frac{D_p G}{\mu}\right)^{0.6}\left(\frac{\mu}{\rho D_i}\right)^{1/3}\right] \qquad (1)$$

$$h = \frac{D_i}{D_p}\left[2 + 1.1\left(\frac{D_p G}{\mu}\right)^{0.6}\left(\frac{C_P \mu}{k}\right)^{1/3}\right] \qquad (2)$$

Because the gas is dilute in benzene, use the properties of air in the coefficient correlations.
At 70°F, $\mu = 183$ micropoise = 1.83×10^{-5} kg/m-s
$k = 0.0256$ J/m-s-K
$C_P = 1.09$ kJ/kg-K = 1090 J/kg-K
From Perry's Handbook, at 32°F, the diffusivity of benzene in air at 1 atm = 0.077 cm^2/s.
From Eq. (3-36), the diffusivity is proportional to T to the 1.75 power.
Therefore, $D_i = 0.077[(70 + 460)/(32 + 460)]^{1.75} = 0.0877$ $cm^2/s = 0.0877 \times 10^{-4}$ m^2/s.
From the ideal gas law, $\rho = \frac{PM}{RT} = \frac{101.3(29)}{8.314(530/1.8)} = 1.20$ kg / m^3

$$N_{\mathrm{Pr}} = \frac{C_P \mu}{k} = \frac{1090(1.83\times10^{-5})}{0.0256} = 0.779$$

$$N_{\mathrm{Sc}} = \frac{\mu}{\rho D_i} = \frac{1.83\times10^{-5}}{1.20(0.0877\times10^{-4})} = 1.74$$

Exercise 15.16 (continued)

Analysis (continued)

In the Reynolds number, G = mass flow rate/bed cross-sectional area

bed cross-sectional area = $A_b = \pi D^2/4 = 3.14(2)^2/4 = 3.14$ ft^2 or 0.292 m^2

Air flow rate = 25 lb/min = 25/60 = 0.417 lb/s or 0.417/29 = 0.0144 lbmol/s

Benzene flow rate = (0.005/0.995)0.0144 = 0.000072 lbmol/s or 0.000072(78.11) = 0.0056 lb/s

Total gas mass flow = 0.417 + 0.0056 = 0.423 lb/s or 0.192 kg/s

Gas mass velocity = G = 0.192/0.292 = 0.658 kg/m^2-s

N_{Re} = 0.00264(0.658)/1.83 x 10^{-5} = 94.9

All dimensionless groups and the particle diameter are in the specified ranges of applicability of the correlations of Eqs (1) and (2). Therefore, using those two equations,

$$k_c = \frac{0.0877\times10^{-4}}{0.00264}\left[2+1.1(94.9)^{0.6}(1.74)^{1/3}\right] = 0.0741 \text{ m/s}$$

$$h = \frac{0.0256}{0.00264}\left[2+1.1(94.9)^{0.6}(0.779)^{1/3}\right] = 170.1 \text{ J/m}^2\text{-s-K}$$

Exercise 15.17

Estimation of external gas-to-particle mass-transfer and heat-transfer coefficients in a fixed-bed adsorption column.

Given: Fixed bed of 12.06-cm inside diameter packed with 3.3-mm-diameter Alcoa F-200 activated alumina beads with an external void fraction of 0.442. Gas is air containing water vapor, which flows through the bed at a flow rate of 1.327 kg/min.

Find: External gas-to-particle mass-transfer and heat-transfer coefficients at a location in the bed where the pressure is 653.3 kPa, temperature is 21°C , and the dew-point temperature = 11.2°C.

Analysis: D_p = 3.3 mm = 0.0033 m. Provided that the dimensionless groups are in the specified ranges of the correlations, Eqs. (15-65) and (15-66) can be used to estimate the coefficients:

$$k_c = \frac{D_i}{D_p}\left[2 + 1.1\left(\frac{D_p G}{\mu}\right)^{0.6}\left(\frac{\mu}{\rho D_i}\right)^{1/3}\right] \qquad (1)$$

$$h = \frac{D_i}{D_p}\left[2 + 1.1\left(\frac{D_p G}{\mu}\right)^{0.6}\left(\frac{C_P \mu}{k}\right)^{1/3}\right] \qquad (2)$$

At the dew-point temperature, the vapor pressure of water = 0.192 psi or 1.32 kPa. Therefore, at 653.3 kPa, the mole fraction of water in the air is only 1.32/653.3 = 0.002. Because the gas is so dilute in water vapor, use the properties of air in the coefficient correlations.

At 21°C = 70°F, μ = 183 micropoise = 1.83 x 10^{-5} kg/m-s

k = 0.0256 J/m-s-K

C_P = 1.09 kJ/kg-K = 1090 J/kg-K

From Perry's Handbook, at 32°F, the diffusivity of water vapor in air at 1 atm = 0.22 cm^2/s.

From Eq. (3-36), the diffusivity is proportional to T to the 1.75 power and inversely proportional to the pressure. Therefore,

$D_i = 0.22(101.3/653.3)[(70 + 460)/(32 + 460)]^{1.75} = 0.0388\ cm^2/s = 0.0388 \times 10^{-4}\ m^2/s$.

At the high pressure of 653.3 kPa, the compressibility factor of air = 0.998. From the generalized gas law, $\rho = \dfrac{PM}{ZRT} = \dfrac{653.3(29)}{0.998(8.314)(530/1.8)} = 7.75\ kg/m^3$

$$N_{Pr} = \frac{C_P \mu}{k} = \frac{1090(1.83\times10^{-5})}{0.0256} = 0.779$$

$$N_{Sc} = \frac{\mu}{\rho D_i} = \frac{1.83\times10^{-5}}{7.75(0.0388\times10^{-4})} = 0.609$$

Exercise 15.17 (continued)

Analysis (continued)

In the Reynolds number, G = mass flow rate/bed cross-sectional area

Bed cross-sectional area = $A_b = \pi D^2/4 = 3.14(0.1206)^2/4 = 0.0114$ m^2

Gas flow rate = 1.327 kg/min = 1.327/60 = 0.0221 kg/s

Gas mass velocity = $G = 0.0221/0.0114 = 1.94$ kg/m^2-s

$N_{Re} = 0.0033(1.94)/1.83 \times 10^{-5} = 350$

All dimensionless groups and the particle diameter are in the specified ranges of applicability of the correlations of Eqs (1) and (2). Therefore, using those two equations,

$$k_c = \frac{0.0388\times10^{-4}}{0.0033}\left[2+1.1(350)^{0.6}(0.609)^{1/3}\right] = 0.0392 \text{ m/s}$$

$$h = \frac{0.0256}{0.0033}\left[2+1.1(350)^{0.6}(0.779)^{1/3}\right] = 280 \text{ J/m}^2\text{-s-K}$$

Exercise 15.18

Subject: Effective diffusivity of acetone in the pores of activated carbon.

Given: Activated carbon with $\rho_p = 0.85$ g/cm^3, $\varepsilon_p = 0.48$, $d_p = 25$ Angstroms $= 25 \times 10^{-8}$ cm, and tortuosity $= \tau = 2.75$. Diffusion of acetone vapor in nitrogen, where from Example 15.7, temperature = 297 K, pressure = 136 kPa, and molecular (bulk) diffusivity $= D_i = 0.085 \times 10^{-4}$ m^2/s or 0.085 cm^2/s.
Assumptions: Negligible surface diffusion.

Find: Effective diffusivity of acetone vapor through nitrogen in the pores, accounting for bulk (molecular) diffusion and Knudsen diffusion.

Analysis: From a modification of Eq. (15-75), omitting surface diffusion,

$$D_e = \frac{\varepsilon_p}{\tau}\left(\frac{1}{\frac{1}{D_i}+\frac{1}{D_K}}\right) = \frac{0.48}{2.75}\left(\frac{1}{\frac{1}{0.085}+\frac{1}{D_K}}\right) = \frac{0.175}{11.76+\frac{1}{D_K}} \qquad (1)$$

From Eq. (14-21), using 58 for the molecular weight of acetone,
$D_K = 4850\, d_p(T/M_i)^{1/2} = 4850(25 \times 10^{-8})(297/58)^{1/2} = 0.00274$ cm^2/s
Substituting this value into Eq. (1) gives:

$$D_e = \frac{0.175}{11.76+\frac{1}{0.00274}} = \frac{0.175}{11.76+364} = 4.66\times10^{-4} \text{ cm}^2/\text{s}$$

It is noted that Knudsen diffusion is very important and largely controls diffusion.

Exercise 15.19

Subject: Effective diffusivity of benzene vapor in the pores of silica gel.

Given: Silica gel with ρ_p = 1.15 g/cm^3 = 71.8 lb/ft^3 , ε_p = 0.48, d_p = 30 Angstroms = 30 x 10^{-8} cm, and tortuosity = τ = 3.2. Diffusion of benzene vapor in air in the pores, where from Exercise 15.16, temperature = 70°F and pressure = 1 atm. Differential heat of adsorption = -11,000 cal/mol. Adsorption equilibrium constant from Eq. (1) of Example 15.10 = K = 5,120 (lb/ft^3 particles)/(lb/ft^3 gas).

Find: Effective diffusivity of benzene vapor through air in the pores, accounting for bulk (molecular) diffusion, Knudsen diffusion, and surface diffusion.

Analysis: From Eq. (15-75), for all three mechanisms of internal diffusion,

$$D_e = \frac{\varepsilon_p}{\tau}\left\{\left[\frac{1}{\frac{1}{D_i}+\frac{1}{D_K}}\right]+(D_i)_s\frac{\rho_p K}{\varepsilon_p}\right\} = \frac{0.48}{3.2}\left\{\left(\frac{1}{\frac{1}{D_i}+\frac{1}{D_K}}\right)+(D_i)_s\frac{\rho_p K}{0.48}\right\} \qquad (1)$$

From Perry's Handbook, at 32°F, the diffusivity of benzene in air at 1 atm = 0.077 cm^2/s.
From Eq. (3-36), the diffusivity is proportional to T to the 1.75 power.
Therefore, D_i = 0.077[(70 + 460)/(32 + 460)]$^{1.75}$ = 0.0877 cm^2/s.
From Eq. (14-21), using 78 for the molecular weight of benzene and T = 70°F = 294 K ,
$D_K = 4850\, d_p(T/M_i)^{1/2}$ = 4850(30 x 10^{-8})(294/78)$^{1/2}$ = 0.00282 cm^2/s
From Eq. (15-76), using m =1 because silica gel is an insulating adsorbent,

$$(D_i)_s = 0.016\exp\left[\frac{-0.45(-\Delta H_{ads})}{mRT}\right] = 0.016\exp\left[\frac{-0.45(11{,}000)}{(1)(1.987)(294)}\right] = 3.34\times10^{-6}\ \text{cm}^2/\text{s}$$

In Eq. (1), the units of K are (g adsorbed/g adsorbent)/(g solute/cm^3 of gas). Therefore, converting the units of the given K, $K = (5{,}120/\rho_p)[62.4\ (\text{lb/ft}^3)/(\text{g/cm}^3)]$ = 5,120(62.4)/71.8 = 4,450 (g adsorbed/g adsorbent)/(g solute/cm^3 of gas).
Substituting the above values of D_i , D_K, $(D_i)_s$, and K into Eq. (1) gives:

$$D_e = \frac{0.48}{3.2}\left\{\left[\frac{1}{\frac{1}{0.0877}+\frac{1}{0.00282}}\right]+\left(3.12\times10^{-6}\right)\frac{(1.15)(4{,}450)}{0.48}\right\}$$

$$= 0.15\left\{\left(\frac{1}{11.40+355}\right)+0.0333\right\} = 0.15(0.00273+0.0333) = 0.0054\ \text{cm}^2/\text{s}$$

Note that the internal diffusion process is controlled by surface diffusion.

Exercise 15.20

Subject: Effective diffusivity of water vapor in the pores of activated alumina.

Given: Activated alumina with $\rho_p = 1.38$ g/cm^3, $\varepsilon_p = 0.52$, $d_p = 60$ Angstroms $= 60 \times 10^{-8}$ cm, and tortuosity $= \tau = 2.3$. Diffusion of water vapor in air in the pores, where from Exercise 15.17, temperature = 21°C and pressure = 653.3 kPa.

Find: Effective diffusivity of water vapor through air in the pores, accounting for bulk (molecular) diffusion and Knudsen diffusion, but not surface diffusion.

Analysis: From a modification of Eq. (15-75),

$$D_e = \frac{\varepsilon_p}{\tau}\left(\frac{1}{\frac{1}{D_i}+\frac{1}{D_K}}\right) = \frac{0.52}{2.3}\left(\frac{1}{\frac{1}{D_i}+\frac{1}{D_K}}\right) \qquad (1)$$

From Perry's Handbook, at 32°F, the diffusivity of water vapor in air at 1 atm = 0.22 cm^2/s.
From Eq. (3-36), the diffusivity is proportional to T to the 1.75 power and inversely proportional to the pressure. Therefore,
$D_i = 0.22(101.3/653.3)[(70 + 460)/(32 + 460)]^{1.75} = 0.0388$ cm^2/s
From Eq. (14-21), using 18 for the molecular weight of water and $T = 21$°C $= 294$ K ,
$D_K = 4850\, d_p(T/M_i)^{1/2} = 4850(60 \times 10^{-8})(294/18)^{1/2} = 0.0118$ cm^2/s
Substituting the above values of D_i and D_K into Eq. (1) gives:

$$D_e = \frac{0.52}{2.3}\left(\frac{1}{\frac{1}{0.0388}+\frac{1}{0.0118}}\right) = 0.226\left(\frac{1}{25.8+84.7}\right) = 0.226(0.00905) = 0.00205 \text{ cm}^2/\text{s}$$

Note that Knudsen diffusion is somewhat more important than molecular diffusion.

Exercise 15.21

Subject: Comparison of batch, continuous, and semicontinuous modes of slurry adsorption for removal of trichloroethylene (TCE) from water with activated carbon.

Given: Feed of water at 25°C containing 3.3 mg/L of TCE. Activated carbon with an average particle diameter of 1.5 mm = 0.15 cm and the following Freundlich adsorption isotherm for TCE at 25°C:
$q = 67\ c^{0.564}$ where q = mg TCE adsorbed/g carbon and c = mg TCE/L solution.
Sherwood number = 30. Particle external surface area = 5 m^2/kg.
Assumptions: Mass-transfer resistance in the pores is negligible compared to the external resistance.

Find: For an effluent of 0.01 mg TCE/L,

(a) Minimum amount of adsorbent needed per liter of feed solution.

(b) For batch mode with twice the minimum amount of adsorbent, the contact time.

(c) For continuous mode with twice the minimum amount of adsorbent, the required residence time.

(d) For semicontinuous mode at a feed rate of 50 gpm and a liquid residence time of 1.5 times that in Part (c), the amount of activated carbon to give a reasonable vol% solids in the tank and run time of not less than 10 times the liquid residence time.

Analysis: (a) The minimum amount of adsorbent corresponds to equilibrium with a solution of the effluent concentration of 0.01 mg TCE/L. From the Freundlich equation, the equilibrium loading is given by: $q = 67(0.01)^{0.564} = 4.99$ mg TCE/g carbon.
By material balance on the TCE, $c_F\, Q = c_{\text{final}}\, Q + q\, S_{\min}$
Solving for $S_{\min}$, for a basis of 1 L of solution,

$$S_{\min} = \frac{Q\left(c_F - c_{\text{final}}\right)}{q} = \frac{1.0(3.3-0.01)}{4.99} = 0.66 \text{ g carbon/L solution}$$

(b) For batch mode, use 2(0.66) = 1.32 g carbon/L solution = 1.32 kg/m^3 = S/Q
Combining Eqs. (15-77), (15-78), and (15-79), to eliminate q and c^*,

$$-\frac{dc}{dt} = k_L a\left\{c - \left[\frac{Q(c_F - c)}{Sk}\right]^n\right\} = k_L a\left\{c - \left[\frac{(3.3-c)}{(1.32)(67)}\right]^{1/0.564}\right\} = k_L a\left\{c - \left[\frac{(3.3-c)}{88.4}\right]^{1.773}\right\} \qquad (1)$$

From Eq. (15-65), k_L in cm/s = $N_{\text{Sh}}\, D_i / D_p = 30\, D_i / 0.15 = 200\, D_i$ (in cm^2/s)
From the Wilke-Chang Eq. (3-39),

$$D_{\text{A,B}} = \frac{7.4\times10^{-8}\left(\phi_{\text{B}} M_{\text{B}}\right)^{1/2} T}{\mu_{\text{B}} v_{\text{A}}^{0.6}} \qquad (2)$$

Exercise 15.21 (continued)

Analysis: (b) (continued)

From Table 3.2, $v_A = v_{TCE} = (2)14.8 + 3.7 + 3(21.6) = 98.1 \times 10^{-3}$ m^3/kmol = 98.1 cm^3/mol

Solvent water viscosity at 25°C = 0.94 cP, $M_B = 18$, and $\phi_B = 2.6$. Substitution into Eq. (2) gives,

$$D_{A,B} = \frac{7.4\times10^{-8}(2.6\times18)^{1/2}298}{0.94(98.1)^{0.6}} = 1.02\times10^{-5}\ \text{cm}^2/\text{s} = D_i$$

Therefore, $k_L = 200(1.02 \times 10^{-5}) = 0.00204$ cm/s

The units of a in Eq. (1) are cm^2 of external surface area of adsorbent/ cm^3 of solution.

Therefore, $a = 5$ m^2/kg (S/Q) = 5(1.32) = 6.60 m^2/m^3 of solution = 0.066 cm^2/cm^3.

Therefore, $k_L a = 0.00204(0.066) = 1.35 \times 10^{-4}$ s^{-1}

Eq. (1) becomes:

$$-\frac{dc}{dt} = 1.35\times10^{-4}\left\{c - \left[\frac{(3.3-c)}{88.4}\right]^{1.773}\right\}$$ where c is in mg TCE/L solution, and t is in seconds.

This equation represents an initial value problem in ODEs, which can be solved by the Euler method using a spreadsheet if a small time step is taken. The Euler form, where j is the iteration number, is,

$$c^{(j+1)} = c^{(j)} - (\Delta t)\ 1.35\times10^{-4}\left\{c^{(j)} - \left[\frac{(3.3-c^{(j)})}{88.4}\right]^{1.773}\right\} \qquad (3)$$

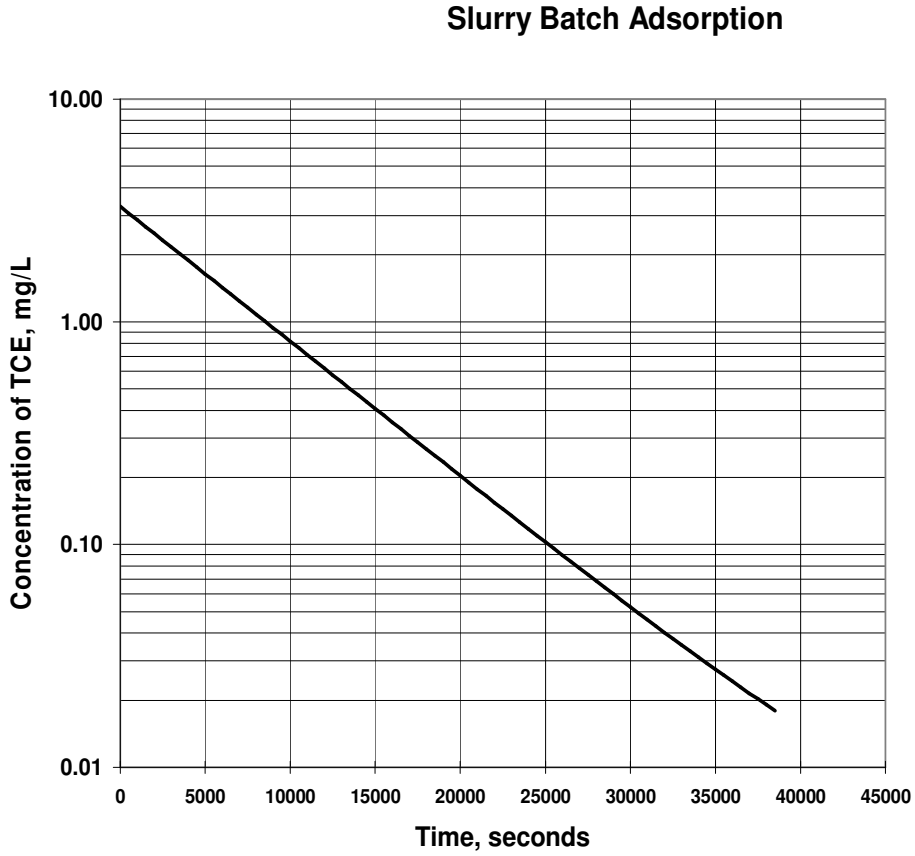
If a time step, Δt, of 500 s is used to find the time when c becomes 0.01 mg/L, the first 10 values of c are as follows:

Time, s	c of TCE, mg/L
0	3.300
500	3.077
1000	2.870
1500	2.676
2000	2.495
2500	2.327
3000	2.170
3500	2.023
4000	1.887
4500	1.760
5000	1.641

The time required is found to be 44,000 s = 733 minutes = 12.2 h. A plot of c vs. t is given on the next page, where semi-log coordinates gives almost a straight line.

Exercise 15.21 (continued)

Analysis: (b) (continued)



Exercise 15.21 (continued)

Analysis: (continued)

(c) For continuous slurry adsorption, assume a solution feed rate, Q, of 1 L/h. Therefore, the adsorbent feed rate, from Part (a) = S = 2(0.66) = 1.32 g carbon/h. A rearrangement of Eq. (15-86) gives the residence time as:

$$t_{res} = \frac{c_F - c_{out}}{k_L a\left(c_{out} - c^*\right)} = \frac{3.3 - 0.01}{1.35\times10^{-4}\left(0.01 - c^*\right)} \qquad (4)$$

The quantity c^* is the ficticious concentration in equilibrium with q_{out}, which is obtained by material balance, Eq. (15-87), which after rearrangement is:

$$q_{out} = \frac{Q\left(c_F - c_{out}\right)}{S} = \frac{1(3.3 - 0.01)}{1.32} = 2.42 \text{ mg/g}$$

Then, from a rearrangement of the given Freundlich adsorption isotherm,

$$c^* = \left(\frac{q_{out}}{67}\right)^{1/0.564} = \left(\frac{2.42}{67}\right)^{1.773} = 0.00277 \text{ mg/L}$$

Substitution into Eq. (4) gives,

$$t_{res} = \frac{3.3 - 0.01}{1.35\times10^{-4}\left(0.01 - 0.00277\right)} = 3{,}370{,}000 \text{ s} = 56{,}200 \text{ minutes} = 936 \text{ h} = 39.0 \text{ days}.$$

This very large residence time is due to the very low exit concentration of TCE in the solution, making the continuous mode impractical.

(d) Semicontinuous mode.

Average residence time of the solution in the tank = 1.5(57,370) = 86,100 min.

Flow rate of the solution = 50 gal/min or 50(3.785) = 189 L/min.

The volume of solution in the tank = 189(86,100) = 16,300,000 L or 16,300 m^3.

For a cylindrical tank with height = diameter, this gives a tank diameter of 27.5 m, which is probably impractical, although many smaller tanks in parallel could be used.

In the tank, where the solid adsorbent charge resides, the variation of the loading, q, with run time is given by Eq. (15-91), which for time in minutes is,

$$S\frac{dq}{dt} = k_L a\left(c_{out} - c^*\right)t_{res}Q = 1.35\times10^{-4}(60)\left(c_{out} - c^*\right)(86{,}100)(189) = 132{,}000\left(c_{out} - c^*\right) \qquad (5)$$

where S is in g, q is in mg TCE/g, and t is in min.

From Eq. (15-86),

$$c_{out} = \frac{c_F + k_L a t_{res} c^*}{1 + k_L a t_{res}} = \frac{3.3 + 1.35\times10^{-4}(60)(86{,}100)c^*}{1 + 1.35\times10^{-4}(60)(86{,}100)} = 0.00473 + 0.99857c^* \qquad (6)$$

Exercise 15.21 (continued)

Analysis: (d) (continued)

From the given Freundlich equation, $c^* = (q/67)^{1.773} = 0.000579\, q^{1.773}$ (7)

Combining Eqs. (5), (6), and (7), gives,

$$S\frac{dq}{dt} = 132{,}000\left(0.00473 + 0.99857c^* - c^*\right) = 624.36 - 188.76c^* = 624.36 - 0.1093q^{1.773} \qquad (8)$$

Let the volume of solids in the tank = 2.5 vol%. The solids-free volume of liquid in the tank = 16,300 m^3. Therefore, the solids volume = (2.5/97.5)(16,300) =418 m^3. Assume a particle density = 850 kg/m^3. Therefore, S = 418 (850) = 355,000 kg = 3.55 x 10^8 g and Eq. (8) becomes,

$$\frac{dq}{dt} = 1.76\times10^{-6} - 3.08\times10^{-10}q^{1.773} \qquad (9)$$

Now, compute the run time to achieve a cumulative c_{out} = 0.01 mg/L, where,

$$c_{cum} = 0.01 = \frac{\int_0^t c_{out}\,dt}{t} \qquad (10)$$

Eq. (9) represents an initial value problem in ODEs, which can be solved by the Euler method using a spreadsheet, if a small time step is taken. The Euler form, with j as the iteration index, is,

$$q^{(j+1)} = q^{(j)} + (\Delta t)\left[1.76\times10^{-6} - 3.08\times10^{-10}\left(q^{1.773}\right)^{(j)}\right] \qquad (11)$$

The total run time is specified to be not less than 10 times the average liquid residence time; thus, 10(86,100) = 861,000 minutes. Try a Δt of 100,000 minutes. From the spreadsheet, the first 5 and last 5 values are:

t, min.	q, mg/g	c^*, mg/L	c out	c cum
0	0	0	0.00473	0
100,000	0.176	2.66E-05	0.00476	0.00474
200,000	0.352	9.09E-05	0.00482	0.00477
300,000	0.528	0.000187	0.00492	0.00480
400,000	0.704	0.000311	0.00504	0.00484
500,000	0.880	0.000462	0.00519	0.00490
3,200,000	5.625	0.012377	0.01709	0.00919
3,300,000	5.800	0.013069	0.01778	0.00944
3,400,000	5.975	0.013778	0.01849	0.00970
3,500,000	6.151	0.014502	0.01921	0.00996
3,600,000	6.326	0.015243	0.01995	0.01023

Thus, the run time is just more over 3,500,000 minutes (2,430 days), which is greater than the above 861,000 minutes. Unfortunately, the vessel size is enormous.

Exercise 15.22

Subject: Comparison of batch, continuous, and semicontinuous modes of slurry adsorption for removal of benzene (B) and m-xylene (X) from water with activated carbon.

Given: Feed of water at 25°C containing 0.324 mg/L of B and 0.630 mg/L of X. Activated carbon with an average particle diameter of 1.5 mm = 0.15 cm and the following Freundlich adsorption isotherms at 25°C: $q = 32\, c^{0.428}$ for B and $q = 125\, c^{0.333}$ for X, where q = mg adsorbed/g carbon and c = mg in solution/L solution.
Sherwood number = 30. Particle external surface area = 5 m^2/kg.
Assumptions: Mass-transfer resistance in the pores is negligible compared to the external resistance.

Find: For an effluent of 0.002 mg each of B and X,

(a) Minimum amount of adsorbent needed per liter of feed solution.

(b) For batch mode with twice the minimum amount of adsorbent, the contact time.

(c) For continuous mode with twice the minimum amount of adsorbent, the required residence time.

(d) For semicontinuous mode at a feed rate of 50 gpm and a liquid residence time of 1.5 times that in Part (c), the amount of activated carbon to give a reasonable vol% solids in the tank and run time of not less than 10 times the liquid residence time.

Analysis: (a) The minimum amount of adsorbent corresponds to equilibrium with a solution of the effluent concentration of 0.002 mg of B or X, with the other solute at a lower concentration.. Must determine which solute controls. From the Freundlich equation for B, the equilibrium loading is given by: $q = 32(0.002)^{0.428} = 2.24$ mg B/g carbon.
By material balance on B, $c_F\, Q = c_{final}\, Q + q\, S_{min}$
Solving for S_{min}, for a basis of 1 L of solution,

$$S_{min} = \frac{Q(c_F - c_{final})}{q} = \frac{1.0(0.324 - 0.002)}{2.24} = 0.144 \text{ g carbon/L solution}$$

From the Freundlich equation for X, the equilibrium loading is given by: $q = 125(0.002)^{0.333} =$ 15.78 mg X/g carbon.By material balance on X, $c_F\, Q = c_{final}\, Q + q\, S_{min}$
Solving for S_{min}, for a basis of 1 L of solution,

$$S_{min} = \frac{Q(c_F - c_{final})}{q} = \frac{1.0(0.630 - 0.002)}{15.78} = 0.0398 \text{ g carbon / L solution}$$

Therefore B controls and the minimum amount of adsorbent = 0.144 g carbon/L solution.

(b) For batch mode, use 2(0.144) = 0.288 g carbon/L solution = 0.288 kg/m^3 = S/Q
Combining Eqs. (15-77), (15-78), and (15-79) and applying them to B, to eliminate q and c*,

Exercise 15.22 (continued)

Analysis: (a) (continued)

$$-\frac{dc}{dt} = k_L a\left\{c - \left[\frac{Q(c_F - c)}{Sk}\right]^n\right\} = k_L a\left\{c - \left[\frac{(0.324 - c)}{(0.288)(32)}\right]^{1/0.428}\right\} = k_L a\left\{c - \left[\frac{(0.324 - c)}{9.22}\right]^{2.336}\right\} \quad (1)$$

From Eq. (15-65), k_L in cm/s = $N_{Sh}\, D_i / D_p = 30\, D_i / 0.15 = 200\, D_i$ (in cm^2/s)
From the Wilke-Chang Eq. (3-39),

$$D_{A,B} = \frac{7.4\times10^{-8}(\phi_B M_B)^{1/2} T}{\mu_B v_A^{0.6}} \quad (2)$$

From Table 3.2, $v_A = v_B = (6)14.8 + 6(3.7) - 15 = 96 \times 10^{-3}$ m^3/kmol = 96 cm^3/mol
Solvent water viscosity at 25°C = 0.94 cP, $M_B = 18$, and $\phi_B = 2.6$. Substitution into Eq. (2) gives,

$$D_{A,B} = \frac{7.4\times10^{-8}(2.6\times18)^{1/2}298}{0.94(96)^{0.6}} = 1.04\times10^{-5}\ cm^2/s = D_i$$

Therefore, $k_L = 200(1.04 \times 10^{-5}) = 0.0021$ cm/s
The units of a in Eq. (1) are cm^2 of external surface area of adsorbent/ cm^3 of solution.
Therefore, $a = 5$ m^2/kg (S/Q) = 5(0.288) = 1.44 m^2/m^3 of solution = 0.0144 cm^2/cm^3.
Therefore, $k_L a = 0.0021(0.0144) = 3.02 \times 10^{-5}$ s^{-1}
Eq. (1) becomes:

$$-\frac{dc}{dt} = 3.02\times10^{-5}\left\{c - \left[\frac{(0.324 - c)}{9.22}\right]^{2.336}\right\}$$ where c is in mg B/L solution, and t is in seconds.

This equation represents an initial value problem in ODEs, which can be solved by the Euler method using a spreadsheet if a small time step is taken. The Euler form, where j is the iteration number, is,

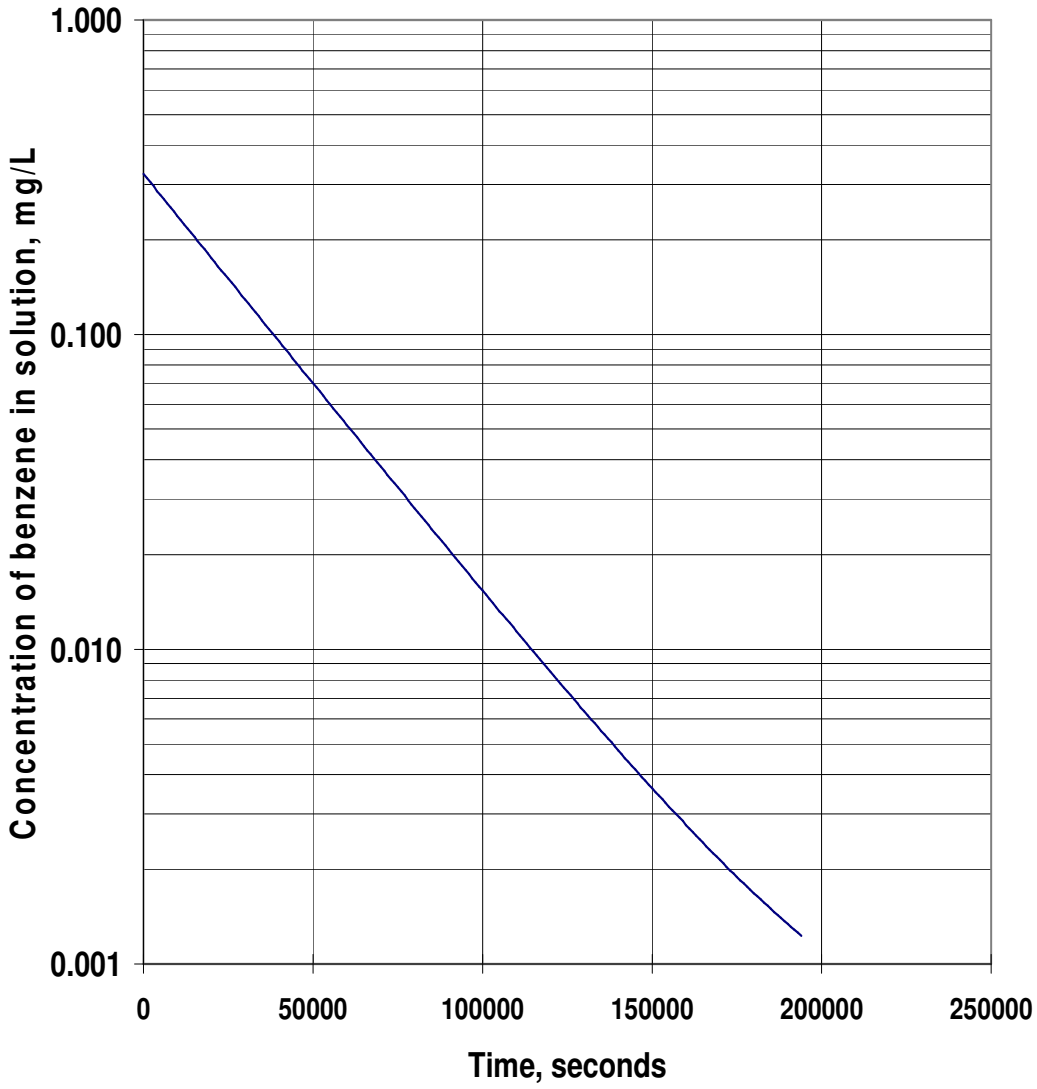
$$c^{(j+1)} = c^{(j)} - (\Delta t)\ 3.02\times10^{-5}\left\{c^{(j)} - \left[\frac{(0.324 - c^{(j)})}{9.22}\right]^{2.336}\right\} \quad (3)$$

If a time step, Δt, of 1,000 s is used to find the time when c becomes 0.002 mg/L, the first 7 values of c for B are as follows:

Time, s	c of B, mg/L
0	0.324
1,000	0.314
2,000	0.305
3,000	0.296
4,000	0.287
5,000	0.278
6,000	0.270

Exercise 15.22 (continued)

Analysis: (b) (continued)
The time required is found to be 172,000 s = 2,870 minutes = 47.8 h. A plot of *c* vs. *t* follows, where semi-log coordinates gives almost a straight line.



Exercise 15.22 (continued)

Analysis: (continued)

(c) For continuous slurry adsorption, assume a solution feed rate, Q, of 1 L/h. Therefore, the adsorbent feed rate, from Part (a) = S = 2(0.144) = 0.288 g carbon/h. A rearrangement of Eq. (15-86) gives the residence time as:

$$t_{res} = \frac{c_F - c_{out}}{k_L a\left(c_{out} - c^*\right)} = \frac{0.324 - 0.002}{3.02\times10^{-5}\left(0.002 - c^*\right)} \qquad (4)$$

The quantity c^* is the ficticious concentration in equilibrium with q_{out}, which is obtained by material balance, Eq. (15-87), which after rearrangement is:

$$q_{out} = \frac{Q\left(c_F - c_{out}\right)}{S} = \frac{1(0.324 - 0.002)}{0.288} = 1.118 \text{ mg / g}$$

Then, from a rearrangement of the given Freundlich adsorption isotherm,

$$c^* = \left(\frac{q_{out}}{32}\right)^{1/0.428} = \left(\frac{1.118}{32}\right)^{2.336} = 0.000395 \text{ mg / L}$$

Substitution into Eq. (4) gives,

$$t_{res} = \frac{0.324 - 0.002}{3.02\times10^{-5}\left(0.002 - 0.000395\right)} = 6,640,000 \text{ s} = 110{,}700 \text{ minutes} = 1{,}845 \text{ h} = 76.9 \text{ days}.$$

This very large residence time is due to the very low exit concentration of benzene in the solution, making the continuous mode impractical.

(d) Semicontinuous mode.

Average residence time of the solution in the tank = 1.5(110,700) = 166,100 min.

Flow rate of the solution = 50 gal/min or 50(3.785) = 189 L/min.

The volume of solution in the tank = 189(166,100) = 31,400,000 L or 31,400 m^3.

For a cylindrical tank with height = diameter, this gives a tank diameter of 34.2 m, which is probably impractical, although many smaller tanks in parallel could be used.

In the tank, where the solid adsorbent charge resides, the variation of the loading, q, with run time is given by Eq. (15-91), which for time in minutes is,

$$S\frac{dq}{dt} = k_L a\left(c_{out} - c^*\right)t_{res}Q = 3.02\times10^{-5}(60)\left(c_{out} - c^*\right)(166{,}100)(189) = 56{,}900\left(c_{out} - c^*\right) \qquad (5)$$

where S is in g, q is in mg B/g, and t is in min.

Exercise 15.22 (continued)

Analysis: (d) (continued)

From Eq. (15-86),

$$c_{\text{out}} = \frac{c_F + k_L a t_{\text{res}} c^*}{1 + k_L a t_{\text{res}}} = \frac{0.324 + 3.02\times10^{-5}(60)(166{,}100)c^*}{1 + 3.02\times10^{-5}(60)(166{,}100)} = 0.00107 + 0.99669c^* \qquad (6)$$

From the given Freundlich equation, $c^* = (q/32)^{2.336} \qquad = 0.000305\, q^{2.336}$ (7)

Combining Eqs. (5), (6), and (7), gives,

$$S\frac{dq}{dt} = 56{,}900\left(0.00107 + 0.99669c^* - c^*\right) = 60.88 - 188.34c^* = 60.88 - \ 0.0574q^{2.336} \qquad (8)$$

Let the volume of solids in the tank = 2.5 vol%. The solids-free volume of liquid in the tank = 31,400 m^3. Therefore, the solids volume = (2.5/97.5)(31,400) =805 m^3. Assume a particle density = 850 kg/m^3. Therefore, S = 805 (850) = 684,000 kg = 6.84 x 10^8 g and Eq. (8) becomes,

$$\frac{dq}{dt} = 8.90\times10^{-8} - 8.39\times10^{-11}q^{2.336} \qquad (9)$$

Now, compute the run time to achieve a cumulative c_{out} = 0.002 mg/L, where,

$$c_{\text{cum}} = 0.002 = \frac{\int_0^t c_{\text{out}}\,dt}{t} \qquad (10)$$

Eq. (9) represents an initial value problem in ODEs, which can be solved by the Euler method using a spreadsheet, if a small time step is taken. The Euler form, with j as the iteration index, is,

$$q^{(j+1)} = q^{(j)} + (\Delta t)\left[8.90\times10^{-8} - 8.39\times10^{-11}\left(q^{2.336}\right)^{(j)}\right] \qquad (11)$$

The total run time is specified to be not less than 10 times the average liquid residence time; thus, 10(166,100) = 1,661,000 minutes. Try a Δt of 500,000 minutes. From the spreadsheet, the first 6 and last 6 values are:

t, min.	q, mg/g	c^*, mg/L	c out	c cum
0	0	0	0.00154	0
500000	0.04450	2.12E-07	0.00154	0.00154
1000000	0.08900	1.07E-06	0.00154	0.00154
1500000	0.13500	2.76E-06	0.00155	0.00154
2000000	0.17800	5.41E-06	0.00155	0.00154
2500000	0.22250	9.11E-06	0.00155	0.00154
20000000	1.77815	0.001170	0.00270	0.00189
20500000	1.82249	0.001239	0.00277	0.00191
21000000	1.86682	0.001311	0.00284	0.00193
21500000	1.91114	0.001385	0.00292	0.00195
22000000	1.95545	0.001461	0.00299	0.00198
22500000	1.99974	0.001539	0.00307	0.00200

Thus, the run time is 22,500,000 minutes (15,600 days), which is much greater than the above 1,661,000 minutes. Unfortunately, the vessel size is enormous.

Exercise 15.23

Subject: Comparison of batch, continuous, and semicontinuous modes of slurry adsorption for removal of chloroform (C) from water with activated carbon.

Given: Feed of water at 25°C containing 0.223 mg/L of C. Activated carbon with an average particle diameter of 1.5 mm = 0.15 cm and the following Freundlich adsorption isotherm for C at 25°C: $q = 10\,c^{0.564}$ where q = mg C adsorbed/g carbon and c = mg C/L solution.
Sherwood number = 30. Particle external surface area = 5 m^2/kg.
Assumptions: Mass-transfer resistance in the pores is negligible compared to the external resistance.

Find: For an effluent of 0.01 mg C/L,

(a) Minimum amount of adsorbent needed per liter of feed solution.

(b) For batch mode with twice the minimum amount of adsorbent, the contact time.

(c) For continuous mode with twice the minimum amount of adsorbent, the required residence time.

(d) For semicontinuous mode at a feed rate of 50 gpm and a liquid residence time of 1.5 times that in Part (c), the amount of activated carbon to give a reasonable vol% solids in the tank and run time of not less than 10 times the liquid residence time.

Analysis: (a) The minimum amount of adsorbent corresponds to equilibrium with a solution of the effluent concentration of 0.01 mg TCE/L. From the Freundlich equation, the equilibrium loading is given by: $q = 10(0.01)^{0.564} = 0.745$ mg C/g carbon.
By material balance on the C, $c_F\,Q = c_{final}\,Q + q\,S_{min}$
Solving for S_{min}, for a basis of 1 L of solution,

$$S_{min} = \frac{Q\left(c_F - c_{final}\right)}{q} = \frac{1.0(0.223-0.01)}{0.745} = 0.286 \text{ g carbon/L solution}$$

(b) For batch mode, use 2(0.286) = 0.572 g carbon/L solution = 0.572 kg/m^3 = S/Q
Combining Eqs. (15-77), (15-78), and (15-79), to eliminate q and c^*,

$$-\frac{dc}{dt} = k_L a\left\{c - \left[\frac{Q(c_F - c)}{Sk}\right]^n\right\} = k_L a\left\{c - \left[\frac{(0.223-c)}{(0.572)(10)}\right]^{1/0.564}\right\} = k_L a\left\{c - \left[\frac{(0.223-c)}{5.72}\right]^{1.773}\right\} \quad (1)$$

From Eq. (15-65), k_L in cm/s = $N_{Sh}\,D_i/D_p = 30\,D_i/0.15 = 200\,D_i$ (in cm^2/s)
From the Wilke-Chang Eq. (3-39),

$$D_{A,B} = \frac{7.4\times10^{-8}\left(\phi_B M_B\right)^{1/2} T}{\mu_B v_A^{0.6}} \quad (2)$$

Exercise 15.23 (continued)

Analysis: (b) (continued)

From Table 3.2, $\upsilon_A = \upsilon_{TCE} = 14.8 + 3.7 + 3(21.6) = 83.3 \times 10^{-3}$ m^3/kmol = 83.3 cm^3/mol
Solvent water viscosity at 25°C = 0.94 cP, $M_B = 18$, and $\phi_B = 2.6$. Substitution into Eq. (2) gives,

$$D_{A,B} = \frac{7.4\times10^{-8}(2.6\times18)^{1/2}298}{0.94(83.3)^{0.6}} = 1.13\times10^{-5}\ \text{cm}^2/\text{s} = D_i$$

Therefore, $k_L = 200(1.13 \times 10^{-5}) = 0.00226$ cm/s
The units of a in Eq. (1) are cm^2 of external surface area of adsorbent/ cm^3 of solution.
Therefore, $a = 5$ m^2/kg (S/Q) = 5(0.572) = 2.86 m^2/m^3 of solution = 0.0286 cm^2/cm^3.
Therefore, $k_L a = 0.00226(0.0286) = 6.46 \times 10^{-5}$ s^{-1}
Eq. (1) becomes:

$$-\frac{dc}{dt} = 6.46\times10^{-5}\left\{c - \left[\frac{(0.223-c)}{5.72}\right]^{1.773}\right\}$$ where c is in mg C/L solution, and t is in seconds.

This equation represents an initial value problem in ODEs, which can be solved by the Euler method using a spreadsheet if a small time step is taken. The Euler form, where j is the iteration number, is,

$$c^{(j+1)} = c^{(j)} - (\Delta t)\ 6.46\times10^{-5}\left\{c^{(j)} - \left[\frac{(0.223-c^{(j)})}{5.72}\right]^{1.773}\right\} \qquad (3)$$

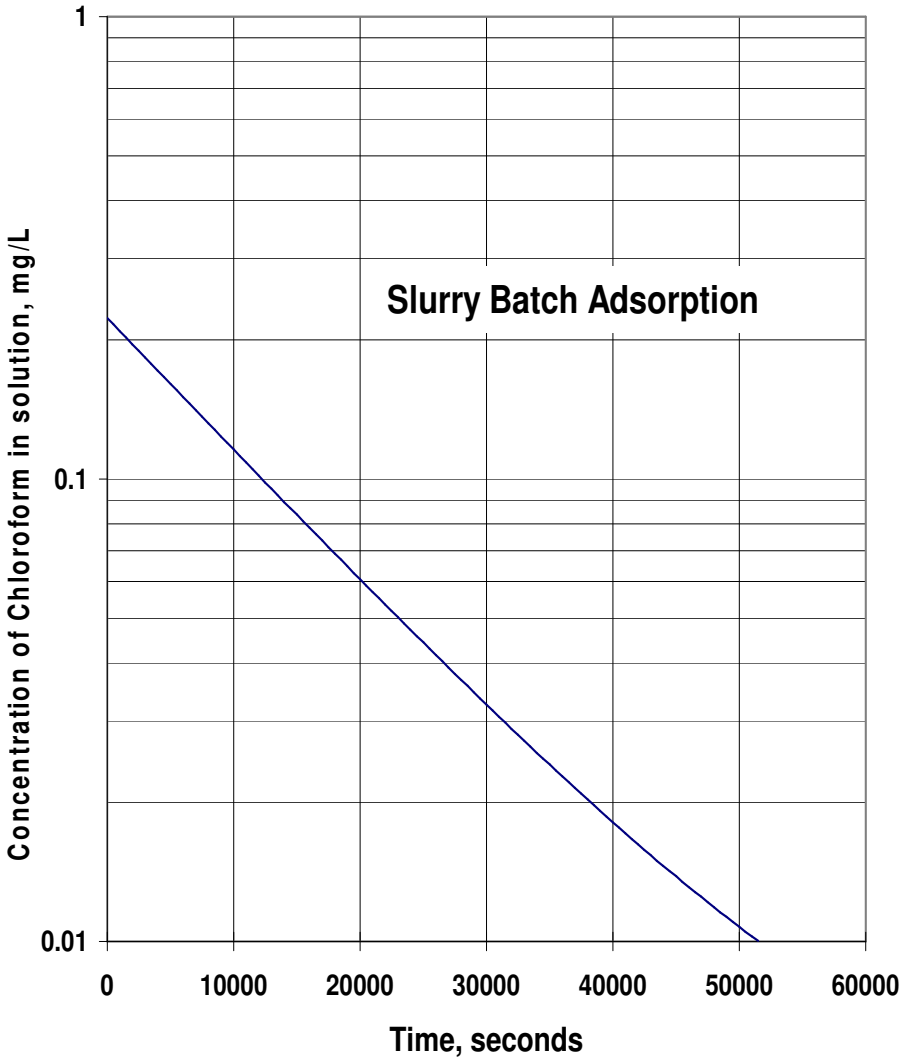
If a time step, Δt, of 500 s is used to find the time when c becomes 0.01 mg/L, the first 10 values of c are as follows:

Time, s	c of C, mg/L
0	0.223
500	0.216
1000	0.209
1500	0.202
2000	0.196
2500	0.189
3000	0.183
3500	0.177
4000	0.172
4500	0.166
5000	0.161

The time required is found to be 51,500 s = 858 minutes = 14.3 h. A plot of c vs. t is given on the next page, where semi-log coordinates gives almost a straight line.

Exercise 15.23 (continued)

Analysis: (b) (continued)



Exercise 15.23 (continued)

Analysis: (continued)

(c) For continuous slurry adsorption, assume a solution feed rate, Q, of 1 L/h. Therefore, the adsorbent feed rate, from Part (a) = S = 2(0.286) = 0.572 g carbon/h. A rearrangement of Eq. (15-86) gives the residence time as:

$$t_{\text{res}} = \frac{c_F - c_{\text{out}}}{k_L a\left(c_{\text{out}} - c^*\right)} = \frac{0.223 - 0.01}{6.46\times10^{-5}\left(0.01 - c^*\right)} \qquad (4)$$

The quantity c^* is the ficticious concentration in equilibrium with q_{out}, which is obtained by material balance, Eq. (15-87), which after rearrangement is:

$$q_{\text{out}} = \frac{Q\left(c_F - c_{\text{out}}\right)}{S} = \frac{1(0.223 - 0.01)}{0.572} = 0.372 \text{ mg/g}$$

Then, from a rearrangement of the given Freundlich adsorption isotherm,

$$c^* = \left(\frac{q_{\text{out}}}{10}\right)^{1/0.564} = \left(\frac{0.372}{10}\right)^{1.773} = 0.00292 \text{ mg/L}$$

Substitution into Eq. (4) gives,

$$t_{\text{res}} = \frac{0.223 - 0.01}{6.46\times10^{-5}\left(0.01 - 0.00293\right)} = 466{,}000 \text{ s} = 7{,}770 \text{ minutes} = 130 \text{ h} = 5.4 \text{ days}.$$

This is a large residence time compared to the batch time in Part (b).

(d) Semicontinuous mode.

Average residence time of the solution in the tank = 1.5(7,700) = 11,600 min.

Flow rate of the solution = 50 gal/min or 50(3.785) = 189 L/min.

The volume of solution in the tank = 189(11,600) = 2,190,000 L or 2,200 m^3.

For a cylindrical tank with height = diameter, this gives a tank diameter of 14.1 m, which is probably impractical, although many smaller tanks in parallel could be used.

In the tank, where the solid adsorbent charge resides, the variation of the loading, q, with run time is given by Eq. (15-91), which for time in minutes is,

$$S\frac{dq}{dt} = k_L a\left(c_{\text{out}} - c^*\right)t_{\text{res}}Q = 6.46\times10^{-5}(60)\left(c_{\text{out}} - c^*\right)(11{,}600)(189) = 8{,}500\left(c_{\text{out}} - c^*\right) \qquad (5)$$

where S is in g, q is in mg C/g, and t is in min.

From Eq. (15-86),

$$c_{\text{out}} = \frac{c_F + k_L a t_{\text{res}} c^*}{1 + k_L a t_{\text{res}}} = \frac{0.223 + 6.46\times10^{-5}(60)(11{,}600)c^*}{1 + 6.46\times10^{-5}(60)(11{,}600)} = 0.00485 + 0.97826c^* \qquad (6)$$

Exercise 15.23 (continued)

Analysis: (d) (continued)

From the given Freundlich equation, $c^* = (q/10)^{1.773}$ $= 0.01687\ q^{1.773}$ (7)

Combining Eqs. (5), (6), and (7), gives,

$$S\frac{dq}{dt} = 8{,}500\left(0.00485 + 0.97826c^* - c^*\right) = 41.2 - 184.79c^* = 41.2 - 3.12q^{1.773} \quad (8)$$

Let the volume of solids in the tank = 2.5 vol%. The solids-free volume of liquid in the tank = 2,200 m^3. Therefore, the solids volume = (2.5/97.5)(2,200) =56.4 m^3. Assume a particle density = 850 kg/m^3. Therefore, S = 56.4 (850) = 48,000 kg = 4.8 x 10^7 g and Eq. (8) becomes,

$$\frac{dq}{dt} = 8.58\times10^{-7} - 6.5\times10^{-8}q^{1.773} \quad (9)$$

Now, compute the run time to achieve a cumulative c_{out} = 0.01 mg/L, where,

$$c_{cum} = 0.01 = \frac{\int_0^t c_{out}\,dt}{t} \quad (10)$$

Eq. (9) represents an initial value problem in ODEs, which can be solved by the Euler method using a spreadsheet, if a small time step is taken. The Euler form, with j as the iteration index, is,

$$q^{(j+1)} = q^{(j)} + (\Delta t)\left[8.58\times10^{-7} - 6.5\times10^{-8}\left(q^{1.773}\right)^{(j)}\right] \quad (11)$$

The total run time is specified to be not less than 10 times the average liquid residence time; thus, 10(7,770) = 77,700 minutes. Try a Δt of 25,000 minutes. From the spreadsheet, the first 6 and last 6 values are:

t, min.	q, mg/g	c^*, mg/L	c out	c cum
0	0	0	0.00485	0
25,000	0.0215	1.86E-05	0.00487	0.00486
50,000	0.0429	6.34E-05	0.00491	0.00487
75,000	0.0643	0.000130	0.00498	0.00490
100,000	0.0858	0.000217	0.00506	0.00493
125,000	0.1072	0.000322	0.00516	0.00497
975,000	0.8208	0.011887	0.01648	0.00910
1,000,000	0.8411	0.012413	0.01699	0.00929
1,025,000	0.8614	0.012948	0.01752	0.00949
1,050,000	0.8816	0.013491	0.01805	0.00968
1,075,000	0.9017	0.014043	0.01859	0.00988
1,100,000	0.9218	0.014602	0.01913	0.01009

By interpolation, the run time is 1,090,000 minutes (757 days), which is greater than the above 77,700 minutes. Unfortunately, the vessel size is very large.

Exercise 15.24

Subject: Use of three beds in a cycle to adsorb 1,2-dichloroethane from water, with application of the MTZ concept.

Given: Three fixed-bed adsorbers, each containing 10,000 lb of activated carbon of $\rho_b = 30$ lb/ft^3, to be used to reduce the concentration of 1,2-dichloroethane (D) in 250 gpm of water from 4.6 mg/L to 0.001 mg/L. Each bed has an $H/D = 2$. Two beds in series for adsorption (a lead bed and a trailing bed). One bed being regenerated by replacing the spent carbon. When the lead bed is saturated, it is regenerated, the trailing bed becomes the lead bed, and the regenerated bed becomes the trailing bed. The adsorption equilibrium isotherm is $q = 8\ c^{0.57}$, with q in mg/g and c in mg/L.

Assumptions: Constant pattern front so that the width of the MTZ is a constant.

Find: How often must the carbon in a bed be replaced. The maximum width of the MTZ to allow saturation of the lead bed.

Analysis: Volume of each bed = V = mass of carbon/ρ_b = 10,000/30 = 333 ft^3

For $H = 2D$, $V = 333 = \pi D^3/2$. Solving, $D = 6.0$ ft and $H = 2(6) = 12.0$ ft.

For ideal equilibrium adsorption from Eq. (15-92), the time for the ideal wave front to move through one of the three beds is $t_b = \dfrac{q_F S}{Q_F c_F}$ (1)

From the adsorption isotherm, the loading in equilbrium with the feed = $q_F = 8\ c_F^{0.57} = 8(4.6)^{0.57}$ = 19.1 mg/g. The grams of adsorbent in each bed = S = 10,000(453.6) = 4,536,000 g

The volumetric feed rate = Q_F = 250(3.785) = 946 L/min, and c_F = 4.6 mg/L

Therefore, from Eq. (1), $t_b = \dfrac{19.1(4{,}536{,}000)}{946(4.6)} = 19{,}900$ minutes = 332 hours = 13.8 days

The lead bed must be replaced every 13.8 days. The width of the MTZ zone can not exceed the height of a bed or 12 ft. Otherwise, breakthrough will occur before the trailing bed becomes the lead bed.

Exercise 15.25

Subject: Use of three or more beds in a cycle to adsorb benzene and m-xylene from water, with application of the MTZ concept.

Given: Three fixed-bed adsorbers, each containing 10,000 lb of activated carbon of $\rho_b = 30$ lb/ft^3, to be used to remove 0.185 mg/L of benzene (B) and 0.583 mg/L of m-xylene (X) from 250 gpm of water. Each bed has an $H/D = 2$. Two or more beds in series for adsorption (at least a lead bed and a trailing bed). One bed being regenerated by replacing the spent carbon. When the lead bed is saturated, it is regenerated, the trailing bed becomes the lead bed, and the regenerated bed becomes the trailing bed. The adsorption equilibrium isotherms are: $q_B = 32\ c_B^{0.428}$ and $q_X = 125\ c_X^{0.333}$, with q in mg/g and c in mg/L. Widths of the mass-transfer zones are $MTZ_B = 2.5$ ft and $MTZ_X = 4.8$ ft.

Assumptions: Constant pattern front so that the widths of the MTZs are constant.

Find: How often must the carbon in a bed be replaced.

Analysis: Volume of each bed = V = mass of carbon/ρ_b = 10,000/30 = 333 ft^3

For $H = 2D$, $V = 333 = \pi D^3/2$. Solving, $D = 6.0$ ft and $H = 2(6) = 12.0$ ft.

For ideal equilibrium adsorption from Eq. (15-92), the time for the ideal wave front to move through one of the three beds for one of the solutes is: $t_b = \dfrac{q_F S}{Q_F c_F}$ (1)

From the adsorption isotherm of B. the loading in equilbrium with the feed = $q_F = 32\ c_F^{0.428} = 32(0.185)^{0.428} = 15.5$ mg/g.

From the adsorption isotherm of X. the loading in equilbrium with the feed = $q_F = 125\ c_F^{0.333} = 125(0.583)^{0.333} = 104.4$ mg/g.

The grams of adsorbent in each bed = S = 10,000(453.6) = 4,536,000 g

The volumetric feed rate = Q_F = 250(3.785) = 946 L/min.

For benzene, with $c_F = 0.185$ mg/L, and

from Eq. (1), $t_b = \dfrac{15.5(4{,}536{,}000)}{946(0.185)} = 402{,}000$ minutes = 6,700 hours = 279 days

For m-xylene, with $c_F = 0.583$ mg/L, and

from Eq. (1), $t_b = \dfrac{104.4(4{,}536{,}000)}{946(0.583)} = 859{,}000$ minutes = 14,300 hours = 596 days

So, benzene controls. A satisfactory bed arrangement is to use two beds in series for adsorption with a time of 279 days to change the beds. Because the MTZs are less than the bed height of 12 ft, no breakthrough will occur. The lead bed will become saturated with benzene but not with m-xylene.

Exercise 15.26

Subject: Comparison of equilibrium model to mass-transfer model for fixed-bed adsorption of water vapor from air with silica gel.

Given: Feed of air with a relative humidity of 80% at 80°F and 1 atm, with a superficial velocity of 100 ft/min in a fixed bed of 2.8-mm-diameter spherical particles of silica gel (ρ_b = 39 lb/ft^3). Bed height = H = 5 ft. Linear adsorption isotherm for water vapor = q = 15.9 p, where q is in lb H_2O/lb gel, and p = partial pressure of water vapor in atm. Effective diffusivity of water vapor in the adsorbent particle = 0.05 cm^2/s. Exit humidity of water vapor to be 0.0009 lb H_2O/lb dry air.

Assumptions: Isothermal and isobaric operation.

Find: Time to breakthrough for the equilibrium model.
Time to breakthrough for the mass-transfer model of Klinkenberg.
Set of breakthrough curves for the mass-transfer model of Klinkenberg.
Approximate width of the MTZ.
Average loading of the bed at breakthrough.

Analysis: First determine the moisture content of the entering air. From a psychrometric chart, the entering humidity for 80% R.H., 80°F, and 1 atm is 0.0177 lb H_2O/lb dry air or a water vapor content of 0.0177/1.0177 x 100% = 1.739 wt%. By Dalton's law, partial pressure of water vapor in the entering air = (1)[0.0177/18.02]/[0.0177/18.02 + 1/28.97] = 0.0277 atm. The mole fraction of water vapor in the entering air = 0.0277.
Assume a bed cross-sectional area of 1 ft^2. Then, entering gas rate = 100 ft^3/min. Bed volume = (1)(5) = 5 ft^3. Bed contains 5(39) = 195 lb silica gel.
The MW of the entering gas = 18.02(0.0277) + 28.97(0.9723) = 28.67.
From the ideal gas law, density of entering gas = PM/RT = (1)(28.67)/[(0.7302)(540)] = 0.0727 lb/ft^3. Therefore, the entering gas flow rate = 100(0.0727) = 7.27 lb/min with a water vapor flow rate of 0.01739(7.27) = 0.1264 lb H_2O/min. For the dilute conditions, the desired c/c_F = 0.0009/0.0177 = 0.05. So use this as the breakthrough value.
Equilibrium model: Equilibrium loading based on entering feed = 15.9(0.0277) = 0.440 lb H_2O/lb silica gel.
Therefore, can adsorb 0.440(195) = 85.8 lb H_2O. The ideal time for breakthrough = 85.8/0.1264 = 679 min = 11.3 h.

Alternatively, can apply Eq. (15-92), with L_{ideal}/L_B = 1, so $t_{ideal} = \dfrac{q_F S}{Q_F c_F} = \dfrac{0.440(195)}{0.1264} = 679 \text{ min.}$

Mass-transfer model using Klinkenberg equations:

From Eq. (15-106), $$\frac{1}{kK} = \frac{R_p}{3k_c} + \frac{R_p^2}{15D_e} \qquad (1)$$

R_p = 0.28/2 = 0.14 cm = 0.0014 m, D_e = 0.05 cm^2/s = 5 x 10^{-6} m^2/s

Exercise 15.26 (continued)

Analysis: (continued)

From Eq. (15-65), $k_c = \frac{D_i}{D_p}\left[2 + 1.1\left(\frac{D_p G}{\mu}\right)^{0.6}\left(\frac{\mu}{\rho D_i}\right)^{1/3}\right]$ (2)

From Perry's Handbook, at 32°F, the diffusivity of water vapor in air at 1 atm = 0.22 cm^2/s.
From Eq. (3-36), the diffusivity is proportional to T to the 1.75 power. Therefore,
$D_i = 0.22[(80 + 460)/(32 + 460)]^{1.75} = 0.26$ $cm^2/s = 0.26 \times 10^{-4}$ m^2/s.
From above, $\rho = 0.0727$ lb/ft^3 = 1.16 kg/m^3.
From a handbook, μ of air at 80°F = 1.75×10^{-5} kg/m-s.
The mass velocity = G = 7.29/1.0 = 7.27 lb/min-ft^2 = 0.592 kg/m^2-s

$$N_{Sc} = \frac{\mu}{\rho D_i} = \frac{1.75\times10^{-5}}{1.16(0.26\times10^{-4})} = 0.580$$

$$N_{Re} = \frac{D_p G}{\mu} = \frac{0.0028(0.592)}{1.75\times10^{-5}} = 94.7$$

From Eq. (2), $k_c = \frac{0.26\times10^{-4}}{0.0028}\left[2 + 1.1(94.7)^{0.6}(0.58)^{1/3}\right] = 0.149$ m/s

From Eq. (1), $\frac{1}{kK} = \frac{0.0014}{3(0.149)} + \frac{(0.0014)^2}{15(0.05\times10^{-4})} = 0.0031 + 0.0261 = 0.0292$ s

The equilibrium constant, K, the given value is 15 lb H_2O/lb gel-atm. We need to convert this to units of (lb H_2O/ft^3 gel)/(lb H_2O/ft^3 gas).
From Table 15.2, assume small-pore silica gel with $\varepsilon_b = 0.47$. Therefore, the particle density from a rearrangement of Eq. (15-4) is $\rho_p = \frac{\rho_b}{1-\varepsilon_b} = \frac{39}{(1-0.47)} = 73.6$ lb gel/ft^3 of particles.

When the partial pressure of H_2O = 0.0277 atm, we have 0.1264/100 = 0.001264 lb H_2O/ft^3 gas.
Therefore, K = 15(73.6)(0.0277)/0.001264 = 24,200. The equilibrium adsorption isotherm is now, q in lb H_2O/ft^3 silica gel particles = 24,200 c in lb H_2O/ft^3 gas
From above, k = 1/[0.0292 K] = 1/[0.0292(24,200)] = 1.42×10^{-3} s^{-1} or 0.0849 min^{-1}

The Klinkenberg Eq. (15-114) is: $\frac{c}{c_F} \approx \frac{1}{2}\left[1 + \left(\sqrt{\tau} - \sqrt{\xi} + \frac{1}{8\sqrt{\tau}} + \frac{1}{8\sqrt{\xi}}\right)\right]$ (3)

where, from Eq. (15-115), $\xi = \frac{kKz}{u}\left(\frac{1-\varepsilon_b}{\varepsilon_b}\right)$ (4)

u = actual (interstitial velocity) = superficial velocity/ε_b = 100/0.47 = 213 ft/min = 1.08 m/s

From Eq. (4), $\xi = \frac{\left(\frac{1}{0.0292}\right)z}{1.08}\left(\frac{1-0.47}{0.47}\right) = 35.8z$ (in meters) (5)

Exercise 15.26 (continued)

Analysis: (continued)
From Eq. (15-116),

$$\tau = k\left(t - \frac{z}{u}\right) = 0.0849\left(t - \frac{z}{1.08(60)}\right) = 0.0849t(\text{in minutes}) - 0.00131z(\text{in meters}) \qquad (6)$$

The maximum value of z, the distance through the bed, is the bed height = 5 ft = 1.524 m.
At breakthrough, c/c_F = 0.05 at z = 1.524 m and, therefore, $\xi = 35.8(1.524) = 54.6$
and $\tau = 0.0849t - 0.00131(1.524) = 0.0849t$ (in minutes) - 0.00200

Must solve Eq. (1) for t at c/c_F = 0.05 and ξ= 54.6. The time will be less than the ideal equilibrium time above of 679 minutes. Can do this by trial and error with a spreadsheet or with a nonlinear solver that can handle the error function, erf. From a spreadsheet, breakthrough time = 451 minutes.

To obtain the width of the MTZ, solve Eq. (1) for z at c/c_F = 0.95 and t = 451 minutes. By trial and error from a spreadsheet, at breakthrough, the MTZ extends from z = 0.718 m to z =1.524 m. Therefore, the width of the MTZ = 1.524 - 0.718 = 0.81 m = 2.6 ft.

Breakthrough curves similar to Figs. 15.30 and 15.31, but in terms of distance, z, through the bed and time, instead of the dimensionless groups, ξ and τ, are shown on the next two pages. They are computed with a spreadsheet from Eq. (3) above for gas concentration and Eq. (15-119) for adsorbent loading, together with Eqs. (5) and (6) to convert from ξ and τ to z and t, respectively. With the spreadsheet, the error function, erf, must be used carefully, noting that erf(-x) = -erf(x). Thus, when the argument of the error function is negative, the argument should be made positive and the result should be multiplied by -1.

To compute the average loading of the bed at the breakthrough time of 451 minutes, use the equation in Example 15.11:

$$\bar{q}_{\text{avg}} = \frac{\int_0^{1.524} \bar{q}\,dz}{1.524} \quad , \text{ where } z \text{ is in meters.} \qquad (7)$$

A spreadsheet is used with Eq. (15-119) to compute $\bar{q}$ as a function of z for t = 451 minutes (breakthrough time) and q_F^* = 0.440 lb H_2O/lb silica gel from above (value in equilibrium with the feed. The results are:

$\bar{q}$, lb/lb	0.440	0.440	0.433	0.382	0.260	0.125	0.042	0.018
z, meters	0.2	0.4	0.6	0.8	1.0	1.2	1.4	1.524

Solving Eq. (7) numerically by the trapezoid method,

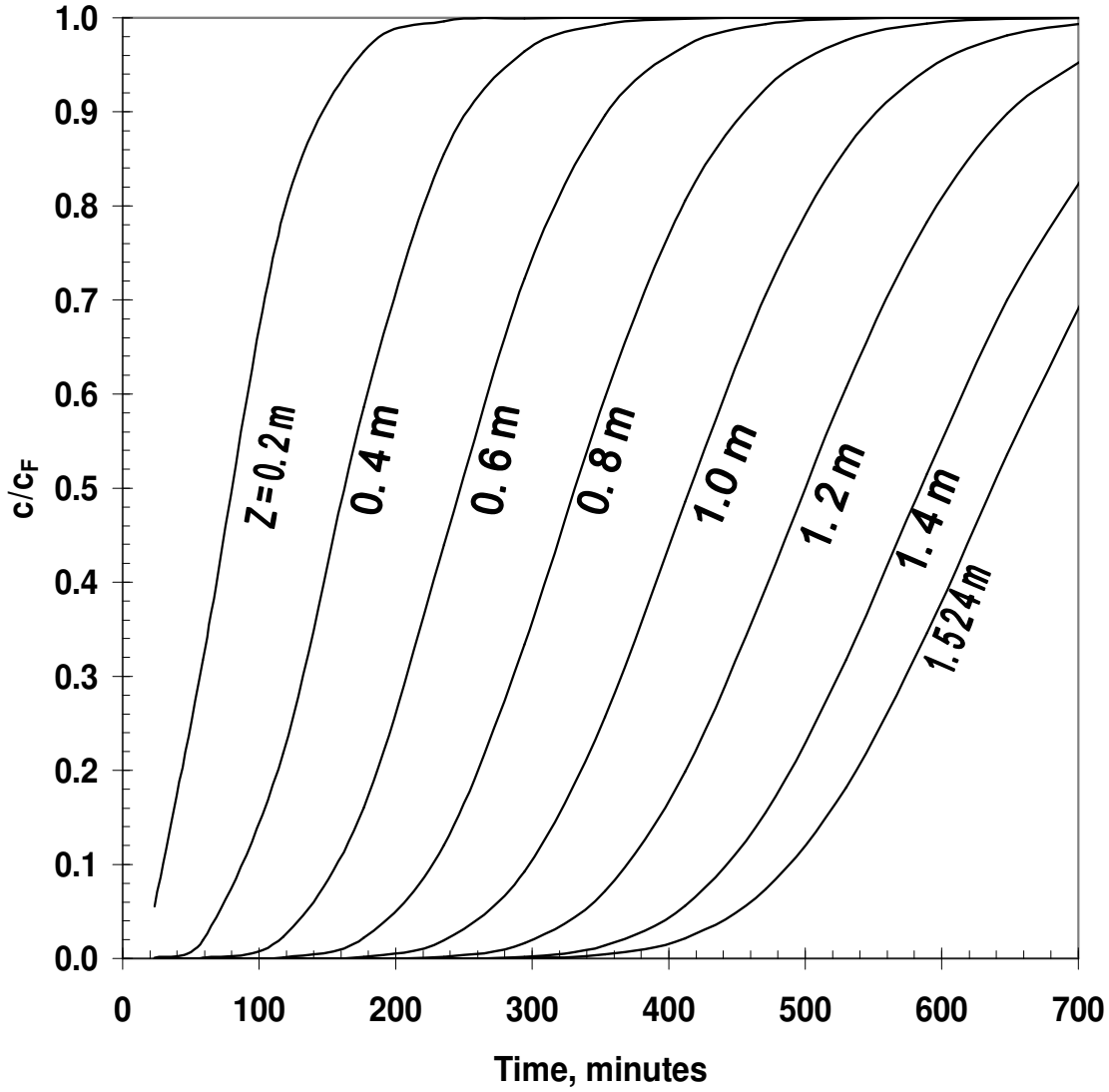
$\bar{q}_{\text{avg}}$ = [0.440(0.2) + 0.440(0.2) + 0.4365(0.2) + 0.4075(0.2) + 0.321(0.2) + 0.1925(0.2) + 0.0835(0.2) + 0.030(0.124)]/1.524 = 0.468/1.524 = 0.307 lb H_2O/lb silica gel.

Thus, 0.307/0.440 x 100% = 70% utilization of the bed.

Exercise 15.26 (continued)

Analysis: (continued)

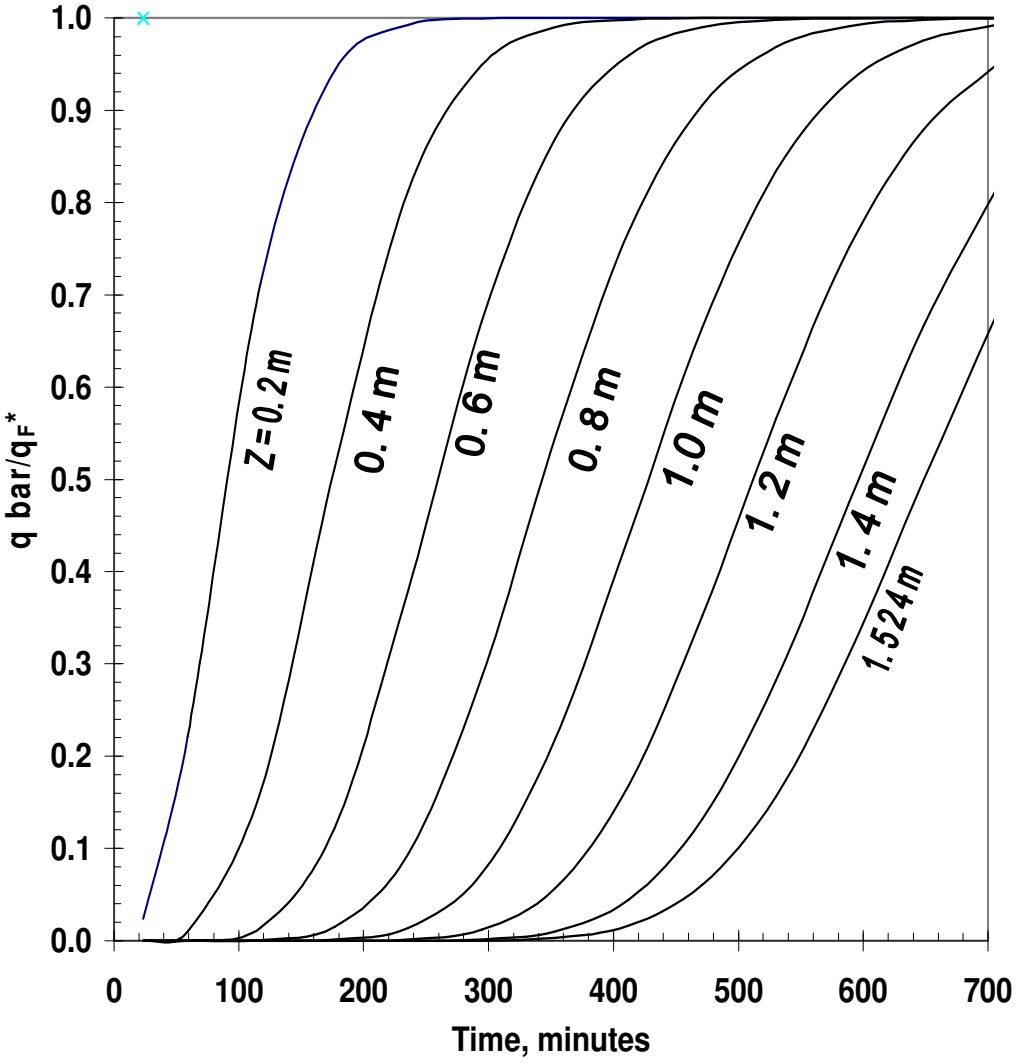
Concentration profiles



Exercise 15.26 (continued)

Analysis: (continued)

Loading Profiles



Exercise 15.27

Subject: Reduction of nitroglycerine (NG) content of wastewater by fixed-bed adsorption with activated carbon in a train of 55-gallon cannisters

Given: Train of four 55-gallon cannisters of activated carbon (ρ_b = 32 lb/ft^3), each with an inside diameter of 2 ft and containing 200 lb of carbon. Flow rate of wastewater = 400 gph with 2,000 ppm (by weight) of NG. When effluent from the first cannister reaches 1 ppm of NG, that cannister is removed and a fresh one added to the end of the train. The following test results are available for one cannister: water flow rate = 10 gpm with 1,020 ppm of NG by weight. Breakthrough time in hours = $t_B = 3.90\,L - 2.05$ for 1ppm NG, with L = bed depth in ft.

Assumptions: Plug flow.

Find: Number of cannisters needed each month. Monthly cannister cost at $700/cannister.

Analysis: Bed volume of activated carbon = 200/32 = 6.25 ft^3 = $V = \pi D^2 L/4$.
Solving for L, with D = 2 ft, gives L = 2 ft.
Rearrange the breakthrough correlation for the test, by solving for L,
$L = t_B/3.90 + 2.05/3.90 = 0.256\,t_B + 0.526$
This is the same form as Eq. (15-120), where the term 0.256 t_B is LES and the term 0.526 is LUB.
Assume that the width of the MTZ = constant, independent of flow rate.
Therefore, LUB is constant at 0.526 ft.
From Eq. (15-122), LES is directly proportional to the feed rate, Q_F. If a linear adsorption isotherm is assumed, then LUB is independent of the ratio q_F/c_F in Eq. (15-122).
That is, for the proposed operation, the higher value of c_F (2,000 ppm compared to 1,020 ppm for the test) is of no consequence. The higher concentration of NG in the feed, c_F, is couterbalanced by the higher loading in equilbrium with the feed, q_F. The breakthrough equation becomes:

$$L = 0.256\left(\frac{Q_F \text{ of operation}}{Q_F \text{ of test}}\right)t_B + 0.526 = 0.256\left(\frac{400}{600}\right)t_B + 0.526 = 0.171\,t_B + 0.526$$

Solving for t_B, with L of operation also equal to 2 ft,

$$t_B = \frac{L - 0.526}{0.171} = 5.86L - 3.08 = 5.86(2) - 3.08 = 8.64 \text{ hours} = 8.64/24 = 0.36 \text{ day}$$

Assume a month of 30 days. Then need 30/0.36 = 84 cannisters per month.

Cost = $700(84) = $58,800/month

Exercise 15.28

Subject: Sizing of fixed-bed adsorption unit for removal of ethyl acetate (EA) from air with activated carbon (C), using adsorption equilibrium isotherm and breakthrough data

Given: Gas feed is 12,000 scfm (60°F and 1 atm) containing 0.5 mol% EA and 99.5 mol% air. Adsorbent is C (ρ_b = 30 lb/ft^3 and d_p = 0.011 ft. Adsorption equilibrium data at 100°F. Breakthrough lab data at a gas superficial velocity of 60 ft/min in a 2-ft high bed at 100°F and 1 atm.

Assumptions: Plug flow.

Find: Diameter and height of carbon bed for a time-to-breakthrough of 8 h, for the same conditions of flow rate, temperature, and pressure as the lab data.

Analysis: Use a continuity equation, similar to Eq. (6-43) to compute the bed diameter:

$$m = u_s A\rho = Q\rho \quad \text{or} \quad A = \frac{\pi D^2}{4} = \frac{Q}{u_s} \qquad (1)$$

At operating conditions, Q = 12,000(560/520) = 12,900 ft^3/min. u_s = 60 ft/min
From Eq. (1), A = 12,900/60 = 215 ft^2. D = [4(215)/3.14]$^{1/2}$ = 16.5 ft.
Use Eq. (15-122) to compute the ideal bed length, LES:

$$\text{LES (in ft)} = \frac{c_F Q_F t_B}{q_F \rho_b A} = \frac{c_F (12{,}900)(8\times 60)}{q_F (30)(215)} = 960\frac{c_F}{q_F} \qquad (2)$$

Want c_F in lb EA/ft^3 inlet gas. MW of EA = 88.1. One scf of gas contains 379 lbmol. Therefore, have 12,000/379 = 31.66 lbmol/min. The mole fraction of EA = 0.005. Concentration of EA in the entering gas of 0.005(31.66)(88.1)/12,900 = 0.00108 lb EA/ft^3 gas.
From the given equilibrium data, for p_{EA} = 0.005 atm, q_F = 0.270 lb EA/lb C.
From Eq. (2),

$$\text{LES} = 960\left(\frac{0.00108}{0.270}\right) = 3.85 \text{ ft}$$

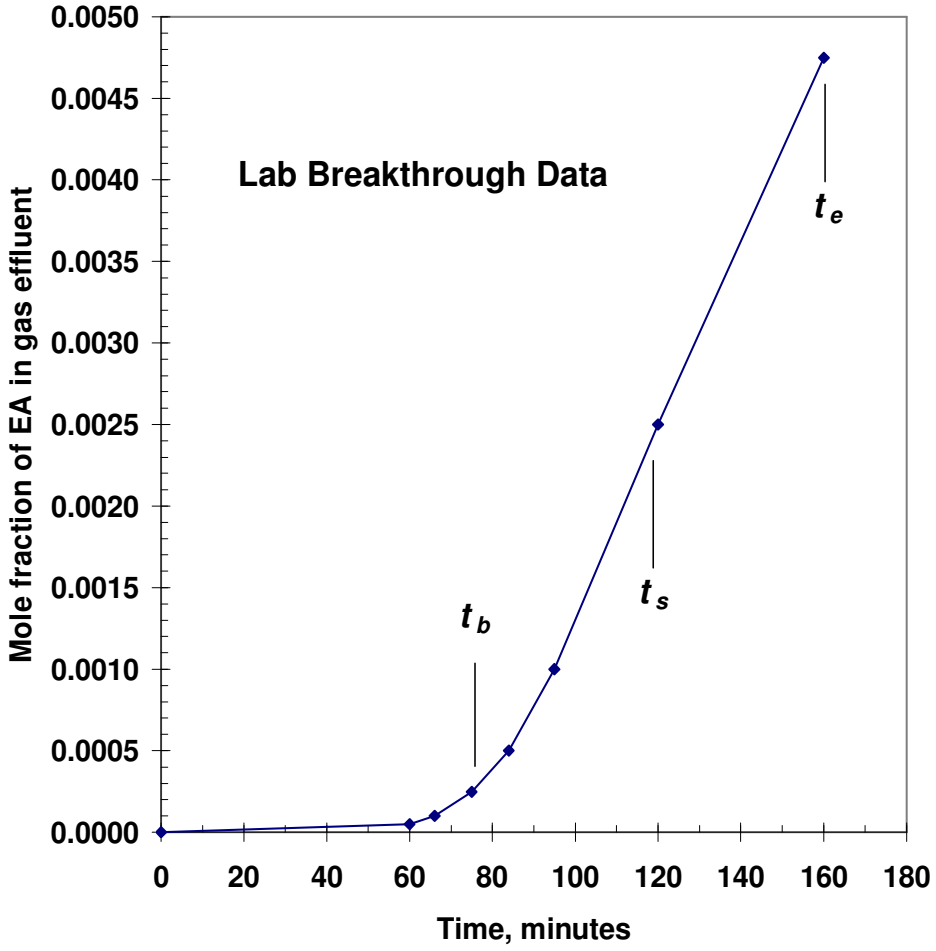
From Eq. (15-120), the required bed length taking into account the MTZ is,
L_B = LES + LUB, where LUB is given by Eq. (15-121).

The breakthrough data for L_e = 2 ft are plotted on the next page as y_{EA} out against time in minutes. The data are almost straight in the mole fraction range of 0.00475 (c/c_F = 0.95), where time = t_e = 160 minutes, to 0.00025 (c/c_F = 0.05), where time = t_b = 75 minutes. Therefore, the midpoint time, t_s = (160 + 75)/2 = 117.5 minutes. Alternatively, t_s can be evaluated by integration, using Eq. (15-123).

From Eq. (15-121), LUB = (t_s - t_b)L_e/t_s = (117.5 - 75)2/117.5 = 0.72 ft.
Therefore, L_B = 3.85 + 0.72 = 4.57 ft. So the bed is 16.5 ft in diameter by 4.57 ft high. This is a poor bed height-to-diameter ratio. Might increase the breakthrough time by a factor of 4 to get a bed height approximately equal to the bed diameter.

Exercise 15.28 (continued)

Analysis: (continued)



Exercise 15.29

Subject: Desorption of benzene from silica gel using air under isothermal, isobaric conditions.

Given: Values are given in a table below for dimensionless benzene concentration, ϕ, and loading, ψ, profiles in a bed following adsorption. Bed is 2 feet in diameter and 30 ft high. Bed contains silica gel adsorbent. Desorption by air at 1 atm and 145°F at an interstitial velocity, u, of 98.5 ft/min. Bed porosity = $\varepsilon_b = 0.5$. During desorption, mass-transfer coefficient = $k = 0.206$ min^{-1} and Henry's law equilibrium adsorption constant = 1,000 in Eq. (1) on p. 837.

Assumptions: Plug flow with a constant interstitial velocity equal to the given inlet value. Negligible axial dispersion. Desorption air is passed up the bed, opposite in direction to the initial flow of benzene-air feed mixture during adsorption.

Find: Desorption time required to remove 90% of the benzene from the bed.

Analysis: First, compute the initial amount of benzene adsorbed in the bed.

Bed volume = $V = \pi D^2 L/4 = 3.14(2)^2(30)/4 = 94.2$ ft^3

Volume of SG particles = $(1-\varepsilon_b)V = (1-0.5)(94.2 = 47.1$ ft^3

During adsorption at 70°F, from Example 15.10, the concentration of benzene in the entering air-benzene mixture = 0.00181 lb benzene/ft^3 = c_F. The adsorbent loading in equilibrium with the feed, as given in Example 15.10, is $q_F^* = 5{,}120\ c_F = 5{,}120(0.00181) = 9.27$ lb benzene/ft^3 of silica gel particles. If the bed were completely saturated with the feed, the benzene in the bed would be 9.27(47.1) = 437 lb benzene. If the breakthrough occurred for c just greater than zero at the given 641 minutes for adsorption (i.e. all of the benzene in the feed were adsorbed), then with a feed flow rate, from Example 15.10, of 310 ft^3/min, the benzene loading would be:

310(641)(0.00181) = 360 lb benzene, which, as expected, is less than complete saturation. However, the breakthrough at 641 minutes corresponds to $\phi = c/c_F = 0.05$ and not at 0. Therefore, it is best to integrate the given loading data at the end of adsorption to obtain a more accurate value of benzene loading. Using the given data on the next page, compute the average value of ψ by numerical integration. Note that because the flow of desorption agent is opposite to the feed gas, the bed distances below are given as $z' = 30$ ft - z.

$$\psi_{avg} = \frac{0.5\psi_{z'=0} + \sum_{z'=1}^{29} \psi_{\text{at } z'} + 0.5\psi_{z'=30}}{30} = \frac{0.022 + 24.079 + 0.500}{30} = 0.820$$

Therefore, the amount of benzene on the adsorbent in the bed at the end of the adsorption period is: 0.820(9.27)(47.1) = 358.0 lb benzene, which is very close to the above rough estimate of 360. The desorption period must be long enough to reduce the loading to (1-0.90)(358) = 35.8 lb benzene.

Exercise 15.29 (continued)

Analysis: (continued)
Given conditions at the beginning of the desorption period:

z, ft	z' = 30 - z, ft	$\phi = c/c_F$	$\psi = q/q_F$*
30	0	0.050	0.044
29	1	0.090	0.081
28	2	0.150	0.137
27	3	0.235	0.217
26	4	0.343	0.321
25	5	0.468	0.444
24	6	0.599	0.575
23	7	0.722	0.701
22	8	0.825	0.808
21	9	0.901	0.890
20	10	0.951	0.944
19	11	0.978	0.975
18	12	0.992	0.990
17	13	0.997	0.997
16	14	0.999	0.999
15	15	1.000	1.000
14 to 0	16 to 30	1.000	1.000

The desorption calculations utilize the following forms of Eqs. (15-123) and (15-124):

$$\frac{\partial\phi}{\partial t} = -u\frac{\partial\phi}{\partial z'} - \left(\frac{1-\varepsilon_b}{\varepsilon_b}\right)kK(\phi-\psi) = -98.5\frac{\partial\phi}{\partial z'} - \left(\frac{1-0.5}{0.5}\right)(0.206)(1{,}000)(\phi-\psi)$$

$$= -98.5\frac{\partial\phi}{\partial z'} - 206(\phi-\psi) \qquad (1)$$

$$\frac{\partial\psi}{\partial t} = 0.206(\phi-\psi) \qquad (2)$$

Conditions for ϕ and ψ at $t = 0$ are given as a function of z' in the above table.
Condition for ϕ at $z' = 0$ is 0 because the desorption gas contains no benzene.

Equations (1) and (2) can be solved for $\phi\{t,z'\}$ and $\psi\{t,z'\}$ for $z' = 0$ to 30 ft and $t > 0$ by various means, including:
(1) A FORTRAN code similar to that on for Example 15-13, with the method of lines and a stiff integrator in connection with Eqs. (15-127) to (15-133).
(2) Use of the windows code PDESOL (www.pdesol.com), which also utilizes the method lines in connection with a number of different integrators and discretization schemes for $\frac{\partial\phi}{\partial z'}$.

Exercise 15.29 (continued)

Analysis: (continued)

(3) Use of a spreadsheet with a finite-difference method where backward differences are used for $\frac{\partial \phi}{\partial z'}$ and an Euler predictor-corrector method is used for the time derivatives, as discussed by D. D. Fry, Chem. Eng. Education, Fall 1990, pp 204-207.

The PDESOL program is particularly convenient and easy to use, and was applied to this exercise. The solution method selected from the many options provided by PDESOL was the same as that described for TSA. Thus, the method of lines was used with Eqs. (15-127) and (15-128). The $\frac{\partial \phi}{\partial z'}$ derivative was approximated by a 5-point, biased, upwind, finite-difference approximation, and a stiff integrator, LODES, was used on the resulting system of ODEs with time derivatives of ϕ and ψ. To obtain accuracy, 121 grid points were used over the 30 ft length for the spatial domain in z'. For the time domain, an arbitrary 800 minutes was chosen for the final time of desorption, with an output as a function of z' every 50 minutes. The initial conditions for ϕ and ψ, given in the table above were inputted as text files, which were interpolated by PDESOL to obtain values for the 121 grid points.

The resulting PDE program equations were as follows, where the symbols ϕ and ψ were replaced by c and q, respectfully, and z' was replaced by x, with xL =0 and xU = 30 ft.

```
c_x = dxu(c,1)          'Uses the 5-point, biased, upwind finite difference approximation
c_t = -98.5*c_x - 206*(c - q)
q_t = 0.206*(c - q)
c@xL = 0
c@t0 = lintc("c_init.txt",x)    'Calls the file c_init.txt for the initial values of c
q@t0 = lintc("q_init.txt",x)    'Calls the file q_init.txt for the initial values of q
```

The form of the two .txt files were as follows, using the above table:

c_init.txt

x	c at t = 0
0	0.050
1	0.090
2	0.150
3	0.235
4	0.343
etc.	etc.
etc.	etc.
15	1.000
30	1.000

q_init.txt

x	q at t = 0
0	0.044
1	0.081
2	0.137
3	0.217
4	0.321
etc.	etc.
etc.	etc.
15	1.000
30	1.000

Exercise 15.29 (continued)

Analysis: (continued)

The results of the calculations are given in the following tables and graphs, in increments of 50 minutes, where by 400 minutes the fronts have almost left the bed, indicating that the desorption time is less than 400 minutes.

Profiles for $\phi = c/c_F$ during desorption:

x = z', ft	c = ϕ at t = 0 minutes	c = ϕ at t = 50 minutes	c = ϕ at t = 100 minutes	c = ϕ at t = 150 minutes	c = ϕ at t = 200 minutes	c = ϕ at t = 250 minutes	c = ϕ at t = 300 minutes	c = ϕ at t = 350 minutes	c = ϕ at t = 400 minutes
0	0.0500	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
1	0.0900	0.0006	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2	0.1500	0.0032	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
3	0.2350	0.0108	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
4	0.3430	0.0271	0.0007	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
5	0.4680	0.0551	0.0024	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
6	0.5990	0.0975	0.0064	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000
7	0.7220	0.1559	0.0147	0.0005	0.0000	0.0000	0.0000	0.0000	0.0000
8	0.8250	0.2312	0.0295	0.0015	0.0000	0.0000	0.0000	0.0000	0.0000
9	0.9010	0.3217	0.0531	0.0038	0.0001	0.0000	0.0000	0.0000	0.0000
10	0.9510	0.4234	0.0879	0.0082	0.0004	0.0000	0.0000	0.0000	0.0000
11	0.9780	0.5300	0.1354	0.0162	0.0009	0.0000	0.0000	0.0000	0.0000
12	0.9920	0.6341	0.1964	0.0295	0.0022	0.0001	0.0000	0.0000	0.0000
13	0.9970	0.7287	0.2701	0.0498	0.0047	0.0002	0.0000	0.0000	0.0000
14	0.9990	0.8087	0.3543	0.0788	0.0091	0.0006	0.0000	0.0000	0.0000
15	1.0000	0.8719	0.4451	0.1181	0.0166	0.0013	0.0001	0.0000	0.0000
16	1.0000	0.9185	0.5379	0.1682	0.0284	0.0027	0.0001	0.0000	0.0000
17	1.0000	0.9507	0.6277	0.2292	0.0459	0.0052	0.0003	0.0000	0.0000
18	1.0000	0.9716	0.7103	0.2997	0.0704	0.0095	0.0008	0.0000	0.0000
19	1.0000	0.9844	0.7824	0.3776	0.1032	0.0163	0.0015	0.0001	0.0000
20	1.0000	0.9918	0.8423	0.4597	0.1450	0.0267	0.0030	0.0002	0.0000
21	1.0000	0.9959	0.8897	0.5427	0.1960	0.0418	0.0054	0.0004	0.0000
22	1.0000	0.9980	0.9255	0.6229	0.2557	0.0627	0.0094	0.0009	0.0001
23	1.0000	0.9991	0.9514	0.6974	0.3228	0.0904	0.0156	0.0017	0.0001
24	1.0000	0.9996	0.9694	0.7637	0.3952	0.1256	0.0248	0.0031	0.0003
25	1.0000	0.9998	0.9813	0.8206	0.4706	0.1688	0.0379	0.0055	0.0005
26	1.0000	0.9999	0.9890	0.8675	0.5462	0.2197	0.0558	0.0091	0.0010
27	1.0000	1.0000	0.9937	0.9048	0.6194	0.2776	0.0793	0.0147	0.0018
28	1.0000	1.0000	0.9965	0.9335	0.6878	0.3414	0.1093	0.0228	0.0032
29	1.0000	1.0000	0.9981	0.9544	0.7492	0.4094	0.1464	0.0344	0.0054
30	1.0000	1.0000	0.9989	0.9692	0.8023	0.4792	0.1909	0.0505	0.0090

Exercise 15.29 (continued)

Analysis: (continued)

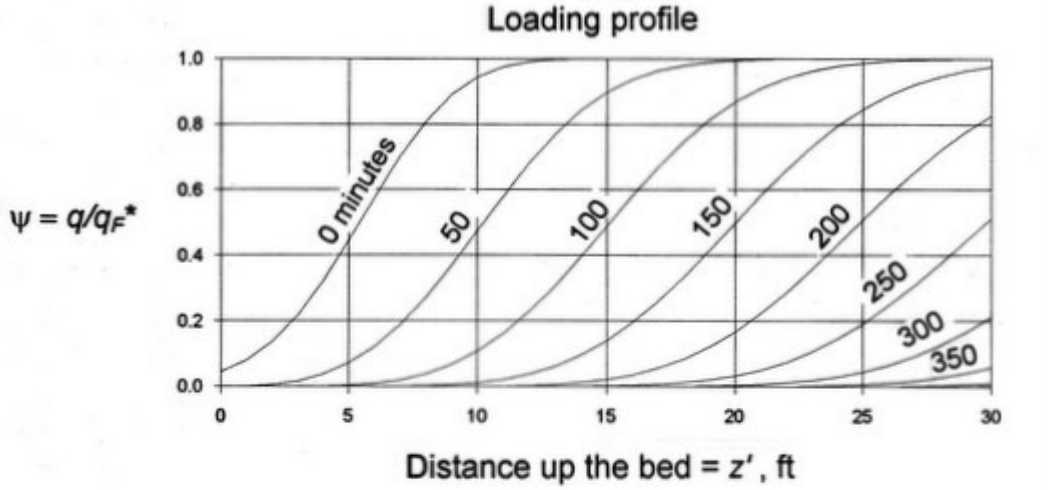
Profiles for $\psi = q/q_F^*$ during desorption:

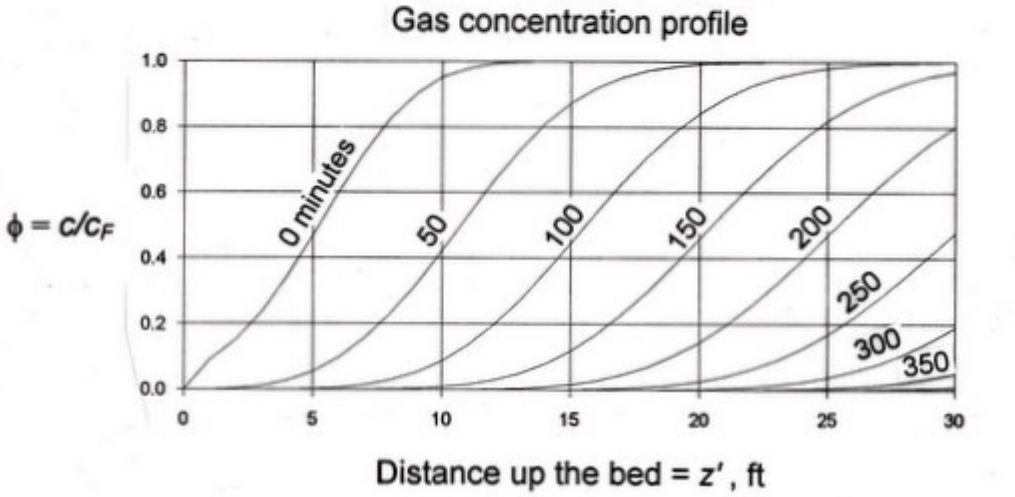
x = z', ft	q = ψ at t = 0 minutes	q = ψ at t = 50 minutes	q = ψ at t = 100 minutes	q = ψ at t = 150 minutes	q = ψ at t = 200 minutes	q = ψ at t = 250 minutes	q = ψ at t = 300 minutes	q = ψ at t = 350 minutes	q = ψ at t =400 minutes
0	0.0440	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
1	0.0810	0.0011	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2	0.1370	0.0053	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
3	0.2170	0.0162	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
4	0.3210	0.0374	0.0011	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
5	0.4440	0.0718	0.0036	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
6	0.5750	0.1214	0.0092	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000
7	0.7010	0.1879	0.0200	0.0008	0.0000	0.0000	0.0000	0.0000	0.0000
8	0.8080	0.2710	0.0384	0.0022	0.0001	0.0000	0.0000	0.0000	0.0000
9	0.8900	0.3680	0.0669	0.0053	0.0002	0.0000	0.0000	0.0000	0.0000
10	0.9440	0.4737	0.1074	0.0111	0.0005	0.0000	0.0000	0.0000	0.0000
11	0.9750	0.5809	0.1614	0.0212	0.0013	0.0000	0.0000	0.0000	0.0000
12	0.9900	0.6820	0.2287	0.0374	0.0030	0.0001	0.0000	0.0000	0.0000
13	0.9970	0.7707	0.3081	0.0614	0.0062	0.0003	0.0000	0.0000	0.0000
14	0.9990	0.8430	0.3964	0.0951	0.0119	0.0008	0.0000	0.0000	0.0000
15	1.0000	0.8980	0.4893	0.1394	0.0211	0.0018	0.0001	0.0000	0.0000
16	1.0000	0.9371	0.5819	0.1948	0.0353	0.0036	0.0002	0.0000	0.0000
17	1.0000	0.9631	0.6692	0.2607	0.0558	0.0067	0.0005	0.0000	0.0000
18	1.0000	0.9794	0.7475	0.3354	0.0840	0.0120	0.0010	0.0001	0.0000
19	1.0000	0.9891	0.8140	0.4160	0.1210	0.0203	0.0020	0.0001	0.0000
20	1.0000	0.9944	0.8679	0.4994	0.1672	0.0327	0.0039	0.0003	0.0000
21	1.0000	0.9973	0.9095	0.5819	0.2226	0.0503	0.0069	0.0006	0.0000
22	1.0000	0.9987	0.9401	0.6601	0.2861	0.0742	0.0118	0.0012	0.0001
23	1.0000	0.9994	0.9617	0.7311	0.3563	0.1054	0.0192	0.0022	0.0002
24	1.0000	0.9997	0.9764	0.7932	0.4307	0.1443	0.0301	0.0040	0.0004
25	1.0000	0.9999	0.9859	0.8454	0.5069	0.1913	0.0452	0.0069	0.0007
26	1.0000	1.0000	0.9918	0.8876	0.5819	0.2458	0.0656	0.0113	0.0013
27	1.0000	1.0000	0.9954	0.9205	0.6534	0.3068	0.0921	0.0179	0.0023
28	1.0000	1.0000	0.9975	0.9453	0.7190	0.3730	0.1252	0.0274	0.0040
29	1.0000	1.0000	0.9986	0.9630	0.7770	0.4424	0.1657	0.0408	0.0067
30	1.0000	1.0000	0.9993	0.9754	0.8262	0.5126	0.2133	0.0590	0.0110

Exercise 15.29 (continued)

Analysis: (continued)

Plots of profiles for $\psi = q/q_F^*$ and profiles for $\phi = c/c_F$ during desorption:





Exercise 15.29 (continued)

Analysis: (continued)

To determine from the above profiles the time for 90% of the benzene to be desorbed, compute the average value of loading, ψ, for each of the desorption times, by numerical integration, using,

$$\psi_{avg} = \frac{0.5\psi_{z'=0} + \sum_{z'=1}^{29} \psi_{at\ z'} + 0.5\psi_{z'=30}}{30}$$

Then, from above, the loading in lb benzene = ψ_{avg} (9.27 lb benzene at sat'n/ft^3)(47.1ft^3)
From above, the desired value is 35.8 lb benzene. Using the above table of loadings as a function of time and location in the bed, the following values for benzene loading are obtained:

Desorption time, minutes	Lb benzene not desorbed	% of benzene desorbed
0	358.0	0.0
50	286.5	20.0
100	214.9	40.0
150	144.0	59.8
200	79.4	22.2
250	33.0	90.8
300	9.8	97.3
350	2.1	99.4
400	0.3	99.9

From the above results, the required desorption time is almost 250 minutes.

Exercise 15.30

Subject: Pressure-swing adsorption cycles to approach a cyclic steady state

Given: Design basis in Example 15.13.

Assumptions: Plug flow with a constant interstitial velocity equal to the given inlet value. Negligible axial dispersion.

Find: PSA cycle results that approach the cyclic steady state starting from:
(a) a clean bed.
(b) a bed saturated with the feed.
Are the two cyclic steady states essentially the same?

Analysis: Mole fraction of DMMP in the feed gas = 236/1,000,000 = 0.000236
Feed gas superficial velocity $= u_s = u\varepsilon_\beta = 10.465(0.43) = 4.5$ cm/s
Cross-sectional area of bed = $A = 3.14(1.1)^2/4 = 0.95$ cm^2
Volumetric feed gas flow rate = $Q = u_s A = 4.5(0.95) = 4.275$ cm^3/s
From the ideal gas law at 3.06 atm and 294 K, molar feed gas flow rate =
$n = PQ/RT = (3.06)(4.275)/[(82.06)(294)] = 0.000542$ mol/s
Because the feed is so dilute, the product gas is almost equal to the feed gas.
Therefore, for the desorption step, the gas used for 20 minutes will be pure air at 41.6% of that for the adsorption step or (0.416)(0.000542)(60)(20) = 0.270 mol.
This will be used for 20 min at a flow rate of 0.270/[(20)(60)] = 0.000225 mol/s
At the conditions of desorption, 1.07 atm and 294 K,
$Q = nRT/P = 0.000225(82.06)(294)/1.07 = 5.073$ cm^3/s
Superficial velocity for desorption = 5.073/0.95 = 5.34 cm/s
Interstitial velocity for desorption = 5.34/0.43 = 12.42 cm/s

Convert the adsorption isotherm into the form consistent with the following equations, which are modifications of Eqs. (15-98) and (15-105), in terms of the gas concentration and loading of DMMP:

$$\frac{\partial c}{\partial t} = -u\frac{\partial c}{\partial z} - \left(\frac{1-\varepsilon_b}{\varepsilon_b}\right)k\left(q^* - \bar{q}\right)$$

$$\frac{\partial \bar{q}}{\partial t} = k\left(q^* - \bar{q}\right)$$

where, the units are:
c in g/cm^3 of gas
t in minutes
u in cm/min
k in min^{-1}
q in g/cm^3 of particles

Exercise 15.30 (continued)

Analysis: (continued)

The given Langmuir isotherm is:

$$q^* = \frac{48{,}360\,p}{1+98{,}700\,p}\ ,\quad \text{where } q^* \text{ is in g/g of adsorbent and } p \text{ is partial pressure in atm.}$$

This isotherm must be converted to units of g/cm^3 of particles for q^* and the variable c in g/cm^3 of gas must be substituted for the partial pressure in atm. First consider q^*.

The bed volume = 0.95(12.80) = 12.16 cm^3

The particle volume = (1-0.43)(12.16) = 6.93 cm^3

Particle density = 5.25/6.93 = 0.758 g/cm^3 of particles

The molecular weight of DMMP, dimethyl methylphosphonate, $CH_3PO(OCH_3)_2 = M = 124.08$

Assuming the ideal gas law, $p = cRT/M = c\,(82.06)(294)/124.08 = 194.4\,c$

Therefore, the Langmuir isotherm becomes:

$$q^* = 0.738\frac{48{,}360(194.4)c}{1+98{,}700(194.4)c} = \frac{6.94\times10^6 c}{1+19.19\times10^6 c}\ ,\quad \text{where } q^* \text{ is in g/cm}^3 \text{ of particles and } c \text{ is g/cm}^3$$

The initial conditions for adsorption step of the first cycle are: $c = 0$ for $t = 0$ and $\bar{q} = 0$ at $t = 0$

The boundary condition for all adsorption steps is:

$c_F = y_F PM/RT = (0.000236)(3.06)(124.08)/[(82.06)(294)] = 3.72 \times 10^{-6}$ g/cm^3 at $z = 0$.

The cycle calculations are conveniently carried out by a modification of the FORTRAN program in Table 15.9, based on using the method of lines to obtain a set of ODEs, similar to the equations for TSA, with a stiff integrator, such as LSODES. The program in Table 15.9, which is for TSA, consists of:

Main program to:
- Set initial parameters.
- Call LSODE
- Perform cycles for:
  - Adsorption step
  - Desorption step
- Write cycle results

Subroutine FEX to:
- Compute derivatives of the set of ODEs

For PSA, the program must add:
- Depressurization step
- Repressurization step

Exercise 15.31

Subject: Three cycles of vacuum-swing adsorption.

Given: Design basis in Example 15.13, except that P_L = 0.12 atm and interstitial velocity during the desorption step corresponds to 44.5% of the product gas from the adsorption step.

Assumptions: Plug flow with a constant interstitial velocity equal to the given inlet value. Negligible axial dispersion.

Find: Result of the third VSA cycle starting from a clean bed.

Analysis: Mole fraction of DMMP in the feed gas = 236/1,000,000 = 0.000236

Feed gas superficial velocity = $u_s = u\varepsilon_\beta$ = 10.465(0.43) = 4.5 cm/s

Cross-sectional area of bed = $A = 3.14(1.1)^2/4 = 0.95$ cm^2

Volumetric feed gas flow rate = $Q = u_s A = 4.5(0.95) = 4.275$ cm^3/s

From the ideal gas law at 3.06 atm and 294 K, molar feed gas flow rate =

$n = PQ/RT$ = (3.06)(4.275)/[(82.06)(294)] = 0.000542 mol/s

Because the feed is so dilute, the product gas is almost equal to the feed gas.

Therefore, for the desorption step, the gas used for 20 minutes will be pure air

44.5% of that for the adsorption step or (0.445)(0.000542)(60)(20) = 0.289 mol.

This will be used for 20 min at a flow rate of 0.289/[(20)(60)] = 0.000241 mol/s

At the conditions of desorption, 0.12 atm and 294 K,

$Q = nRT/P$ = 0.000241(82.06)(294)/0.12 = 48.45 cm^3/s

Superficial velocity for desorption = 48.45/0.95 = 51.0 cm/s

Interstitial velocity for desorption = 51.0/0.43 = 118.6 cm/s

Convert the adsorption isotherm into the form consistent with the following equations, which are modifications of Eqs. (15-98) and (15-105), in terms of the gas concentration and loading of DMMP:

$$\frac{\partial c}{\partial t} = -u\frac{\partial c}{\partial z} - \left(\frac{1-\varepsilon_b}{\varepsilon_b}\right)k\left(q^* - \overline{q}\right)$$

$$\frac{\partial \overline{q}}{\partial t} = k\left(q^* - \overline{q}\right)$$

where, the units are:

c in g/cm^3 of gas

t in minutes

u in cm/min

k in min^{-1}

q in g/cm^3 of particles

Exercise 15.31 (continued)

Analysis: (continued)

The given Langmuir isotherm is:

$$q^* = \frac{48{,}360\,p}{1+98{,}700\,p}\ , \quad \text{where } q^* \text{ is in g/g of adsorbent and } p \text{ is partial pressure in atm.}$$

This isotherm must be converted to units of g/cm^3 of particles for q^* and the variable c in g/cm^3 of gas must be substituted for the partial pressure in atm. First consider q^*.

The bed volume = 0.95(12.80) = 12.16 cm^3

The particle volume = (1-0.43)(12.16) = 6.93 cm^3

Particle density = 5.25/6.93 = 0.758 g/cm^3 of particles

The molecular weight of DMMP, dimethyl methylphosphonate, $CH_3PO(OCH_3)_2 = M = 124.08$

Assuming the ideal gas law, $p = cRT/M = c\,(82.06)(294)/124.08 = 194.4\,c$

Therefore, the Langmuir isotherm becomes:

$$q^* = 0.738\frac{48{,}360(194.4)c}{1+98{,}700(194.4)c} = \frac{6.94\times10^6 c}{1+19.19\times10^6 c}\ , \quad \text{where } q^* \text{ is in g/cm}^3 \text{ of particles and } c \text{ is g/cm}^3$$

The initial conditions for adsorption step of the first cycle are: $c = 0$ for $t = 0$ and $\bar{q} = 0$ at $t = 0$

The boundary condition for all adsorption steps is:

$c_F = y_F PM/RT$ = (0.000236)(3.06)(124.08)/[(82.06)(294)] = 3.72 x 10^{-6} g/cm^3 at $z = 0$.

The cycle calculations are conveniently carried out by a modification of the FORTRAN program in Table 15.9, based on using the method of lines to obtain a set of ODEs, similar to the equations for TSA, with a stiff integrator, such as LSODES. The program in Table 15.9, which is for TSA, consists of:

Main program to:
- Set initial parameters.
- Call LSODE
- Perform cycles for:
  - Adsorption step
  - Desorption step
- Write cycle results

Subroutine FEX to:
- Compute derivatives of the set of ODEs

For VSA, the program must add:
- Depressurization step
- Repressurization step

Exercise 15.32

Subject: Model equations for the separation of air by PSA

Given: Feed of air to be separated into oxygen-rich and nitrogen-rich products in fixed isothermal, adiabatic beds, with mass-transfer resistances and extended Langmuir isotherms.

Assumptions: Constant fluid velocity and negligible axial dispersion.

Find: Model equations for the two main steps and a numerical procedure for solving the equations.

Analysis: Let subscripts X = oxygen and N = nitrogen.

Species Mass Balances:

From a modification of Eq. (15-102),

$$u\frac{\partial c_X}{\partial z}+\frac{\partial c_X}{\partial t}+\left(\frac{1-\varepsilon_b}{\varepsilon_b}\right)\frac{\partial \overline{q}_X}{\partial t}=0$$

$$u\frac{\partial c_N}{\partial z}+\frac{\partial c_N}{\partial t}+\left(\frac{1-\varepsilon_b}{\varepsilon_b}\right)\frac{\partial \overline{q}_N}{\partial t}=0$$

Total Mass Balance:

$$\frac{\partial c_t}{\partial t}+\left(\frac{1-\varepsilon_b}{\varepsilon_b}\right)\left(\frac{\partial \overline{q}_X}{\partial t}+\frac{\partial \overline{q}_N}{\partial t}\right)=0 \qquad \text{where, } c_t = c_X + c_N$$

Component Mass-Transfer Rates:

From Eq. (105) for the LDF model,

$$\frac{\partial \overline{q}_X}{\partial t}=k_X\left(q_X^*-\overline{q}_X\right)$$

$$\frac{\partial \overline{q}_N}{\partial t}=k_N\left(q_N^*-\overline{q}_N\right)$$

Extended Langmuir Isotherms:

$$q_X^*=\frac{q_{m_X}K_X c_X}{1+K_X c_X+K_N c_N}$$

$$q_N^*=\frac{q_{m_N}K_N c_N}{1+K_X c_X+K_N c_N}$$

Exercise 15.32 (continued)

Analysis: (continued)

Boundary conditions for starting adsorption with a clean bed:

$$\overline{q}_X(z,0) = c_X(z,0) = 0$$
$$\overline{q}_N(z,0) = c_N(z,0) = 0$$
$$c_X(0,t) = c_{F_X}$$
$$c_N(0,t) = c_{F_N}$$

Boundary conditions for desorption are the conditions in the bed at the end of adsorption and a feed containing purge gas.

The equations can be solved by the Method of Lines in a manner similar to that described on for TSA, letting:

$$\phi_i = c_i / c_{F_i}$$
$$\psi_i = \overline{q}_i / q^*_{F_i}$$

Exercise 15.33

Subject: Descriptions and possible uses of cycling operations of (1) parametric pumping and (2) cycling zone adsorption.

Given: Reference to an article by Sweed, based on inventions by Wilhelm and by Pigford and their co-workers.

Find: Detailed descriptions of (1) parametric pumping and (2) cycling zone adsorption. Can either or both be used for gas-phase and liquid-phase adsorption?

Analysis: Parametric Pumping:

The separation of binary liquid or gas mixtures by parametric pumping was first proposed, analyzed, and substantiated by experiments in articles by R. H. Wilhelm, A. W. Rice, and A. R. Bendelius, I&EC Fundamentals, 5, 141-144 (1966), and R. H. Wilhelm, A. W. Rice, R. W. Rolke, and N. H. Sweed, I&EC Fundamentals, 7, 337-349 (1968). The technique is based on differences in the extent of equilibrium adsorption of the two components in the feed mixture, and a significant decrease in equilibrium adsorption as the temperature is increased. Two different basic equipment arrangements and operations have been proposed, both in a closed-system operation, as shown in the sketches on the next page. Both consist of a fixed-bed column packed with adsorbent particles, a bottom piston-reservoir, and a top piston-reservoir. In a direct mode, the column is jacketed so that the column may be alternately heated or cooled. In a recuperative mode, heat exchangers (one for heating and one for cooling) are provided at opposite ends of an adiabatically operated column.

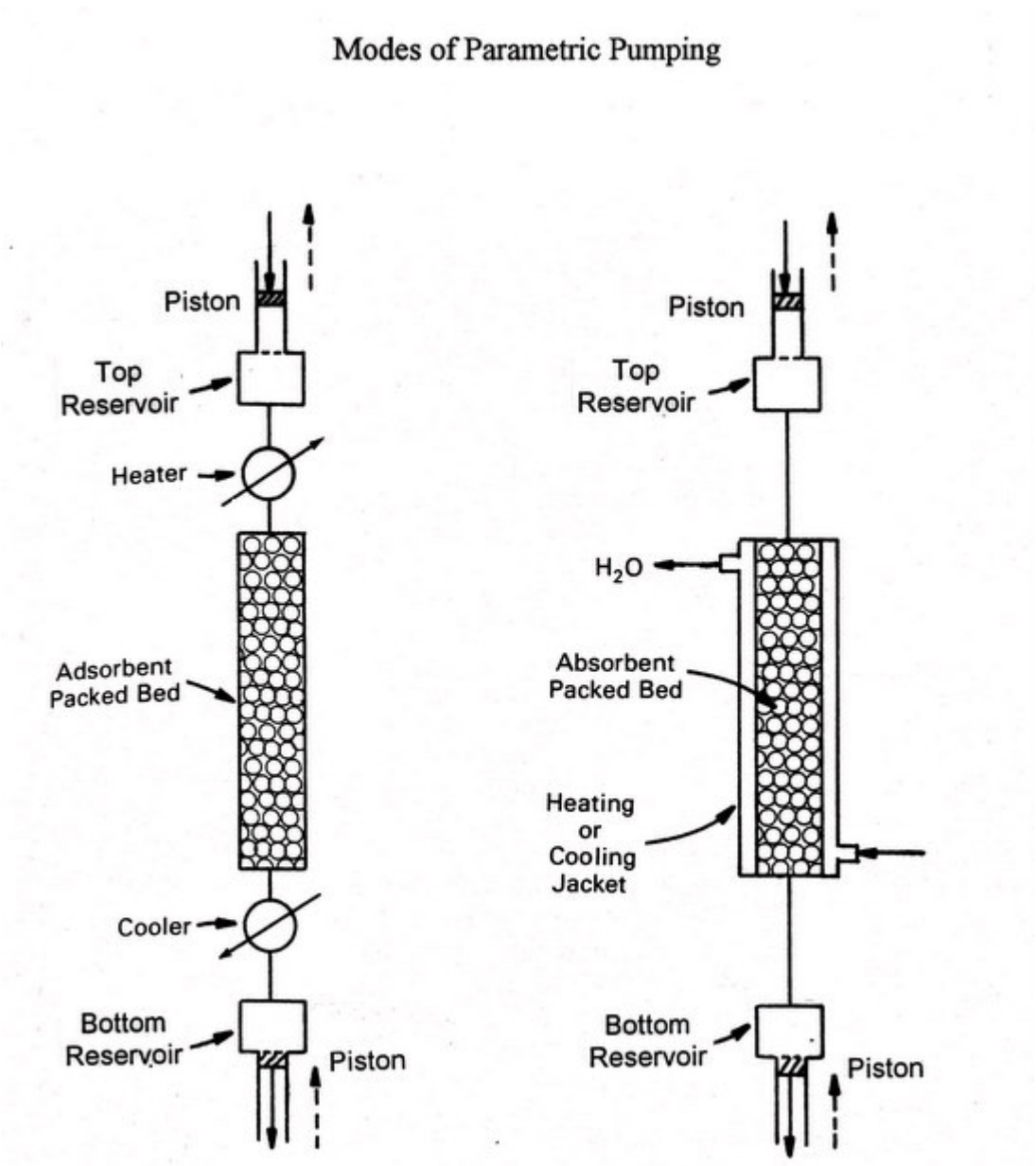
Consider the direct mode, in the context of the example of the experiment reported in the second literature reference above. The column, at ambient temperature, T_1, and packed with silica gel particles, is charged with a liquid feed mixture of 20 vol% toluene and 80 vol% n-heptane and brought to equilibrium. The bottom reservoir is also filled with the same feed mixture, but the top reservoir is initially empty. The toluene is more strongly adsorbed than the n-heptane. The column is heated by the jacket to temperature T_2 and the fluid in the bottom reservoir is pushed into the column by upword movement of the driving piston. At the same time, fluid is drawn into the upper reservoir as the driven piston is forced upward. Because the capacity of the adsorbent is less at the higher temperature and because the adsorbent is more selective for the toluene, the fluid entering the upper reservoir is more concentrated in toluene. This constitutes the first heating half cycle. The direction of fluid flow is now reversed for the first cooling half cycle. The column is cooled to T_1 by the jacket and the top piston becomes the driving piston, pushing the fluid from the top reservoir down into the column. At the lower temperature, the toluene is more selectively adsorbed so that the fluid entering the bottom reservoir is richer in n-heptane. Thus, after one cycle, a partial separation is achieved. Further separation occurs by conducting additional cycles, perhaps 50, after which the reservoirs are emptied into product receivers. Experimental results indicate that although the toluene is almost completely removed from the n-heptane, a nearly pure toluene is not achieved (i.e. high recovery, but not a high purity).

In the recuperative mode, the top of the column is maintained at a hot temperature, T_2, and the bottom is maintained at a cooler temperature, T_1. Again the fluid is pushed first to the

top and then to the bottom for a number of cycles to achieve a separation.

Exercise 15.33 (continued)

Analysis: (continued)



Exercise 15.33 (continued)

Analysis: (continued)

Cycling Zone Adsorption:

The separation of binary liquid or gas mixtures by cycling zone adsorption was first proposed, analyzed, and substantiated by experiments in two articles by R. L. Pigford, B. Baker, and D.E. Blum, I&EC Fundamentals, 8, 848 -851 (1969) and I&EC Fundamentals, 8, 144 (1969). As with parametric pumping, the technique uses fixed beds and is based on differences in the extent of equilibrium adsorption of the two components (A and B) in the feed mixture, and a significant decrease in equilibrium adsorption as the temperature is increased. However, while parametric pumping involves periodic reversals of flow direction and temperature, cycling zone adsorption involves only reversals in temperature. Unlike other fixed-bed schemes, batch-type regeneration of the adsorbent is not required.

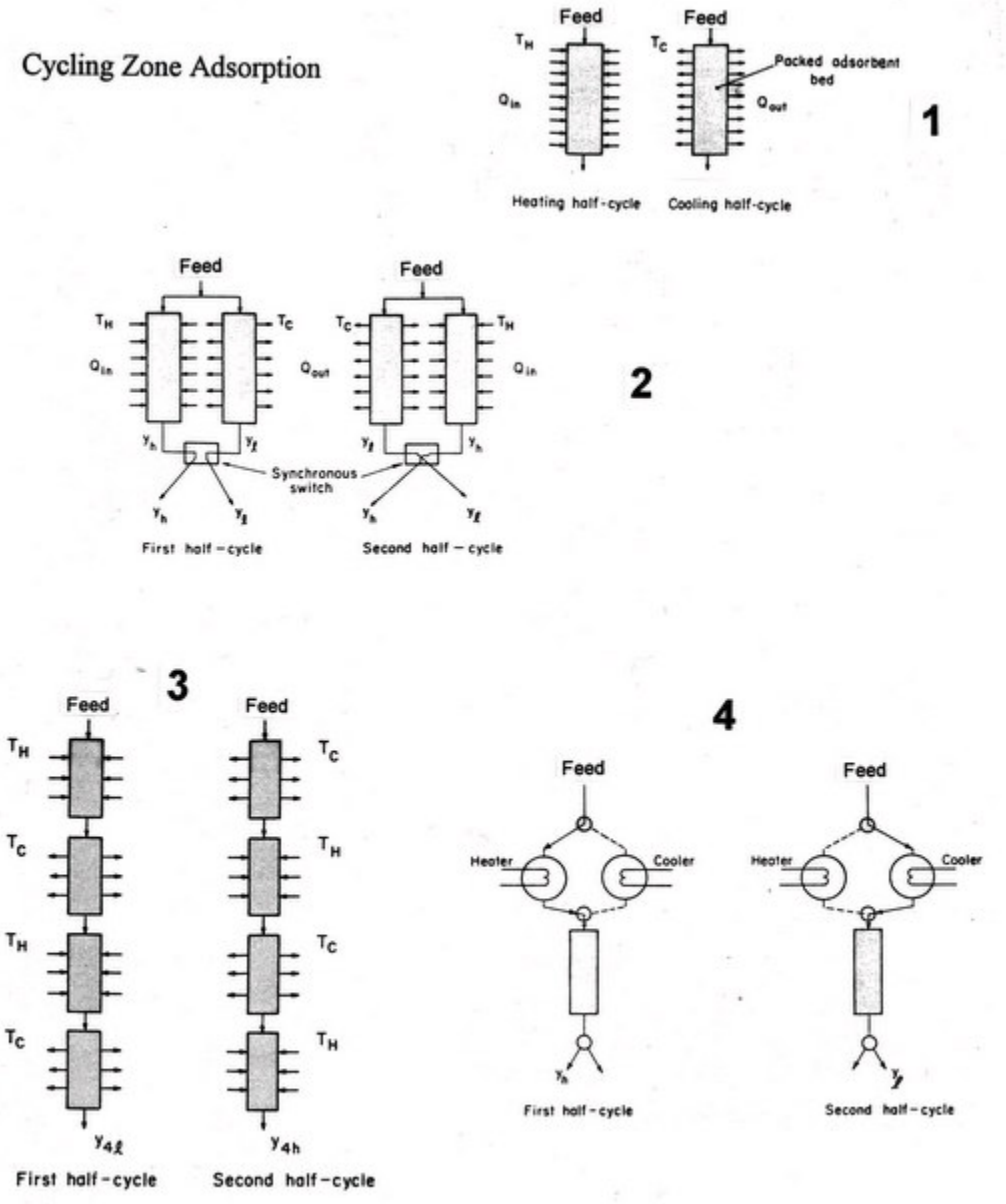
The first sketch on the following page shows the basic idea of cycling zone adsorption. Feed fluid of a fixed composition enters a jacketed fixed bed, maintained at low temperature, T_C, causing component A to be adsorbed to a greater extent than B. At breakthrough, the composition of the exiting fluid approaches that of the feed and the bed temperature is raised to T_H , which causes the adsorbate, rich in component A, to be expelled, raising the concentration of A in the exiting fluid. After a time, the effluent composition again approaches that of the feed. To continuously produce two products, one richer in A, y_h, than the feed, and the other leaner in A than the feed, y_l, two fixed beds are employed, as shown in the second sketch on the following page. One bed is exactly one-half cycle out of phase with the other. The output of each column is periodically switched, but the degree of separation is limited.

The degree of separation is significantly improved by employing two or more beds, called zones, in series, as in the third sketch on the following page. Compared to parametric pumping, theoretical analysis predicts that n cycling zones is equivalent to n parametric pumping cycles. Thus, much more equipment is required for cycling zone adsorption than for parametric pumping. However, with the former, products are produced continuously, instead of in batches. A further simplification in operation is achieved by replacing the jacketed beds by heat exchangers in the manner of the two recuperative mode in parametric pumping, as shown in the fourth sketch.

In the review article by N. H. Sweed, AIChE Symp. Series, 80, No. 233, 44-53 (1984), parametric pumping and cycling zone adsorption, after more than 15 years following their invention, are found to have remained laboratory curiosities, despite their early promise. This is probably due to difficulties in swinging the temperature, and the popularity of PSA for gas.

Exercise 15.33 (continued)

Analysis: (continued)



Exercise 15.34

Subject: Separation of propylene from propane by continuous, countercurrent adsorption.

Given: Feed gas mixture of 55 mol% propane (C3) and 45 mol% propylene (C3=). Continuous, countercurrent adsorption at 25°C and 1 atm with silica gel. Equilibrium data in Exercise 15.9.

Find: Using the McCabe-Thiele method,
(a) Adsorbent flow rate per 1,000 m^3 of gas if 1.2 times the minimum flow rate is used.
(b) Number of theoretical stages needed.

Analysis: First compute the material balance on the gas, taking a basis of one hour. From the ideal gas law, the gas feed rate is

$$F = \frac{P\upsilon}{RT} = \frac{(1)(1{,}000)(10^6)}{(82.06)(298)} = 40{,}900 \text{ mol / h of gas}$$

This gas contains 0.45(40,900) = 18,400 mol/h C3= and 40,900 - 18,400 = 22,500 mol/h C3. Assume a configuration analogous to that for liquid-liquid extraction with reflux, as shown in Fig. 8.26b. Entering solvent, S_B, becomes the adsorbent: raffinate, R, becomes the propane-rich product; Stream $D + L_R$ is desorbed from the adsorbent in the desorber (analogous to the Solvent removal step in extraction), with D becoming the propylene-rich product and L_R, becoming the Extract reflux. The upward movement of adsorbent and adsorbate is V and the downward movement of non-adsorbed gas is L. Other configurations are possible, but the one just described is used here.

From the experimental equilibrium data of Exercise 15.9, assume that at 1atm, the total adsorbent loading remains constant at a value of 2.0 mmol/g = 2.0 mol of combined C3 and C3= adsorbed at equilibrium per kg of adsorbent. Also, in Exercise 15.9, although the mixture data scatter, a relative selectivity = $\alpha_{C3=,C3} = (y_{C3=}/x_{C3=})/(y_{C3}/x_{C3})$ = approximately 2.5, with mole fractions y in the adsorbate an mole fractions x in the non-adsorbed gas. With these two assumptions, a relatively simple McCabe-Thiele method is used to solve this exercise.

Because the flow rate of adsorbent is constant throughout the stages, both below and above the gas feed entry, let V = adsorbate (adsorbent-free) flow rate. Then, because of the assumption of constant loading, V is constant throughout the stages. The non-adsorbed gas flow rate, L, is constant above the feed at a flow rate of L_R;. below the feed, it is R. Thus, on a McCabe-Thiele diagram, the operating lines have constant slopes. By a C3 material balance around the system, followed by a total material balance,

$$Fx_{F_{C3}} = 40{,}900(0.55) = 22{,}500 = y_{D_{C3}}D + x_{B_{C3}}B = 0.10D + 0.90B \qquad (1)$$

$$F = 40{,}900 = D + B \qquad (2)$$

Solving Eqs (1) and (2), D = 17,900 mol/h and B = 23,000 mol/h

Exercise 15.34 (continued)

Analysis: (continued)

The McCabe-Thiele diagram is shown on the following page in mole fractions of C3=, where the equilibrium curve is computed from Eq. (7-3), $y = \alpha x/[1+x(\alpha-1)]$. The q-line is vertical, because the adsorbent that passes over the feed stage is already loaded with adsorbate, so that no change in the adsorbate flow rate, V, occurs. To determine the minimum adsorbent flow rate, the usual minimum reflux construction, shown below, is made (corresponding to an infinite number of stages), with an operating line that starts at $y = x = 0.90$ and terminating at the intersection with the equilibrium line and the q-line x = 0.45 and x = 0.45 and $y = 0.6716$ from the equilibrium equation. Thus, the slope of this operating line = (0.90-0.6716)/(0.9-0.45) = 0.5706. The equation for this operating line is obtained from a C3= material balance around a portion of the upper section of stages, from the top stage (but below the desorber) to an intermediate stage above the feed, in a manner similar to that for distillation on p. 363, where S is the adsorbent flow rate in kg/h and $2S$ is the equilibrium loading of adsorbate in mol/h,

$$2Sy_{C3=} + L_R x_{D_{C3=}} = 2Sy_{D_{C3=}} + L_R x_{C3=}$$

$$\text{Solving, } \quad y_{C3=} = \frac{L_R}{2S} x_{C3=} - \frac{L_R}{2S} x_{D_{C3=}} + y_{D_{C3=}}$$

Thus, the slope of the operating line = $L_R/2S = 0.5706$. Therefore, $L_R = 1.0152\ S$.
Also, $V = 2S$ and by adsorbate material balance around the desorber and divider,
$V = L_R + D = L_R + 17{,}900$. Solving these three equations for the minimum adsorbent condition,
$S = S_{min} = 18{,}200$ kg/h, $V = 2(18{,}200) = 36{,}400$ mol/h, and $L_R = 1.0152(18{,}200) = 18{,}500$ mol/h.

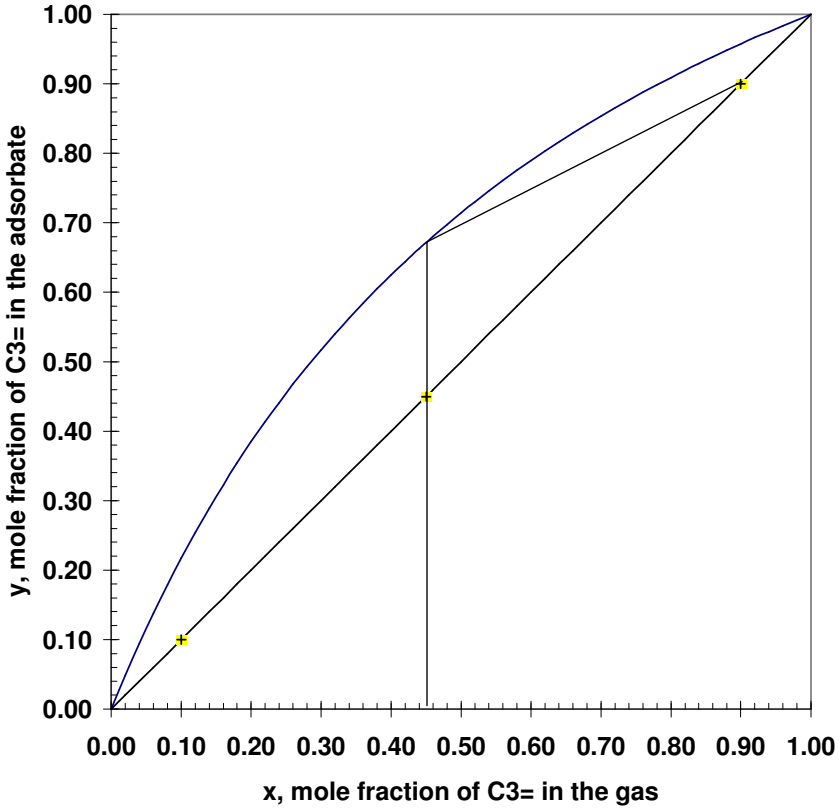
(a) For an adsorbent rate = 1.2 S_{min}, $S = 1.2(18{,}200) = 21{,}850$ kg/h.
Then, $V = 2S = 2(21{,}850) = 43{,}700$ mol/h and $L_R = V - 17{,}900 = 43{,}700 - 17{,}900 = 25{,}800$ mol/h.
The slope of the resulting operating line = $L_R/2S = 25{,}800/[2(21{,}850)] = 0.590$.

(b) This operating line, together with resulting operating line for the lower section is shown in the second McCabe-Thiele diagram below, where 10 equilibrium stages are stepped for the optimal feed-stage location.

Exercise 15.34 (continued)

Analysis: (continued)

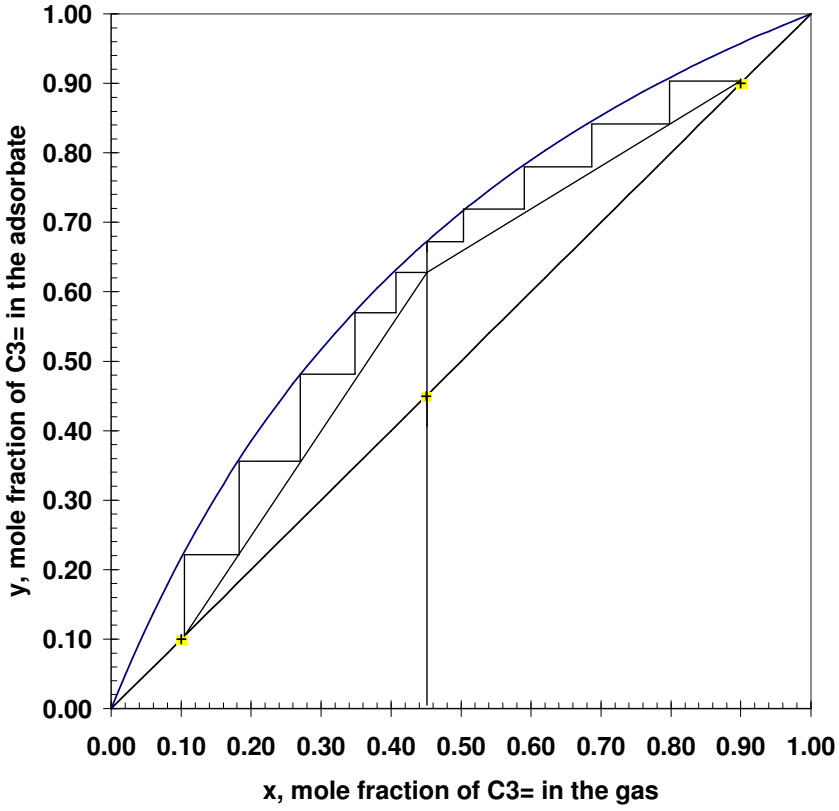
McCabe-Thiele diagram for minimum adsorbent rate



Exercise 15.34 (continued)

Analysis: (continued)

McCabe-Thiele diagram for adsorbent rate
Equal to 1.2 times minimum value



Exercise 15.35

Subject: Softening of hard water in a fixed-bed ion exchange column

Given: Feed at 25°C containing 400 ppm (by wt) $CaCl_2$ and 50 ppm (by wt) NaCl. Bed of 8.5 ft diameter by 10 ft high of gel resin with a cation capacity of 2.3 eq/L of bed volume. Wetted resin void fraction = $\varepsilon_b = 0.38$. 15 gal/min-ft^2 for loading; 1.5 gal/min-ft^2 for displacement, washing , and regeneration. Displacement and regeneration solutions are aq. saturated NaCl (26 wt%).

Assumption: Because of dilute conditions, feed solution contains 1,000 g H_2O/L

Find: (a) Feed solution flow rate, L/min.
(b) Loading time to breakthrough, h
(c) Loading wave front velocity, cm/min
(d) Regeneration solution flow rate, L/min
(e) Displacement time, h
(f) Additional time for regeneration, h

Analysis:

M of $CaCl_2$ = 110.99 M of NaCl = 58.45

Concentration of $CaCl_2$ = 400(1000)/[110.99(1,000,000)] = 0.00360 mol/L = 0.00720 eq/L

Concentration of NaCl = 50(1000)/[58.45(1,000,000)] = 0.000855 mol/L = 0.000855 eq/L

(a) Bed cross-sectional area = $3.14(8.5)^2/4 = 56.7$ ft^2

Feed solution flow rate = 15(56.7) = 851 gpm = 3,219 L/min

(b) Behind the loading wave front in the feed,

equivalent fraction of $Ca^{2+} = x_{Ca^{2+}} = 0.0072 / (0.0072 + 0.000855) = 0.9883$

Since no NaCl in the feed is exchanged, $C_L = 0.0072$ eq/L $Q = 2.3$ eq/L

From Table 15.5, $K_{Ca^{2+},Na^+} = 5.2 / 2 = 2.6$

From Eq. (15-181), $$2.6\left(\frac{2.3}{0.0072}\right) = 830.6 = \frac{\left(y_{Ca^{2+}}\right)(1-0.8938)}{(0.8938)\left(1-y_{Ca^{2+}}\right)} = 0.1188\frac{\left(y_{Ca^{2+}}\right)}{\left(1-y_{Ca^{2+}}\right)}$$

Solving, $y_{Ca^{2+}} = 0.99986$ equivalent fraction

Bed volume = (56.7)(10) = 567 ft^3 or 16,060 L

Total Bed Capacity = 2.3 (16,060) = 36,940 eq

Ca^{2+} absorbed by resin = 0.99986(36,940) = 36,935 eq

Ca^{2+} entering bed in feed solution = 0.0072(3,219) = 23.18 eq/min

Ideal loading time to breakthrough = $t_L = \frac{36,935}{23.18} = 1,593$ min = 26.6 h

Exercise 15.35 (continued)

Analysis: (continued)

(c) Loading wave front velocity = $u_L = L/t_L$ = 10/1,593 = 0.00628 ft/min or 0.191 cm/min

(d) Flow rate of regeneration solution = $\frac{1.5}{15}(3{,}219)$ = 321.9 L/min

(e) Displacement time = time for 321.9 L/min to displace liquid in the voids

Void volume = 0.38 (16,060) = 6,103 L

Displacement time $t_D = \frac{6103}{321.9}$ = 19 min

(f) For a 26 wt% NaCl solution at 25°C, the density from Perry's Chemical Engineers' Handbook = 1.19443 g/cm^3

Flow rate of Na^+ in regeneration solution = $\frac{321.9(1{,}000)(1.19443)(0.26)}{58.45}$ = 1,710 eq/min

NaCl concentration in regenerating solution = $\frac{1{,}710}{321.9}$ = 5.31 eq/L = c_R = C in Eq. (15-139)

From Eq. (15-181), noting conditions in Fig. 15.50b:

$$K_{Ca^{2+},Na^+}\left(\frac{Q}{c_R}\right) = 2.6\left(\frac{2.3}{5.31}\right) = 1.126$$

Unfortunately, this is > 1. Therefore, equilibrium is not as favorable as desired. Also the regeneration wave may not sharpen quickly. Nevertheless, assume a shock wave-like front. From Eq. (15-181):

$$1.126 = \frac{(0.99986)\left(1-x^*_{Ca^{2+}}\right)}{x^*_{Ca^{2+}}(1-0.99986)} = 7{,}142\frac{\left(1-x^*_{Ca^{2+}}\right)}{x^*_{Ca^{2+}}}$$

Solving:

$$x^*_{Ca^{2+}} = 0.99984$$

So downstream of the regeneration wave front, but upstream of the displacement wave front, the liquid contains very few sodium ions. However, this will not be quite so because the wave will not be sharp.

Exercise 15.36

Subject: Separation of glutamic acid, glycine, and valine, in an aqueous solution, by a fixed-bed chromatographic column, using equilibrium theory.

Given: Aqueous solution, buffered to a 3.4 pH by sodium citrate and containing 20 mol/m^3 each of glutamic acid (GA), glycine (G), and valine (V). Chromatographic column, packed with Dowex 50W-X8 in the sodium form to a depth of 470 mm = 47 cm. Resin is 0.07 mm in diameter and is packed to a void fraction, ε_b , of 0.374. All three solutes follow Henry's law, $q = Kc$, where the values of K are 1.18 for GA, 1.74 for G, and 2.64 for V. Superficial solution velocity = u_s = 0.025 cm/s.

Assumptions: Equilibrium theory.

Find: Pulse duration to achieve complete separation. Time duration of the elution step before the second pulse begins.

Analysis: Interstitial velocity = $u = u_s/\varepsilon_b = 0.025/0.374 = 0.0668$ cm/s.

From Eq. (15-183), solute wave velocity = $u_i = \dfrac{u}{1+\left(\dfrac{1-\varepsilon_b}{\varepsilon_b}\right)K_i} = \dfrac{0.0668}{1+\left(\dfrac{1-0.374}{0.374}\right)K_i} = \dfrac{0.0668}{1+1.674K_i}$

Solute	K_i	u_i, cm/s
GA	1.18	0.0225
G	1.74	0.0171
V	2.64	0.0123

From the K values, V is the most strongly adsorbed. Therefore, the solutes will leave the column in the order of GA first, then G, and V last.

First, assume that the separation between GA and G controls, as analogous to Fig. 15.49, where 182 cm is replaced by 47 cm. Thus, at the end of the column, the trailing edge of GA will coincide with the leading edge of G. From Example 15.20,

$$t_P + \frac{47}{0.0225} = \frac{47}{0.0171} \qquad \text{Solving, } t_P = 47\left(\frac{1}{0.0171} - \frac{1}{0.0225}\right) = 660 \text{ s}$$

Thus, the time for the trailing edge of the GA wave to reach the end of the column at 47 cm = t_P + 47/0.0225 = 660 + 2,089 = 2,749 s. At that time, will the G and V waves be separated? The trailing edge of the G wave will be at (2,089)(0.0171) = 35.7 cm, while the leading edge of the V wave will be at (2,749)(0.0123) = 33.8 cm. Therefore, the G and V waves will be separated.

Now assume that the separation between G and V controls. Thus, at the end of the column, the trailing edge of G will coincide with the leading edge of V. From Example 15.20,

$$t_P + \frac{47}{0.0171} = \frac{47}{0.0123} \qquad \text{Solving, } t_P = 47\left(\frac{1}{0.0123} - \frac{1}{0.0171}\right) = 1{,}073 \text{ s}$$

Exercise 15.36 (continued)

Analysis: (continued)

Thus, the time for the trailing edge of the G wave to reach the end of the column at 47 cm = = t_P + 47/0.0171 = 1,073 + 2,749 = 3,822 s. At that time, will the G and GA waves be separated? The leading edge of the G wave will be at a hypothetical distance outside of the column of (3,822)(0.0171) = 65.4 cm. The trailing edge of the GA wave will be at a hypothetical distance outside of the column at 2,749(0.0225) = 61.9 cm. Thus, the G and GA waves are not separated. Therefore, the pulse duration = 660 seconds.

To determine the elution time, compute the time for the trailing edge of the slow V wave to reach 47 cm. This time = 660 + 47/0.0123 = 4,481 s.
The time for the leading edge of the second pulse of GA to reach 47 cm so that V and GA are just separated = 47/0.0225 = 2,089 s.
The difference is 4,481 - 2,089 = 2,392 s before the second pulse starts. But 660 s of this is the first pulse. Therefore, the elution time = 2,392 - 660 = 1,732 s.

Thus, the ideal cycle is:

Pulse:	660 s
Elute:	1,732 s
Pulse:	660 s
Elute:	1,732 s
etc.	

Exercise 15.37

Subject: Separation of glutamic acid, glycine, and valine, in an aqueous solution, by a fixed-bed chromatographic column, accounting for mass transfer resistances.

Given: Aqueous solution, buffered to a 3.4 pH by sodium citrate and containing 20 mol/m^3 each of glutamic acid (GA), glycine (G), and valine (V). Chromatographic column, packed with Dowex 50W-X8 in the sodium form to a depth of 470 mm = 47 cm. Resin is 0.07 mm in diameter and is packed to a void fraction, ε_b , of 0.374. All three solutes follow Henry's law, $q = Kc$, where the values of K are given below. Superficial solution velocity = u_s = 0.025 cm/s. Effective diffusivities of the three solutes are given below. External mass-transfer coefficient = 1.5 x 10^{-3} cm/s for each solute.

Assumptions: Application of Carta's equation, which accounts for mass transfer.

Find: A cycle of feed pulses and elution periods that result in the separation of the three solutes.

Analysis: Interstitial velocity = $u = u_s/\varepsilon_b$ = 0.025/0.374 = 0.0668 cm/s. From Eq. (15-140), the solute wave velocities, u_i, can be computed for ε_b = 0.374 and the following values of K, giving:

Solute	K	D_e , cm^2 /s	u_i, cm/s
GA	1.18	1.94 x 10^{-7}	0.0225
G	1.74	4.07 x 10^{-7}	0.0171
V	2.64	3.58 x 10^{-7}	0.0123

Thus, the GA wave will leave first, followed by G and then V.
From the results of Exercise 15.36 for the equilibrium theory, the pulse time is 660 s and the elution time is 1732 s. It is expected that with mass transfer taken into account, a shorter pulse time and a longer elution time will be required to avoid significant overlap of the solute waves.
Calculate the fixed solute parameters in Carta's equation.
Particle radius = R_p = 0.07/2 = 0.035 mm = 0.00 35 cm
From Eq. (15-154), the overall mass-transfer coefficient =

$$k = \frac{1}{\frac{R_p}{3k_c} + \frac{R_p^2}{15D_e}} = \frac{1}{\frac{0.0035}{3(1.5\times10^{-3})} + \frac{0.0035^2}{15D_e}} = \frac{1}{0.778 + \frac{8.167\times10^{-7}}{D_e}} \qquad (1)$$

From Eq. (15-194), with ε_b = 0.374, $\beta = \frac{\varepsilon_b}{(1-\varepsilon_b)K} = \frac{0.374}{(1-0.374)K} = \frac{0.597}{K}$ (2)

From Eq. (15-192), with z = 47 cm, $n_f = \frac{(1-\varepsilon_b)}{\varepsilon_b}\frac{kz}{u} = \frac{(1-0.374)k(47)}{0.374(0.0668)} = 1{,}178k$ (3)

Exercise 15.37 (continued)

Analysis: (continued)

Calculations with the given values of K and D_e, and Eqs. (1), (2), and (3) give:

Solute	k, s^{-1}	k/K, s^{-1}	β	n_f
GA	0.2005	0.170	0.506	236
G	0.359	0.206	0.343	423
V	0.327	0.124	0.226	385

Now, we must choose a pulse time, t_F, and elution time, t_E. Assume a pulse time that is 50% of that computed by the equilibrium theory of Exercise 15.36, namely 0.5(660) = 330 s. For now, leave the elution time at 1732 s because it does not affect the first set of solute waves. Compute values of c/c_F as a function of time using Carta's infinite-series equation (15-46) using a spreadsheet, being careful to include a sufficient number of terms in the series to obtain a converged result. In this exercise, that number in Eq. (15-46) is not more than $m = 20$. The result is that with $t_F = 330$ s, the GA and G waves overlap significantly at $z = 47$ cm.

Try $t_F = 0.5(330) = 165$ cm. Now, as seen in the table on the next page and the plot on the following page, only a small overlap of the GA and G waves occurs. An even smaller overlap of the G and V waves is evident. However, although not shown, a significant overlap of the first V wave and the second GA wave occurs with $t_E = 1{,}732$ s. Therefore, we must increase the value of t_E. If it is increased to 2,732 s, the results are acceptable, as shown in the table and plot below, where the first set of solute waves and the second wave for GA are shown. Thus, a possible cycle, taking into account mass transfer is:

Pulse:	165 s
Elute:	2,732 s
Pulse:	165 s
Elute:	2,732 s
etc.	

Because of the short pulse time and the long elution time, this is probably not a desirable cycle.

Exercise 15.37 (continued)

Analysis: (continued)

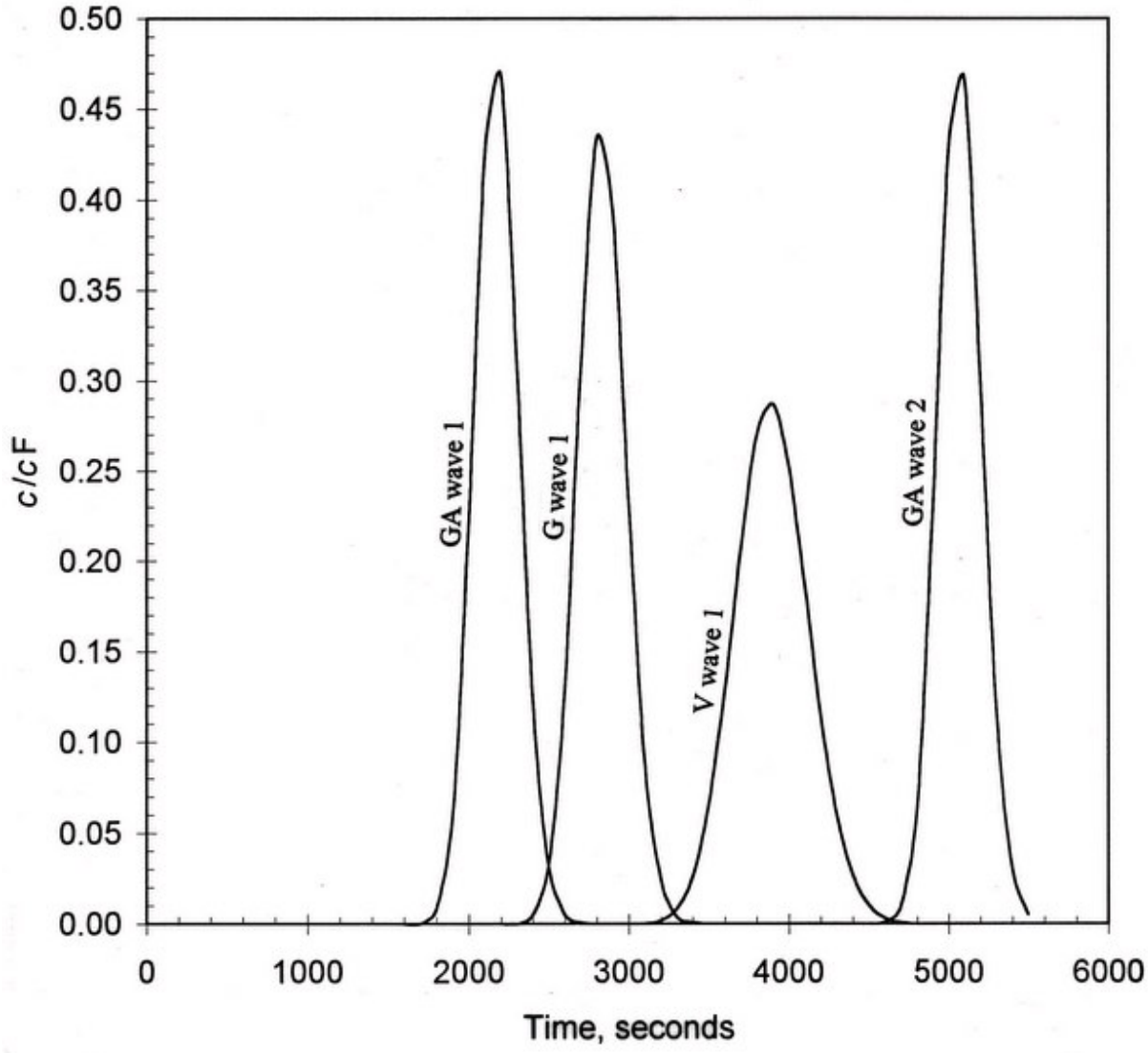
Z = 47 cm, t_F = 165 s, t_E = 2,732 s

	Values of c/c_F		
t, s	GA	G	V
1500	0.000	0.000	0.000
1600	0.000	0.000	0.000
1700	0.000	0.000	0.000
1800	0.008	0.000	0.000
1900	0.060	0.000	0.000
2000	0.218	0.000	0.000
2100	0.425	0.000	0.000
2200	0.469	0.000	0.000
2300	0.308	0.000	0.000
2400	0.124	0.005	0.000
2500	0.032	0.032	0.000
2600	0.005	0.129	0.000
2700	0.001	0.302	0.000
2800	0.000	0.434	0.000
2900	0.000	0.395	0.000
3000	0.000	0.233	0.000
3100	0.000	0.091	0.000
3200	0.000	0.024	0.002
3300	0.000	0.004	0.008
3400	0.000	0.001	0.026
3500	0.000	0.000	0.065
3600	0.000	0.000	0.129
3700	0.000	0.000	0.207
3800	0.000	0.000	0.269
3900	0.000	0.000	0.287
4000	0.000	0.000	0.253
4100	0.000	0.000	0.186
4200	0.000	0.000	0.115
4300	0.000	0.000	0.060
4400	0.000	0.000	0.027
4500	0.000	0.000	0.010
4600	0.001	0.000	0.003
4700	0.009	0.000	0.001
4800	0.063	0.000	0.000
4900	0.225	0.000	0.000
5000	0.429	0.000	0.000
5100	0.467	0.000	0.000
5200	0.301	0.000	0.000
5300	0.120	0.000	0.000
5400	0.030	0.000	0.000
5500	0.005	0.000	0.000

GA wave 1 (2000–2300)
GA wave 2 (4900–5300)
G wave 1 (2700–3000)
V wave 1 (3700–4100)

Exercise 15.37 (continued)

Analysis: (continued)



Exercise 15.38

Subject: Separation of a dilute feed of 3-phenyl-1-propanol (A) and 2-phenyl ethanol (B) in a methanol-water mixture in a 4-section laboratory simulated moving bed.

Given: A liquid feed rate of 0.16 mL/min containing 0.091 g/L of A and 0.115 g/L of B, with the balance being a 60/40 wt% methanol-water mixture. Henry's law applies, in the form, $q_i = K_i c_i$, with $K_A = 2.36$ and $K_B = 1.40$ for the given adsorbent, q and c are concentrations per unit volume. Assume that neither methanol nor water adsorb. External void fraction of the adsorbent beds = $\varepsilon_b = 0.572$. Switching time = 10 minutes.

Find: Using the steady-state, local-composition TMB model for a perfect separation of A from B with a margin, β, of 1.15, estimate initial values for the volumetric flow rates of the extract (E), raffinate (R), desorbent (D), circulation (C), and the solid particles (S). Use those values to determine the recirculation rate for the SMB and the resulting volumetric liquid flow rates in each of the four sections.

Analysis: Carry out the calculations using volumetric flow rates as shown in Figure 15.45. Because, $K_B < K_A$, B will appear in the raffinate and A will appear in the extract. First make calculations for a TMB. Using (15-149) to (15-151), with $Q_F = 0.16$ mL/min,

$$Q_S = \frac{Q_F}{\frac{K_A}{\beta} - K_B\beta} = \frac{0.16}{\frac{2.36}{1.15} - 1.40(1.15)} = 0.362 \text{ mL/min}$$

$$Q_E = Q_S\left(K_A - K_B\right)\beta = 0.362\left(2.36 - 1.40\right)1.15 = 0.400 \text{ mL/min}$$

$$Q_R = \frac{Q_S\left(K_A - K_B\right)}{\beta} = \frac{0.362\left(2.36 - 1.40\right)}{1.15} = 0.302 \text{ mL/min}$$

Using (15-154), $Q_D = Q_E + Q_R - Q_F = 0.400 + 0.302 - 0.160 = 0.542 \text{ mL/min}$

Using (15-153), $Q_C = Q_S K_A \beta - Q_D = 0.362\left(2.36\right)(1.15) - 0.542 = 0.442 \text{ mL/min}$

Now, make calculations for the SMB, where the solid particles do not flow down through the unit, but are in stationary beds.

Referrring to Figure 15.45, the volumetric flow rate in section I of the TMB is,

$$\left(Q_I\right)_{TMB} = Q_C + Q_D = 0.442 + 0.542 = 0.984 \text{ mL/min}$$

Exercise 15.38 (continued)

Analysis: (continued)

From (15-175),

$$(Q_{\mathrm{I}})_{\mathrm{SMB}} = (Q_{\mathrm{I}})_{\mathrm{TMB}} + \left(\frac{\varepsilon_b}{1-\varepsilon_b}\right)(Q_S)_{\mathrm{TMB}} = 0.984 + \left(\frac{0.572}{1-0.572}\right)0.362 = 1.468 \text{ mL/min}$$

Then, $(Q_{\mathrm{II}})_{\mathrm{SMB}} = (Q_{\mathrm{I}})_{\mathrm{SMB}} - Q_E = 1.468 - 0.400 = 1.068$ mL/min

$(Q_{\mathrm{III}})_{\mathrm{SMB}} = (Q_{\mathrm{II}})_{\mathrm{SMB}} + Q_F = 1.068 + 0.160 = 1.228$ mL/min

$(Q_{\mathrm{IV}})_{\mathrm{SMB}} = (Q_{\mathrm{III}})_{\mathrm{SMB}} - Q_R = 1.228 - 0.302 = 0.926$ mL/min

Exercise 15.39

Subject: Effect of mass-transfer coefficients on the steady-state TMB results of Example 15.17 for the separation of fructose from glucose.

Given: Data in Examples 15.16 and 15.17.

Find: The compositions of the extract and raffinate.

Analysis: In Example 15.17, the component mass-transfer coefficients (MTC) for A and B are 10 min^{-1}. Using Aspen Chromatography, increase the value to 1000 min^{-1}. The following results are obtained, compared to those from Example 15.17.

Concentrations in g/L

Component	**Extract MTC = 10 min^{-1}**	**Extract MTC = 1000 min^{-1}**	**Raffinate MTC = 10 min^{-1}**	**Raffinate MTC = 1000 min^{-1}**
Fructose	211.6	223.2	12.7	3.9
Glucose	8.4	2.6	295.3	303.3
Water	861.7	858.9	795.8	796.1

Some improvement in the separation is noted. Additional improvement may be possible by altering the switching time, the fluid circulation flow rate, and the extract and raffinate flow rates.

Exercise 16.1

Subject: Mass balance check on test data around a leaching unit.

Given: Feed rate to extractor of 6.375 lb/h with 10.67 wt% moisture and 0.2675 g oil per g dry, oil-free flakes. Solvent rate to extractor of 10.844 lb/h. Extract of 7.313 lb/h with 15.35 wt% oil. Leached solids with 0.0151 g oil per g dry, oil-free flakes.

Assumptions: Solvent is n-hexane. Extract contains no solids. Leached solids contain all of the moisture in the feed and are wet with solvent.

Find: Check on mass balances around the leaching unit for oil and hexane. Mass ratio of oil to flakes in leached solids.

Analysis: Make calculations with AE units, noting that g/g is the same as lb/lb. Calculate the flow rates of components in the feed:

Moisture = 0.1067(6.375) = 0.680 lb/h moisture
Dry flakes = 6.375 – 0.680 = 5.695 lb/h dry flakes
Oil = [0.2675/(0.2675 + 1.00)] 5.695 = 1.202 lb/h oil
Dry, oil-free flakes = 5.695 – 1.202 = 4.493 lb/h dry, oil-free flakes

Calculate flow rates in the leached solids, assuming all dry, oil-free flakes are in the leached solids:

Oil = 0.0151(4.493) = 0.068 lb/h oil

Therefore, by mass balance around the leaching unit,

Oil in the extract = 1.202 – 0.068 = 1.134 lb/h oil

Compare this to data given for the extract:

Oil in the extract = 0.1535(7.313) = 1.123 lb/h oil

This number is 99% of the mass balance number, which is an excellent check.

A similar check cannot be made for the hexane, but we can calculate the amount of hexane contained in the wet leached solids.

Hexane = 10.844 – (7.313 – 1.123) = 4.654 lb/h hexane in the wet leached solids.

Mass ratio of oil to wet leached solids = 0.068/(0.068 + 4.493 + 0.680 + 4.654) = 0.0069

Summary of mass balance in lb/h:

Component	Feed	Solvent	Wet, leached solids	Extract
Moisture	0.680	0.000	0.680	0.000
Oil	1.202	0.000	0.068	1.134
n-Hexane	0.000	10.844	4.654	6.190
Dry, oil and solvent-free flakes	4.493	0.000	4.493	0.000

Exercise 16.2

Subject: Manufacture of insoluble barium carbonate by precipitation of barium sulfide in an aqueous solution with sodium carbonate, followed by washing with water to remove sodium sulfide.

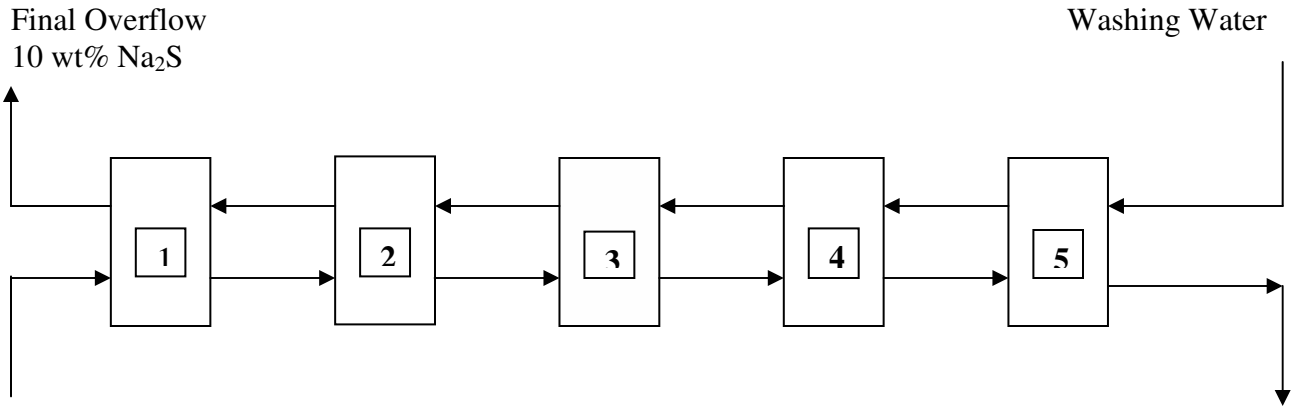
Given: Specifications given below for a 5-stage countercurrent flow system, where precipitation occurs in the first stage and washing is done in four stages of thickeners.

Assumptions: No solids in the overflows. Liquid in the underflow and liquid in the overflow leaving a stage have the same composition. Stoichiometric amounts for the precipitation reaction.

Find: (a) A schematic diagram of the process. (b) The flow rates of sodium carbonate and wash water required. The flow rates of barium carbonate and sodium sulfide produced. (c) The wt% of sodium sulfide leaving in the liquid in the underflow from each stage. The flow rate of sodium sulfide in the barium carbonate after drying.

Analysis: Because the underflow liquid is given as a mass ratio of Na_2S-free water to the solid $BaCO_3$ in the underflow, use Na_2S compositions in the liquid as mass ratios, X, to water.

(a) Schematic diagram of the process with given information.



(b) Na_2CO_3 requirement and $BaCO_3$ and Na_2S produced by stoichiometry:

	$BaS\,(aq)$	+ $Na_2CO_3\,(s)$	= $BaCO_3\,(s)$	+ $Na_2S\,(aq)$
Molecular Weight:	169.42	106.00	197.37	78.05

Exercise 16.2 (continued)

Flow rate of Na_2CO_3 required = 40,000(106.00/169.42) = 25,027 kg/d
Flow rate of $BaCO_3$ produced = 40,000(197.37/169.42) = 46,599 kg/d
Flow rate of Na_2S produced = 40,000(78.05/169.42) = 18,428 kg/d

Determination of fresh water needed washing:

Final underflow contains all of the solid $BaCO_3$ = 46,599 kg/d

Water in the final underflow = 2(46,599) = 93,198 kg/d

Since the precipitation reaction is complete and under stoichiometric conditions, the final overflow contains only water and Na_2S.

Need to write mass balances for Na_2S for each stage. Best to write these in terms of mass ratios of Na_2S because underflow ratios are given as parts of H_2O (rather than parts solution) per part of solid $BaCO_3$.

Let: Y_i = mass ratio of Na_2S to water in the overflow from Stage i
X_i = mass ratio of Na_2S to water in the underflow from Stage i
V_i = kg/d of water in the overflow from Stage i.
L_i = kg/d of water in the underflow from Stage i.
S = kg/d of wash water entering Stage 5.

Then: $Y_1 = 0.1/0.9 = 0.1111 = X_1$ and all $Y_i = X_i$.

Since the flow rate of water in the underflows is constant,

$$L_1 = L_2 = L_3 = L_4 = L_5 = 93{,}198 \text{ kg/d of water}$$

Overall water balance:

$$120{,}000 + S = V_1 + 93{,}198 \quad \text{or} \quad S = V_1 - 26{,}802$$

A water balance around each stage results in,

$$V_2 = V_3 = V_4 = V_5 = V_1 - 26{,}802 = S$$

Mass balances for Na_2S around each stage:

Stage 1: $18{,}428 + Y_2V_2 = X_1L_1 + Y_1V_1$

or $18{,}428 + Y_2S = 0.1111(93{,}148) + 0.1111(S + 26{,}802)$ (1)

Stage 2: $X_1L_1 + Y_3V_3 = X_2L_2 + Y_2V_2$

or $0.1111(93{,}198) + Y_3S = Y_2(93{,}198) + Y_2S$ (2)

Stage 3: $X_2L_2 + Y_4V_4 = X_3L_3 + Y_3V_3$

or $Y_2(93{,}198) + Y_4S = Y_3(93{,}198) + Y_3S$ (3)

Stage 4: $X_3L_3 + Y_5V_5 = X_4L_4 + Y_4V_4$

or $Y_3(93{,}198) + Y_5S = Y_4(93{,}198) + Y_4S$ (4)

Stage 5: $X_4L_4 = X_5L_5 + Y_5V_5$

or $Y_4(93{,}198) = Y_5(93{,}198) + Y_5S$ (5)

We have five linear equations in five variables: S, Y_2, Y_3, Y_4, and Y_5

Solving with Polymath, S = 130,600 kg/d and Y_i values from Stage 2 to 5 are 0.07207, 0.04421, 0.02433, and 0.01013.

(c) Since $Y_i = X_i$ and Wt% Na_2S in an underflow = $[X_i/(1 + X_i)](100\%) = [Y_i/(1 + Y_i)](100\%)$,

the Wt% values from Stage 2 to 5 are: 6.72%, 4.23%, 2.37%, and 1.00%.

The final dried underflow contains 0.01013(93,198) = 944 kg/d of Na_2S. Therefore, purity of the final dried $BaCO_3$ is 46,599/(944 + 46,599) = 0.980 or 98.0%.

Exercise 16.3

Subject: Precipitation of $CaCO_3$ from the reaction of solid CaO and an aqueous solution of Na_2CO_3, followed by two stages of washing.

Given: A process consisting of a precipitation vessel followed by a two-stage, continuous, countercurrent washing system using water. Slurry of 100,000 lb/h from the precipitation tank is 5 wt% solid $CaCO_3$, 0.1 wt% NaOH, and 94.9 wt% water. Wash is 20,000 lb/h of water. Underflow from each of the two washing stages is 20 wt% solids.

Assumptions: No solids in the overflows. Liquid in the underflow and liquid in the overflow leaving a stage have the same composition.

Find: The percent recovery of NaOH in the final overflow (extract) and the wt% NaOH in the dried $CaCO_3$. Also, is it worthwhile to add a third washing stage?

Analysis: Because the slurry composition and flow rate are given, it is not necessary to consider the precipitation reaction, which is:

$$CaO\ (s) + Na_2CO_3\ (aq) + H_2O\ (l) = CaCO_3\ (s) + 2\ NaOH\ (aq)$$

First compute the component flow rates in the slurry leaving the precipitation vessel and entering washing Stage 1.

Component	Wt%	Flow rate, lb/h
$CaCO_3$	5.0	5,000
NaOH	0.1	100
Water	94.9	94,900

Now consider the underflows. Each underflow will contain all of the solid $CaCO_3$ or 5,000 lb/h of solids. Therefore, the liquid in each underflow of 20% solids will be 20,000 lb/h of aqueous NaOH. Because the underflow basis is on total solution (not just the water), use mass fractions to express the NaOH composition in the overflow and the liquid in the underflow.

Let: y_i = mass fraction of NaOH in the overflow from Stage i
x_i = mass fraction of NaOH in the underflow from Stage i
V_i = lb/h of liquid in the overflow from Stage i.
L_i = lb/h of liquid in the underflow from Stage i.
S = lb/h of fresh wash water entering Stage 2.

Then: $x_i = y_i$
L_i = 20,000 lb/h

Overall mass balance for the two washing stages gives:

$$100{,}000 + 20{,}000 = 5{,}000 + 20{,}000 + V_1$$

Solving, V_1 = 95,000 lb/h

Total mass balance around Stage 2 gives:

$$20{,}000 + 5{,}000 + 20{,}000 = 5{,}000 + 20{,}000 + V_2$$

Solving V_2 = 20,000 lb/h

Exercise 16.3 (continued)

Mass balances for NaOH for each stage:

Stage 1 (to which the slurry from precipitation enters):

$$100 + y_2V_2 = y_1V_1 + x_1L_1$$

or, $100 + y_2(20{,}000) = y_1(95{,}000) + y_1(20{,}000)$ (1)

Stage 2 (to which the fresh wash water is sent):

$$0 + x_1L_1 = y_2V_2 + x_2L_2$$

or, $y_1(20{,}000) = y_2(20{,}000) + y_2(20{,}000)$ (2)

We have two linear equations in two variables: y_1 and y_2.
Solving (1) and (2), gives: $y_1 = x_1 = 0.000952$ and $y_2 = x_2 = 0.000476$

Flow rate of NaOH in final overflow = $y_1V_1 = 0.000952(95{,}000) = 90.44$ lb/h
Therefore, the recovery of NaOH in the extract = 90.44/100 = 0.9044 or 90.44%

Flow rate of NaOH in the dried solids = 100 – 90.44 = 9.56 lb/h
Therefore, the wt% NaOH in the dried solids = 9.56/(9.56 + 5,000) = 0.00191 or 0.191 wt%.

If a third washing stage is added, the three mass balance equations for NaOH are:

Stage 1: $20{,}000\ y_2 + 100 = 20{,}000\ y_1 + 95{,}000\ y_1$
Stage 2: $20{,}000\ y_3 + 20{,}000\ y_1 = 20{,}000\ y_2 + 20{,}000\ y_2$
Stage 3: $0 + 20{,}000\ y_2 = 20{,}000\ y_3 + 20{,}000\ y_3$

Solving these three linear equations, $y_1 = x_1 = 0.000984$
$y_2 = x_2 = 0.000656$
$y_3 = x_3 = 0.000328$

The % recovery of NaOH in the extract = (95,000)(0.000984)/100 = 0.9348 or 93.48%

The lb/h NaOH in the dry solids = 100 – 93.48 = 6.52 lb/h
The wt% NaOH in the dry solids = 6.52/(6.52 + 5,000) = 0.00130 or 0.130 wt%

The use of three stages does give a significantly increased recovery of NaOH or a significantly increased purity of $CaCO_3$.

Exercise 16.4

Subject: Recovery of zinc from a ZnS ore by oxidizing the ZnS to ZnO, followed by leaching with aq. H_2SO_4 to produce a decanted sludge of water soluble $ZnSO_4$ and insoluble residue called gangue.

Given: 20,000 kg/h of decanted sludge, consisting of 5 wt% water, 10 wt% $ZnSO_4$, and 85 wt% gangue. A leaching stage and a continuous, countercurrent washing system, using wash water to produce an extract (strong solution) of 10 wt% $ZnSO_4$ in water with a $ZnSO_4$ recovery of 98%.

Assumptions: Each underflow consists of two parts of water ($ZnSO_4$-free basis) per part gangue. No solids in the overflows. Liquid in the underflow and liquid in the overflow leaving a stage have the same composition.

Find: The number of stages

Analysis: Because the underflow liquid is given as a mass ratio of $ZnSO_4$-free water to the solid gangue in the underflow, use $ZnSO_4$ compositions in the liquid as mass ratios, X, to water, and liquid flow rates on a $ZnSO_4$-free basis.

Let: Y_i = mass ratio of $ZnSO_4$ to water in the overflow from Stage i
X_i = mass ratio of $ZnSO_4$ to water in the underflow from Stage i
V_i = kg/h of water in the overflow from Stage i
L_i = kg/h of water in the underflow from Stage i
S = kg/h of wash water entering the last stage

Decanted sludge consists of:
0.05(20,000) = 1,000 kg/h of water
0.10(20,000) = 2,000 kg/h of $ZnSO_4$
0.85(20,000) = 17,000 kg/h of solid gangue

$ZnSO_4$ in the extract = 0.98(2,000) = 1,960 kg/h
Water in the extract of 90% water = (9/1)(1,960 = 17,640 kg/h
Final underflow is: 17,000 kg/h of gangue
2(17,000) = 34,000 kg/h of water
2,000 – 1,960 = 40 kg/h of soluble $ZnSO_4$

By overall water mass balance, flow rate of wash water = 34,000 + 17,640 – 1,000 = 50,640 kg/h
Use (16-8) of the McCabe-Thiele algebraic method to determine the number of stages. That equation is in terms of mass fractions, but it also applies to the use of mass ratios. Thus,

$$N = \frac{\log\left[\dfrac{X_N - Y_{N+1}}{Y_L - Y_1}\right]}{\log\left(\dfrac{L}{V}\right)} \qquad (1)$$

where the subscripts on the symbols refer to Figure 16.7. Thus, the countercurrent system consists of one leaching stage, L, and N washing stages for a total of N+1 stages.

Exercise 16.4 (continued)

From the calculations above, $X_N = 40/34{,}000 = 0.001176$

Also, $Y_{N+1} = 0$
$Y_L = 10/90 = 0.1111$
$S = 17{,}000$ kg/h leaving each stage
Therefore, $L = 2(17{,}000) = 34{,}000$ kg/h, constant from each stage
And, by mass balance for each washing stage, $V = 50{,}640$ kg/h, a constant

Obtain Y_1 by a $ZnSO_4$ mass balance around just the leaching stage, L:

$$Y_1V_1 + 2{,}000 = 1{,}960 + X_LL_L$$

But, $V_1 = V$, $L_L = L$, and $X_L = Y_L$, and therefore,

$$Y_1(50{,}640) + 2{,}000 = 1{,}960 + 0.1111(34{,}000)$$

Solving, $Y_1 = 0.0738$

Now apply (1) to calculate the number of washing stages:

$$N = \frac{\log\left[\dfrac{0.001176 - 0}{0.1111 - 0.0738}\right]}{\log\left(\dfrac{34{,}000}{50{,}640}\right)} = 8.7$$

Therefore, need 9 ideal washing stages plus a leaching stage or 10 stages total.

Exercise 16.5

Subject: Leaching of oil from flaked soybeans with n-hexane in a continuous, countercurrent system consisting of a leaching stage and three washing stages.

Given: 50,000 kg/h of flaked soybeans containing 20 wt% oil and 80 wt% insoluble solids. 50,000 kg/h of n-hexane solvent for washing. From experiments, all underflows contain 0.8 kg of liquid/kg of oil-free soybeans.

Assumptions: No solids in the overflows. Liquid in the underflow and liquid in the overflow leaving a stage have the same composition.

Find: (a) The % recovery of oil in the final extract, if all leaching takes place in the leaching stage.

(b) The % recovery of oil in the final extract, if leaching takes 3 of the total of 4 stages, with the amount of leaching divided equally among the three stages.

Analysis: Because the underflow basis is on total liquid (not just the hexane), use mass fractions to express the oil composition in the overflow and in the liquid in the underflow.

Let: y_i = mass fraction of oil in the overflow from Stage i
x_i = mass fraction of oil in the underflow from Stage i
V_i = kg/h of liquid in the overflow from Stage i
L_i = kg/h of liquid in the underflow from Stage i
S = kg/h of fresh n-hexane entering the last stage

(a) This part can be solved from oil mass balances around each stage or by applying (16-8) of the McCabe-Thiele algebraic method. In either method: (1) the flowsheet of Figure 16.7 applies with a leaching stage, L, and N = 3 washing stages; and (2) the leaching stage is computed separately. Solve with (16-8).

For both methods, 40,000 kg/h of insoluble solids appear in each underflow.
Therefore, all $L = 0.8(40{,}000) = 32{,}000$ kg/h.
The total final underflow = 40,000 + 32,000 = 72,000 kg/h
The total flow rate of flaked soybeans = 50,000 kg/h
The flow rate of entering n-hexane solvent = 50,000 kg/h

Therefore, by overall total mass balance, $V_L = 50{,}000 + 50{,}000 - 72{,}000 = 28{,}000$ kg/h
However, since all $L = 32{,}000$ kg/h, total mass balances around each washing stage give:

$V = 50{,}000$ kg/h for all stages except the overflow leaving the leaching stage.

Oil mass balance around the leaching stage:

$$y_1V_1 + 10{,}000 = y_LV_L + x_LL_L$$

or, since $x_L = y_L$, $\quad y_1(50{,}000) + 10{,}000 = y_L(28{,}000) + y_L(32{,}000) = y_L(60{,}000)$ (1)

Because there are two unknowns, we cannot compute y_L. We need more equations.
A total oil mass balance around all stages gives:

$$10{,}000 + 0 = x_3(32{,}000) + y_L(28{,}000) \quad (2)$$

Exercise 16.5 (continued)

From (16-8),

$$N = \frac{\log\left[\dfrac{x_3 - y_{N+1}}{y_L - y_1}\right]}{\log\left(\dfrac{L}{V}\right)}$$

or, $3 = \dfrac{\log\left[\dfrac{x_3 - 0}{y_L - y_1}\right]}{\log\left(\dfrac{32{,}000}{50{,}000}\right)}$ or rearranging, $\dfrac{x_3}{y_L - y_1} = 10^{3\log(0.64)} = 0.262$ (3)

Equations (1) to (3) are three linear equations in three unknowns: y_1, y_L, and x_3
Solving with Polymath,

$$y_1 = 0.1794, \quad y_L = 0.3162, \quad x_3 = 0.03585$$

Oil in the final extract = $y_L V_L$ = 0.3162(28,000) = 8,854 kg/h
The % recovery of oil = 8,854/10,000 = 0.8854 or 88.54%

(b) We cannot use (16-8) for this part because the leaching is divided equally among the leaching stage and the first 2 washing stages. Until the oil is leached, it is part of the solid. However, because the underflow from each stage is given as 0.8 kg liquid/kg of oil-free soybeans, values of V and L remain the same as in Part (a) and $x_i = y_i$ still applies.

Write oil mass balances for each stage, using the nomenclature of Figure 16.7, noting that the following flow rates apply for unleached oil in the underflows:

10,000 – (1/3)(10,000) = 6, 667 kg/h to Stage 1
6,667 – (1/3)(10,000) = 3,333 kg/h to Stage 2
3,333 – (1/3)(10,000) = 0 kg/h to Stage 3

Stage L: $y_1V_1 + 10{,}000 = y_LV_L + x_LL_L + 6{,}667$
or, $y_1(50{,}000) + 10{,}000 = y_L(28{,}000) + y_L(32{,}000) + 6{,}667$ (4)
Stage 1: $y_2V_2 + x_LL_L + 6{,}667 = y_1V_1 + x_1L_1 + 3{,}333$
or, $y_2(50{,}000) + y_L(32{,}000) + 6{,}667 = y_1(50{,}000) + y_1(32{,}000) + 3{,}333$ (5)
Stage 2: $y_3V_3 + x_1L_1 + 3{,}333 = y_2V_2 + x_2L_2$
or, $y_3(50{,}000) + y_1(32{,}000) + 3{,}333 = y_2(50{,}000) + y_2(32{,}000)$ (6)
Stage 3: $0 + x_2L_2 = y_3V_3 + x_3L_3$
or, $y_2(32{,}000) = y_3(50{,}000) + y_3(32{,}000)$ (7)

Solving linear Equations (4) to (7) with Polymath for the four unknowns of y_L, y_1, y_2, and y_3,

$y_L = 0.2736$, $y_1 = 0.2616$, $y_2 = 0.1873$, $y_1 = 0.0731$

Therefore % recovery of oil to the final extract = 0.2736(28,000)/10,000 = 0.766 or 76.6%

Exercise 16.6

Subject: Leaching and washing of Na_2CO_3 from a solid mixture with insoluble solids in a continuous, countercurrent system.

Given: 100 tons/h of feed of 20 wt% water-soluble Na_2CO_3 and 80 wt% insoluble solids. Final extract contains 15 wt% solute. Recovery of solute is 98%. Underflow contains 0.5 lb solution/lb insoluble solids. Washing is with pure water.

Assumptions: One ideal leaching stage. No solids in the overflows. Liquid in the underflow and liquid in the overflow leaving a stage have the same composition.

Find: Number of ideal washing stages required.

Analysis: First compute the overall mass balance from the given data:

Feed is 20 tons/h of Na_2CO_3 and 80 tons/h insoluble solids.

Final extract contains 0.98(20) = 19.6 tons/h of Na_2CO_3.

Water rate in final extract = (85/15)19.6 = 111.1 tons/h

Final underflow contains 20 -19.6 = 0.4 tons/h, 80 tons/h of insoluble solids, and 0.5(80) = 40 tons/h of solution. The solution contains 40 – 0.4 = 39.6 tons/h of water.

By overall water balance, the fresh wash water flow rate = 111.1 + 39.6 = 150.7 tons/h

Summary of overall mass balance in tons/h:

Component	Feed	Wash Water	Final Underflow	Final Extract
Na_2CO_3	20.0		0.4	19.6
Insolubles	80.0		80.0	
Water		150.7	39.6	111.1
Total	100.0	150.7	120.0	130.7

Because the underflow basis is on total liquid (not just the water), use mass fractions to express the Na_2CO_3 composition in the overflow and in the liquid in the underflow.

Let: y_i = mass fraction of Na_2CO_3 in the overflow from Stage i

x_i = mass fraction of Na_2CO_3 in the underflow from Stage i

V_i = tons/h of liquid in the overflow from Stage i

L_i = tons/h of liquid in the underflow from Stage i

All flow rates of L = 40 tons/h and by total mass balance around each washing stage, all V = 150.7 tons/h. Also, $y_i = x_i$. Also for the last washing stage, $x_N = 0.4/40 = 0.01$

Calculate the leaching stage by a Na_2CO_3 mass balance, referring to Figure 16.7:

$$20 + y_1 V_1 = 19.6 + x_L(40)$$

$$\text{or,}\quad 20 + y_1(150.7) = 19.6 + 0.15(40)$$

Solving, $y_1 = 0.0372$

From (16-8),
$$N = \frac{\log\left[\dfrac{x_N - y_{N+1}}{y_L - y_1}\right]}{\log\left(\dfrac{L}{V}\right)} = \frac{\log\left[\dfrac{0.01-0}{0.150-0.0372}\right]}{\log\left(\dfrac{40}{150.7}\right)} = 1.8 \text{ or 2 washing stages}$$

Exercise 16.7

Subject: Production of pure, insoluble TiO_2 by leaching and washing soluble impurities with water in a continuous, countercurrent system.

Given: Feed contains 50 wt% TiO_2, 20 wt% soluble salts, and 30 wt% water. Final product after filtering and drying is 200,000 kg/h of 99.9 wt% TiO_2. Pure wash water flow rate = feed flow rate on a mass-flow basis.

Assumptions: One ideal leaching stage. No solids in the overflows. Liquid in the underflow and liquid in the overflow leaving a stage have the same composition.

Find: (a) Number of washing stages if the underflow from each stage = 0.4 kg solution/kg TiO_2.

(b) Number of washing stages if the underflow from each stage in terms of retention of solution to solid TiO_2 in underflow depends on concentration of solutes/kg solution as follows (note the linear relationship):

Solute Concentration, kg solutes/kg solution	**Retention of Solution, kg solution/kg TiO_2**
0.0	0.30
0.2	0.34
0.4	0.38
0.6	0.42

Analysis: Because the underflow basis is on total liquid (not just the water), use mass fractions to express the solutes composition in the overflow and in the liquid in the underflow.

Let: y_i = mass fraction of solutes in the overflow from Stage i

x_i = mass fraction of solutes in the underflow from Stage i

V_i = kg/h of liquid in the overflow from Stage i

L_i = kg/h of liquid in the underflow from Stage i

(a) First compute the overall mass balance:

Final underflow from Stage N is 0.999(200,000) = 199,800 kg/h of TiO_2 and 200 kg/h of solutes. Solution in the final underflow = 0.4(199,800) = 79,920 kg/h. Water in the final underflow = 79,920 – 200 = 79,720 kg/h. Therefore, x_N = 200/79,920 = 0.00250.

Feed to the system is 199,800 kg/h TiO_2, (20/50)199,800 = 79,920 kg/h of solutes, and (30/50)199,800 = 119,880 kg/h of water.

Fresh water flow rate = total feed flow rate = 199,800 + 79,920 + 119,880 = 399,600 kg/h

Therefore, by overall mass balances,

Water in final extract = 119,880 + 399,600 – 79,720 = 439,660 kg/h

Solutes in final extract = 79,920 -200 = 79,720 kg/h

Summary of overall mass balance in kg/h:

Component	**Feed**	**Wash Water**	**Final Underflow**	**Final Extract**
TiO_2	199,800		199,800	
Solutes	79,920		200	79,720
Water	119,880	399,600	79,720	439,760
Total	399,600	399,600	279,720	519,480

Exercise 16.7 (continued)

Referring to Figure 16.7, all underflow liquid flow rates = L = 79,920 kg/h. All overflow liquid flow rates, except for the leaching stage = V = 399,600 kg/h. $x_L = y_L$ = 79,720/519,480 = 0.153. Calculate the solute mass balance for just the leaching stage:

$$79{,}920 + y_1 V_1 = 79{,}720 + x_L(79{,}920)$$

or, $$79{,}920 + y_1(399{,}600) = 79{,}720 + 0.153(79{,}920)$$

Solving, $y_1 = 0.0301$

From (16-8), $$N = \frac{\log\left[\frac{x_N - y_{N+1}}{y_L - y_1}\right]}{\log\left(\frac{L}{V}\right)} = \frac{\log\left[\frac{0.00250 - 0}{0.153 - 0.0301}\right]}{\log\left(\frac{79{,}920}{399{,}600}\right)} = 2.4$$ or 3 washing stages

Therefore, need 1 ideal leaching stage and 3 ideal washing stages.

(b) Because the flow rate of liquid in the underflow depends on the solute concentration and, therefore, varies from stage to stage, we can not apply the McCabe-Thiele algebraic method used in Part (a). Instead, we must set up solute mass balances for each washing stage. The relationship between the retention of solution on the solids = R_i in kg solution/kg TiO_2 and the mass fraction, x_i, of solutes/kg solution is linear and we can develop the following equation from the given data in the above table:

$$R_i = 0.2\, x_i + 0.30 \qquad (1)$$

First compute the overall mass balance:

Final underflow from Stage N is 0.999(200,000) = 199,800 kg/h of TiO_2 and 200 kg/h of solutes. From Part (a), the final underflow will likely have a $x_N < 0.01$. Therefore, let R_N = 0.3. Therefore, solution in the final underflow = 0.3(199,800) = 59,940 kg/h. Water in the final underflow = 59,940 – 200 = 59,740 kg/h. Therefore, x_N = 200/59,940 = 0.00334 is the target.

Feed to the system is 199,800 kg/h TiO_2, (20/50)199,800 = 79,920 kg/h of solutes, and (30/50)199,800 = 119,880 kg/h of water.

Fresh water flow rate = total feed flow rate = 199,800 + 79,920 + 119,880 = 399,600 kg/h

Therefore, by overall mass balances,

Water in final extract = 119,880 + 399,600 – 59,740 = 439,660 kg/h

Solutes in final extract = 79,920 - 200 = 79,720 kg/h

Summary of overall mass balance in kg/h:

Component	Feed	Wash Water	Final Underflow	Final Extract
TiO_2	199,800		199,800	
Solutes	79,920		200	79,720
Water	119,880	399,600	59,740	459,740
Total	399,600	399,600	259,740	539,460

Refer to Figure16.7. Calculate the leaching stage. $x_L = y_L$ = 79,720/539,460 = 0.148.

A solute mass balance gives:

$$79{,}920 + y_1 V_1 = 79{,}720 + x_L L_L$$

or, $$y_1 V_1 = -200 + 0.148 L_L \qquad (2)$$

Exercise 16.7 (continued)

A solution mass balance gives:

$$V_1 + 79{,}920 + 119{,}800 = L_L + 79{,}720 + 459{,}460$$

$$\text{or,} \quad V_1 = L_L + 339{,}460 \qquad (3)$$

We have 2 equations in 3 unknowns. However, from (1),

$$R_L = L_L/199{,}800 = 0.2\, x_L + 0.3 = 0.2(0.148) + 0.3 = 0.3296$$

$$\text{or,} \quad L_L = 65{,}850 \text{ kg/h}$$

From (3), $V_1 = 65{,}850 + 339{,}460 = 405{,}310$ kg/h

From (2), $y_1 = [-200 + 0.148(65{,}850)]/405{,}310 = 0.0236 = x_1$

Now compute Stage 1:

From (1), $R_1 = L_1/199{,}800 = 0.2x_1 + 0.3 = 0.2(0.0236) + 0.3 = 0.3047$

Therefore, $L_1 = 60{,}880$ kg/h

From a liquid flow balance around Stage 1, $L_L + V_2 = L_1 + V_1$

or, $V_2 = 60{,}880 + 405{,}310 - 65{,}850 = 400{,}340$ kg/h

From a solute balance around Stage 1, $x_L L_L + y_2 V_2 = x_1 L_1 + y_1 V_1$

or, $y_2 = [0.0236(60{,}880) + 0.0236(405{,}310) - 0.148(65{,}850)]/400{,}340 = 0.00314$

Therefore, $x_2 = y_2 = 0.00314$

But, x_2 is already below the target of 0.00334. Therefore, 2 washing stages is sufficient together with the leaching stage or a total of 3 stages.

Exercise 16.8

Subject: Rate of leaching of solute from a flake when the internal resistance to mass transfer is negligible, such that mass transfer is controlled by the external resistance of the solvent.

Find: Derive Equation (16-20)

Analysis: For diffusion from either side of a flake when the rate of mass transfer is controlled by the external resistance, (16-13), gives for mass-transfer from the surface of the solid to the solvent surrounding the solid,

$$n_i = k_c A\left[\left(Y_i\right)_s - \left(Y_i\right)_b\right] \tag{1}$$

where,

n_i = rate of mass transfer of solute from the flake to the solvent, mass/time

k_c = external mass-transfer coefficient on a concentration driving force basis,

A = area for mass transfer at the surface of the flake

$\left(Y_i\right)_s$ = concentration of solute in the solvent at the surface of the flake, mass solute/volume of solvent

$\left(Y_i\right)_b$ = concentration of solute in the bulk of the solvent, mass solute/volume of solvent

Also, let,

$\left(X_i\right)$ = concentration of solute in the solid, mass solute/volume of flake

$\left(X_i\right)_o$ = initial concentration of solute in the solid, mass solute/volume of flake

Because the mass-transfer resistance of the solid is negligible, values of $\left(X_i\right)$ stay uniform throughout the solid, but decrease with time, t.

Let the equilibrium ratio for the solute concentration between the flake and solvent be,

$$Y_i = mX_i \tag{2}$$

Combining (1) and (2),

$$n_i = k_c A\left[X_i - \left(Y_i\right)_b\right] \tag{3}$$

A differential mass balance on the solute is given by,

$$n_i = -Aa\frac{dX_i}{dt} \tag{4}$$

Where, a = the half thickness of the slice

Combining (3) and (4), and separating variables,

$$\frac{dX_i}{X_i - \dfrac{\left(Y_i\right)_b}{m}} = -\frac{k_c m}{a}dt \tag{5}$$

Integrating between the limits of $(X_i)_o$ at $t = 0$ and X_i at $t = t$,

$$\ln\left[\frac{X_i - \dfrac{\left(Y_i\right)_b}{m}}{\left(X_i\right)_o - \dfrac{\left(Y_i\right)_b}{m}}\right] = -\frac{k_c m t}{a} \quad \text{or} \quad \frac{X_i - \dfrac{\left(Y_i\right)_b}{m}}{\left(X_i\right)_o - \dfrac{\left(Y_i\right)_b}{m}} = \exp\left(-\frac{k_c m t}{a}\right) \quad \text{which is (16-20)}$$

Exercise 16.9

Subject: Rate of leaching of solute from a cossette when the external resistance to mass transfer is negligible, such that mass transfer is controlled by the internal resistance of the solid.

Find: Derive Equation (16-24)

Analysis: Treat the cossette as an infinite slab and ignore mass transfer from assumed thin edges. For diffusion from both sides of the slab when the rate of mass transfer is controlled by the internal resistance, with a Fourier number for mass transfer, $\left(N_{\mathrm{Fo}}\right)_M = \dfrac{D_e t}{a^2}$, (16-21) applies,

$$\ln E_{\mathrm{avg_{slab}}} = \ln\left(\frac{8}{\pi^2}\right) - \frac{\pi^2}{4}\left(N_{\mathrm{Fo}}\right)_M \tag{1}$$

where,

D_e = effective diffusivity for the solute in the solid

t = time

a = half thickness of solid

$E_{\mathrm{avg_{slab}}}$ = fractional unaccomplished approach to equilibrium for leaching, which decreases with time

From (16-22), the time for leaching is given by,

$$t = \int_{E_{\mathrm{in}}}^{E_{\mathrm{out}}} \frac{dE}{\left(\dfrac{dE}{dt}\right)} \tag{2}$$

Differentiating (1), using the definition of the Fourier number for mass transfer, gives,

$$\frac{dE}{dt} = -\frac{\pi^2 D_e E}{4a^2} \tag{3}$$

Separating variables and integrating (3),

$$t = -\int_{E_{\mathrm{in}}}^{E_{\mathrm{out}}} \frac{4a^2 dE}{\pi^2 D_e E} = -\frac{4a^2}{\pi^2 D_e}\left[\ln\left(\frac{E_{\mathrm{out}}}{E_{\mathrm{in}}}\right)\right] \tag{4}$$

Rearranging (4) gives,

$$t = \frac{4a^2}{\pi^2 D_e}\left[\ln\left(\frac{E_{\mathrm{in}}}{E_{\mathrm{out}}}\right)\right] \qquad \text{which is (16-24)}$$

Exercise 16.10

Subject: Determination, from a set of experimental data for leaching of oil from soybeans by n-hexane, of the effective diffusivity to determine if it is constant with time

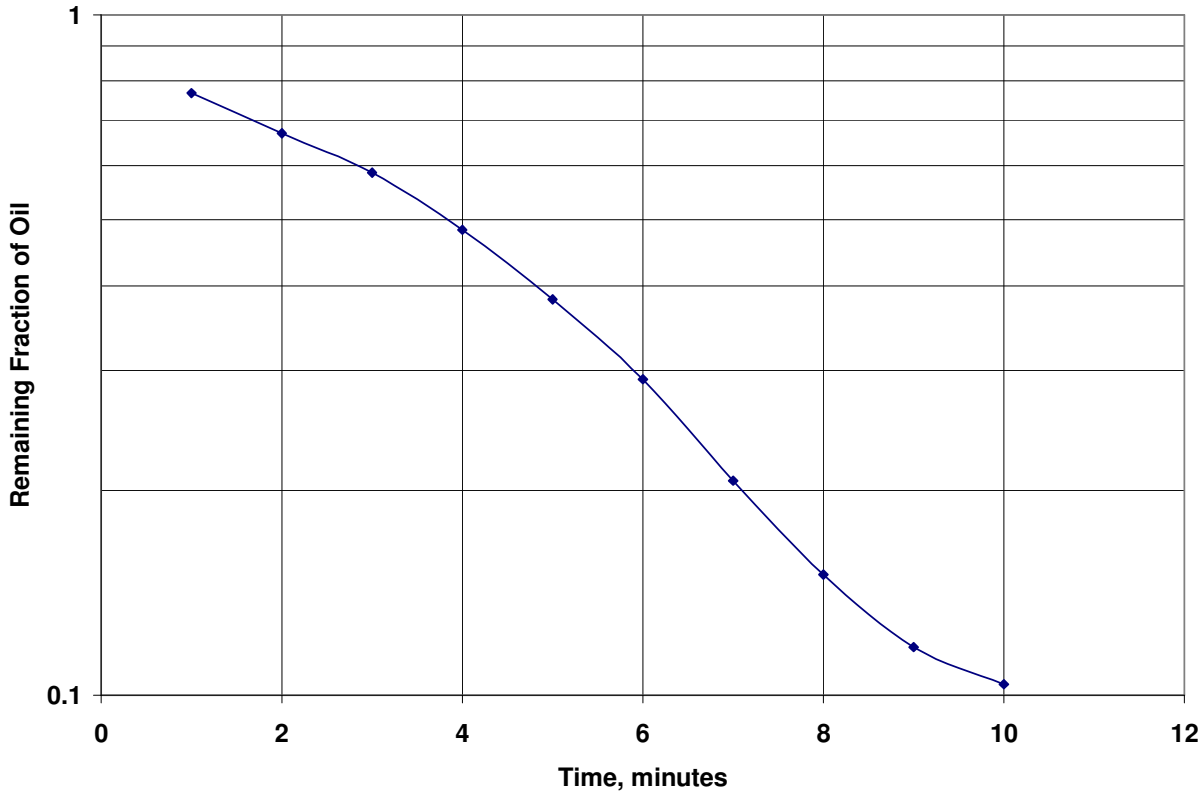
Given: A table of data for the average oil content of soybeans with respect to time

Assumptions: Effective diffusivity is constant

Find: Determine whether the effective diffusivity is constant

Analysis: According to (16-21), if $\left(N_{\mathrm{Fo}}\right)_M = \dfrac{D_e t}{a^2} > 0.10$, a plot of $\ln E_{\mathrm{avg_{slab}}}$ versus t should be a straight line with a slope of $-\dfrac{\pi^2 D_e}{4a^2}$, if D_e is a constant.

A plot of the data, using a spreadsheet is as shown below, where it is seen that a straight line is not obtained. Therefore, the effective diffusivity is not constant.



Exercise 16.11

Subject: Estimation of the molecular diffusivity of sucrose in water at infinite dilution at 80°C.

Given: Value of the molecular diffusivity of 0.54 x 10^{-5} cm^2/s at 25°C.

Assumptions: Applicability of the Wilke-Chang equation (3-39)

Find: The diffusivity value at 80°C and compare it to the value given in Example 16.6.

Analysis: From (3-9), D_{AB} is proportional to $\dfrac{T \text{ in K}}{\mu_{H_2O}}$

Therefore, estimated $D_{AB_{80^\circ C}} = 0.54\times10^{-5}\left(\dfrac{273+80}{273+25}\right)\left(\dfrac{0.89 \text{ cP at } 25^\circ C}{0.35 \text{ cP at } 80^\circ C}\right) = 1.63\times10^{-5}$

However, in Example 16.6, the diffusivity value is given as 1.1×10^{-6} or 0.11×10^{-5} cm^2/s

This is more than an order-of-magnitude less than the estimated value.

A possible explanation for the difference is that in Example 16.6, we don't have the diffusion of sucrose in water, but we have the diffusion of sucrose through water and insoluble fiber, where the fibers may offer an enhanced resistance to molecule movement.

Exercise 16.12

Subject: Time to leach 95% of the sucrose from ground coffee particles with water at 25°C.

Given: Coffee particles of average diameter = 2 mm. Diffusivity of sucrose in the particles = 1.0 x 10^{-6} cm^2/s.

Assumptions: Leaching is controlled by internal mass transfer in the particles. Particles are spheres. If $N_{Fo} > 0.10$,

$$E_{avg} = \frac{6}{\pi^2}\exp\left(\frac{-\pi^2 D_e t}{a^2}\right) \qquad (1)$$

Find: Time to leach 95% of the sucrose.

Analysis: a = particle radius = 1 mm = 0.1 cm.
Want $E_{avg} = 1 - 0.95 = 0.05$
Rearranging (1) and using cgs units,

$$t = \frac{a^2}{\pi^2 D_e}\ln\left(\frac{6}{\pi^2 E_{avg}}\right) = \frac{0.1^2}{3.14^2\left(1\times10^{-6}\right)}\ln\left[\frac{6}{3.14^2\left(0.05\right)}\right] = 2{,}530 \text{ s} = 42.2 \text{ min}$$

Check the Fourier number for mass transfer to see if (1) is valid.

$$N_{Fo} = \frac{D_e t}{a^2} = \frac{1\times10^{-6}\left(2530\right)}{0.1^2} = 0.25 \text{ which is} > 0.10$$ Therefore, (1) is valid.

Exercise 16.13

Subject: Effect of particle size on the leaching of CuO from copper ore by sulfuric acid in Example 16.8, using the shrinking-core model.

Given: Particles ranging in size from 0.5 mm to 50 mm (or 0.05 to 5.0 cm). Data from Example 16.8.

Assumptions: Applicability of the shrinking-core model. CuO is uniformly distributed in the particles. Pseudo-steady-state assumption is valid.

Find: Effect of particle size on leaching time for 98% of the Cu.

Analysis: Equation (16-34) is applied:

$$t = \frac{\rho_B r_s^2}{6 D_e b M_B c_{A_b}} \left[1 - 3\left(\frac{r_c}{r_s}\right)^2 + 2\left(\frac{r_c}{r_s}\right)^3 \right] \tag{1}$$

where, the leaching reaction is assumed to be that of Eq. (1) in Example 16.8.
Using cgs units and data from Example 16.8, the symbols are:

t = time in s
ρ_B = mass of CuO per volume of ore = 0.054 g/cm^3
r_s = radius of particle in cm
r_c/r_s = radius ratio corresponding to 2% of the particle volume = $(0.02)^{1/3}$ = 0.271
D_e = effective diffusivity of the hydrogen ion of the H_2SO_4 = 0.6 x 10^{-6} cm^2/s
b = stoichiometric coefficient of the solid reactant, CuO in Eq. (1) of Example 16.8 = 0.5
M_B = molecular weight of CuO = 79.6
c_{A_b} = concentration of H^+ in bulk fluid = 0.001 mol/cm^3

Substituting these values into (1), gives:

$$t = 376{,}900 r_s^2 \left[0.819\right] \tag{2}$$

Calculations for particle diameters of 0.05, 0.5, and 5 cm give the following results:

Particle diameter, cm	0.05	0.5	5.0
Time, seconds	193	19,300	1,930,000

All values are consistent with the assumption of a pseudo-steady-state necessary for the validity of Eq. (1), as shown in Example 16.8.

Exercise 16.14

Subject: Effect of % recovery of copper on the leaching of CuO from copper ore by sulfuric acid in Example 16.8, using the shrinking-core model.

Given: Particles of 10 mm (1.0 cm) in diameter. Data from Example 16.8.

Assumptions: Applicability of the shrinking-core model. CuO is uniformly distributed in the particles. Pseudo-steady-state assumption is valid.

Find: Effect of % recovery over the range of 50 to 100% of Cu on leaching time.

Analysis: Equation (16-34) is applied:

$$t = \frac{\rho_B r_s^2}{6 D_e b M_B c_{A_b}} \left[1 - 3\left(\frac{r_c}{r_s}\right)^2 + 2\left(\frac{r_c}{r_s}\right)^3 \right] \tag{1}$$

where, the leaching reaction is assumed to be that of Eq. (1) in Example 16.8.
Using cgs units and data from Example 16.8, the symbols are:

t = time in s
ρ_B = mass of CuO per volume of ore = 0.054 g/cm^3
r_s = radius of particle in cm
r_c/r_s = radius ratio corresponding to 50 to 100% of the particle volume = (1 – fraction recovered)$^{1/3}$
D_e = effective diffusivity of the hydrogen ion of the H_2SO_4 = 0.6 x 10^{-6} cm^2/s
b = stoichiometric coefficient of the solid reactant, CuO in Eq. (1) of Example 16.8 = 0.5
M_B = molecular weight of CuO = 79.6
c_{A_b} = concentration of H^+ in bulk fluid = 0.001 mol/cm^3

Substituting these values into (1), gives:

$$t = 94,200 \left[1 - 3\left(\frac{r_c}{r_s}\right)^2 + 2\left(\frac{r_c}{r_s}\right)^3 \right] \tag{2}$$

Calculations for % recoveries of 50, 70, 90, and 100% give the following results:

% Recovered	[1 – fraction recovered]$^{1/3}$	Time, s
50	0.7937	10,380
70	0.6694	24,080
90	0.4642	52,170
100	0.0000	94,200

Exercise 16.15

Subject: Recovery of copper by the leaching of Cu_2O from copper ore with sulfuric acid, by the method of Example 16.8, using the shrinking-core model.

Given: Particles of 10 mm (1.0 cm) in diameter and an ore with 3 wt% Cu_2O instead of 2 wt% CuO as in Example 16.8. Other data from Example 16.8.

Assumptions: Applicability of the shrinking-core model. Cu_2O is uniformly distributed in the particles. Pseudo-steady-state assumption is valid.

Find: Time for 98% leaching of the copper.

Analysis: Equation (16-34) is applied:

$$t = \frac{\rho_B r_s^2}{6 D_e b M_B c_{A_b}} \left[1 - 3\left(\frac{r_c}{r_s}\right)^2 + 2\left(\frac{r_c}{r_s}\right)^3 \right] \qquad (1)$$

where, the leaching reaction is now: $\frac{1}{2}Cu_2O_{(s)} + H^+_{(aq)} = Cu^+_{(aq)} + \frac{1}{2}H_2O_{(l)}$

Using cgs units and data from Example 16.8, the symbols are:

t = time in s

ρ_B = mass of Cu_2O per volume of ore = 0.03(2.7) = 0.081 g/cm^3

r_s = radius of particle in 0.5 cm

r_c/r_s = radius ratio corresponding to 98% of the particle volume = (1 – fraction recovered)$^{1/3}$ = (1 – 0.98)$^{1/3}$ = 0.271

D_e = effective diffusivity of the hydrogen ion of the H_2SO_4 = 0.6 x 10^{-6} cm^2/s

b = stoichiometric coefficient of the solid reactant, Cu_2O in Eq. (1) of Example 16.8 = 0.5

M_B = molecular weight of Cu_2O = 143.14

c_{A_b} = concentration of H^+ in bulk fluid = 0.001 mol/cm^3

The only changes from Example 16.8 are ρ_B and M_B. Therefore, instead of using Eq. (1), we can just ratio from the result in Example 16.8. Therefore,

$$t = 21.4 \text{ hours} \left(\frac{0.081}{0.054}\right)\left(\frac{79.6}{143.14}\right) = 17.9 \text{ hours}$$

Exercise 16.16

Subject: Leaching of a spherical particle where the rate is controlled by a first-order reaction at the interface of the shrinking core.

Given: Spherical particle with a shrinking core as leaching proceeds.

Find: Derive the expression:

$$t = \frac{\rho_B r_s^2}{bM_B kc_{A_b}}\left(1 - \frac{r_c}{r_s}\right) \tag{1}$$

Analysis:

The reaction occurs at the outer boundary of the shrinking core at $r = r_c$, where the initial radius of the particle is r_s. The rate of reaction is

$$\text{Rate} = -kc_{A_b}\left(4\pi r_c^2\right) \tag{2}$$

where the term in parentheses is the surface area at the outer boundary of the shrinking core.

The rate of reaction is also given by a mass balance on the shrinking core:

$$\text{Rate} = \frac{\rho_B}{bM_B}\left(4\pi r_c^2\right)\frac{dr}{dt} \tag{3}$$

Equating (2) and (3) and separating variables, followed by integration, gives:

$$\frac{-\rho_B}{bM_B kc_{A_b}}\int_{r_s}^{r_c} dr = \int_0^t dt \tag{4}$$

Integrating (4) and rearranging the result gives (1).

Exercise 17.1

Subject: Estimation of sphericities

Given: (a) a cylindrical needle with height = 5 times the diameter.
(b) a rectangular prism of sides a, $2a$, and $3a$.

Find: The sphericities

Analysis: The sphericity, ψ, is defined by (17-1) and (17-2):

$$\psi = \frac{\text{surface area of a sphere of same volume as the particle}}{\text{surface area of particle}} = \frac{6}{D_p}\left(\frac{V_{\text{particle}}}{S_{\text{particle}}}\right) \qquad (1)$$

(a) Let the diameter of the needle be D and the height be $H = 5D$

The volume of the needle = $V_{\text{needle}} = \dfrac{\pi D^2 H}{4} = \dfrac{\pi D^2 (5D)}{4} = \dfrac{5\pi D^3}{4}$

The surface area of the needle = $S_{\text{needle}} = \pi DH + 2\left(\dfrac{\pi D^2}{4}\right) = \pi D(5D) + \dfrac{\pi D^2}{2} = \dfrac{11}{2}\pi D^2$

Substitution into (1), gives: $\psi = \dfrac{6}{D_p}\dfrac{\left(\frac{5\pi D^3}{4}\right)}{\left(\frac{11}{2}\pi D^2\right)} = \dfrac{15}{11}\dfrac{D}{D_p}$ (2)

From the definition of the sphericity, $V_{\text{needle}} = V_{\text{sphere}}$ or $\dfrac{5\pi D^3}{4} = \dfrac{\pi D_p^3}{6}$

Therefore, $\dfrac{D_p}{D} = \left(\dfrac{30}{4}\right)^{1/3} = 1.96$ and from (2), $\psi = \dfrac{15}{11}\left(\dfrac{1}{1.96}\right) = 0.696$

(b) Let the sides of the prism be a, $2a$, and $3a$.

The volume of the prism = $V_{\text{prism}} = a(2a)(3a) = 6a^3$

The surface area of the prism = $S_{\text{prism}} = 2\left[(a)(2a) + (a)(3a) + (2a)(3a)\right] = 22a^2$

Substitution into (1) gives: $\psi = \dfrac{6}{D_p}\left(\dfrac{6a^3}{22a^2}\right) = \dfrac{36}{22}\left(\dfrac{a}{D_p}\right)$

From the definition of the sphericity, $V_{\text{prism}} = V_{\text{sphere}}$ or $6a^3 = \dfrac{\pi D_p^3}{6}$

Therefore, $\dfrac{D_p}{a} = \left(\dfrac{36}{3.14}\right)^{1/3} = 2.55$ and from (2), $\psi = \dfrac{36}{22}\left(\dfrac{1}{2.25}\right) = 0.727$

Exercise 17.2

Subject: Sphericity of a thin circular plate

Given: Circular plate of thickness, t, and diameter, D, with sphericity, ψ, equal to 0.594

Find: The ratio of t to D.

Analysis: The sphericity, ψ, is defined by (17-1) and (17-2):

$$\psi = \frac{\text{surface area of a sphere of same volume as the particle}}{\text{surface area of particle}} = \frac{6}{D_p}\left(\frac{V_{\text{particle}}}{S_{\text{particle}}}\right) \tag{1}$$

The volume of the plate = $V_{\text{plate}} = \dfrac{\pi D^2 t}{4}$

The surface area of the plate = $S_{\text{plate}} = 2\left(\dfrac{\pi D^2}{4}\right) + \pi D t = \dfrac{\pi D^2}{2} + \pi D t$

Substitution into (1), gives: $\psi = \dfrac{6}{D_p}\dfrac{\left(\dfrac{\pi D^2 t}{4}\right)}{\left(\dfrac{\pi D^2}{2} + \pi D t\right)} = \dfrac{6}{D_p}\left(\dfrac{tD}{2D + 4t}\right)$ (2)

From the definition of the sphericity, $V_{\text{sphere}} = V_{\text{plate}}$ or $\dfrac{\pi D_p^3}{6} = \dfrac{\pi D^2 t}{4}$

Therefore, $D_p^3 = \dfrac{3}{2} D^2 t$ and from (2), $\psi = 0.594 = \dfrac{6}{\left(\dfrac{3}{2} D^2 t\right)^{1/3}}\left(\dfrac{tD}{2D + 4t}\right)$ (3)

Let $R = t/D$ Therefore, $t = RD$
Substitution into (3) gives:

$$0.594 = \frac{6}{\left(\dfrac{3}{2} D^3 R\right)^{1/3}} \frac{RD^2}{(2D + 4RD)} = 5.24\left(\frac{R}{R^{1/3}(2 + 4R)}\right)$$

which can be rewritten as, $0.297 R^{1/3} + 0.594 R^{4/3} - 1.31 = 0$ (4)

Solving (4), a nonlinear equation, with Polymath, for an initial guess of 0.3, $R = t/D = 0.166$

Exercise 17.3

Subject: Differential and cumulative undersize plots of a screen analysis for crystals of sodium thiosulfate.

Given: U.S. Screen analysis.

Assumptions: particles approximate spheres

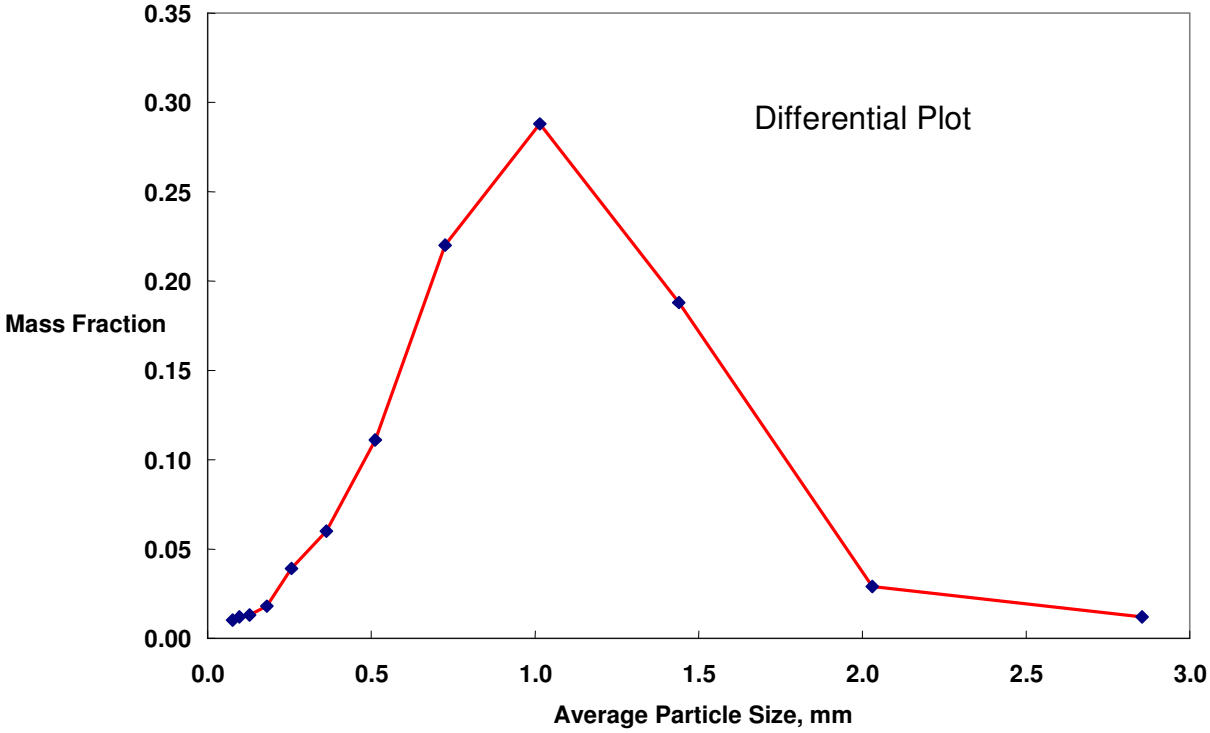
Find: Differential and cumulative undersize plots of the data

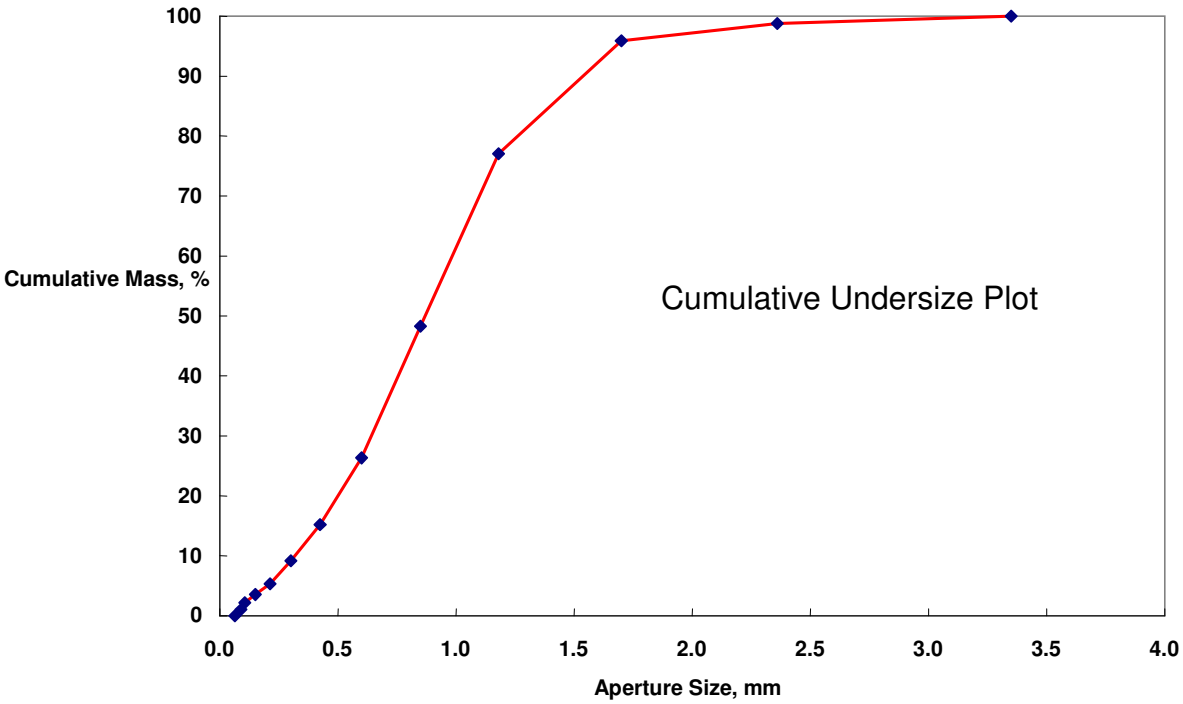
Analysis: Use a spreadsheet with apertures for U.S. Mesh from Table 17.4. Results are as follows with the two plots on the next page. Arithmetic plots are preferred here.

Differential and Cumulative Undersize Screen Analyses

				Differential Analysis		Cumulative Undersize Analysis	
U.S. Mesh Number	Aperture, Dp, mm	Mass retained, grams	% Mass retained	Average Particle Size, mm	Mass Fraction, xi	Aperture, Dp, mm	Cumulative Undersize wt%
6	3.350	0.0	0.00			3.350	100.00
8	2.360	8.8	1.20	2.855	0.0120	2.360	98.80
12	1.700	21.3	2.90	2.030	0.0290	1.700	95.90
16	1.180	138.2	18.80	1.440	0.1880	1.180	77.10
20	0.850	211.6	28.79	1.015	0.2879	0.850	48.31
30	0.600	161.7	22.00	0.725	0.2200	0.600	26.31
40	0.425	81.6	11.10	0.513	0.1110	0.425	15.21
50	0.300	44.1	6.00	0.363	0.0600	0.300	9.21
70	0.212	28.7	3.90	0.256	0.0390	0.212	5.31
100	0.150	13.2	1.80	0.181	0.0180	0.150	3.51
140	0.106	9.6	1.31	0.128	0.0131	0.106	2.20
170	0.090	8.8	1.20	0.098	0.0120	0.090	1.01
230	0.063	7.4	1.01	0.077	0.0101	0.063	0.00
Total		735.0	100.00		1.0000		

Exercise 17.3 (continued)





Exercise 17.4

Subject: Mean particle diameter from a particle-size analysis

Given: Particle-size analysis in terms of the number of particles in each size fraction

Assumptions: All particles have the same shape

Find: Expressions for the surface-mean and mass-mean diameters based on numbers of particles, N_i, rather than mass fractions, x_i, for each size range.

Analysis: It is important to note that regardless of whether the expression is in terms of mass fractions or numbers of particles, the numerical result for the mean diameter is the same.

Surface-mean diameter:

From (17-7), the surface-mean diameter in terms of mass fractions is:

$$\overline{D}_S = \frac{1}{\sum_{i=1}^{n} \frac{x_i}{\overline{D}_{p_i}}} \tag{1}$$

From (17-10), mass fraction is related to number of particles by,

$$x_i = \frac{N_i f_v \left(\overline{D}_{p_i}\right)^3 \rho_p}{M_t} \tag{2}$$

Substituting (2) into (1) gives,

$$\overline{D}_S = \frac{1}{\frac{f_v \rho_p}{M_t} \sum_{i=1}^{n} N_i \overline{D}_{p_i}^2} \tag{3}$$

Summing (2) over all mass fractions gives,

$$\frac{f_v \rho_p}{M_t} = \frac{1}{\sum_{i=1}^{n} N_i \overline{D}_{p_i}^3} \tag{4}$$

Substituting (4) into (3) gives the desired expression for surface-mean diameter:

$$\overline{D}_S = \frac{\sum_{i=1}^{n} N_i \overline{D}_{p_i}^3}{\sum_{i=1}^{n} N_i \overline{D}_{p_i}^2}$$

Exercise 17.4 (continued)

Mass-mean diameter:

From (17-8), the mass-mean diameter in terms of mass fractions is:

$$\overline{D}_W = \sum_{i=1}^{n} x_i \overline{D}_{p_i} \tag{5}$$

Substitution of (2) into (5) gives,

$$\overline{D}_W = \frac{f_v \rho_p}{M_t} \sum_{i=1}^{n} N_i \left(\overline{D}_{p_i} \right)^4 \tag{6}$$

Substitution of (4) into (6) gives the desired expression for mass-mean diameter:

$$\overline{D}_W = \frac{\sum_{i=1}^{n} N_i \overline{D}_{p_i}^4}{\sum_{i=1}^{n} N_i \overline{D}_{p_i}^3}$$

It may be noted that expressions for the other two mean diameters in terms of numbers of particles are given as (17-9) for arithmetic mean and as (17-14) for the volume mean.

Exercise 17.5

Subject: Calculation of mean particle diameters from a screen analysis.

Given: Screen analysis of sodium thiosulfate crystals from Exercise 17.3.

Assumptions: All particles have the same sphericity and volume shape factor.

Find: Surface-mean, mass-mean, arithmetic-mean, and volume-mean diameters

Analysis: The following equations apply for n screen fractions, i:

Surface-mean diameter, (17-7): $$\overline{D}_S = \frac{1}{\sum_{i=1}^{n} \frac{x_i}{\overline{D}_{p_i}}}$$ where $\overline{D}_{p_i}$ is average aperture

Mass-mean diameter, (17-8): $$\overline{D}_W = \sum_{i=1}^{n} x_i \overline{D}_{p_i}$$

Arithmetic-mean diameter, (17-12): $$\overline{D}_N = \frac{\sum_{i=1}^{n} \left(\frac{x_i}{\overline{D}_{p_i}^2} \right)}{\sum_{i=1}^{n} \left(\frac{x_i}{\overline{D}_{p_i}^3} \right)}$$

Volume-mean diameter, (17-15): $$\overline{D}_V = \frac{1}{\left[\sum_{i=1}^{n} \left(\frac{x_i}{\overline{D}_{p_i}^3} \right) \right]^{1/3}}$$

The calculations are made with a spreadsheet on the following page where mesh apertures are obtained from Table 17.4.

Exercise 17.5 (continued)

Differential Analysis

Average Particle Size, mm Dp	Mass Fraction, xi		x/Dp	xDp	x/Dp^2	x/Dp^3
2.855	0.0120		0.0042	0.0342	0.0015	0.0005
2.030	0.0290		0.0143	0.0588	0.0070	0.0035
1.440	0.1880		0.1306	0.2708	0.0907	0.0630
1.015	0.2879		0.2836	0.2922	0.2794	0.2753
0.725	0.2200		0.3034	0.1595	0.4185	0.5773
0.513	0.1110		0.2166	0.0569	0.4227	0.8247
0.363	0.0600		0.1655	0.0218	0.4566	1.2596
0.256	0.0390		0.1525	0.0100	0.5958	2.3274
0.181	0.0180		0.0992	0.0033	0.5482	3.0287
0.128	0.0131		0.1020	0.0017	0.7972	6.2281
0.098	0.0120		0.1222	0.0012	1.2466	12.7209
0.077	0.0101		0.1316	0.0008	1.7204	22.4885
	1.0000	Sums	1.7258	0.9110	6.5847	49.7974

Surface-mean diameter = $\overline{D}_S = \dfrac{1}{1.7258} = 0.579$ mm

Mass-mean diameter = $\overline{D}_W = 0.911$ mm

Arithmetic-mean diameter = $\overline{D}_N = \dfrac{6.5847}{49.7974} = 0.132$ mm

Volume-mean diameter = $\overline{D}_V = \dfrac{1}{49.7974^{1/3}} = 0.272$ mm

Exercise 17.6

Subject: Particle size analysis from data in terms of numbers of particles of each size range

Given: Table of particle-size distribution for perfect spheres of silica of size from 1 to almost 100 microns.

Find: (a) Differential and cumulative plots
(b):
(1) Surface mean diameter (same as surface-mean diameter)
(2) Arithmetic-mean diameter
(3) Mass-mean diameter
(4) Volume-mean diameter

Analysis: Use a spreadsheet to do the calculations and prepare the plots. The equations for Part (b) are as follows by calculations using the spreadsheet values on the next page for the sums:

(1) Surface mean diameter from solution to Exercise 17.4:

$$\overline{D}_S = \frac{\sum_{i=1}^{n} N_i \overline{D}_{p_i}^3}{\sum_{i=1}^{n} N_i \overline{D}_{p_i}^2} = \frac{5,680,872}{222,058} = 25.6 \text{ microns}$$

(2) Arithmetic-mean diameter from (17-9):

$$\overline{D}_N = \frac{\sum_{i=1}^{n} N_i \overline{D}_{p_i}}{\sum_{i=1}^{n} N_i} = \frac{12,256}{1,000} = 12.2 \text{ microns}$$

(3) Mass-mean diameter from solution to Exercise 17.4:

$$\overline{D}_W = \frac{\sum_{i=1}^{n} N_i \overline{D}_{p_i}^4}{\sum_{i=1}^{n} N_i \overline{D}_{p_i}^3} = \frac{190,270,428}{5,680,872} = 33.5 \text{ microns}$$

(4) Volume-mean diameter for (17-14):

$$\overline{D}_V = \left(\frac{\sum_{i=1}^{n} N_i \overline{D}_{p_i}^3}{\sum_{i=1}^{n} N_i} \right)^{1/3} = \left(\frac{5,680,872}{1,000} \right)^{1/3} = 17.8 \text{ microns}$$

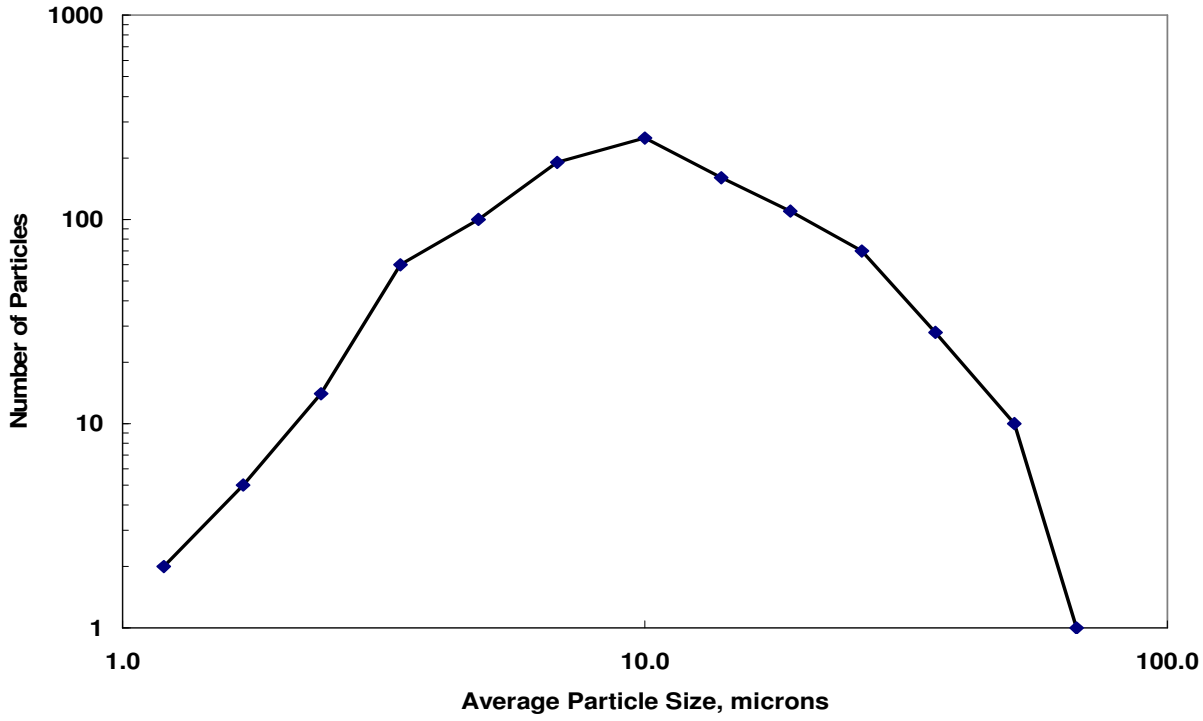
Exercise 17.6 (continued)

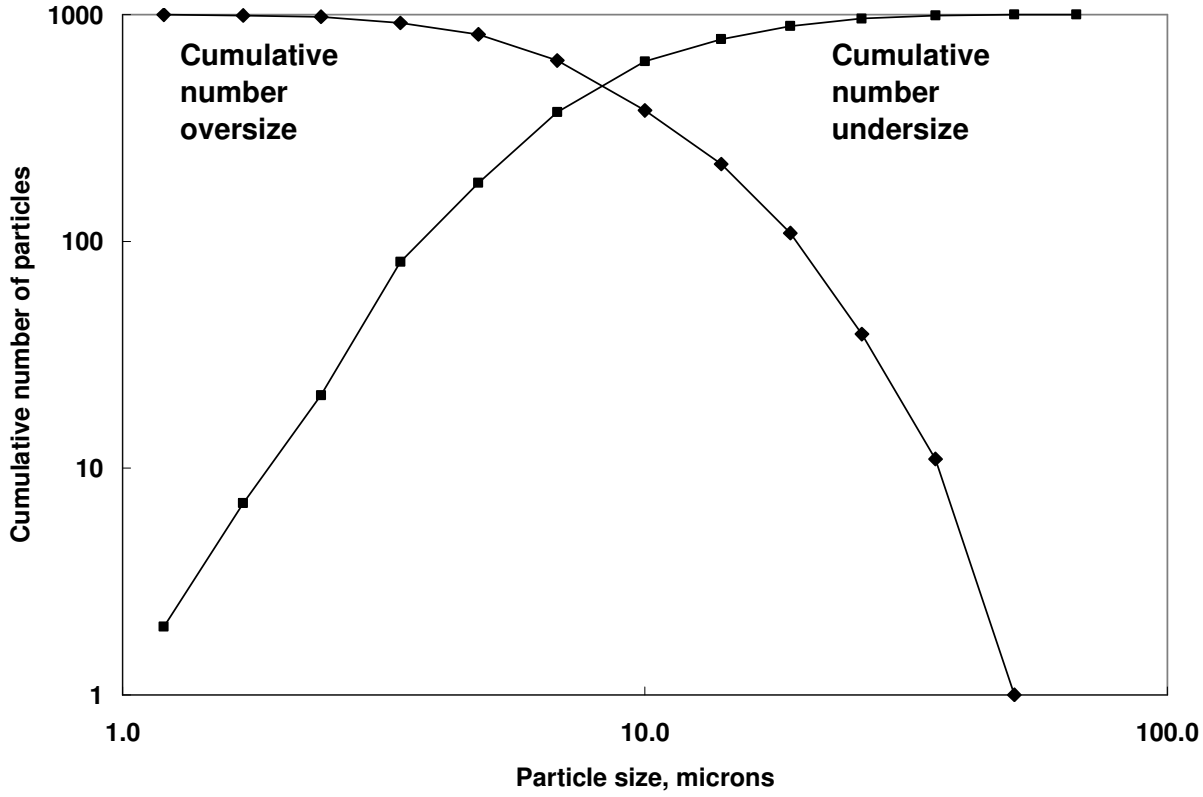
Exercise 17.6
Differential and Cumulative Undersize Screen Analyses

Differential Analysis						**Cumulative Undersize Analysis**		**Cumulative Oversize Analysis**
Average Particle size, microns	No. of Particles, Ni	NDp	NDp^2	NDp^3	NDp^4	Average Size, Dp microns	Cumulative number Undersize	Cumulative number Oversize
						1.2	998	2
1.2	2	2.4	2.9	3.5	4.1	1.7	993	7
1.7	5	8.5	14.5	24.6	41.8	2.4	979	21
2.4	14	33.6	80.6	193.5	464.5	3.4	919	81
3.4	60	204.0	693.6	2358.2	8018.0	4.8	819	181
4.8	100	480.0	2304.0	11059.2	53084.2	6.8	629	371
6.8	190	1292.0	8785.6	59742.1	406246.1	10.0	379	621
10.0	250	2500.0	25000.0	250000.0	2500000.0	14.0	219	781
14.0	160	2240.0	31360.0	439040.0	6146560.0	19.0	109	891
19.0	110	2090.0	39710.0	754490.0	14335310.0	26.0	39	961
26.0	70	1820.0	47320.0	1230320.0	31988320.0	36.0	11	989
36.0	28	1008.0	36288.0	1306368.0	47029248.0	51.0	1	999
51.0	10	510.0	26010.0	1326510.0	67652010.0	67.0	0	1000
67.0	1	67.0	4489.0	300763.0	20151121.0			
Sums:	1000	12256	222058	5680872	190270428			

Differential and cumulative plots of the above spreadsheet analysis are given on the following page.

Exercise 17.6 (continued)





Exercise 17.7

Subject: Plots of screen analysis and average diameters of a sample of glauber's salt from a commercial crystallizer.

Given: U.S. screen analysis

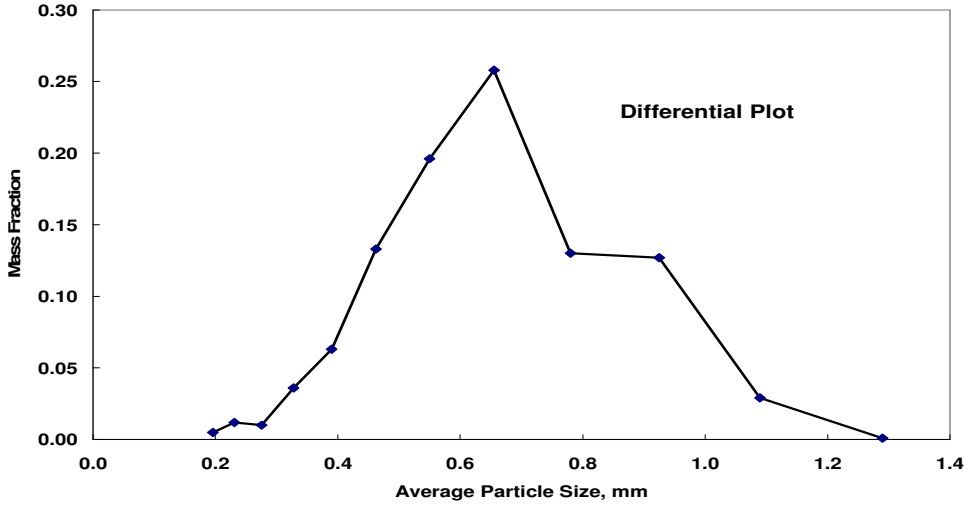
Assumptions: All particles have the same sphericity and volume shape factor.

Find: Differential and cumulative undersize and oversize plots. Surface-mean, mass-mean, arithmetic-mean, and volume-mean diameters.

Analysis: Use a spreadsheet with apertures for U.S. Mesh from Table 17.4. Results are:

Differential Analysis

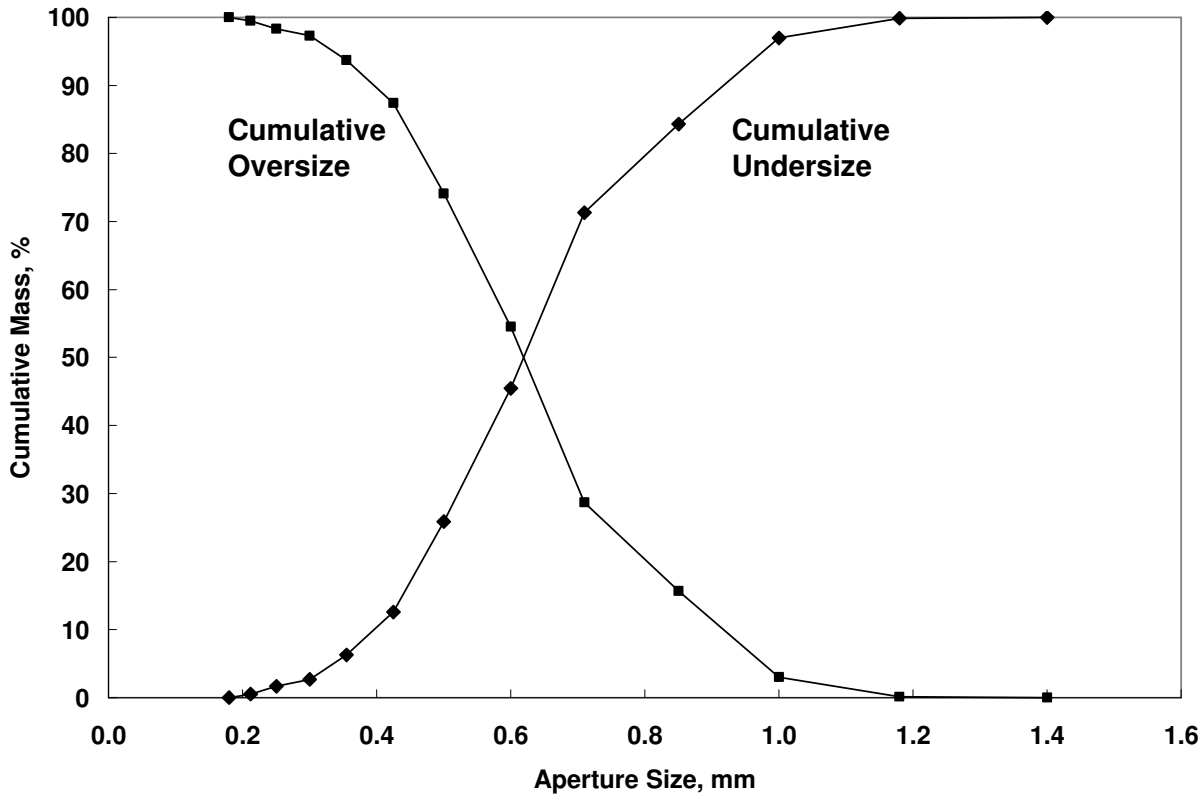
U.S. Mesh Number	Aperture, Dp, mm	Mass retained, grams	% Mass retained	Average Particle Size, mm	Mass Fraction, xi	x/Dp	xDp	x/Dp^2	x/Dp^3
14	1.400	0.0	0.00						
16	1.180	0.9	0.10	1.290	0.0010	0.0008	0.0013	0.0006	0.0005
18	1.000	25.4	2.90	1.090	0.0290	0.0266	0.0316	0.0244	0.0224
20	0.850	111.2	12.70	0.925	0.1270	0.1373	0.1175	0.1484	0.1604
25	0.710	113.9	13.01	0.780	0.1301	0.1668	0.1015	0.2138	0.2741
30	0.600	225.9	25.80	0.655	0.2580	0.3938	0.1690	0.6013	0.9180
35	0.500	171.7	19.61	0.550	0.1961	0.3565	0.1078	0.6482	1.1785
40	0.425	116.5	13.30	0.463	0.1330	0.2876	0.0615	0.6219	1.3447
45	0.355	55.1	6.29	0.390	0.0629	0.1613	0.0245	0.4137	1.0607
50	0.300	31.5	3.60	0.328	0.0360	0.1098	0.0118	0.3354	1.0241
60	0.250	8.7	0.99	0.275	0.0099	0.0361	0.0027	0.1314	0.4777
70	0.212	10.5	1.20	0.231	0.0120	0.0519	0.0028	0.2247	0.9727
80	0.180	4.4	0.50	0.196	0.0050	0.0256	0.0010	0.1308	0.6673
Total		875.7	100.00		1.0000	1.7543	0.6330	3.4945	8.1012



Exercise 17.7 (continued)

Cumulative Analyses

U.S. Mesh Number	Aperture, Dp, mm	Mass retained, grams	% Mass retained	Aperture, Dp, mm	Cumulative Undersize wt%	Cumulative Oversize wt%
14	1.400	0.0	0.00		100.000	0.0000
16	1.180	0.9	0.10	1.4	99.897	0.1028
18	1.000	25.4	2.90	1.18	96.997	3.0033
20	0.850	111.2	12.70	1	84.298	15.7017
25	0.710	113.9	13.01	0.85	71.292	28.7085
30	0.600	225.9	25.80	0.71	45.495	54.5050
35	0.500	171.7	19.61	0.6	25.888	74.1121
40	0.425	116.5	13.30	0.5	12.584	87.4158
45	0.355	55.1	6.29	0.425	6.292	93.7079
50	0.300	31.5	3.60	0.355	2.695	97.3050
60	0.250	8.7	0.99	0.3	1.701	98.2985
70	0.212	10.5	1.20	0.25	0.502	99.4975
80	0.180	4.4	0.50	0.212	0.000	100.0000
Total		875.7	100.00			



Exercise 17.7 (continued)

The following equations apply for n screen fractions, i:

Surface-mean diameter, (17-7): $\overline{D}_S = \dfrac{1}{\sum_{i=1}^{n} \dfrac{x_i}{\overline{D}_{p_i}}}$ where $\overline{D}_{p_i}$ is average aperture

Mass-mean diameter, (17-8): $\overline{D}_W = \sum_{i=1}^{n} x_i \overline{D}_{p_i}$

Arithmetic-mean diameter, (17-12): $\overline{D}_N = \dfrac{\sum_{i=1}^{n} \left(\dfrac{x_i}{\overline{D}_{p_i}^2} \right)}{\sum_{i=1}^{n} \left(\dfrac{x_i}{\overline{D}_{p_i}^3} \right)}$

Volume-mean diameter, (17-15): $\overline{D}_V = \dfrac{1}{\left[\sum_{i=1}^{n} \left(\dfrac{x_i}{\overline{D}_{p_i}^3} \right) \right]^{1/3}}$

The calculations are made from results of the spreadsheet calculations given above.

Surface-mean diameter = $\overline{D}_S = \dfrac{1}{1.7543} = 0.570$ mm

Mass-mean diameter = $\overline{D}_W = 0.633$ mm

Arithmetic-mean diameter = $\overline{D}_N = \dfrac{3.4945}{8.1012} = 0.431$ mm

Volume-mean diameter = $\overline{D}_V = \dfrac{1}{8.1012^{1/3}} = 0.498$ mm

Exercise 17.8

Subject: Dissolution of sparingly soluble solids.

Given: Mixing of 1,000 grams of water, 50 grams of Ag_2CO_3, and 100 grams of AgCl at 25°C.

Assumptions: Attainment of equilibrium. Solids have an activity of one.

Find: Concentrations of Ag^+, Cl^-, $CO_3^=$, and grams of solids Ag_2CO_3 and AgCl.

Analysis: From Table 17.6, Ag_2CO_3 and AgCl are both sparingly soluble in water, with the following solubility products:

$$Ag_2CO_{3\,(s)} = 2Ag^+_{(aq)} + CO_3^{=}{}_{(aq)} \qquad \text{with} \qquad K_c = \left(c_{Ag^+}\right)^2 \left(c_{CO_3^=}\right) = 6.15\times10^{-12} \tag{1}$$

$$AgCl_{\,(s)} = Ag^+_{(aq)} + Cl^-_{(aq)} \qquad \text{with} \qquad K_c = \left(c_{Ag^+}\right)\left(c_{Cl^-}\right) = 1.56\times10^{-10} \tag{2}$$

$$\text{By stoichiometry,} \qquad c_{Ag^+} = c_{Cl^-} + 2c_{CO_3^=} \tag{3}$$

Solving (1), (2), and (3), which constitute a system of nonlinear equations, by Polymath, using the constrained option and noting a high sensitivity to initial guesses, the following results are obtained by assuming initial values for all three concentrations of 1.0 x 10^{-5} mol/L:

$c_{Ag^+} = 2.311\times10^{-4}$ mol/L

$c_{CO_3^=} = 1.152\times10^{-4}$ mol/L

$c_{Cl^-} = 6.751\times10^{-7}$ mol/L

Therefore, the concentration of dissolved AgCl = $c_{Cl^-} = 6.751\times10^{-7}$ mol/L , and

The concentration of dissolved Ag_2CO_3 = $c_{CO_3^=} = 1.152\times10^{-4}$ mol/L

Now compute the amount of solids. The molecular weights are 143.32 for AgCl and 275.74 for Ag_2CO_3. Since we have 1 L of water, the amounts that dissolve are:

6.751×10^{-7} (143.32) = 0.000097 g of dissolved AgCl

1.152×10^{-4} (275.74) = 0.0318 g of dissolved Ag_2CO_3

Amount of solid AgCl = 100 – 0.000097 = 99.999903 g

Amount of solid Ag_2CO_3 = 50 – 0.0318 = 49.9682 g

Exercise 17.9

Subject: Crystallization of $(NH_4)_2SO_4$ from water by a combination of cooling and evaporation.

Given: 5,000 lb/h of a saturated aqueous solution of $(NH_4)_2SO_4$ at 80°C. Evaporate 50% of the water and cool the solution to 30°C.

Assumptions: Equilibrium

Find: The lb/h of crystals formed.

Analysis: From Table 17.7, the solubility of $(NH_4)_2SO_4$ at 80°C = 95.3 g/100 g water

Therefore, have $\frac{95.3}{95.3+100}(5,000) = 2,440$ lb/h of $(NH_4)_2SO_4$

and 5,000 – 2,440 = 2,560 lb/h of water

Evaporate 0.5(2,560) = 1,280 lb/h of water leaving 1,280 lb/h of water in solution

From Table 17.7, the solubility of $(NH_4)_2SO_4$ at 30°C = 78 g/100 g water and the crystals of $(NH_4)_2SO_4$ have no water of hydration.

Therefore, in solution at 30°C, we have $\frac{78}{100}(1,280) = 998$ lb/h of $(NH_4)_2SO_4$

Therefore, we have 2,440 – 998 = 1,442 lb/h of crystals of $(NH_4)_2SO_4$

Exercise 17.10

Subject: Crystallization of the hexahydrate of $FeCl_3$ from an aqueous solution by cooling.

Given: 7,500 lb/h of a 50 wt% solution of $FeCl_3$ at 100°C. Cooled to 20°C. The solubilities of $FeCl_3$ in g/100 g water are 540 at 100°C and 91.8 at 20°C.

Assumptions: Equilibrium

Find: The lb/h of $FeCl_3 \cdot 6\ H_2O$ crystals formed

Analysis: At 100°C, have a solution of 3,750 lb/h of $FeCl_3$ and 3,750 lb/h of water. Note that this amount of $FeCl_3$ is far below its solubility at that temperature.

The molecular weights are: 162.22 for $FeCl_3$ and 270.32 for $FeCl_3 \cdot 6\ H_2O$

The final solution will contain less water than the initial solution because of the water of hydration in the crystals.

Let x = lb/h of water in the final aqueous solution. Then, $3{,}750 - x$ = water in crystals.

The crystals are $\frac{162.22}{270.32}(100\%) = 60.0\%$ $FeCl_3$ and 40.0% water

A mass balance for $FeCl_3$ at 20°C gives,

$$3{,}750 = \frac{91.8}{100}x + (3{,}750 - x)\left(\frac{162.22}{270.32 - 162.22}\right) \qquad (1)$$

Solving (1), gives x = 3,222 lb/h of water in solution and, therefore, 3,750 – 3,222 = 528 lb/h of water in crystals.

Therefore, the $FeCl_3$ still in the solution = 0.918(3,222) = 2,958 lb/h

Crystals of $FeCl_3 \cdot 6\ H_2O$ = 3,750 – 2,958 + 528 = 1,320 lb/h

Exercise 17.11

Subject: Continuous vacuum crystallization of $MgSO_4$.

Given: Feed to the crystallizer consisting of a mixture of 5,870 lb/h of aqueous 35 wt% $MgSO_4$ at 180°F and 25 psia as a concentrate from an evaporator, and 10,500 lb/h of saturated aqueous recycle filtrate of $MgSO_4$ at 80°F and 25 psia. The vacuum crystallizer operates at 85°F and 0.58 psia to produce steam and a magma of 25 wt% crystals and 75 wt% saturated solution.

Assumptions: Equilibrium in the crystallizer.

Find: Evaporation rate of water in the crystallizer in lb/h and the production rate of crystals in tons/day (dry basis for 2,000 lb/ton)

Analysis: First compute the total feed to the crystallizer.

Concentrate: 0.35(5,870) = 2,055 lb/h $MgSO_4$
5,870 – 2,055 = 3,815 lb/h water
At 189°F, from Fig. 17.2, solubility of $MgSO_4$ = 39 wt%.
So, all of the sulfate is in solution.

Filtrate: From Fig. 17.2, the solubility of $MgSO_4$ in water at 80°F = 27.5 wt%
0.275(10,500) = 2,888 lb/h $MgSO_4$
10,500 – 2,888 = 7,612 lb/h water

Total feed: 2,055 + 2,888 = 4,943 lb/h $MgSO_4$
3,815 + 7,612 = 11,427 lb/h water

Compute the mass balance around the crystallizer.
From Fig. 17.2, the solubility of $MgSO_4$ in water = 28 wt% and $MgSO_4$ is crystallized as the heptahydrate.

Let: L = lb/h of solution in the magma
V = lb/h of water vaporized in the crystallizer
S = lb/h of crystals in the magma

MW of $MgSO_4$ = 120.4. MW of $MgSO_4 \cdot 7H_2O$ = 246.4
Crystals are 120.4/246.4 = 0.4886 mass fraction $MgSO_4$ and 0.5114 mass fraction water.
Magma is 25 wt% crystals and 75 wt% of a solution of 28 wt% $MgSO_4$.
$MgSO_4$ mass balance around the crystallizer:

$$4{,}943 = 0.28\,L + 0.4886\,S \qquad \text{But, } S = 0.25(S + L)$$

Solving these two equations, L = 11,160 lb/h and S = 3,720 lb/h
Therefore, the tons/day of crystals = 3,720(24)/2,000 = 44.6 tons/day

Total mass balance around the crystallizer:

$$4{,}943 + 11{,}427 = V + L + S = V + 11{,}160 + 3{,}720$$

Solving, V = 1,490 lb/h of water vapor produced in the crystallizer.

Exercise 17.12

Subject: Crystallization of urea from an aqueous solution by cooling and evaporation.

Given: Feed is a 90% saturated solution of urea in water at 100°C. Final solution at 30°C with 90% crystallization of the urea in the anhydrous form.

Assumptions: Equilibrium in the crystallizer.

Find: Fraction of water that must be evaporated.

Analysis: From Table 17.7, solubility of urea in water at 100°C = 730 g/100 g water, and
solubility of urea in water at 30°C = 135 g/100 g water

Take a basis of 1,000 kg of feed.
Therefore, have 0.90(730) = 657 g urea/100 g water
Therefore, feed is: [657/(657 + 100)]1,000 = 868 kg urea
1,000 – 868 = 132 kg water

Urea crystals formed at 30°C = 0.90(868) = 781 kg
Urea remaining in solution = 868 – 781 = 87 kg
Therefore, water in solution = [100/135]87 = 64.4 kg

By overall mass balance, water evaporated = 132 – 64.4 = 67.6 kg

Fraction of water evaporated = 67.6/132 = 0.512

Exercise 17.13

Subject: Heat addition to the feed of a crystallizer

Given: Data from Examples 17.3 and 17.5. Crystallizer feed is 4,466 lb/h of 37.75 wt% $MgSO_4$ in water at 170°F and 20 psia. Instead of adding 246,000 Btu/h of heat to recirculating magma in the vacuum, evaporating crystallizer, that heat is to be added to the feed.

Assumptions: Linear extrapolation of the enthalpy chart of Figure 17.10.

Find: Exit temperature from the feed heat exchanger.

Analysis: Use the enthalpy-concentration chart for aqueous solutions of $MgSO_4$ in Figure 17.10.

$H_{\text{feed in}}$ = -20 Btu/lb for 37.75 wt% $MgSO_4$ at 170°F

By an enthalpy balance on the heat exchanger,

$H_{\text{feed out}}$ = -20 + 246,000/4,466 = 35.1 Btu/lb

For 37.75 wt% $MgSO_4$, this enthalpy is off the chart of Figure 17.10. Therefore, make a linear extrapolation, assuming a constant specific heat for the solution. For the temperature range of 170°F to 230°F, the enthalpy change is -20 to 18 Btu/lb. Therefore, the average specific heat = [18 – (-20)]/(230 – 170) = 0.63 Btu/lb-°F.

Using this specific heat, $T_{\text{feed out}}$ = 170 + 246,000/[4,466(0.63)] = 257°F.

This is a much higher temperature than the temperature of 85°F in the crystallizer. Therefore, a much higher heating-medium temperature would be required. Furthermore, the pressure of the feed would have to be increased to suppress vaporization in the heat exchanger.

The conclusion is that a heat exchanger on the recirculating magma is preferred over a heat exchanger on the feed.

Exercise 17.14

Subject: Rate of heat addition to a crystallizer

Given: Data from Exercise 17.11. Feed of 5,870 lb/h of 35 wt% $MgSO_4$ in water at 180°F and 25 psia. Recycle of 10,500 lb/h of saturated $MgSO_4$ at 80°F and 25 psia. From calculations made in Exercise 17.11, three phases leave the crystallizer at 85°F and 0.58 psia in the vapor space: 1,490 lb/h of steam; 3,720 lb/h of crystals of $MgSO_4 \cdot 7H_2O$; and 11,160 lb/h of a saturated solution of 28 wt% $MgSO_4$.

Assumptions: No heat losses from the crystallizer

Find: Rate of heat addition to the crystallizer.

Analysis: Use Figure 17.10 for enthalpies of liquid and crystals. Use steam table for steam.
An enthalpy balance around the crystallizer gives,

$$m_{\text{feed}} H_{\text{feed}} + m_{\text{recycle}} H_{\text{recycle}} + Q_{\text{in}} = m_{\text{steam}} H_{\text{steam}} + m_{\text{liquid}} H_{\text{liquid}} + m_{\text{crystals}} H_{\text{crystals}} \quad (1)$$

Substituting given flow rates and Figure 17.10 enthalpies into (1) gives,

$5{,}870(-3) + 10{,}500(-44) + Q_{\text{in}} = 1{,}490(1{,}099) + 11{,}160(-43) + 3{,}720(-148)$

Solving, $Q_{\text{in}} = 1{,}087{,}000$ Btu/h

Exercise 17.15

Subject: Rate of heat removal from a cooling crystallizer

Given: Feed of saturated oxalic acid in water at 100°C. From Example 17.4, solution is cooled to 10.6°C to crystallize 95% of the oxalic acid.

Assumptions: No heat losses from the crystallizer.

Find: Required rate of heat removal.

Analysis: Use cgs units. Assume a thermodynamic path of cooling to 10.6°C, followed by crystallization to the dihydrate.

From Example 17.4, using a basis of 100 grams of water in the feed, the oxalic acid in the feed is 84.4 grams from Table 17.7. Also, the amount of oxalic acid remaining in the solution at 10.6C is 4.2 g. Therefore, 84.4 – 4.2 = 80.2 g of oxalic acid is crystallized.

MW of oxalic acid = 90.0.
Therefore the mols of oxalic acid crystallized = 80.2/90 = 0.891 mols

From Perry's Handbook, the estimated feed specific heat = 0.76 cal/g-°C.
Therefore, to cool the solution, must remove:

$$(100 + 84.4)(0.76)(100 - 10.6) = 12{,}530 \text{ cal/100 g water in feed}$$

Also, the heat of exothermic crystallization = 8,580 cal/mol
Therefore, must remove an additional 0.891(8,580) = 7,650 cal/100 g water in feed

The total amount of heat that must be removed is:

$$12{,}530 + 7{,}650 = 20{,}180 \text{ cal/100 g water in the feed}$$

Exercise 17.16

Subject: Effect of crystal size on solubility

Given: Crystals of KCl, $BaSO_4$, and sucrose at 25°C , together with values of their interfacial tensions in water, $\sigma_{s,L}$ of 0.028, 0.13, and 0.01 J/m^2, respectively.

Assumptions: Spherical crystals

Find: Effect of crystal size, say from 0.01 to 10 microns on the solubility in water

Analysis: From (17-16),

$$\ln\left(\frac{c}{c_s}\right)=\frac{4v_s\sigma_{s,L}}{\upsilon RTD_p} \qquad (1)$$

From a handbook,

Component	MW	Density, kg/m^3	v_s, m^3/kmol	υ
KCl	74.6	1,980	0.0376	2
$BaSO_4$	233.42	4,499	0.0519	2
Sucrose	342.30	1,588	0.216	1

Use SI units in (1).

KCl:

Solubility at 25°C from Table 17.5 by interpolation = c_s = 35.5 g/100 g water
Results from Example 17.7 are:

D_p, microns	D_p, m	c/c_s	c, g/100 g water
0.01	0.00000001	1.0085	35.80
0.10	0.0000001	1.00085	35.53
1.00	0.000001	1.000085	35.50
10.00	0.00001	1.0000085	35.50

$BaSO_4$:

Calculate solubility from solubility product in Table 17.6 assuming value of 0.87 x 10^{-7} at 18°C equals that at 25°C.

$$K_c=\left(c_{Ba^{++}}\right)\left(c_{SO_4^{=}}\right)=\left(c_{BaSO_4}\right)^2=0.87\times10^{-10}$$

Solving, $\left(c_{BaSO_4}\right)$ = 0.93 x 10^{-5} mol/L water or

c_s = 0.93 x 10^{-5} (0.1)(233.42) = 2.2 x 10^{-4} g/100 g water

From (1), $$\ln\left(\frac{c}{c_s}\right)=\frac{4(0.0519)(0.13)}{2(8315)(298)(D_p \text{ in m})} \qquad (2)$$

Exercise 17.16 (continued)

Solving (2) for a range of crystal size,

D_p, microns	D_p, m	c/c_s	c, g/100 g water
0.01	0.00000001	1.716	0.00038
0.10	0.0000001	1.055	0.00023
1.00	0.000001	1.0054	0.00022
10.00	0.00001	1.00054	0.00022

Sucrose: Solubility at 25°C from Table 17.7 by interpolation = c_s = 212 g/100 g water

From (1), $$\ln\left(\frac{c}{c_s}\right)=\frac{4(0.0216)(0.01)}{1(8315)(298)(D_p \text{ in m})} \qquad (3)$$

Solving (3) for a range of crystal size,

D_p, microns	D_p, m	c/c_s	c, g/100 g water
0.01	0.00000001	1.417	300
0.10	0.0000001	1.0355	219.5
1.00	0.000001	1.0035	212.7
10.00	0.00001	1.00035	212.1

The results show that the effect on solubility is greatest for the smallest crystals.

Exercise 17.17

Subject: Required supersaturation ratio.

Given: Crystals of sucrose of 0.5 microns diameter. Properties of sucrose: MW = 342; crystal density = 1,590 kg/m^3; and interfacial tension, $\sigma_{s,L}$ = 0.01 J/m^2

Assumptions: Spherical crystals. Temperature of 25^{o}C.

Find: Supersaturation ratio, $S = c/c_s$ required for the crystals to grow.

Analysis: Use (17-16) with SI units:

$$\ln S = \ln\left(\frac{c}{c_s}\right) = \frac{4v_s\sigma_{s,L}}{\upsilon RTD_p} \tag{1}$$

Substituting into (1) gives,

$$S = \exp\left(\frac{4\left(\frac{342}{1,590}\right)(0.01)}{1(8315)(298)\left(\frac{0.5}{10^6}\right)}\right) = 1.007$$

Exercise 17.18

Subject: Explanation for the experimental maximum in the crystal solubility curve with crystal size.

Given: Surface energy of crystals may depend on surface electrical charge as well as on interfacial tension. Relationship for electrical charge effect.

Assumptions: Spherical crystals.

Find: A modification of (17-16) that predicts the maximum.

Analysis: From (17-16),

$$\ln S = \ln\left(\frac{c}{c_s}\right) = \frac{4v_s\sigma_{s,L}}{\upsilon RTD_p} \tag{1}$$

To predict a maximum, modify (1) by incorporating the given electrical charge effect, as follows:

$$\ln S = \ln\left(\frac{c}{c_s}\right) = \left[\frac{4v_s\sigma_{s,L}}{\upsilon RTD_p} - \frac{2q^2v_s}{\pi KRTD_p^4}\right] \tag{2}$$

Equation (2) is of the form:

$$\ln\left(\frac{c}{c_s}\right) = \frac{v_s}{RT}\left[\frac{A}{D_p} - \frac{B}{D_p^4}\right] \tag{3}$$

Differentiate (3) with respect to D_p to find min/max:

$$\frac{d}{dD_p}\left(\ln\frac{c}{c_s}\right) = \frac{v_s}{RT}\left[-\frac{A}{D_p^2} + \frac{4B}{D_p^5}\right] = 0 \tag{4}$$

Solving (4) for D_p,

$$D_p = \left(\frac{4B}{A}\right)^{1/3} = \left(\frac{2q^2\upsilon}{\pi K\sigma_{s,L}}\right)^{1/3}$$, which can be shown to be a maximum

Exercise 17.19

Subject: Effect of supersaturation ratio on rate of primary homogeneous nucleation.

Given: Aqueous solutions of $AgNO_3$, $NaNO_3$, and KNO_3 at 25°C, together with values for crystal density and interfacial tension.

Assumptions: Spherical crystals.

Find: Rates of primary homogeneous nucleation over the range of supersaturation ratio, $S = c/c_s$, of 1.005 to 1.02.

Analysis: Use (17-18) with SI units in the exponential term:

$$B^o,\ \text{number of nuclei formed/cm}^3\text{-s} = 10^{30} \exp\left[\frac{-16\pi v_s \sigma_{s,L}^3 N_a}{3\upsilon^2 (RT)^3 (\ln S)^2}\right] \qquad (1)$$

The properties are:

Component	υ	MW	ρ, kg/m^3	v_s = MW/ρ	$\sigma_{s,L}$, J/m^2
$AgNO_3$	2	169.6	4,350	0.0390	0.0025
$NaNO_3$	2	85.0	2,260	0.0376	0.0015
KNO_3	2	101.1	2,110	0.0479	0.0030

N_a = Avagadro's number = 6.022 x 10^{26} molecules/kmol
R = 8315 J/kmol-K
T = 298 K

Use of a spreadsheet gives the following results from (1):

Rate of primary nucleation, B^o , nuclei/s-cm^3

Component	S = 1.02	S = 1.01	S = 1.005
$AgNO_3$	4.37 x 10^{25}	5.43 x 10^{12}	1.91 x 10^{-39}
$NaNO_3$	1.33 x 10^{29}	3.39 x 10^{26}	1.54 x 10^{16}
KNO_3	4.20 x 10^{18}	8.72 x 10^{-16}	4.50 x 10^{-150}

Exercise 17.20

Subject: Primary homogeneous nucleation of $BaSO_4$.

Given: Crystal density of 4.50 g/cm^3 and interfacial tension of 0.12 J/m^2.

Assumptions: Spherical crystals.

Find: Effect of relative supersaturation on primary nucleation from an aqueous solution at 25°C.

Analysis: Since from Table 17.6, $BaSO_4$ is sparingly soluble in water, a high supersaturation ratio will be needed. Try values of supersaturation ratio, S, of 50, 40, and 30; noting that the relative supersaturation, s, from (17-17) is $s = S - 1$, so that in this case the two supersaturations are approximately the same.

Use (17-18) with SI units in the exponential term:

$$B^{\circ},\ \text{number of nuclei formed/cm}^3\text{-s} = 10^{30} \exp\left[\frac{-16\pi v_s \sigma_{s,L}^3 N_a}{3\upsilon^2 (RT)^3 (\ln S)^2}\right] \qquad (1)$$

The properties are:

Component	υ	MW	ρ, kg/m^3	v_s = MW/ρ	$\sigma_{s,L}$, J/m^2
$BaSO_4$	2	233.4	4,500	0.0519	0.120

N_a = Avagadro's number = 6.022 x 10^{26} molecules/kmol
R = 8315 J/kmol-K
T = 298 K

Use of a spreadsheet gives the following results from (1):

Rate of primary nucleation, B°, nuclei/s-cm^3

Component	S = 50	S = 40	S = 30
$BaSO_4$	1.38 x 10^8	2.59 x 10^5	12.0

Exercise 17.21

Subject: Crystal growth and the controlling resistance.

Given: Data in Example 17.9, except that solution velocity past crystal face = 1 cm/s.

Assumptions: Crystal growth controlled by mass transfer to the face, surface reaction, or a combination of the two. No primary or secondary nucleation.

Find: Crystal growth rate and its controlling mechanism.

Analysis: A review of the results of Example 17.9 shows that with a solution velocity past the crystal face of 5 cm/s, crystal growth is controlled mainly by surface reaction because the measured growth rate was given as 0.005 mm/min, while a rate calculated on the basis of control by mass transfer is higher, namely: 0.029 mm/min for the largest crystal size of 400 microns. Since, the solution velocity in this exercise is lower by a factor of 5, maybe mass transfer will be more important.

First, calculate new mass transfer coefficients from (15-62), using ratios from the results in Example 17.9.

$$N_{\mathrm{Sh}} = \frac{k_c D_p}{D} = 2 + 0.6\left(\frac{D_p v \rho}{\mu}\right)^{1/2}\left(\frac{\mu}{\rho D}\right)^{1/3}$$

The only change from Example 17.9 is the velocity, v, in the Reynolds number. For each crystal diameter, the Reynold's numbers here are 1/5 of those in Example 17.9. The resulting mass transfer coefficients are as follows:

Crystal size, microns	k_c, cm/s in Ex. 17.9	k_c, cm/s here
50	0.019	0.011
400	0.006	0.003

Take the smallest value, $k_c = 0.003$ cm/s. As in Example 17.9, the growth rate is,

$$\frac{dr}{dt} = 0.008k_c = 0.008(0.003) = 0.000024 \text{ cm/s} = 0.0144 \text{ mm/min}$$

This growth rate is still larger than the measured value of 0.005 mm/min. Thus, the growth rate will be more at the lower solution velocity.
To determine more quantitatively the effect of mass transfer on the growth rate, use the results of Example 17.9 to compute an approximate value of k_i in (17-23).

From (17-23), rewrite the growth rate in terms of an overall coefficient,

$$\frac{dr}{dt} = 0.008K_c = 0.005 \text{ mm/min}$$

Exercise 17.21 (continued)

Therefore, K_c = 0.005/0.008 = 0.625 mm/min = 0.00104 cm/s
From Example 17.9, the average k_c = (0.019 + 0.006)/2 = 0.0125 cm/s
From (17-23),

$$K_c = 0.00104 = \frac{1}{\frac{1}{k_c} + \frac{1}{k_i}} = \frac{1}{\frac{1}{0.0125} + \frac{1}{k_i}} \qquad (1)$$

Solving (1), k_i = 0.00113 cm/s.

Now assume that this value of k_i holds for this exercise. For this exercise, the average k_c = 0.007 cm/s.
From (17-13),

$$K_c = \frac{1}{\frac{1}{k_c} + \frac{1}{k_i}} = \frac{1}{\frac{1}{0.007} + \frac{1}{0.00113}} = 0.00097 \text{ cm/s},$$

which is about 7% lower than in Example 17.9.

Thus, here the crystal growth rate is still controlled by surface reaction, but mass transfer does make a small contribution with about 14% of the resistance.

Exercise 17.22

Subject: Heat transfer area of a cooling crystallizer.

Given: Feed of 2,000 kg/h of 30 wt% Na_2SO_4 in water at 40°C; cooled to a temperature at which 50% of the sulfate is crystallized as the decahydrate. Overall heat transfer coefficient = 15 Btu/h-ft^2-°F. Specific heat of solution = 0.80 cal/g-°C. Coolant is chilled water in countercurrent flow, entering at 10°C and exiting so as to give a log-mean temperature driving force of 10°C.

Assumptions: Equilibrium and no heat loss.

Find: Heat transfer area in m^2.

Analysis: First compute the mass balance around the crystallizer.

Feed is 600 kg/h of Na_2SO_4 and 1,400 kg/h of water.

From Table 17.5, at 40°C, the solubility of 48.8 g/100 g of water.

Since the feed contains 42.9 g/100 g of water, the feed is below solubility

MW of Na_2SO_4 = 142.1

MW of $Na_2SO_4 \cdot 10H_2O$ = 322.2

Therefore, the crystals are 142.1/322.2 = 0.441 mass fraction Na_2SO_4

Na_2SO_4 crystallized = 0.5(600) = 300 kg/h

Water of crystallization = (0.559/0.441)300 = 380 kg/h

Therefore, have exiting, 680 kg/h of crystals and a solution of 300 kg/h Na_2SO_4 and 1,400 – 380 = 1,020 kg/h of water. This gives a solubility of (300/1,020)100 = 29.4 g/100 g

From Table 17.5, the temperature corresponding to that solubility is, by interpolation, approximately 25°C.

Now compute the heat transfer rate by an enthalpy balance.

From Table 17.5, the heat of solution at 25°C = +18,700 cal/mol of compound

Therefore, the heat of crystallization is exothermic at 18,700 kcal/kmol.

Since the final temperature is also 25°C, assume a thermodynamic path of cooling the feed from 40°C to 25°C and then crystallizing at 25°C.

Therefore, in cgs units,

Q to be transferred to chilled water = 2,000(1,000)(0.80)(40 – 25) + (680/322.2)(18,700)(1,000) = 24,000,000 + 39,500,000 = 63,500,000 cal/h

Now apply the heat transfer rate equation, $Q = UA\,\Delta T_{LM}$ in SI units

Q = 63,500,000(4.185) = 266,000 kJ/h

U = 15(20.44) = 307 kJ/h-m^2-K

ΔT_{LM} = 10°C = 10 K

Therefore, heat transfer area = A = 266,000/[307(10)] = 87 m^2

Exercise 17.23

Subject: Number of cooling crystallizer units

Given: Two tons (4,000 lb) per hour of $Na_3PO_4 \cdot 12H_2O$ to be produced in a cooling crystallizer from a saturated aqueous solution entering at 40°C and exiting at 20°C. Countercurrent chilled water enters at 10°C and exits at 25°C. Average specific heat of the solution = 0.80 cal/g-°C. Overall heat transfer coefficient = 20 Btu/h-ft^2-°F.

Assumptions: Equilbrium and no heat loss. Linear temperature profile on both sides of the heat transfer surface.

Find: (a) The tons/h of required feed solution.
(b) Heat transfer area in ft^2.
(c) The number of crystallizer units needed, if each has 30 ft^2 of heat transfer surface.

Analysis:

(a) First, compute the mass balance around the crystallizer.
Take a basis of 100 g of water in the entering feed.
From Table 17.5, the solubility of Na_3PO_4 at 40°C = 31 g/100 water.
At 20°C, the solubility is 11 g/100 g water.
Let x = g water exiting in the crystals
Then water left in solution = $100 - x$ and the amount of Na_3PO_4 in the exiting solution = $11(100 - x)/100$
MW of Na_3PO_4 = 163.97
MW of $Na_3PO_4 \cdot 12H_2O$ = 380.16
Therefore, the crystals are 163.97/380.16 = 0.431 mass fraction Na_3PO_4
A mass balance on Na_3PO_4 gives,

$$31 = 11\frac{(100 - x)}{100} + x\frac{0.431}{0.569} \qquad (1)$$

Solving (1), x = 30.8 g water in the crystals with 30.8(0.431/0.569) = 23.3 g Na_3PO_4
Therefore, 100 g water in the feed gives 30.8 + 23.3 = 54.1 g crystals.
For a production rate of 4,000 lb/h of crystals, we need a feed containing 7,390 lb/h of water and 2,290 lb/h of dissolved Na_3PO_4 or a total feed of 4.84 tons/h

(b) Now, compute the rate of heat to be removed. Assume a thermodynamic path of cooling from 40°C to 20°C, followed by crystallization at 20°C.
From Table 17.5, heat of solution = +15,000 cal/mol of compound at room temperature
Therefore, the heat of crystallization is exothermic at 15,000(1.8) = 27,000 Btu/lbmol
Q to be removed = 9,680(0.80)[(40 – 20)(1.8)] + 27,000(4,000/380.16) =
279,000 + 284,000 = 563,000 Btu/h

Exercise 17.23 (continued)

Now apply the heat transfer rate equation, $Q = UA\,\Delta T_{LM}$ in American Engineering units
For countercurrent flow with linear temperature profiles,

$$\Delta T_{LM} = \frac{(40-25)-(20-10)}{\ln\dfrac{(40-25)}{(20-10)}} = 12.3^{o}\text{C} = 22.1^{o}\text{F}$$

U = 20 Btu/h-ft^2-^{o}F

Therefore, heat transfer area = A = 563,000/[20(22.1)] = 1,270 ft^2

(c) The number of crystallizer units needed = 1,270/30 = 43 units.

Exercise 17.24

Subject: MSMPR Crystallizer model.

Given: An aqueous feed of 10,000 kg/h of saturated $BaCl_2$ at 100°C enters an MSMPR crystallizer. Negligible evaporation. Magma leaves at 20°C with crystals of the dihydrate. The volume of the vapor-space-free crystallizer = 2.0 m^3. Experimental crystal growth = G = 4.0 x 10^{-7} m/s.

Assumptions: Equilibrium

Find: (a) The kg/h of crystals in the magma product.
(b) The predominant crystal size in mm.
(c) The mass fraction of crystals in the size range for U.S. Standard 20 mesh to 25 mesh.

Analysis:

(a) First carry out a mass balance around the crystallizer.

From Table 17.5, solubility of $BaCl_2$ at 100°C = 58.3 g/100 g water, and at 20°C, solubility = 35.7 g/100 g water

Therefore, the feed contains 10,000[58.3/(58.3 + 100)] = 3,680 kg/h of $BaCl_2$, and 10,000 – 3,680 = 6,320 kg/h of water.

MW of $BaCl_2$ = 208.27

MW of $BaCl_2 \cdot 2H_2O$ = 244.31

Therefore, the crystals are 208.27/244.31 = 0.852 mass fraction $BaCl_2$

Mass balance for $BaCl_2$ around the crystallizer. Let x = kg/h of water in the crystals.

$$3,680 = (6,320 - x)\left(\frac{35.7}{100}\right) + x\left(\frac{0.852}{1-0.852}\right) \qquad (1)$$

Solving (1), x = 263 kg/h of water in the crystals.

$BaCl_2$ in the crystals = 263(0.852/0.148) = 1,514 kg/h

Therefore, the product crystals in the magma = 263 + 1,514 = 1,777 kg/h

(b) Next calculate the volumetric flow rate of the magma, so we can compute the residence time in the crystallizer.

The flow rate of solution in the magma = 10,000 – 1,777 = 8,223 kg/h

From Perry's Handbook, the density of $BaCl_2 \cdot 2H_2O$ crystals = 3,097 kg/m^3, and the density of the solution in the magma = 1,279 kg/m^3

The volumetric flow rate of the magma is,

8,223/1,279 + 1,777/3,097 = 7.00 m^3/h

Average residence time, τ, of crystals in the crystallizer = 2.0/7.0 = 0.286 h = 17 minutes

Growth rate, G = 4.0 x 10^{-7} m/s = 0.0024 cm/min

From (17-49), the predominant crystal size is given by,

$L_{pd} = 3G\tau$ = 3(4.0 x 10^{-7})[17(60)] = 0.00122 m = 0.122 cm = 1.22 mm

Exercise 17.24 (continued)

(c) Now estimate the mass fraction of crystals in the size range from 10 to 25 mesh.
From Table 17.4,

20 mesh has an aperture of 0.850 mm = 0.085 cm
25 mesh has an aperture of 0.710 mm = 0.071 cm

Calculate the dimensionless crystal size from (17-48), $z = L/G\tau$

For 20 mesh, z = 0.085/[(0.0024)(17)] = 2.08
For 25 mesh, z = 0.071/[(0.0024)(17)] = 1.74

From Table 17.9, the cumulative mass fraction of crystals smaller than size L, is:

$$x_m = 1 - \left[1 + z + \frac{z^2}{2} + \frac{z^3}{6}\right]\exp(-z) \qquad (2)$$

For L = 0.085 cm, z = 2.08. Substitution into (2), gives,

$$x_m = 1 - \left[1 + 2.08 + \frac{2.08^2}{2} + \frac{2.08^3}{6}\right]\exp(-2.08) = 0.158$$

For L = 0.071 cm, z = 1.74. Substitution into (2), gives,

$$x_m = 1 - \left[1 + 1.74 + \frac{1.74^2}{2} + \frac{1.74^3}{6}\right]\exp(-1.74) = 0.099$$

Therefore, we have 15.8 wt% crystals smaller than 0.085 cm, and
9.9 wt% crystals smaller than 0.071 cm

Therefore, the mass fraction of crystals between 20 and 25 U.S. mesh =
0.158 = 0.099 = 0.059 or 5.9 wt%

Exercise 17.25

Subject: Operation of an MSMPR crystallizer

Given: Feed of 5,000 kg/h of 40 wt% sodium acetate in water. Monoclinic crystals of the trihydrate are formed. 20% of the water in the feed is evaporated at 40°C. Crystal growth rate, G, is 0.0002 m/h. Predominant crystal size, L_{pd}, is 20 U.S. standard mesh. Solubility of sodium acetate at 40°C = 65.5 g/100 g water. Crystal density = 1.45 g/cm^3. Mother liquid density = 1.20 g/cm^3.

Assumptions: Equilibrium and applicability of the MSMPR model.

Find: (a) The kg/h of crystals in the exiting magma.
(b) The kg/h of mother liquor in the exiting magma.
(c) The volume in m^3 of magma in the crystallizer.

Analysis: (a) and (b) Compute a mass balance around the crystallizer.
The feed contains 0.4(5,000) = 2,000 kg/h of sodium acetate and 3,000 kg/h of water.
MW of sodium acetate = 82.04.
MW of sodium acetate trihydrate = 136.09.
Let x = kg/h of water in the crystals.
Sodium acetate mass balance:

$$2{,}000 = \frac{65.5}{100}\left(3{,}000 - 600 - x\right) + x\left(\frac{82.04}{136.09 - 82.04}\right)$$

Solving, x = 496 kg/h of water in the crystals
Therefore, water in the mother liquor = 3,000 – 600 – 496 = 1,904 kg/h
Sodium acetate in the mother liquor = 0.655(1,904) = 1,247 kg/h
Sodium acetate in the crystals = 2,000 – 1,247 = 753 kg/h
Therefore, the flow rate of crystals in the exiting magma = 496 + 753 = 1,249 kg/h
The flow rate of mother liquor in the exiting magma = 1,904 + 1,247 = 3,151 kg/h

(c) The total volumetric flow rate of exiting magma is:

$$\frac{1{,}249}{1.45(100)} + \frac{3{,}151}{1.20(100)} = 3.49 \text{ m}^3\text{/h}$$

From Table 17.4, for 20 mesh, L_{pd} = 0.850 mm = 0.000850 m
From (17-49), $L_{pd} = 3G\tau$

Therefore, $\tau = \dfrac{L_{pd}}{3G} = \dfrac{0.00085}{3(0.0002)} = 1.42$ h

Therefore, volume of magma in the crystallizer = 3.49(1.42) = 4.96 m^3

Exercise 17.26

Subject: Design of an MSMRP crystallizer

Given: Production of 2,000 lb/h of crystals of $MgSO_4 \cdot 7H_2O$ with an L_{pd} of U.S. 35 mesh. Magma is 15 vol% crystals. Crystallizer temperature = 50°C. Residence time, $\tau = 2$ h. Crystal density = 1.68 g/cm^3. Mother liquor density = 1.32 g/cm^3.

Assumptions: Equilibrium.

Find: (a) Volumetric flow rates of crystals, mother liquor, and magma.
(b) Crystallizer volume if vapor space = magma space.
(c) Crystallizer dimensions if height = twice the diameter.
(d) Required crystal growth rate, G, in ft/h.
(e) Necessary nucleation rate in nuclei/h-ft^3 of mother liquor.
(f) Number of crystals produced /h.
(g) Predicted cumulative and differential screen analyses of product crystals.
(h) Plots of the predicted screen analyses

Analysis:

a) Volumetric flow rate of crystals = 2,000/[1.68(62.4)] = 19.1 ft^3/h.
Volumetric flow rate of mother liquor = 19.1(85/15) = 108.2 ft^3/h
Volumetric flow rate of magma = 19.1 + 108.2 = 127.3 ft^3/h

(b) Volume of magma in crystallizer = 127.3(2) = 254.6 ft^3
Total crystallizer volume = 2(254.6) = 509 ft^3 or 509/7.48 = 68.1 gal

(c) $H = 2D$, $V = \pi D^2 H/4 = \pi D^3/2 = 509$ ft^3

Solving, $D = 6.87$ ft and $H = 2(6.87) = 13.74$ ft.

(d) From Table 17.4, L_{pd} = 35 U.S. mesh = 0.0197 in = 0.00164 ft.
From (17-49), $L_{pd} = 3G\tau$

Therefore, $G = L_{pd}/3\tau = 0.00164/[3(2)] = 0.000273$ ft/h

(e) From (17.60), assuming a shape factor, $f_v = 0.5$

$$B^\circ = \frac{9C}{2 f_v \rho_p V_{ML} L_{pd}^3} = \frac{9(2{,}000)}{2(0.5)[1.68(62.4)][108.2(2)](0.00164)^3} = 1.80\times10^8 \text{ nuclei/h-ft}^3$$

(f) Crystals produced per hour = $1.80\times10^8 (108.2)(2) = 3.9 \times 10^{10}$ crystals/h

Exercise 17.26 (continued)

(g) For predicting the screen analysis, use Table 17.9 for the third moment, where,

$$x_m = 1 - \left(1 + z + \frac{z^2}{2} + \frac{z^3}{6}\right)\exp(-z) \quad \text{for Cumulative fraction smaller} \tag{1}$$

$$\frac{dx_m}{dz} = \frac{z^3}{6}\exp(-z) \quad \text{which must be normalized for 100\% total} \tag{2}$$

where z is a dimensionless particle size.

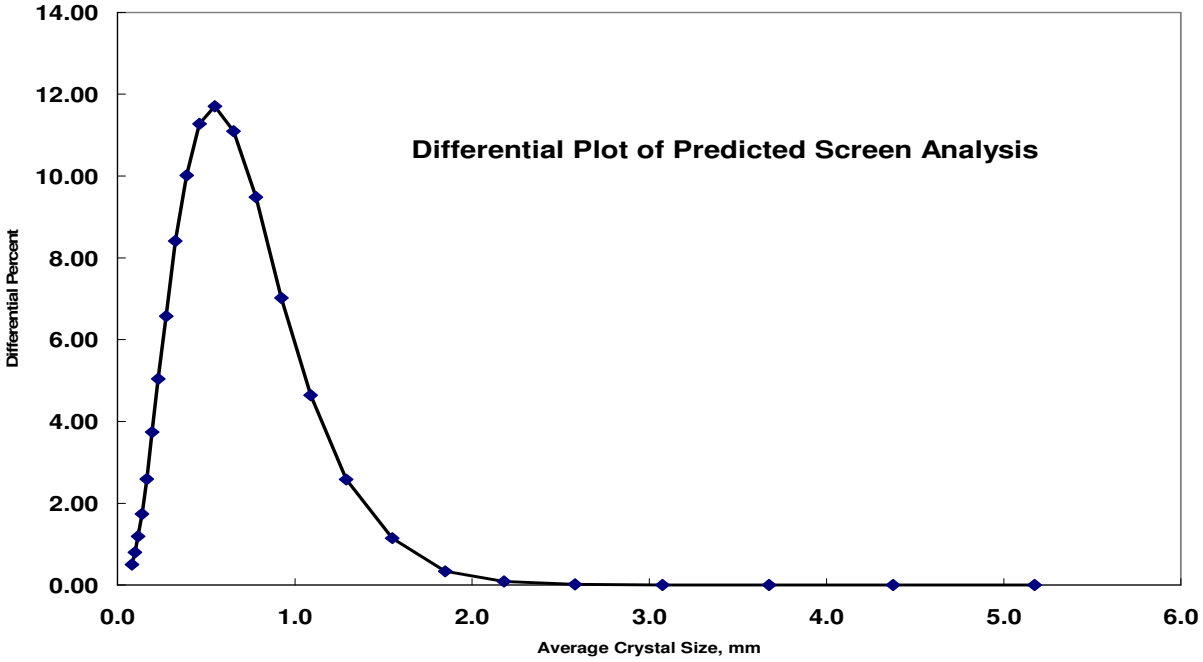
$$z = L/G\tau = L/[0.000273(2)] = 1{,}832\ L \text{ in ft or } 6.01\ L \text{ in mm}$$

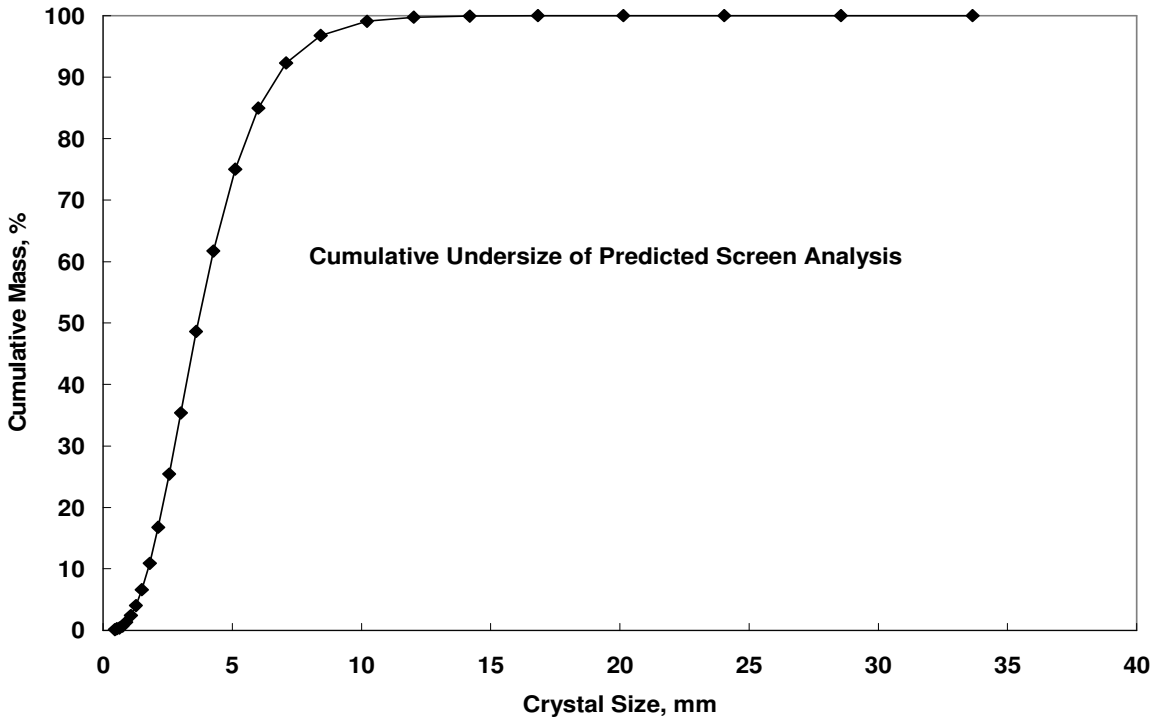
Using a spreadsheet, the following results are obtained using (1) and (2):

			Cumulative Analysis	**Differential Analysis**		
U.S. Mesh Number	Aperture, Dp, mm	z, Dimensionless Length, mm	xm, Mass Percent smaller	Average Particle Size, mm	dxm/dz	Mass Percent Differential
3.5	5.600	33.656	100.00			
4	4.750	28.548	100.00	5.175	0.00	0.000
5	4.000	24.040	100.00	4.375	0.00	0.000
6	3.350	20.134	100.00	3.675	0.00	0.000
7	2.800	16.828	100.00	3.075	0.00	0.002
8	2.360	14.184	99.96	2.580	0.00	0.017
10	2.000	12.020	99.77	2.180	0.00	0.091
12	1.700	10.217	99.12	1.850	0.01	0.339
14	1.400	8.414	96.80	1.550	0.02	1.150
16	1.180	7.092	92.29	1.290	0.05	2.583
18	1.000	6.010	84.97	1.090	0.09	4.638
20	0.850	5.109	74.99	0.925	0.13	7.017
25	0.710	4.267	61.69	0.780	0.18	9.486
30	0.600	3.606	48.61	0.655	0.21	11.088
35	0.500	3.005	35.39	0.550	0.22	11.704
40	0.425	2.554	25.41	0.463	0.22	11.281
45	0.355	2.134	16.77	0.390	0.19	10.013
50	0.300	1.803	10.92	0.328	0.16	8.410
60	0.250	1.503	6.60	0.275	0.13	6.573
70	0.212	1.274	4.06	0.231	0.10	5.037
80	0.180	1.082	2.44	0.196	0.07	3.737
100	0.150	0.902	1.35	0.165	0.05	2.590
120	0.125	0.751	0.73	0.138	0.03	1.742
140	0.106	0.637	0.41	0.116	0.02	1.190
170	0.090	0.541	0.23	0.098	0.02	0.802
200	0.075	0.451	0.12	0.083	0.01	0.508
Total					1.9142	100.0000

Exercise 17.26 (continued)

(h) The following plots are obtained from the spreadsheet:





Exercise 17.27

Subject: Precipitation using the MSMPR model

Given: Continuous precipitation of $BaSO_4$ from the mixing of aqueous solutions of Na_2SO_4 and $BaCl_2$ at stoichiometric ratio to give a NaCl concentration of 0.15 mol/L. Perfect mixing in a 1.8 L crystallizer. Data for mixing at 200 rpm fits the equation, $\ln n = 26.3 - 0.407\,L$, where n = number density of crystals in nuclei/micron-L, and L = crystal size in microns. Average residence time, τ, is 38 s.

Assumptions: Equilibrium and applicability of the MSMPR model.

Find: (a) n^o
(b) G
(c) B^o
(d) mean crystal length
(e) n_c
(f) whether the results are consistent with the trends in Example 17.12.
(g) From the results here and in Example 17.12, predict G if no agitation.

Analysis:

(a) From (17-38), $\ln n = \ln n^o - L/G\tau$

Comparing this to the given experimental correlation above, $\ln n^o = 26.3$

Therefore, $n^o = \exp(26.3) = 2.64 \times 10^{11}$

(b) Also from the same correlation, $L/G\tau = 0.407\,L$

Therefore, $G\tau = 1/0.407$ and $G = 1/[0.407(38)] = 0.0647$ micron/s

(c) From (17-51), $B^o = Gn^o = 0.0647(2.64 \times 10^{11}) = 1.71 \times 10^{10}$ nuclei/L-s

(d) From (17-42), $L_{mean} = G\tau = 0.0647(38) = 2.46$ microns

(e) From (17-54), $n_c = n^o\tau G = (2.64 \times 10^{11})(38)(0.0647) = 6.49 \times 10^{11}$ crystals/L
or 6.49×10^{8} crystals/m^3

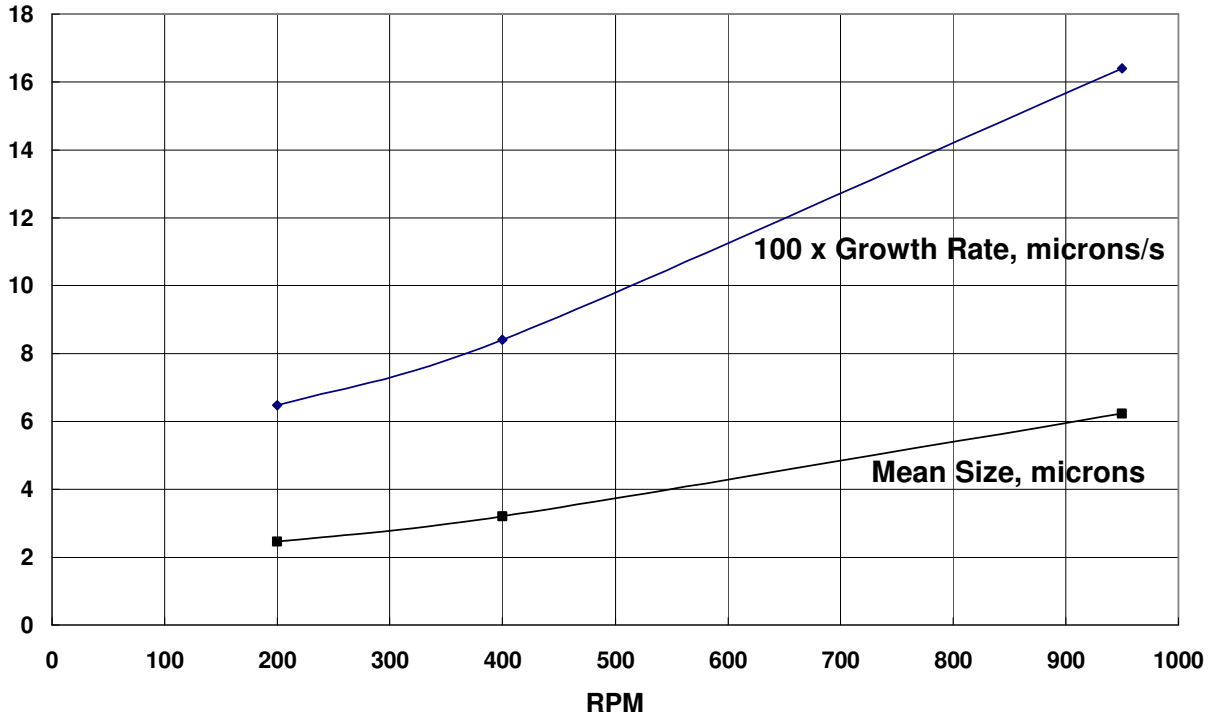
(f) Comparison of results to those of Example 17.12:

Rpm	**950**	**400**	**200**	Consistent ?
n^o, crystals/micron-L	1.11×10^{12}	1.22×10^{11}	2.64×10^{11}	Yes
G, microns/s	0.164	0.0841	0.0647	Yes
B^o, nuclei/L-s	1.89×10^{9}	1.03×10^{10}	1.71×10^{10}	Yes
L_{mean}, microns	6.23	3.20	2.46	Yes
n_c, crystals/m^3	6.92×10^{7}	3.91×10^{8}	6.49×10^{8}	Yes

(g) By extrapolation to an asymptotic value, as shown in the diagram on the next page,

At 0 rpm, $L_{mean} = 2$ microns and $G = L_{mean}/\tau = (2)/(38) = 0.053$ micron/s

Exercise 17.27 (continued)



Exercise 17.28

Subject: Precipitation of $CaCO_3$ as calcite by mixing aqueous solutions of Na_2CO_3 and $CaCl_2$ in an MSMPR crystallizer.

Given: Precipitation conditions of 8.65 pH, an rpm of 800, and a residence time of 100 min. Crystal population density data in Fig. 17.37, which do not fit (17-38).

Assumptions: Equilibrium

Find: (a) An empirical equation that does fit the crystal population density data.
(b) Whether and how nucleation rate and growth rate can be determined from the data.

Analysis:

(a) From Fig. 17.37, values of n in nuclei/m-m^3 for crystal sizes L are read and listed in the table below. Using the nonlinear regression feature of Polymath, a number of different expressions were tried for fitting the data. The best fit, which was not entirely satisfactory, giving an R^2 of 0.986, was:

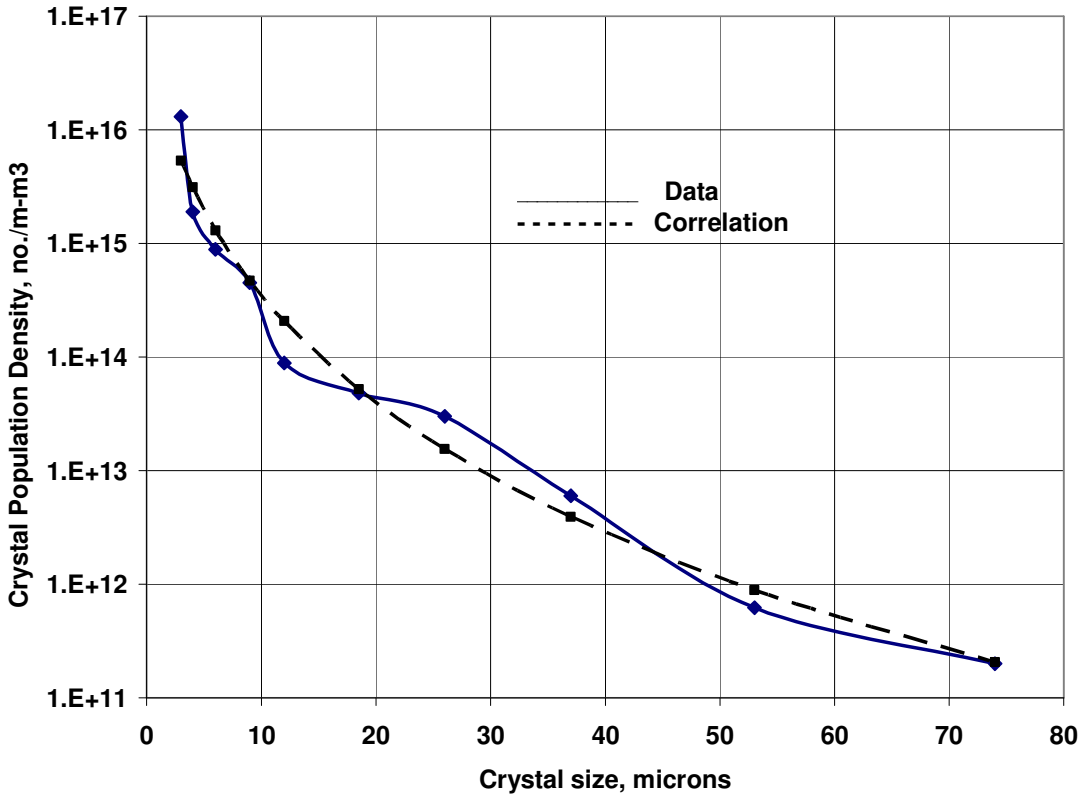
$$\ln n = 40.08 \exp(0.00124\, L - 0.06075\, L^{0.5})$$

The following spreadsheet compares the data points to the predictions of the correlation.

Data:			**Correlation:**	
Crystal size, *L*, microns	*n*, no./m-m3	ln *n*	ln *n*	*n*
3	1.30E+16	37.10	36.21	5.32E+15
4	1.90E+15	35.18	35.67	3.10E+15
6	8.80E+14	34.41	34.80	1.29E+15
9	4.50E+14	33.74	33.78	4.67E+14
12	8.80E+13	32.11	32.96	2.06E+14
18.5	4.80E+13	31.50	31.58	5.18E+13
26	3.00E+13	31.03	30.37	1.54E+13
37	6.00E+12	29.42	29.00	3.92E+12
53	6.20E+11	27.15	27.50	8.80E+11
74	2.00E+11	26.02	26.05	2.06E+11

A comparison of the data to the prediction by the correlation is given on the next page.

Exercise 17.28 (continued)



(b) Because the correlation is not of the form of (17-38), the theory in Section 17 .6 cannot be used to predict nucleation rate and growth rate.

Exercise 17.29

Subject: Precipitation of $Mg(OH)_2$ from mixing of aqueous solutions of $MgCl_2$ and $Ca(OH)_2$ in an MSMPR crystallizer.

Given: Crystallizer volume = 1 L. Operation at 450 rpm and 25°C. Measured crystal size given in Fig. 17.38 for 5 minutes residence time.

Assumptions: Crystal size is proportional to $\exp(-L/G\tau)$ as in (17-38). Assume that n in Fig. 17.38 has units of no./micron-L.

Find:

(a) Growth rate, G
(b) Nucleation rate, B^o
(c) Predominate crystal size, L_{pd}

Analysis:

(a) From (17-52), $$n = \frac{B^o}{G}\exp\left(-\frac{L}{G\tau}\right)$$

or in a straight-line form, $$\log n = \log\left(\frac{B^o}{G}\right) - \frac{L}{2.303G\tau} \qquad (1)$$

Take end points of the line in Fig. 17.38 as: $n = 90$ at $L = 0.55$ and $n = 3$ at $L = 1.35$
Substituting these two data points into (1) with $\tau = 5$ minutes, and solving, gives

$G = 0.047$ microns/min

(b) With this value of G, substitution into (1) for either data point gives,

$B^o = 44$ nuclei/L-min.

(c) From (17-49),

$L_{pd} = 3G\tau = 3(0.047)(5) = 0.705$ micron

Exercise 17.30

Subject: Melt crystallization of naphthalene from a mixture with benzene in a falling-film crystallizer.

Given: Feed of 60 wt% naphthalene and 40 wt% benzene at saturation conditions. Coolant enters at top at 10°C. Physical property data from Example 17.13.

Assumptions: Equilibrium. Crystallization on a planar wall.

Find: Crystal layer thickness for up to 2 cm as a function of time.

Analysis: Assume the major resistance to heat transfer is the crystal layer building up on the wall. Let r_i - r_s = thickness of the crystal layer

$$\text{From (17-66), crystal-layer thickness} = (r_i - r_s) = \left[\frac{2k_c(T_m - T_c)t}{\rho_c \Delta H_f}\right]^{1/2} \qquad (1)$$

From Fig. 17.24, the temperature of the saturated solution at 60 wt% naphthalene = T_m = 44°C.
It is clear from Fig. 17.24 that the crystals will be naphthalene.
Assume that the coolant temperature will not change much, so that T_c = 10°C.

From Example 17.13, ρ_c = 71.4 lb/ft^3
k_c = 0.17 Btu/h-ft-°F
ΔH_f = 63.9 Btu/lb

$$\text{From (1), } (r_i - r_s) \text{ in feet} = \left[\frac{2(0.17)[(44-10)1.8]t}{71.4(63.9)}\right]^{1/2} = 0.0675t^{1/2} \quad \text{with } t \text{ in h.}$$

Results of calculations:

$(r_i - r_s)$, cm	$(r_i - r_s)$, ft	t, h	t, min
0.5	0.0164	0.059	3.5
1.0	0.0328	0.236	14.2
1.5	0.0492	0.531	31.9
2.0	0.0656	0.944	56.6

Exercise 17.31

Subject: Melt crystallization of paradichlorobenzene (PDCB) from a mixture with orthodichlorobenzene (ODCB) in a falling-film crystallizer.

Given: A mixture of 80 wt% PDCB (melts at 53°C) and 20 wt% ODCB (melts at -17.6°C) at the saturation temperature of 43°C. A eutectic forms at 87.5 wt% ODCB and -23°C. Coolant enters at 15°C. Tubes are 8 cm inside diameter. Properties in Perry 's Handbook, except for k_c = 0.15 Btu/h-ft-°F.

Assumptions: Equilibrium. Cylindrical crystallizer with crystallization inside the tube.

Find: Which isomer will crystallizer? Find the time for crystal layer thickness to reach 2 cm.

Analysis: Assume the major resistance to heat transfer is the crystal layer building up on the inside of the cylindrical tube. Let r_i = inside radius of the tube, and r_s = distance from the center of the tube to the surface of the crystal layer, which starts at r_i and decreases with time.

$$\text{From (17-67), } \frac{1}{4}\left(r_i^2 - r_s^2\right) - \frac{r_s^2}{2}\ln\left(\frac{r_i}{r_s}\right) = \frac{k_c\left(T_m - T_c\right)t}{\rho_c \Delta H_f} \qquad (1)$$

It is clear from the given melting and eutectic temperatures that the crystals will be PDCB. Assume that the coolant temperature will not change much, so that T_c = 15°C.

From Perry's Handbook, $\rho_c = 1.458$ g/cm^2

$\Delta H_f = 29.67$ cal/g

Also, $r_i = 4$ cm

$r_s = 2$ cm

$\left(T_m - T_c\right) = 43 - 15 = 28$°C

$k_c = 0.15$ Btu/h-ft-°F or 0.00062 cal/s-cm-°C

Use cgs units in (1),

$$\frac{1}{4}\left(4^2 - 2^2\right) - \frac{2^2}{2}\ln\left(\frac{4}{2}\right) = 1.614 = \frac{0.00062(28)t}{1.458(29.67)}$$

Solving, t = 4,021 s or 1.17 h

Exercise 17.32

Subject: Melt crystallization in a cylindrical tube.

Given: Cylindrical tube with inside radius r_i, inside of which crystallization is occurring due to passage of a coolant on the other side of the tube wall.

Assumptions: The only resistance to heat transfer is the crystal layer.

Find: Derive (17-67):

$$\frac{1}{4}\left(r_i^2 - r_s^2\right) - \frac{r_s^2}{2}\ln\left(\frac{r_i}{r_s}\right) = \frac{k_c\left(T_m - T_c\right)t}{\rho_c \Delta H_f} \tag{1}$$

Analysis: Let r_s = radial distance from tube centerline to the inside surface of the crystal layer.
$T_m - T_c$ = overall temperature driving force (melt to coolant)

For a cylindrical tube, the rate of heat conduction through the crystal layer = heat released by crystallization, based on a shell balance is:

$$\Delta H_f \frac{dm}{dt} = -2\pi r L \rho_c \Delta H_f \frac{dr}{dt} = \frac{k_c\left(T_m - T_c\right)}{r_i - r} A_{\mathrm{LM}} \tag{2}$$

$$\text{where, } A_{\mathrm{LM}} = \frac{2\pi L\left(r_i - r\right)}{\ln\left(\frac{r_i}{r}\right)} \tag{3}$$

Combining (2) and (3), simplifying, separating variables, and integrating both sides,

$$-\int_{r_i}^{r_s} r \ln\left(\frac{r_i}{r}\right) dr = \frac{k_c\left(T_m - T_c\right)}{\rho_c \Delta H_f} \int_0^t dt \tag{4}$$

The left side of (4) becomes,

$$\int_{r_s}^{r_i} \left[r \ln r_i - r \ln r\right] dr = \frac{r^2}{2}\ln r_i\Big|_{r_s}^{r_i} - \frac{r^2}{2}\ln r\Big|_{r_s}^{r_i} + \frac{r^2}{4}\Big|_{r_s}^{r_i} = \frac{r_s^2}{2}\ln\frac{r_s}{r_i} + \frac{1}{4}\left(r_i^2 - r_s^2\right) \tag{5}$$

Combining (4) and (5) and integrating the right side gives (1).

Exercise 17.33

Subject: Zone melting with a single or partial pass.

Given: A crystal layer undergoing zone melting to remove impurities.

Assumptions: Melt zone of width, l, is perfectly mixed with impurity concentration, w. Diffusion of the impurity does not occur in the solid phase. Initial impurity concentration is uniform at w_o. Impurity concentration in the melt zone is in equilibrium with that in the solid phase upstream of the melt zone.

Find: Derive an expression for the average impurity concentration over a particular length of crystal layer, $z_2 - z_1$, after one pass or partial pass of zone melting. Also calculate for Example 17.14, w_{avg} for $z_1 = 0$ and $z_2/l = 9$.

Analysis: The given expression to be derived is:

$$w_{avg} = w_o \left\{ \frac{l(1-K)}{K(z_2 - z_1)} \left[\exp\left(-\frac{z_2 K}{l} \right) - \exp\left(-\frac{z_1 K}{l} \right) \right] + 1 \right\} \tag{1}$$

where, $$K = \frac{\text{impurity concentration in the solid phase}}{\text{impurity concentration in the melt phase}}$$

Using the definition of w_{avg} with (17-73),

$$w_{avg} = \frac{\int_{z_1}^{z_2} w_s \, dz}{z_2 - z_1} = \frac{\int_{z_1}^{z_2} w_o \left[1 - (1-K) \exp\left(-\frac{Kz}{l} \right) \right] dz}{z_2 - z_1} \tag{2}$$

Integrating (2) and applying the limits,

$$w_{avg} = w_o \left\{ \frac{z_2 - z_1}{z_2 - z_1} + \frac{l(1-K)}{K(z_2 - z_1)} \exp\left(-\frac{z_2 K}{l} \right) - \frac{l(1-K)}{K(z_2 - z_1)} \exp\left(-\frac{z_1 K}{l} \right) \right\} ,$$

which simplifies to (1).

From Example 17.14, $K = 0.36$ and $w_o = 0.01$. From above, $(z_2 - z_1)/l = 9$

Substitution into (1) gives,

$$w_{avg} = 0.01 \left\{ \frac{(1-0.36)}{0.36(9)} \left[\exp[-9(0.36] - \exp(0) \right] + 1 \right\} = 0.0081$$

Exercise 17.34

Subject: Zone melting with a single or partial pass.

Given: A crystal layer undergoing the zone melting of Example 17.14, where the last 20% of the crystal layer is removed following the first pass to $z/l = 9$.

Assumptions: Melt zone of width, l, is perfectly mixed with impurity concentration, w. Diffusion of the impurity does not occur in the solid phase. Initial impurity concentration is uniform at w_o. Impurity concentration in the melt zone is in equilibrium with that in the solid phase upstream of the melt zone.

Find: The average impurity concentration in the remaining crystal layer using the expression derived in Exercise 17.33.

Analysis: The expression in Exercise 17.33 is:

$$w_{avg} = w_o \left\{ \frac{l(1-K)}{K(z_2 - z_1)} \left[\exp\left(-\frac{z_2 K}{l}\right) - \exp\left(-\frac{z_1 K}{l}\right) \right] + 1 \right\} \tag{1}$$

where, from Example 17.14, $K = 0.36$, $w_o = 0.01$, $z_1 = 0$, $l/L = 0.1$, and given $z_2 = 0.80$.

Therefore, $\dfrac{l}{z_2 - z_1} = \dfrac{l/L}{z_2/L - z_1/L} = \dfrac{0.1}{0.8 - 0} = \dfrac{0.1}{0.8}$

and, $\dfrac{z_2}{l} = \dfrac{z_2/L}{l/L} = \dfrac{0.8}{0.1} = 8$

Substitution into (1) gives,

$$w_{avg} = 0.01 \left\{ \frac{(1-0.36)(0.1)}{0.36(0.8)} \left[\exp[-8(0.36] - \exp(0) \right] + 1 \right\} = 0.0079$$

Exercise 17.35

Subject: Zone melting with a single pass.

Given: A bar of 98 wt% Al with 2 wt% Fe impurity subjected to one pass of zone refining. K = 0.29 for the impurity. The resulting bar is cut off at $z_2 = 0.75\ z$ and z/l =10.

Assumptions: Melt zone of width, l, is perfectly mixed with impurity concentration, w. Diffusion of the impurity does not occur in the solid phase. Initial impurity concentration is uniform at w_o. Impurity concentration in the melt zone is in equilibrium with that in the solid phase upstream of the melt zone.

Find: The concentration profile for Fe, and the average concentration, using (1) in Exercise 17.33.

Analysis: For the concentration profile, use (17-73),

$$w_s = w_o\left[1-(1-K)\exp\left(-\frac{Kz}{l}\right)\right] = 0.02\left[1-(1-0.29)\exp\left(-\frac{0.29z}{l}\right)\right]$$

Use a spreadsheet to compute the concentration profile for w_s as a function of z/l from 0 to 9. The results are:

z/l	w_s
0	0.0058
1	0.0094
2	0.0120
3	0.0141
4	0.0155
5	0.0167
6	0.0175
7	0.0181
8	0.0186
9	0.0190

The expression in Exercise 17.33 is:

$$w_{avg} = w_o\left\{\frac{l(1-K)}{K(z_2-z_1)}\left[\exp\left(-\frac{z_2K}{l}\right)-\exp\left(-\frac{z_1K}{l}\right)\right]+1\right\} \qquad (1)$$

where, here, $K = 0.29$, $w_o = 0.02$, $z_1 = 0$, take $l/L = 0.1$, and use $z_2 = 0.75\ z$.

Exercise 17.35 (continued)

Therefore, $\dfrac{l}{z_2 - z_1} = \dfrac{l/z}{z_2/z - 0} = \dfrac{1/9}{0.75 - 0} = 0.148$

and, $\dfrac{z_2}{l} = \dfrac{0.75z}{z/9} = 6.75$

Substitution into (1) gives,

$$w_{avg} = 0.02\left\{\frac{(1-0.29)}{0.29}(0.148)\left[\exp\left[-6.75(0.29\right] - \exp(0)\right] + 1\right\} = 0.0138$$

Exercise 17.36

Subject: Desublimation unit of heat exchanger type.

Given: Feed gas of 0.8 mol% benzoic acid (BA) and 99.2 mol% N_2 at 780 torr and 130°C, containing 200 kg/h. Exit temperature is 80°C with no pressure drop. Cooling water flows countercurrently through the inside of the tubes, entering at 40°C and exiting at 90°C. From Example 17.15, tubes are 1 m long and 2.5 cm in outside diameter

Assumptions: Equilibrium

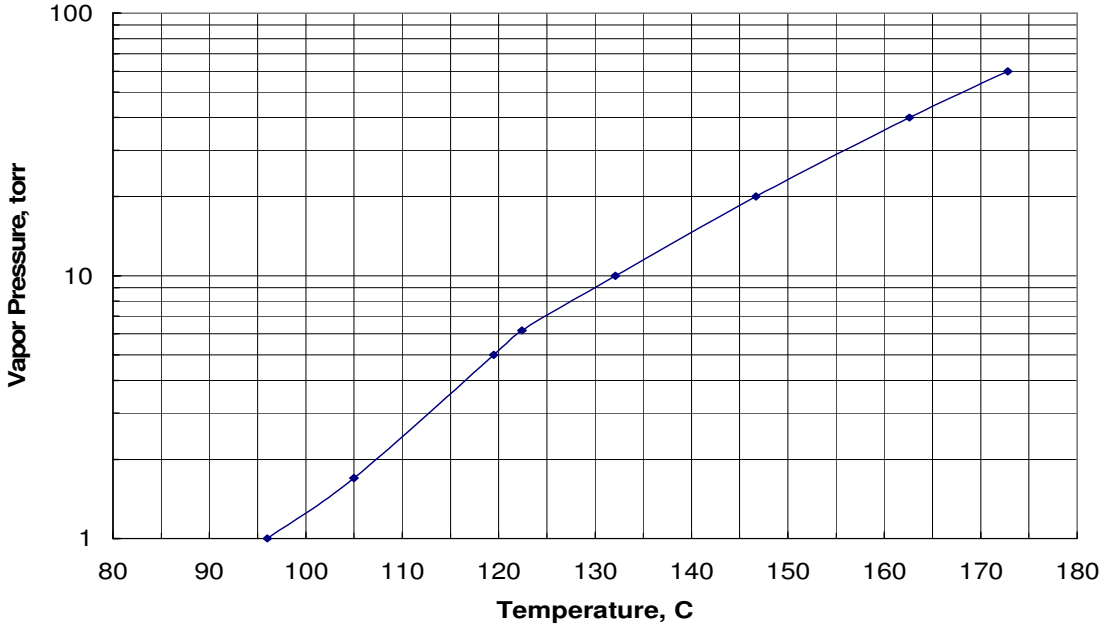
Find: Number of tubes needed and the time to reach the maximum crystal thickness of 1.25 cm.

Analysis: The following properties apply:

MW of BA = 122.12, MW of N_2 = 28.02
Melting point = 122.4°C
Thermal conductivity of BA crystals = 1.4 cal/h-cm-°C
Density of BA crystals = 1.316 g/cm^3
Specific heat of solid and vapor = 0.32 cal/g-°C
Heat of sublimation = 134 cal/g. Therefore, desublimation is exothermic at 134 cal/g
Vapor pressure of BA:

Temp., °C	96	105	119.5	132.1	146.7	162.6	172.8
Vapor Pressure, torr	1 solid	1.7 solid	5 solid	10 liquid	20 liquid	40 liquid	60 liquid

A plot of the vapor pressure data follows:



Exercise 17.36 (continued)

If the thickness of the dusublimate is uniform, mass of BA desublimated =

$$\pi\left(r_s^2 - r_o^2\right) L\rho_c = 3.14\left[(1.25+1.25)^2 - (1.25)^2\right](100)(1.316) = 1{,}940 \text{ g} = 1.94 \text{ kg}$$

Entering gas contains 200 kg/h BA = 200/122.12 = 1.638 kmol/h
Therefore, the N_2 flow rate = 1.638(99.2/0.8) = 203 kmol/h
Partial pressure of BA in entering gas = 0.008(780) = 6.24 torr compared to a BA vapor pressure of 9 torr at 130°C. This confirms that all entering BA is in the vapor phase.

Exit gas temperature is 80°C, which is below the melting point of BA. Therefore, it will desublime as a solid. We must extrapolate the vapor pressure data to estimate the vapor pressure at 80°C. The value is approximately 0.5 torr. Therefore, the flow rate of BA in the exiting gas is

203[0.5/(780 – 0.5)] = 0.13 kmol/h

Therefore, BA desublimes at the rate of 1.638 – 0.130 = 1.508 kmol/h = 184 kg/h.
The ratio of mass of entering gas mixture to entering BA mass =

$$M_r = \frac{28.02(0.992)+122.12(0.008)}{122.12(0.008)} = 29.45$$

Sensible heat + heat of fusion per gram of BA desublimed =

$$M_r C_{P_g}\left(T_{\text{in}} - T_{\text{out}}\right)_g + \Delta H_s = 29.45(0.32)(130-80)+134 = 605 \text{ cal/g}$$

From (17-75), time = $t = \dfrac{1.316(605)}{1.4(40)}\left[\dfrac{(2.5)^2}{2}\ln\left(\dfrac{2.5}{1.25}\right) - \dfrac{1}{4}\left(2.5^2 - 1.25^2\right)\right]$ = 14.2 h

Number of tubes = $\dfrac{184(14.2)}{1.94}$ = 1,350

Exercise 17.37

Subject: Bulk-phase desublimation of benzoic acid from N_2 by injection of water followed by two steps of nitrogen quench.

Given: 3 m^3/h of gas at 1 atm and a temperature of 10°C above the dew point and containing 6.4 mol% benzoic acid (BA) and 93.6 mol% N_2. 150 cm^3/h of water at 25°C is added. Then the gas is further cooled in two steps with N_2 at 1 atm, first with 1.5 m^3/h at 105°C, and secondly with 2.0 m^3/h at 25°C. The following are properties of BA:

Melting point = 122.4°C
Specific heat of solid and gas = 0.32 cal/g-°C
Heat of sublimation = 134 cal/g. Therefore, desublimation is exothermic at 134 cal/g
Vapor pressure of BA:

Temp., °C	96	105	119.5	132.1	146.7	162.6	172.8
Vapor Pressure, torr	1 solid	1.7 solid	5 solid	10 liquid	20 liquid	40 liquid	60 liquid

Assumptions: Equilibrium. Desublimation occurs in the bulk gas. Adiabatic process.

Find: The final gas temperature and the fractional yield of solid benzoic acid crystals.

Analysis: A plot of the vapor pressure data, using a spreadsheet is shown on the following page. Note the change in slope at the melting point.

MW of BA = 122.12
MW of H_2O = 18.02
MW of N_2 = 28.01

First find the entering gas temperature by computing the dew point temperature.
Partial pressure of BA in entering gas = 0.064(760) = 49 torr. From the vapor pressure curve, this is in the liquid region with a temperature of 167.5°C. Therefore, the entering gas temperature is 167.5 + 10 = 177.5°C

Next, calculate the mass flow rate of the entering gas, using SI units.

MW of entering gas = M = 0.064(122.12) + 0.936(28.01) = 34.03
Temperature = 177.5 + 273.2 = 450.7 K
Pressure = 1 atm = 101.3 kPa

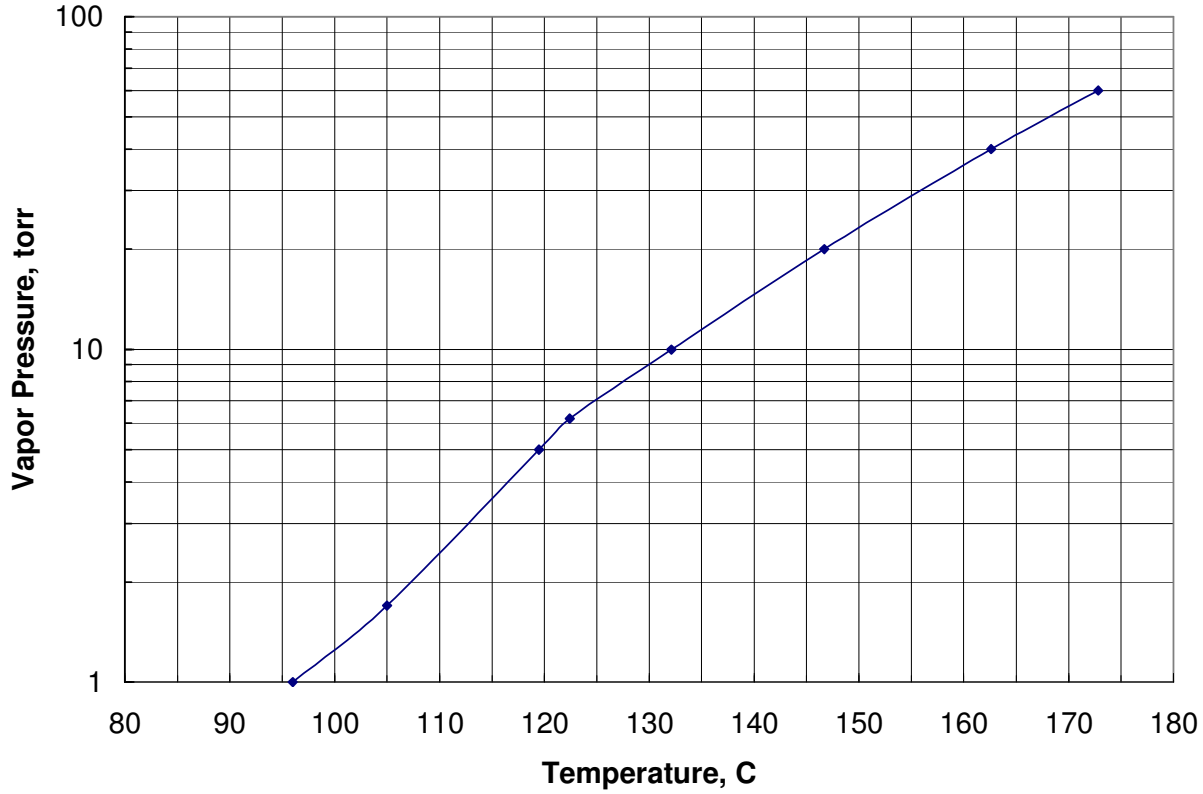
Therefore, from the ideal gas law,

$$\rho = \frac{PM}{RT} = \frac{(101.3)(34.03)}{(8.314)(450.7)} = 0.920 \text{ kg/m}^3$$

Entering gas flow rate = 3(0.920) = 2.76 kg/h or 2.76/34.03 = 0.0811 kmol/h

This gives 0.064(0.0811) = 0.00519 kmol/h or 0.634 kg/h of BA
and 2.76 – 0.634 = 2.126 kg/h of N_2

Exercise 17.37 (continued)



Water at a flow rate of 150 cm^3/h or 0.150 kg/h is now added.
Now add 1.5 m^3/h of N_2 at 105°C and 1 atm. From the ideal gas law,

$$\rho = \frac{PM}{RT} = \frac{(101.3)(28.02)}{(8.314)(378.2)} = 0.903 \text{ kg/m}^3$$

Therefore the mass flow rate of N_2 added = 1.5(0.903) = 1.354 kg/h
Next, add 2.0 m^3/h of N_2 at 25°C and 1 atm. From the ideal gas law,

$$\rho = \frac{PM}{RT} = \frac{(101.3)(28.02)}{(8.314)(298.2)} = 1.145 \text{ kg/m}^3$$

Therefore the mass flow rate of N_2 added = 2.0(1.145) = 2.290 kg/h

Thus, the final exiting combined gas and solid is as follows:

Component	kg/h	kmol/h	Mol fraction	Partial Pressure if no condensation, torr
Benzoic acid	0.634	0.00519	0.0236	17.9
Nitrogen	5.770	0.20600	0.9385	713.3
Water	0.150	0.00832	0.0379	28.8
Total	6.554	0.21951	1.0000	760.0

Exercise 17.37 (continued)

Now determine the exit temperature and the amount of BA desublimed.
Assume that water does not condense.
Let x = fraction of BA desublimed and T be the exiting temperature
Assume a thermodynamic path of all water evaporated at 25°C and BA condensed at the final temperature (however, it doesn't matter because BA and N_2 specific heats are assumed constant regardless of the phase state).

An enthalpy balance can be written as:

Cooling of feed gas to T and desublimation of BA = vaporization of added water and heating of gas of added water and added N_2 to T. Using cgs units, with a heat of vaporization for water = 583 cal/g at 25°C,

$$2{,}760(0.32)(177.5 - T) + 634x(134) =$$
$$150(583) + 150(0.44)(T - 25) + 1{,}354(0.32)(T - 105) + 2{,}290(0.32)(T - 25) \qquad (1)$$

This balance must be consistent with a partial pressure of non-desublimed BA in the gas equal to the vapor pressure at T.

For a set of assumed values of T, compute x and compare the partial pressure of BA to its vapor pressure, using a spreadsheet. We need an interpolating equation for the vapor pressure. A fit of the Clausius-Clapeyron equation from 96 to 105°C with Polymath, gives,

$$\log_{10}\left(P^s_{\text{BA}} \text{ in torr}\right) = 9.679 - \frac{3572}{T\left(^\circ\text{C}\right) + 273}$$

The spreadsheet results are:

T, C	x	Vapor Pressure, torr	kmol/h BA in vapor	Partial Pressure, torr
96	0.804	1.00	0.001018	3.59
97	0.829	1.06	0.000889	3.14
98	0.854	1.12	0.000760	2.69
99	0.878	1.19	0.000631	2.23
100	0.903	1.27	0.000502	1.77
101	0.928	1.34	0.000372	1.32
102	0.953	1.42	0.000243	0.86
103	0.978	1.51	0.000114	0.40
105	1.028	1.70	-0.000145	-0.51

The vapor pressure = the partial pressure at an exit temperature of 101°C with 93% of the BA desublimed.

Check to determine if any water is condensed at this temperature. The vapor pressure of water at 101°C exceeds 760 torr. Since the partial pressure of water in the exiting gas is much less than this, the assumption of no condensation of water is valid.

Exercise 17.38

Subject: Desublimation on the outside of a heat exchanger tube.

Given: Heat exchanger tube with a coolant flowing through the inside and desublimation occurring on the outside surface of the tube.

Assumptions: Rate of desublimation controlled by heat conduction through the deposited crystal layer. Sensible heat effect is negligible compared to the latent heat of desublimation. Temperatures of the gas and the coolant assumed constant over tube length.

Find: Derive (17-75), which gives the time for a crystal layer to grow from the outside tube radius, r_o, to a radius, r_s.

Analysis: Equation (17-75) gives,

$$t = \frac{\rho_c \Delta H_s}{k_c \left(T_g - T_c\right)} \left[\frac{r_s^2}{2} \ln\left(\frac{r_s}{r_o}\right) - \frac{1}{4}\left(r_s^2 - r_o^2\right) \right] \tag{1}$$

Rate of heat released by desublimation = rate of heat conduction through the crystal layer.

$$\text{Therefore, } \Delta H_s \frac{dm}{dt} = \Delta H_s 2\pi r L \rho_c \frac{dr}{dt} = \frac{k_c A_{LM} \left(T_g - T_c\right)}{r - r_o} \tag{2}$$

where, ΔH_s = heat of sublimation

ρ_c = density of the crystal layer
k_c = thermal conductivity of the crystal layer
L = length of the tube
T_g = bulk temperature of the gas carrying the component that desublimes
T_c = bulk temperature of the coolant
A_{LM} = log mean area for conduction through the crystal layer

$$A_{LM} = \frac{2\pi r L - 2\pi r_o L}{\ln\left(\dfrac{2\pi r L}{2\pi r_o L}\right)} \tag{3}$$

Combining (2) and (3), simplifying, separating variables, and putting in integral form,

$$\int_{r_o}^{r_s} r \ln\left(\frac{r}{r_o}\right) dr = \frac{k_c \left(T_g - T_c\right)}{\rho_c \Delta H_s} \int_0^t dt \tag{4}$$

Carrying out the integration and applying the limits gives (1).

Exercise 17.39

Subject: Evaporation of aqueous NaOH in a single-effect evaporator

Given: Feed of 50,000 lb/h of a 20 wt% aqueous solution of NaOH at 120°F. Concentration to 40 wt% NaOH at a pressure of 3.7 psia. Heating medium is saturated steam at a temperature 40°F higher than the solution temperature in the evaporator.

Assumptions: Perfect mixing in the evaporator. No heat losses.

Find: (a) Boiling-point elevation of the solution
(b) Saturated heating steam temperature and pressure
(c) Evaporation rate
(d) Heat transfer rate
(e) Heating steam flow rate
(f) Economy
(g) Heat-transfer area if U = 300 Btu/h-ft^2-°F

Analysis:

(a) From the steam tables, at 3.7 psia, saturated steam temperature = 122.3°F. From the During chart of Fig. 17.32, the boiling temperature of 40 wt% NaOH = 166°F. Therefore the boiling-point elevation = 166 – 122 = 44°F. This result is consistent with Fig. 17.33.

(b) Saturated heating steam temperature = 166 + 40 = 206°F, with a pressure of 13 psia.
Note: Best not to use steam under vacuum. Should change to atmospheric pressure.

(c) NaOH flow rate = 0.2(50,000) = 10,000 lb/h. Entering water rate = 50,000 – 10,000 = 40,000 lb/h. Water in concentrated NaOH = (60/40)10,000 = 15,000 lb/h. Therefore evaporation rate = 40,000 – 15,000 = 25,000 lb/h.

(d) Calculate heat transfer rate by an enthalpy balance around the evaporator using Fig. 17.35 and the steam tables for enthalpies.

$$Q = m_v H_v + m_p H_p - m_f H_f \qquad (1)$$

Note that the vapor produced is superheated steam at 3.7 psia and 166°F.

$$Q = 25{,}000(1{,}133.7) + 25{,}000(145) - 50{,}000(72) = 28{,}400{,}000 \text{ Btu/h}$$

(e) Heating steam = $m_s = Q/\Delta H_s$ = 28,400,000/974.2 = 29,100 lb/h

(f) Economy = 25,000/29,100 = 0.859 = 85.9%

(g) From (17-81),

$$A = \frac{Q}{U\left(T_s - T_p\right)} = \frac{28{,}400{,}000}{300(206-166)} = 2{,}370 \text{ ft}^2$$

Exercise 17.40

Subject: Comparison of single-effect to double-effect evaporation.

Given: Feed of 30,000 lb/h of 10 wt% NaOH at 100°F. Concentrated to 50 wt% using saturated steam at 115 psia.

Assumptions: Perfect mixing in the evaporator. No heat losses. Equal heat-transfer areas for the double-effect system.

Find: (a) Heat-transfer area and economy for a single effect, with U = 400 Btu/h-ft^2-°F and vapor-space pressure of 4 in Hg.

(b) Heat-transfer areas and overall economy for a double-effect system, with forward feed and U = 450 for the first effect and 350 for the second effect. Vapor-space pressure of 4 in Hg for the second effect

Analysis: (a) Single-effect

First compute the mass balance.
NaOH in the feed = 0.1(30,000) = 3,000 lb/h
Water in the feed = 30,000 – 3,000 = 27,000 lb/h
Water in the product solution = (50/50)3,000 = 3,000 lb/h
Water evaporated = 27,000 – 3,000 = 24,000 lb/h

Now, calculate the product solution temperature. At 4 in Hg, water boils at 125.4°F. From Fig. 17.32, the boiling temperature of 50 wt% NaOH = 197°F, consistent with Fig. 17.33.

Calculate heat transfer rate by an enthalpy balance around the evaporator using Fig. 17.35 and the steam tables for enthalpies.

$$Q = m_v H_v + m_p H_p - m_f H_f \tag{1}$$

Note that the vapor produced is superheated steam at 4 in Hg and 197°F.

$$Q = 24{,}000(1{,}148.6) + 6{,}000(222) - 30{,}000(62) = 27{,}000{,}000 \text{ Btu/h}$$

Heating steam = $m_s = Q/\Delta H_s$ = 27,000,000/880.6 = 30,700 lb/h

Economy = 24,000/30,700 = 0.782 = 78.2%

From (17-81),

$$A = \frac{Q}{U\left(T_s - T_p\right)} = \frac{27{,}000{,}000}{400\left(338.1 - 197\right)} = 478 \text{ ft}^2$$

Exercise 17.40 (continued)

(b) Double-effect system with forward feed and equal heat-transfer areas

The overall mass balance is the same as part (a), where the total evaporation rate is 24,000 lb/h. This system is solved iteratively, converging when the two areas are equal.

As a first approximation, assume equal evaporation rates, i.e. 12,000 lb/h each. Solution leaving Effect 1 = 30,000 – 12,000 = 18,000 lb/h with a composition of 3,000 lb/h of NaOH and 15,000 lb/h water, or 16.67 wt% NaOH. Boiling-point elevation from Fig. 17.32 is 10°F for Effect 1, while boiling-point elevation for Effect 2 is still 72°F, giving a temperature of 197°F for streams leaving Effect 2.

With heating steam at 338°F in Effect 1, the overall ΔT for the two effects is 338 – 197 – the boiling-point elevation of 10°F in Effect 1 (because the vapor produced there and used as heating steam in Effect 2 will condense at a temperature less by the boiling-point elevation) = 131°F.

Iteration 1:

Assume that the ΔT for each effect is inversely proportional to U. Thus, $\Delta T_1 = (U_2/U_1)\,\Delta T_2$. Also $\Delta T_1 + \Delta T_2 = 131^\circ$F. Solving these equations simultaneously, $\Delta T_1 = 57^\circ$F and $\Delta T_2 = 74^\circ$F. Therefore, the exiting temperature in Effect 1 = 338 – 57 = 281°F. This reduces the boiling-point elevation in Effect 1 to 8°F. Use this. Therefore, the superheated vapor leaving Effect 1 will condense in Effect 2 at 281 – 8 = 273°F, corresponding to a pressure of 44 psia in Effect 1.

Enthalpy balances for the two effects are:

$$Q_1 = m_s \Delta H_s^{vap} = m_{v_1} H_{v_1} + m_1 H_1 - m_f H_f \tag{2}$$

$$Q_2 = m_{v_1}\left(\Delta H_{v_1} - H \text{ of saturated condensate of } v_1\right) = m_{v_2} H_{v_2} + m_2 H_2 - m_1 H_1 \tag{3}$$

Using Fig. 17.35 and steam tables for enthalpies, these two equations are solved for m_s and m_1: From (2),

$$m_s(880.6) = (30{,}000 - m_1)(1176) + m_1(222) - 30{,}000(62) \tag{4}$$

From (3),

$$(30{,}000 - m_1)(1176 - 242) = (m_1 - 6{,}000)(1148.6) + 6{,}000(222) - m_1(222) \tag{5}$$

Solving (4) and (5), m_1 = 18,000 lb/h which was the guess.

m_s = 18,400 lb/h

Now, solve for the heat-transfer areas:

$$A_1 = \frac{Q_1}{U_1(T_s - T_1)} = \frac{18{,}400(880.6)}{450(338.1 - 281)} = 631 \text{ ft}^2$$

$$A_2 = \frac{Q_2}{U_2(273 - T_2)} = \frac{(30{,}000 - 18{,}000)(1176 - 242)}{350(273 - 197)} = 421 \text{ ft}^2$$

Because the areas are far apart, make another iteration. To do this, adjust the ΔTs, as follows: Assume the heat duties from above will still hold. That is, Q_1 = 18,400(880.6) = 16,200,000 and Q_2 = 12,000(1176 – 242) = 11,200,000, both in Btu/h. Then, for equal Areas, A:

$$A(450)(338 - T_1) = 16{,}200{,}000 \text{ and } A(350)(T_1 - 8 - 197) = 11{,}200{,}000$$

Solving these two equations, T_1 = 268°F, compared to 281°F in the first iteration.

Exercise 17.40 (continued)

Iteration 2:

Equations (4) and (5) now become:

$$m_s(880.6) = (30{,}000 - m_1)(1172) + m_1(210) - 30{,}000(62) \qquad (6)$$

and

$$(30{,}000 - m_1)(1172 - 242) = (m_1 - 6{,}000)(1148.6) + 6{,}000(222) - m_1(210) \qquad (7)$$

Solving (4) and (5), m_1 = 17,900 lb/h

m_s = 18,300 lb/h

Thus, little change in these flow rates from iteration 1.

Now, solve for the heat-transfer areas:

$$A_1 = \frac{Q_1}{U_1(T_s - T_1)} = \frac{18{,}300(880.6)}{450(338.1 - 268)} = 510 \text{ ft}^2$$

$$A_2 = \frac{Q_2}{U_2(273 - T_2)} = \frac{(30{,}000 - 18{,}000)(1172 - 242)}{350(260 - 197)} = 510 \text{ ft}^2$$

Thus, the problem is converged.

Economy = 24,000/18,300 = 1.31 or 131% compared to 78.2% for one effect

Exercise 17.41

Subject: Double-effect evaporation with forward feed.

Given: Feed of 16,860 lb/h of 10 wt% aqueous $MgSO_4$ at 14.7 psia and 70°F. Pressure in the second effect = 2.20 psia. Heating medium is saturated steam at 230°F. Estimated heat transfer coefficients in Btu/h-ft^2-°F are 400 for Effect 1 and 350 for Effect 2. Concentrated solution from Effect 2 is to be 30 wt% $MgSO_4$.

Assumptions: Perfect mixing in the evaporator. No heat losses. Equal heat-transfer areas for the double-effect system. Neglect boiling-point elevations.

Find: (a) The pressure in Effect 1
(b) Percent of total evaporation in Effect 1
(c) Heat-transfer area of each effect
(d) Economy

Analysis: First compute the overall mass balance:

$MgSO_4$ in the feed = 0.1(16,860) = 1,686 lb/h
Water in the feed = 16,860 – 1,686 = 15,174 lb/h
Water in the product solution = (70/30)1,686 = 3,934 lb/h
Water evaporated = 15,174 – 3,934 = 11,240 lb/h
Product solution = 1,686 + 3,934 = 5,620 lb/h

With no boiling-point elevation, from the steam tables, T_2 = 130°F at 2.2 psia
Therefore, the overall $\Delta T = \Delta T_1 + \Delta T_2$ = 230 – 130 = 100°F.

Iteration 1:

Assume that the ΔT for each effect is inversely proportional to U. Thus, $\Delta T_1 = (U_2/U_1)\,\Delta T_2$.
Also $\Delta T_1 + \Delta T_2$ = 100°F. Solving these equations simultaneously, ΔT_1 = 47°F and ΔT_2 = 53°F.
Therefore, the exiting temperature in Effect 1 = T_1 230 – 47 = 183°F.

Enthalpy balances for the two effects are:

$$Q_1 = m_s \Delta H_s^{vap} = m_{v_1} H_{v_1} + m_1 H_1 - m_f H_f \tag{1}$$

$$Q_2 = m_{v_1} \left(\Delta H_{v_1}^{vap}\right) = m_{v_2} H_{v_2} + m_2 H_2 - m_1 H_1 \tag{2}$$

Using Fig. 17.10 and steam tables for enthalpies, these two equations are solved for m_s and m_1:
From (1),

$$m_s(958.8) = (16{,}860 - m_1)(1139.3) + m_1(82) - 16{,}860(6) \tag{3}$$

From (2),

$$(16{,}860 - m_1)(988.5) = (m_1 - 5{,}620)(1117.7) + 5{,}620(-17) - m_1(82) \tag{4}$$

Solving (3) and (4), m_1 = 11,380 lb/h
m_s = 7,388 lb/h

Exercise 17.41 (continued)

Now, solve for the heat-transfer areas:

$$A_1 = \frac{Q_1}{U_1(T_s - T_1)} = \frac{7{,}388(958.8)}{400(47)} = 377 \text{ ft}^2$$

$$A_2 = \frac{Q_2}{U_2(273 - T_2)} = \frac{(16{,}860 - 11{,}380)(988.5)}{350(53)} = 292 \text{ ft}^2$$

Because the areas are far apart, make another iteration. To do this, adjust the ΔTs, as follows: Assume the heat duties from above will still hold. That is, Q_1 = 7,388(958.8) = 7,084,000 and Q_2 = 5480(988.5) = 5,417,000, both in Btu/h. Then, for equal Areas, A:

$A(400)(230 - T_1) = 7{,}084{,}000$ and $A(350)(T_1 - 130) = 5{,}417{,}000$

Solving these two equations, T_1 = 176.6°F, compared to 183°F in the first iteration.

Iteration 2:

Solve (4) for the new temperatures:

$$(16{,}860 - m_1)(992.4) = (m_1 - 5{,}620)(1117.7) + 5{,}620(-17) - m_1(82) \qquad (5)$$

Solving, m_1 = 11,400 lb/h, which is very close to the value of 11,380 lb/h

Thus, essentially no change in these flow rates from iteration 1 and the problem is converged.

Now, solve for the heat-transfer areas:

$$A_1 = \frac{Q_1}{U_1(T_s - T_1)} = \frac{7{,}388(958.8)}{400(230 - 176.6)} = 332 \text{ ft}^2$$

$$A_2 = \frac{Q_2}{U_2(273 - T_2)} = \frac{(16{,}860 - 11{,}400)(988.5)}{350(176.6 - 130)} = 327 \text{ ft}^2$$

(c) The area of each evaporator = 330 ft^2

(a) The pressure in the first effect is that corresponding to 176.6°F. From steam tables, 7 psia.

(b) Evaporation in the Effect 1 = 16,860 – 11,400 = 5,460 lb/h of heating steam.
Therefore, percent of total evaporation in the first effect = 5,560/11,240 = 0.495 or 49.5 %

(e) Heating steam required for Effect 1 is obtained from a revision of (3),

$m_s(958.8) = (16{,}860 - m_1)(1136.8) + m_1(82) - 16{,}860(6)$

Solving, m_s = 7,340 lb/h

Economy = 11,240/7,340 = 1.53 or 153%.

Exercise 18.1

Subject: Selection of dryer for removal of surface moisture from 0.5 mm crystals of NaCl without breakage.

Find: Suitable type continuous, direct-heat dryers. Highest gas feed temperature.

Analysis: Applicable dryers are tunnel dryer or belt dryer.
Inlet gas temperature can be high, to say 1400°F, because of the high melting point of NaCl.

Exercise 18.2

Subject: Batch drying of 100 kg/h of a toxic, temperature-sensitive material of 350 mm size.

Find: Suitable dryers.

Analysis: Select a rotating, double-cone vacuum dryer.

Exercise 18.3

Subject: Drying of a thin, milk-like liquid to produce a powder

Find: Suitable continuous, direct-heat dryer that will restrict temperature to less than 200°F.

Analysis: Select a spray dryer.

Exercise 18.4

Subject: Selection of dryers from conditions of the feed, temperature sensitivity, and form of the dried product

Find: Suitable batch or continuous dryers for different cases.

Analysis: (a) A temperature-insensitive paste that must be maintained in slab form.
Select a batch tray dryer or a continuous belt dryer.

(b) A temperature-insensitive paste that can be extruded.
Select a continuous through-circulation belt or band dryer, or a batch, agitated pan dryer.

(c) A temperature-insensitive slurry.
Select a continuous spray dryer.

(d) A thin liquid from which flakes are to be produced.
Select a continuous drum dryer.

(e) Pieces of lumber.
Select a batch closed container with wood stacked for good flow of air by kiln drying in a chamber with temperature and humidity control.

(f) Pieces of pottery.
Select a continuous tunnel dryer.

(g) Temperature-insensitive inorganic crystals, where particle size is to be maintained and only surface moisture is to be removed.
Select a tunnel dryer, a belt or band dryer, or an indirect-heat, steam-tube rotary dryer.

(h) Orange juice to produce a powder.
Select a batch freeze dryer.

Exercise 18.5

Subject: Solar drying

Find: Advantages and disadvantages of solar drying for organic materials. Other applicable dryers for organic materials and for continuously drying beans.

Analysis: Advantage of solar drying is no cost for energy.
Disadvantage of solar drying is long drying time, variability of weather, lack of control.

Other dryers suitable for organic materials are tunnel dryer and belt or band dryer.

For the continuous drying of beans, can use steam-tube rotary dryer, roto-louvre dryer, screw conveyor dryer, through-circulation or band dryer, and fluidized-bed dryer. Might also consider a column dryer with solids moving down by gravity with countercurrent flow of warm air.

Exercise 18.6

Subject: Fluidized-bed dryer

Find: Advantages of fluidized-bed dryer for vegetables, including potato granules, peas, diced carrots, and onion flakes.

Analysis: Advantage is control and uniformity of temperature of both solids and gas.

Exercise 18.7

Subject: Three-stage process for producing powdered milk from liquid milk

Find: Reasons why the following 3-stage process is better than a single stage of spray drying:
Stage 1: Vacuum evaporation in a falling-film evaporator to a high-viscosity liquid of less than 50 wt% water.
Stage 2: Spray drying to 7 wt% moisture.
Stage 3: Fluidized-bed drying to 3.6 wt% moisture.

Analysis: Since milk is very temperature sensitive, it is best to first concentrate the liquid rapidly at a low temperature. The falling-film evaporator is ideal for this. Then the combination of a spray dryer and fluidized-bed dryer offers efficiency, product control, and flexibility. Because of the large amount of moisture that would have to be removed compared to the final dry-milk powder, it would be difficult to achieve a uniform moisture content with a spray dryer alone.

Exercise 18.8

Subject: Drying pharmaceutical products.

Find: Reasons why a closed-cycle spray dryer using N_2 is a good choice for the drying of materials from a non-aqueous solvent, such as methanol, ethanol, acetone, etc.

Analysis: Closed-cycle spray dryers offer flexibility, scalability, reliability, and controllability. The product from such a dryer is a powder of controlled particle size that is readily compressed into tablets.

Exercise 18.9

Subject: Drying of paper made from a suspension of fibers in water, followed by draining the fibers to a water-to-fiber ratio of 6:1, followed by pressing to a 2:1 ratio.

Find: Type of dryer to produce a continuous sheet to an equilibrium-moisture content of 8 wt% (dry basis).

Analysis: Use a continuous sheeting or rolling dryer with stretched paper that passes over steam-heated rollers.

Exercise 18.10

Subject: Reasons for drying green wood.

Find: Best way to dry green wood to avoid distortion, cracks, splits, and checks. The green wood contains from 40 to 110 wt% moisture (dry basis) and must be dried to just under its equilibrium moisture content, typically 6 to 15 wt% (dry basis).

Analysis: To avoid cracks, splits, and checks, coat the ends with tar. To avoid distortion, dry slowly and uniformly in a chamber with air at a moderate temperature and controlled humidity. Use kiln drying in a closed container. Dry lumber machines better, glues better, and finishes better.

Exercise 18.11

Subject: Drying of wet coal.

Find: Types of direct-heat dryers that are suitable for drying coal to a moisture content less than 20 wt% (dry basis) before it is transported, briquetted, coked, gasified, carbonized, or burned. Can a spouted-bed dryer be used? Does the use of air pose a fire and explosion hazard? Can superheated steam be used?

Analysis: Fluidized-bed and fixed-bed column dryers are suitable, as is a spouted-bed and belt or band dryer. Air does pose a fire and explosion hazard in the presence of coal dust particles. Superheated steam can be used as the heating medium.

Exercise 18.12

Subject: Drying of coated paper, films, tapes, and sheets

Find: Types of dryers for removing solvents from water-based or solvent-based coatings from coated webs, such as coated paper and cardboard, coated plastic films and tape, and coated metallic sheets. Typical coatings are 0.1 mm in wet thickness. Much of the drying time is in the falling-rate period. Can infrared dryers be used?

Analysis: Yes, infrared dryers can be used. Their advantages over hot-air systems are thorough drying that is fast and efficient. Infrared dryers are compact with simple installation and operation, low maintenance, and accurate control.

Exercise 18.13

Subject: Drying of finely divided solvent- or water-wet polymer beads of polymers such as polyvinylchloride, polystyrene, and polymethylmethacrylate, made by suspension or emulsion polymerization at high production rates

Find: Why rotary, fluidized-bed, and spouted-bed dryers are popular choices, using air, inert gas, or superheated steam as the heating medium.

Analysis: Rotary, fluidized-bed, and spouted-bed dryers are good choices because they can handle, at high production rates, low-density polymer beads very well, and can be designed as closed systems with an inert gas or superheated steam if the beads are solvent-wet.

Exercise 18.14

Subject: Comparison of air and superheated steam as heating media.

Find: Advantages and disadvantages of superheated steam compared to air, especially for the drying of lumber.

Analysis: The use of superheated steam is viable for drying lumber. Of particular interest is the use of superheated steam under vacuum conditions to lower the drying temperature so as to avoid problems such as distortion, cracks, splits, and checks. The disadvantage is cost.

Exercise 18.15

Subject: Air conditions from a psychrometric chart and equations.

Given: Air, for a direct-heat dryer, entering at 250°F and 1 atm with a wet-bulb temperature of 105°F.

Find: All of the psychrometric values listed below, using a psychrometric chart, steam tables, and Table 18.3.

Analysis: (a) Humidity

Humidity, $\mathcal{H}$ = 0.0158 lb water/lb dry air

(b) Molal humidity

Molal humidity = $\mathcal{H}_m$ = 0.0158(28.97/18.02) = 0.0254 mol water/mol dry air

(c) Percentage humidity

% humidity, $\mathcal{H}_P$, is not applicable at these conditions because the vapor pressure is greater than the pressure.

(d) Relative humidity

$$\text{Relative humidity, } \mathcal{H}_R = \frac{p_{H_2O}}{p^s_{H_2O}} = \frac{\frac{0.0254}{1.0254}(14.696)}{29.83} = 0.0122 \text{ or } 1.22\%$$

which is in agreement with Fig.18.17.

(e) Saturation humidity is not applicable because vapor pressure is > than pressure.

(f) Humid volume

From (18-10), humid volume us given by,

$$v_H = \frac{RT}{P}\left(\frac{1}{M_{\text{air}}} + \frac{H}{M_{H_2O}}\right) = \frac{0.730(250+460)}{1}\left(\frac{1}{28.97} + \frac{0.0158}{18.02}\right) = 18.3 \text{ ft}^3\text{/lb dry air}$$

which is in agreement with Fig. 18.17.

(g) Humid heat

From (18-11), humid heat is given by,

$$c_s = 0.24 + 0.45(0.0158) = 0.247 \text{ Btu/lb dry air - }^\circ\text{F}$$

(h) Enthalpy

From (18-12) with T_o = 32°F and for water, λ_o = 1075 Btu/lb

H = 0.247(250 – 32) + 1075(0.0158) = 70.8 Btu/lb dry air

Exercise 18.15 (continued)

(i) Adiabatic-saturation temperature

For the air-water system, adiabatic-saturation temperature = wet-bulb temperature = 105^{o}F

(j) Mole fraction of water in the air

Obtain this from the molal humidity.

$$y_{H_2O} = \frac{0.0254}{1.0254} = 0.0248$$

Exercise 18.16

Subject: Air conditions from a psychrometric chart and equations.

Given: Air, for a direct-heat dryer, entering at 200°F and 1 atm with a relative humidity of 15%.

Find: All of the psychrometric values listed below, using a psychrometric chart, steam tables, and Table 18.3.

Analysis: (a) Wet-bulb temperature

T_w = 127.5°F

(b) Adiabatic-saturation temperature

For the air-water system, adiabatic-saturation temperature = wet-bulb temperature = 127.5°F

(c) Humidity

Humidity, $\mathcal{H}$ = 0.0835 lb water/lb dry air

(d) Percentage humidity

From (18-9) using the saturation humidity computed in part (e),

$$\mathcal{H}_P = \frac{0.0835}{2.262} \times 100\% = 3.69\%$$

(e) Saturation humidity

From (18-7), using the vapor pressure of water at 200°F = 11.526 psia,

$$\text{Saturation humidity, } \mathcal{H}_s = \frac{18.02}{28.97}\frac{(11.526)}{(14.696-11.526)} = 2.262 \text{ lb water/lb dry air}$$

(f) Humid volume

From (18-10), humid volume us given by,

$$v_H = \frac{RT}{P}\left(\frac{1}{M_{\text{air}}} + \frac{H}{M_{\text{H}_2\text{O}}}\right) = \frac{0.730(200+460)}{1}\left(\frac{1}{28.97} + \frac{0.0835}{18.02}\right) = 18.9 \text{ ft}^3\text{/lb dry air}$$

which is in agreement with Fig. 18.17.

(g) Humid heat

From (18-11), humid heat is given by,

$$c_s = 0.24 + 0.45(0.0835) = 0.278 \text{ Btu/lb dry air - }^\circ\text{F}$$

Exercise 18.16 (continued)

(h) Enthalpy

From (18-12) with $T_o = 32^oF$ and for water, $\lambda_o = 1075$ Btu/lb

$$H = 0.278(200 - 32) + 1075(0.0835) = 136.5 \text{ Btu/lb dry air}$$

(i) Partial pressure of water in the air. From (18-8),

$$p_{H_2O} = 0.15\, p^s_{H_2O} = 0.15(11.526) = 1.73 \text{ psia}$$

Exercise 18.17

Subject: Air conditions from a psychrometric chart and equations.

Given: From Example 18.1, air at 131°F with a humidity of 0.03 lb water/lb dry air, but with a total pressure for this exercise of 1.5 atm.

Find: All of the psychrometric values listed below, using a psychrometric chart, steam tables, and Table 18.3.

Analysis: (a) Molal humidity. From (18-6),

Molal humidity = $\mathcal{H}_m = 0.03(28.97/18.02) = 0.048$ mol water/mol dry air

(b) Saturation humidity

From (18-7), using the vapor pressure of water at 131°F = 0.155 atm,

$$\text{Saturation humidity, } \mathcal{H}_s = \frac{18.02}{28.97}\frac{(0.155)}{(1.5-0.155)} = 0.072 \text{ lb water/lb dry air}$$

(c) Relative humidity

$$\text{Relative humidity, } \mathcal{H}_R = \frac{p_{H_2O}}{p^s_{H_2O}} = \frac{\frac{0.048}{1.048}(1.5)}{0.155} = 0.443 \text{ or } 44.3\%$$

(d) Percentage humidity

From (18-9) using the saturation humidity computed in part (b),

$$\mathcal{H}_P = \frac{0.03}{0.072}\times 100\% = 41.7\%$$

(e) Humid volume

From (18-10), humid volume us given by,

$$v_H = \frac{RT}{P}\left(\frac{1}{M_{air}} + \frac{H}{M_{H_2O}}\right) = \frac{0.730(131+460)}{1.5}\left(\frac{1}{28.97} + \frac{0.03}{18.02}\right) = 10.4 \text{ ft}^3\text{/lb dry air}$$

(f) and (g) The small pressure change has a negligible effect.

Therefore, $c_s = 0.254$ Btu/lb dry air-°F

And $H = 57.4$ Btu/lb dry air

Exercise 18.18

Subject: Humidity conditions for a mixture of n-hexane and nitrogen.

Given: Gas at 70°F and 1.1 atm with a relative humidity for hexane of 25%.

Find: Humidity conditions given below.

Analysis: At 70°F, from Fig. 2.4, the vapor pressure of n-hexane is 2.4 psia or 0.163 atm.

(a) Partial pressure of hexane.

From (18-8), $p = p^s \mathcal{H}_R = 0.163(0.25) = 0.041$ atm

(b) Humidity

From (18-5), $\mathcal{H} = \dfrac{M_{nC_6}}{M_{N_2}} \dfrac{p_{nC_6}}{\left(P - p_{nC_6}\right)} = \dfrac{86.17}{28.02} \dfrac{0.041}{(1.1 - 0.041)} = 0.119$ lb nC_6/lb dry N_2

(c) Percentage humidity

Need saturation humidity, $\mathcal{H}_s$, from (18-7),

$$\mathcal{H}_S = \frac{M_{nC_6}}{M_{N_2}} \frac{p^s_{nC_6}}{\left(P - p^s_{nC_6}\right)} = \frac{86.17}{28.02} \frac{0.163}{(1.1 - 0.163)} = 0.535 \text{ lb } nC_6\text{/lb dry } N_2$$

From (18-9),

$$\mathcal{H}_P = (0.119/0.535) \text{ x } 100\% = 22.2\%$$

(d) Mole fraction of n-hexane

$$y_{nC_6} = \frac{p_{nC_6}}{P} = \frac{0.041}{1.1} = 0.037$$

Exercise 18.19

Subject: Humidity conditions for a mixture of toluene and air.

Given: Gas at 180°F and 1 atm with a relative humidity for toluene of 15%.

Find: Humidity conditions given below.

Analysis: Use Fig. 18.20 for the air-toluene system at 1 atm.

Using Fig. 18.20: $\mathcal{H}$ = 0.21 lb toluene/lb dry air

T_s = 112°F

To obtain the wet-bulb temperature, which is not equal to the adiabatic saturation temperature for the toluene-air system, a large extrapolation is needed, giving T_w = approximately 118°F.

From Table 18.5, psychrometric ratio = $N_{\text{Le}}^{2/3} = 1.908$

Exercise 18.20

Subject: Wet-solid temperature profile in a continuous, adiabatic, direct-heat dryer

Given: Entering air at $T_o = 180^oF$ and 1 atm, with a relative humidity of 15%. Air flows cocurrently to the water-wet solid, which maintains the wet-bulb temperature of the entering air ($T_s = T_w$). The air exits the dryer at 120^oF. The temperature of the air in the dryer, T_g, experiences an exponential decrease with distance through the dryer according to the relation,

$$T_g = T_s + (T_o - T_s)\exp(-0.1377z) \qquad (1)$$

where, z = distance through the dryer in feet.

Assumptions: Isobaric and adiabatic.

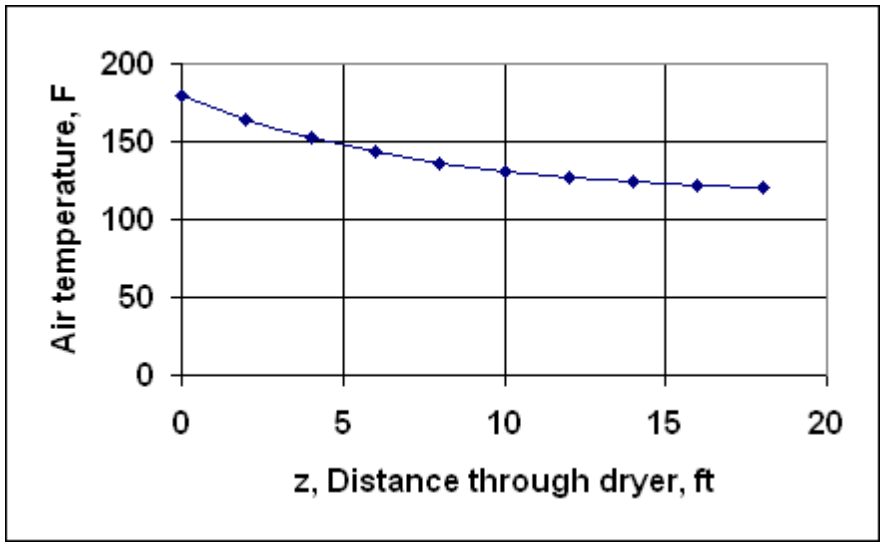
Find: Calculate and plot the variation of the moisture-evaporation temperature, T_v, and the gas temperature as a function of z.

Analysis: From Fig. 18.17, humidity of the entering air = $\mathcal{H}_o = 0.052$ lb water/lb dry air, and the wet-bulb temperature = $T_w = 114.5^oF$

In the dryer, the solid will follow the adiabatic-saturation temperature, which for the air-water system is the same as the entering wet-bulb temperature. Therefore, $T_v = 114.5^oF$.

A spreadsheet is used to compute the gas temperature from (1), using $T_s = T_w = 114.5^oF$.

z, ft	*Tg*, F
0	180.0
2	164.2
4	152.3
6	143.2
8	136.3
10	131.0
12	127.0
14	124.0
16	121.7
18	120.0



Exercise 18.21

Subject: Wet-bulb temperature of high-temperature air

Given: Air at 1,000°F with a humidity of 0.01 kg H_2O/kg dry air.

Assumptions: Wet-bulb temperature = adiabatic-saturation temperature for air-water system

Find: The wet-bulb temperature for pressures of (a) 1 atm, (b) 0.8 atm, and (c) 1.2 atm

Analysis: Note that 1,000°F is way off the humidity chart of Fig. 18.17.
Therefore, use (18-24),

$$T_s = T - \frac{\Delta H_s^{\text{vap}}}{(c_s)_{\text{in}}}(\mathcal{H}_s - \mathcal{H}) \qquad (1)$$

From (18-11), c_s = 0. 24 + 0.45(0.01) = 0.245 Btu/lb-°F
Because $\mathcal{H}_s$ and ΔH_s^{vap} depend on the value of T_s, solve for T_s iteratively.

(a) P = 1 atm

Iteration 1: Assume T_s = 150°F

From steam tables, ΔH_s^{vap} = 1008.2 Btu/lb and P^s = 3.72 psia = 0.253 atm

From (18-7), $\mathcal{H}_s = \dfrac{18.02}{28.97}\left(\dfrac{0.253}{1-0.253}\right) = 0.211$ lb H_2O/lb dry air

Substituting into (1), gives $T_s = 1000 - \dfrac{1008.2}{0.245}(0.211 - 0.01) = 173°\text{F}$ (too high)

Iteration 2: Assume T_s = 152°F

From steam tables, ΔH_s^{vap} = 1007 Btu/lb and P^s = 3.906 psia = 0.266 atm

From (18-7), $\mathcal{H}_s = \dfrac{18.02}{28.97}\left(\dfrac{0.266}{1-0.266}\right) = 0.225$ lb H_2O/lb dry air

Substituting into (1), gives $T_s = 1000 - \dfrac{1007}{0.245}(0.225 - 0.01) = 116°\text{F}$ (too low)

By extrapolation, $T_s = T_w$ = 151°F

(b) P = 0.8 atm

Iteration 1: Assume T_s = 140°F

From steam tables, ΔH_s^{vap} = 1014 Btu/lb and P^s = 2.889 psia = 0.197 atm

Exercise 18.21 (continued)

From (18-7), $\mathcal{H}_s = \dfrac{18.02}{28.97}\left(\dfrac{0.197}{0.8-0.197}\right) = 0.203$ lb H_2O/lb dry air

Substituting into (1), gives $T_s = 1000 - \dfrac{1014}{0.245}(0.203 - 0.01) = 201^\circ\text{F}$ (too high)

Based on interpolation of results for Part (a), $T_s = T_w = 141^\circ\text{F}$

(c) P = 1.2 atm

Iteration 1: Assume $T_s = 158^\circ\text{F}$

From steam tables, $\Delta H_s^{vap} = 1003.5$ Btu/lb and $P^s = 4.519$ psia = 0.3075 atm

From (18-7), $\mathcal{H}_s = \dfrac{18.02}{28.97}\left(\dfrac{0.3075}{1.2-0.3075}\right) = 0.214$ lb H_2O/lb dry air

Substituting into (1), gives $T_s = 1000 - \dfrac{1003.5}{0.245}(0.214 - 0.01) = 164^\circ\text{F}$ (too high)

Based on interpolation of previous results, $T_s = T_w = 158^\circ\text{F}$

Exercise 18.22

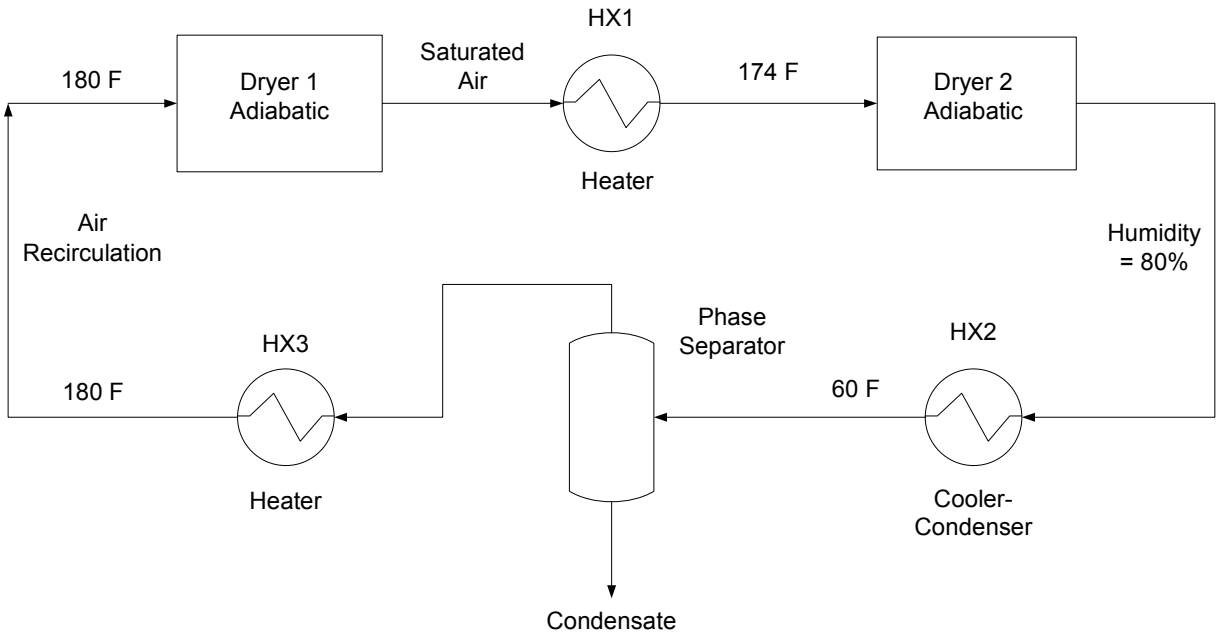
Subject: Drying of paper with two dryers and a recirculating air system

Given: Equipment and process flow conditions shown in the flowsheet below. Pressure is 1 atm throughout the process.

Assumptions: Adiabatic drying conditions and no heat losses in the heat exchangers

Find: (a) Labeled process-flow diagram
(b) lb water evaporated in each dryer per lb of dry air circulated
(c) lb water condensed in the second heat exchanger per lb of dry air circulated

Analysis: (a) Labeled process-flow diagram

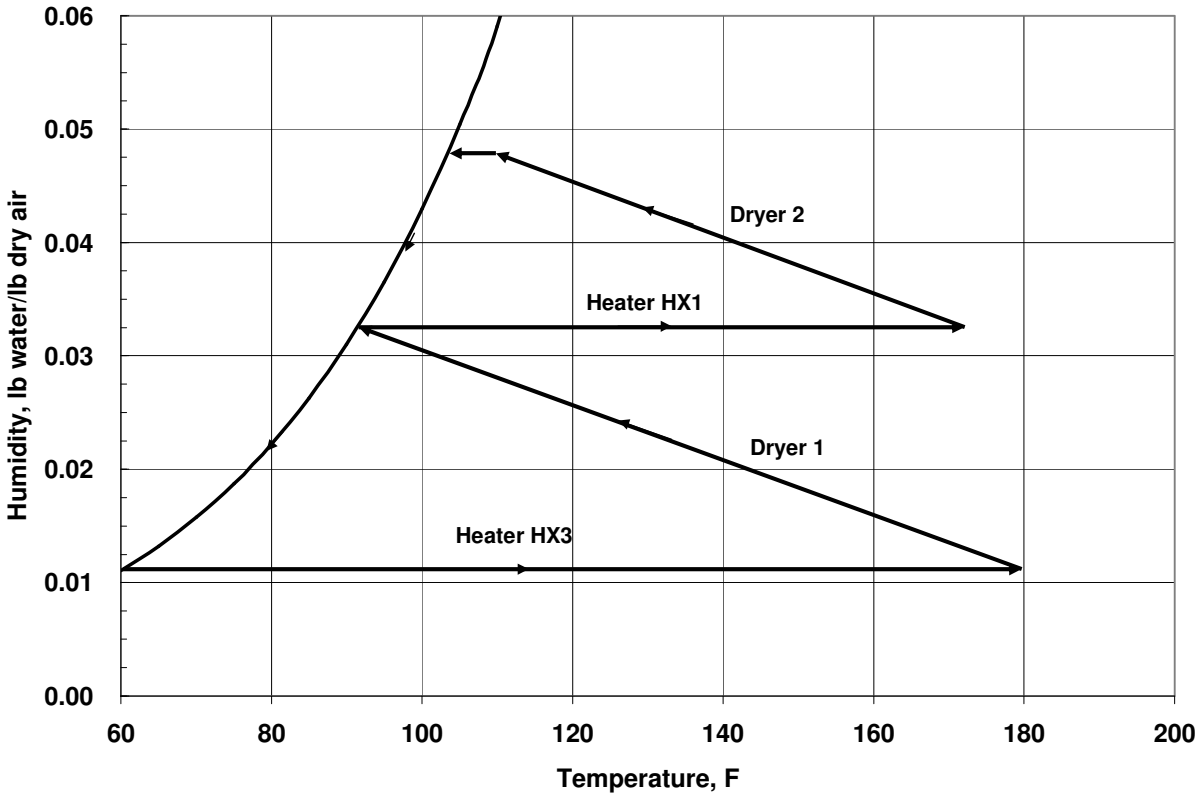


(b) The only place in the process where all conditions are fixed for the air is after the cooler-condenser, HX2, where because of partial condensation of moisture, the air leaving the phase separator is saturated at 60°F and 1 atm. Because the pressure is 1 atm. Fig. 18.17 can be used to follow the process from that point. The process path is shown on a schematic of that figure on the next page. The humidity values from Fig. 18.17 are as follows:

For Dryer 1, $\mathcal{H}_{in}$ = 0.0110 lb/lb dry air, $\mathcal{H}_{out}$ = 0.0325 lb/lb dry air
Therefore, the moisture evaporated = 0.0325 – 0.0110 = 0.0215 lb water/lb dry air
For Dryer 2, $\mathcal{H}_{in}$ = 0.0325 lb/lb dry air, $\mathcal{H}_{out}$ = 0.0478 lb/lb dry air
Therefore, the moisture evaporated = 0.0478 – 0.0325 = 0.0153 lb water/lb dry air

(c) Using conditions from the humidity chart for HX2,
$\mathcal{H}_{in}$ = 0.0478 lb/lb dry air, $\mathcal{H}_{out}$ = 0.0110 lb/lb dry air
Therefore, the moisture condensed = 0.0478 – 0.0110 = 0.0368 lb water/lb dry air

Exercise 18.22 (continued)



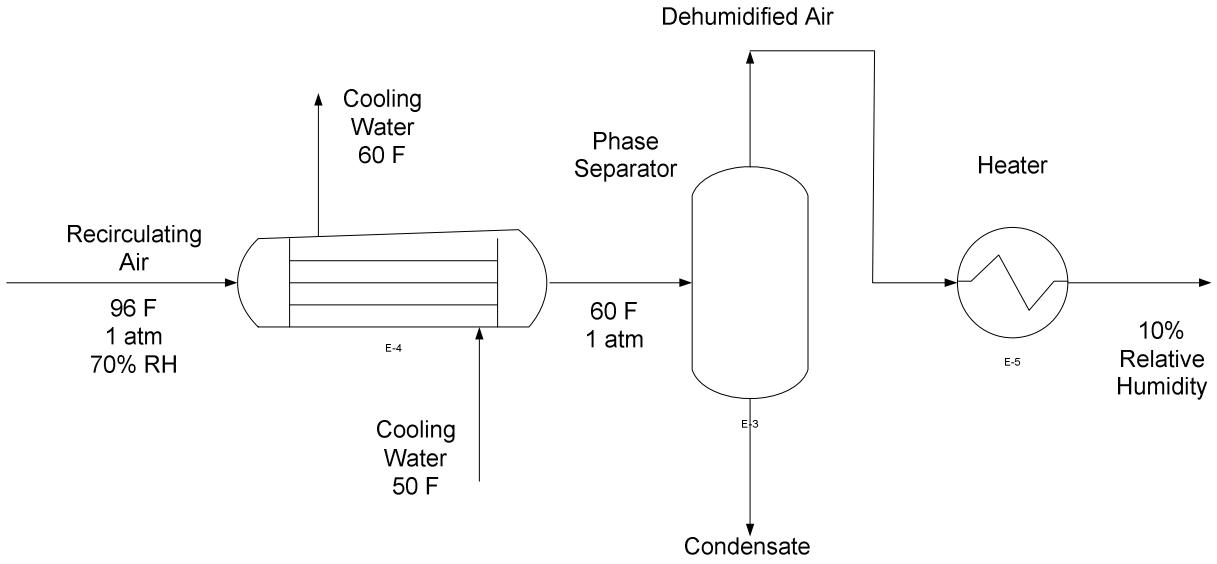
Exercise 18.23

Subject: Dehumidification of air

Given: Air at 96°F, 1 atm, and 70% relative humidity. Dehumidify to 10% relative humidity. Cooling water at 50°F is available

Find: A labeled process-flow diagram for carrying out the dehumidification. Cooling-water requirement in lb water per lb of dry air recirculated.

Analysis: One method of carrying out the dehumidification is to cool the air to 60°F (i.e. 10°F above the entering cooling-water temperature). Assume the cooling water flows countercurrently to the air in a heat exchanger, exiting at 60°F. This gives a temperature-driving force of about 20°F in the exchanger. The labeled process-flow diagram is



From Figure 18.17, the air entering the heat exchanger has a humidity of 0.0257 lb water per lb dry air. At the exit conditions of the heat exchanger, the air is saturated at 60°F and 1 atm. From Figure 18.17, the humidity is now 0.0113 lb water per lb dry air. To achieve a relative humidity of 10%, using Figure 18.17 again, we must heat the air to 136 F.

To make an energy balance around the first exchanger, use (18-12) with a T_o of 32°F. From (18-11), c_s of the entering air = 0.24 + 0.45(0.0257) = 0.252 Btu/lb dry air – °F. At 32°F, the heat of vaporization = 1075 Btu/lb water. Therefore, from (18-12),

Enthalpy of air in = 0.252(96 – 32) + 1075(0.0257) = 43.8 Btu/lb dry air

For the exit air, c_s = 0.24 + 0.45(0.0113) = 0.245 Btu/lb dry air – °F.
Therefore, Enthalpy of air out = 0.245(60 – 32) + 1075(0.0113) = 19.0 Btu/lb dry air
Therefore, the heat duty = 43.8 – 19.0 = 24.8 Btu/lb dry air. Since the cooling water temperature change is 10°F, this amounts to 10 Btu/lb of water. Therefore, need 24.8/10 = 2.48 lb H_2O/lb dry air.

Exercise 18.24

Subject: Drying of nitrocellulose fibers using equilibrium moisture content

Given: Nitrocellulose fibers with initial total water content of 40 wt% on dry basis ($X_{in} = 0.40$). Dried in a tunnel dryer at 1 atm. Fibers brought to equilibrium with air at 25°C and a relative humidity of 30%. Equilibrium moisture content given in Figure 18.24.

Find: The kg of moisture evaporated per kg of bone-dry fibers.

Analysis: From Figure 18.24, the final moisture content = $X_{out} = X^* = 0.07$ lb water/lb dry solid

Therefore, evaporation = $X_{in} - X_{out} = 0.40 - 0.07 = 0{,}33$ lb water/lb dry solid

Exercise 18.25

Subject: Slow drying of lumber using equilibrium moisture content

Given: Initial moisture content = $X_{in} = 0.50$ lb water/lb dry lumber. Final air conditions of 25°C and 1 atm, with a relative humidity of 40%.

Assumptions: Applicability of Figure 18.24, 10 – Lumber.

Find: (a) Unbound moisture before drying
(b) Bound moisture before drying
(c) Free moisture before drying
(d) lb moisture evaporated per lb of bone-dry wood

Analysis: The definitions of moisture content are shown schematically in Figure 18.23.
Total moisture content = $X_T = X_{in} = 0.50$ lb water/lb dry lumber
Figure 18.24 applies at the desired conditions of 25°C and 1 atm.
Bound moisture content = $X_B = 0.306$ lb water/lb dry lumber
Equilibrium moisture content = $X^* = 0.075$ lb water/lb dry lumber

(a) Unbound moisture content = $X_T - X_B = 0.500 - 0.306 = 0.194$ lb water/lb dry lumber

(b) Bound moisture content = $X_B = 0.306$ lb water/lb dry lumber

(c) Free moisture content = $X_T - X^* = 0.500 - 0.075 = 0.425$ lb water/lb dry lumber

(d) Moisture evaporated is the free moisture = 0.425 lb water/lb dry lumber

Exercise 18.26

Subject: Drying of cotton cloth in a closed air system

Given: 50 lb of cotton cloth at 100°F and 1 atm with a total moisture content of 20 wt% (dry basis). Cloth is hung in a closed room containing 4,000 ft^3 of air at 100°F and 1 atm with an initially wet-bulb temperature of 69°F. Air is kept at 100°F and equilibrium is achieved in the room.

Assumptions: Equilibrium moisture content of cotton cloth at 100°F is given by Figure 18.25. Neglect the increase in air pressure. Air is not vented and no new air enters the room.

Find: Final moisture content of the cotton cloth and the final relative humidity of the air. Also, determine the increase in air pressure.

Analysis: The relative humidity of the air will increase, so an iterative solution is required.

Initial composition of the wet cloth:

% water in solid on a wet basis = 20/(20+100) = 0.1667

Therefore, the initial wet solid is:

0.1667(50) = 8.33 lb water

50 – 8.33 = 41.67 lb water-free cotton cloth

Initial air conditions:

From Figure 18.17, humidity = 0.008 lb water/lb dry air

From (18-10), the humid volume is:

$$v_H = \frac{0.730(100+460)}{(1)}\left[\frac{1}{28.97}+\frac{0.008}{18.02}\right] = 14.29 \text{ ft}^3\text{/lb dry air}$$

Therefore, have 4,000/14.29 = 280 lb dry air

Initial moisture in the air = 0.008(280) = 2.24 lb water

Now, perform iterations to determine final equilibrium conditions for a room containing:

41.67 lb water-free cotton cloth

280 lb air on the dry basis

8.33 + 2.24 = 10.57 lb water

If all the water were evaporated, the humidity of the air would be:

10.57/280 = 0.0378 lb water/lb dry air, which, from Figure 18.17 corresponds to 87% relative humidity. This is an upper limit.

Iteration 1:

Assume a relative humidity, $\mathcal{H}_R$, of 60%. From Fig. 18.17, $\mathcal{H}$ = 0.025 lb/lb dry air.

Therefore, moisture in the air = 0.025(280) = 7 lb moisture.

Moisture remaining in the cotton cloth = 10.57 – 7 = 3.57 lb moisture

This gives a moisture content of the solid = 3.57/41.67 = 0.0857 lb H_2O/lb dry air

From Figure 18.25 at 100°F, the equilibrium $\mathcal{H}_R$ = 59%

Exercise 18.26 (continued)

Iteration 2:

Assume a relative humidity, $\mathcal{H}_R$, of 59%. From Fig. 18.17, $\mathcal{H}$ = 0.0245 lb/lb dry air.

Therefore, moisture in the air = 0.0245(280) = 6.86 lb moisture.

Moisture remaining in the cotton cloth = 10.57 – 6.86 = 3.71 lb moisture

This gives a moisture content of the solid = 3.71/41.67 = 0.089 lb H_2O/lb dry air

From Figure 18.25 at 100°F, the equilibrium $\mathcal{H}_R$ = 61%

By interpolation, the final equilibrium moisture content of the solid is 8.8 wt% (dry basis) and the relative humidity of the air is 59.5%.

Now calculate the final pressure in the room. Initially, have:

2.24 lb water = 2.24/18.02 = 0.124 lbmol

280 lb air = 280/28.97 = 9.665 lbmol

Total lbmol of initial gas = 0.124 + 9.665 = 9.789 lbmol

At equilibrium, have:

10.57 – 0.088(41.67) = 6.903 lb water in gas or 6.903/18.02 = 0.383 lbmol

Total lbmol of final gas = 0.383 + 9.665 = 10.048 lbmol

Assuming an ideal gas, final pressure = 1(10.048/9.789) = 1.026 atm

Exercise 18.27

Subject: Batch drying of raw cotton in a cross-circulation tray dryer.

Given: Raw cotton with an initial total moisture content of 95 wt% (dry basis) with a dry density of 43.7 lb/ft^3, to be dried to 10 wt% (dry basis). Dryer trays are 3 cm high with an area of 1.5 m^2 and are filled with cotton. Tray bottoms are insulated. Heating medium is air at 160^{o}F and 1 atm, with a relative humidity of 30%. The air flows at mass velocity across the tray of 500 lb/h-ft^2. Under these conditions, the critical moisture content is 0.4 lb water/lb bone-dry cotton, with a falling-rate drying period like Figure 18.31a, based on free-moisture content.

Assumptions: Applicability of Figure 18.25 for equilibrium moisture content.

Find: (a) Amount of raw cotton in lb (wet basis) that can be dried in one batch for 16 trays.
(b) Drying time for the constant-rate period.
(c) Drying time for the falling-rate period.
(d) Total drying time if preheat period is 1 h.

Analysis: (a) Compute the amount of cotton in 16 full trays.
Assume cotton volume does not change when it is wetted.
Volume of one tray = $3(1.5)(10^4) = 45{,}000$ cm^3
Amount of dry cotton per tray = 45,000(43.7/62.4) = 31,500 g or 69.4 lb
Total mass of wet cotton = 69.4(1.95) = 135 lb of wet cotton
For 16 trays, can dry 16(135) = 2,160 lb of wet cotton

(b) Assume during the constant-rate drying period that the relative humidity and temperature of the air remains constant as it passes over the trays.
For 30% relative humidity at 160^{o}F, from Figure 18.25, X^* = 0.04 lb H_2O/lb dry cotton
Therefore, the initial free-moisture content = 0.95 – 0.04 = 0.91 lb H_2O/lb dry cotton and the free-moisture content at the end of the constant-rate drying period = 0.40 – 0.04 = 0.36.
Therefore, the moisture evaporated from the cotton on one tray =
69.4(0.91 – 0.36) = 38.2 lb H_2O
This moisture is evaporated from an area = 1.5 m^2 or $1.5/0.3048^2$ = 16.2 ft^2
During this period, the temperature of the cotton will be at the wet-bulb temperature of the air, which from Figure 18.17 is 118.7^{o}F.
The heat transfer from the air will have to provide latent heat to evaporate the moisture at 118.7^{o}F and sensible heat to increase the temperature of the evaporated moisture to 160^{o}F.
From the steam tables, the heat of vaporization = 1026.5 Btu/lb and the specific heat of steam = 0.45 Btu/lb-^{o}F. Thus, the heat that must be transferred from the air =
Q = 38.2[1026.5 + 0.45(160 – 118.7)] = 39,900 Btu/tray
Note that if the sensible heat is neglected, Q = 39,200 Btu/tray (just 1.8% less)
Now, compute the rate of heat transfer to each tray from:
$q = hA\Delta T$, where A = 16.2 ft^2 and ΔT = 160 – 118.7 = 41.3 ^{o}F
Obtain h from (1) of Table 18.6:
$h = 0.0204\ G^{0.8}$, where h is in W/m^2-K and G is in kg/h-m^2

Exercise 18.27 (continued)

G = 500 lb/h-ft^2 or 2,440 kg/h-m^2, which is just within the range of the correlation.

Therefore, $h = 0.0204(2{,}440)^{0.8}$ = 10.5 W/m^2-K or 1.85 Btu/h-ft^2-^{o}F

and $q = 1.85(16.2)(41.3)$ = 1,240 Btu/h

Therefore, the drying time for the constant-rate period is,

Q/q = 39,900/1,240 = 32.2 h = t_c

(c) For the falling-rate period based on the curve in Figure 18.31a, (18-41) applies:

$$t_f = \frac{m_s X_c}{A R_c} \ln \frac{X_c}{X} \qquad (1)$$

The rate of drying per unit area in the constant-rate period is,

R_c = 38.2 /[32.2(16.2)] = 0.0732 lb H_2O/h-ft^2

m_s = mass of bone-dry solid per tray = 69.4 lb dry cotton
X_c = critical free-moisture content = 0.40 – 0.04 = 0.36 lb water/lb dry solid
X = final free-moisture content = 0.10 – 0.04 = 0.06 lb water/lb dry solid

Therefore, from (1),

$$t_f = \frac{69.4(0.36)}{(16.2)(0.0732)} \ln\left(\frac{0.36}{0.06}\right) = 37.7 \text{ h}$$

(d) The total drying time = 1.0 + 32.2 + 37.7 = 70.9 h or almost 3 days

Exercise 18.28

Subject: Batchwise drying of slabs of filter cake in trays.

Given: Filter cake of bone-dry density of 1,600 kg/m^3 with an initial free-moisture content of 110% (dry basis). Critical free-moisture content = 70% (dry basis) and final free-moisture content is to be 5% (dry basis). Trays are 1 m long x 0.5 m wide x 3 cm deep. Drying takes place only from the top. Drying air at 160^{o}C and 1 atm, with a wet-bulb temperature of 60^{o}C, passes across the trays at 3.5 m/s. Falling-rate period follows the type curve in Fig. 18.31a, based on free-moisture content.

Assumptions: Assume filter cake fills the trays. Neglect sensible heat to increase the temperature of the evaporated moisture from 60^{o}C to 160^{o}C. Drying-air conditions stay constant as the air passes over the trays. Cake does not shrink as it dries.

Find: (a) Drying time for the constant-rate period.
(b) Drying time for the falling-rate period

Analysis: (a) The constant-rate drying flux, from (18-34) is,

$$R_c = \frac{h\left(T_g - T_w\right)}{\Delta H_w^{\text{vap}}} \tag{1}$$

T_g = Gas temperature = 160^{o}C = 320^{o}F, T_w = drying temperature = 60^{o}C = 140^{o}F
From the steam tables, at 140^{o}F, ΔH_w^{vap} = 1014.1 Btu/lb
For the heat-transfer coefficient, h, use (18-38) in Table 18.6:

$h = 0.0204\, G^{0.8}$, where h is in W/m^2-K and G is in kg/h-m^2
$G = v\rho$, v = 3.5 m/s = 3.5(3600) = 12,600 m/h
The humidity of the air, from a high-temperature humidity chart in Perry's Handbook
$= \mathcal{H}$ = 0.10 lb water/lb dry air.
Use the humid volume to get the air density. From (18-10),

$$v_H = \frac{0.730\left(320+460\right)}{\left(1\right)}\left[\frac{1}{28.97}+\frac{0.10}{18.02}\right] = 24.7 \text{ ft}^3\text{/lb dry air}$$

or 24.7/1.10 = 22.5 ft^3/lb moist air or 1.40 m^3/kg moist air
Therefore, ρ = 1/1.40 = 0.714 kg/m^3
Therefore, $G = v\rho$ = 12,600(0.714) = 9,000 kg/h-m^2, which is within the range of (1) in Table 18.6.
Therefore, h = 0.0204(9,000)$^{0.8}$ = 29.7 W/m^2-K or 5.24 Btu/h-ft^2-^{o}F

Exercise 18.28 (continued)

From (1), $R_c = \dfrac{5.24(320-140)}{1014.1} = 0.93$ lb/h-ft^2

From (18-42),

$$t_c = \frac{m_s}{AR_c}(X_o - X_c) \tag{2}$$

Compute the mass of bone-dry solid in one tray = m_s
Tray volume = 1(0.5)(0.03) = 0.015 m^3
Therefore m_s = 1,600(0.015) = 24 kg = 53 lb of dry solid
The moisture contents are given on a free-moisture-content basis.
The tray area = A = 0.5(1) = 0.5 m^2 = 5.38 ft^2
Substituting into (2),

$$t_c = \frac{53}{5.38(0.93)}(1.10-0.70) = 4.24 \text{ h}$$

(b) For the falling-rate period based on the curve in Figure 18.31a, (18-41) applies:

$$t_f = \frac{m_s X_c}{AR_c} \ln \frac{X_c}{X} \tag{3}$$

X_c = critical free-moisture content = 0.70 lb water/lb dry solid
X = final free-moisture content = 0.05 lb water/lb dry solid

Therefore, from (3),

$$t_f = \frac{53(0.70)}{(5.38)(0.93)} \ln\left(\frac{0.70}{0.05}\right) = 19.6 \text{ h}$$

Exercise 18.29

Subject: Batchwise drying of extrusions of filter cake in trays.

Given: Filter cake of bone-dry density of 1,600 kg/m^3 with an initial free-moisture content of 110% (dry basis). Critical free-moisture content = 70% (dry basis) and final free-moisture content is to be 5% (dry basis). The cake is extruded into cylindrical-shaped pieces measuring ¼-inch in diameter by 3/8-inch long, which are placed in trays that are 6 cm high by 1 m long by 0.5 m wide. Drying air at 160°C and 1 atm, with a wet-bulb temperature of 60°C, passes through the bed of pieces at a superficial velocity of 1.75 m/s. Falling-rate period follows the type curve in Fig. 18.31a, based on free-moisture content. Bed porosity is 50%.

Assumptions: Neglect sensible heat to increase the temperature of the evaporated moisture from 60°C to 160°C. Drying-air conditions stay constant as the air through the pieces on the trays. Cake does not shrink as it dries.

Find: (a) Drying time for the constant-rate period.
(b) Drying time for the falling-rate period.

Analysis: (a) The constant-rate drying flux, from (18-34) is,

$$R_c = \frac{h\left(T_g - T_w\right)}{\Delta H_w^{\text{vap}}} \tag{1}$$

T_g = Gas temperature = 160°C = 320°F, T_w = drying temperature = 60°C = 140°F
From the steam tables, at 140°F, ΔH_w^{vap} = 1014.1 Btu/lb

For the heat-transfer coefficient, h, use (3) or (4) for through-circulation in a packed bed, in Table 18.6, where the choice depends on the value of the bed Reynolds number,

$$N_{\text{Re}} = \frac{d_p G}{\mu} \tag{2}$$

where, from Example 18.8, d_p is the diameter of a sphere of the same surface area as the particle. From (1) of Example 18.8, with particle diameter, D, and particle length, L,

$$\pi d_p^2 = \pi DL + 2\left(\frac{\pi D^2}{4}\right) \text{ or } d_p = \left[DL + \frac{D^2}{2}\right]^{1/2} = \left[\frac{1}{4}\left(\frac{3}{8}\right) + \frac{0.25^2}{2}\right]^{1/2} = 0.354 \text{ in} = 0.00897 \text{ m}$$

The superficial mass velocity = $G = v\rho$, with v = 1.75 m/s = 1.75(3600) = 6,300 m/h
For the gas density, calculate the humid volume.
The humidity of the air, from a high-temperature humidity chart in Perry's Handbook
= $\mathcal{H}$ = 0.10 lb water/lb dry air.

Exercise 18.29 (continued)

From (18-10),

$$v_H = \frac{0.730(320+460)}{(1)}\left[\frac{1}{28.97}+\frac{0.10}{18.02}\right] = 24.7 \text{ ft}^3\text{/lb dry air}$$

or 24.7/1.10 = 22.5 ft^3/lb moist air or 1.40 m^3/kg moist air

Therefore, $\rho = 1/1.40 = 0.714$ kg/m^3

Therefore, $G = v\rho = 6{,}300(0.714) = 4{,}500$ kg/h-m^2

From Example 18.8, take the air viscosity = $\mu = 2 \times 10^{-5}$ kg/m-s or 0.072 kg/m-h

Therefore, bed Reynolds number, from (2) is,

$$N_{\text{Re}} = \frac{0.00897(4{,}500)}{0.072} = 561$$

Therefore, (3) in Table 18.6 applies:

$$h = 0.151\frac{G^{0.59}}{d_p^{0.41}} = 0.151\frac{4500^{0.59}}{0.00897^{0.41}} = 149 \text{ W/m}^2\text{-K or } 26.3 \text{ Btu/h-ft}^2\text{-}^{\circ}\text{F}$$

$$\text{From (1), } R_c = \frac{26.3(320-140)}{1014.1} = 4.67 \text{ lb/h-ft}^2$$

From (18-42), the time for the constant-rate drying period is,

$$t_c = \frac{m_s}{AR_c}(X_o - X_c) \qquad (2)$$

Compute the mass of bone-dry solid in one tray = m_s

Tray volume = 1(0.5)(0.06) = 0.03 m^3

For a porosity of 0.5, m_s = 1,600(0.03)(0.5) = 24 kg = 53 lb of dry solid

The moisture contents are given on a free-moisture-content basis.

The area, A, in (2) is the total area of the particles in the bed on the tray.

Volume of one extrusion = $\pi D^2 L/4 = 3.14(0.25)^2(0.375)/4 = 0.0184$ in^3 or 3.02×10^{-7} m^3

The extrusions on one tray fill a volume of 0.015 m^3 (50% of the tray volume)

Therefore, the number of extrusions = $0.015/3.02 \times 10^{-7} = 49{,}750$

The surface area of one extrusion is,

$$\pi DL + 2\left(\frac{\pi D^2}{4}\right) = 3.14[(0.25)(0.375) + 0.5(0.25)^2] = 0.393 \text{ in}^2 = 0.00273 \text{ ft}^2$$

Therefore, total surface area of the extrusions on a tray = 49,750(0.00273) = 136 ft^2

Substituting into (2),

$$t_c = \frac{53}{136(4.67)}(1.10-0.70) = 0.0334 \text{ h or } 2 \text{ min}$$

Exercise 18.29 (continued)

(b) For the falling-rate period based on the curve in Figure 18.31a, (18-41) applies:

$$t_f = \frac{m_s X_c}{A R_c} \ln \frac{X_c}{X} \tag{3}$$

X_c = critical free-moisture content = 0.70 lb water/lb dry solid
X = final free-moisture content = 0.05 lb water/lb dry solid

Therefore, from (3),

$$t_f = \frac{53(0.70)}{(136)(4.67)} \ln\left(\frac{0.70}{0.05}\right) = 0.154 \text{ h or } 9.2 \text{ min}$$

Exercise 18.30

Subject: Tray drying in the constant- and falling-rate periods

Given: Takes 5 hours to dry a wet solid in a tray from 36 to 8 wt% on dry basis. Critical and equilibrium moisture contents are 15 and 5 wt% dry basis, respectively. Negligible preheat time. Straight-line falling-rate period.

Assumptions: Drying-air conditions stay constant. Cake does not shrink as it dries.

Find: Drying time for same wet material from 40 to 7 wt% on dry basis.

Analysis: From (18-42),

$$t_T = t_c + t_f = \left(\frac{m_s}{AR_c}\right)\left[(X_o - X_c) + X_c \ln\left(\frac{X_c}{X_{\text{final}}}\right)\right] \tag{1}$$

Solve for $\left(\frac{m_s}{AR_c}\right)$ from given data for the 5-hour test. All moisture contents are on a free-moisture basis. Therefore, $X_o = 0.36 - 0.05 = 0.31$, $X_c = 0.15 - 0.05 = 0.10$, $X_{\text{final}} = 0.08 - 0.05 = 0.03$

Substituting into a rearrangement of (1),

$$\left(\frac{m_s}{AR_c}\right) = \frac{t_c + t_f}{\left[(X_o - X_c) + X_c \ln\left(\frac{X_c}{X_{\text{final}}}\right)\right]} = \frac{5}{\left[(0.31-0.10) + 0.10 \ln\left(\frac{0.10}{0.03}\right)\right]} = 15.13 \text{ h}$$

Use this value for the new conditions, with $X_o = 0.40 - 0.05 = 0.35$, $X_c = 0.15 - 0.05 = 0.10$, $X_{\text{final}} = 0.07 - 0.05 = 0.02$

$$t_T = t_c + t_f = (15.13)\left[(0.35-0.10) + 0.10 \ln\left(\frac{0.10}{0.02}\right)\right] = 6.2 \text{ h}$$

Exercise 18.31

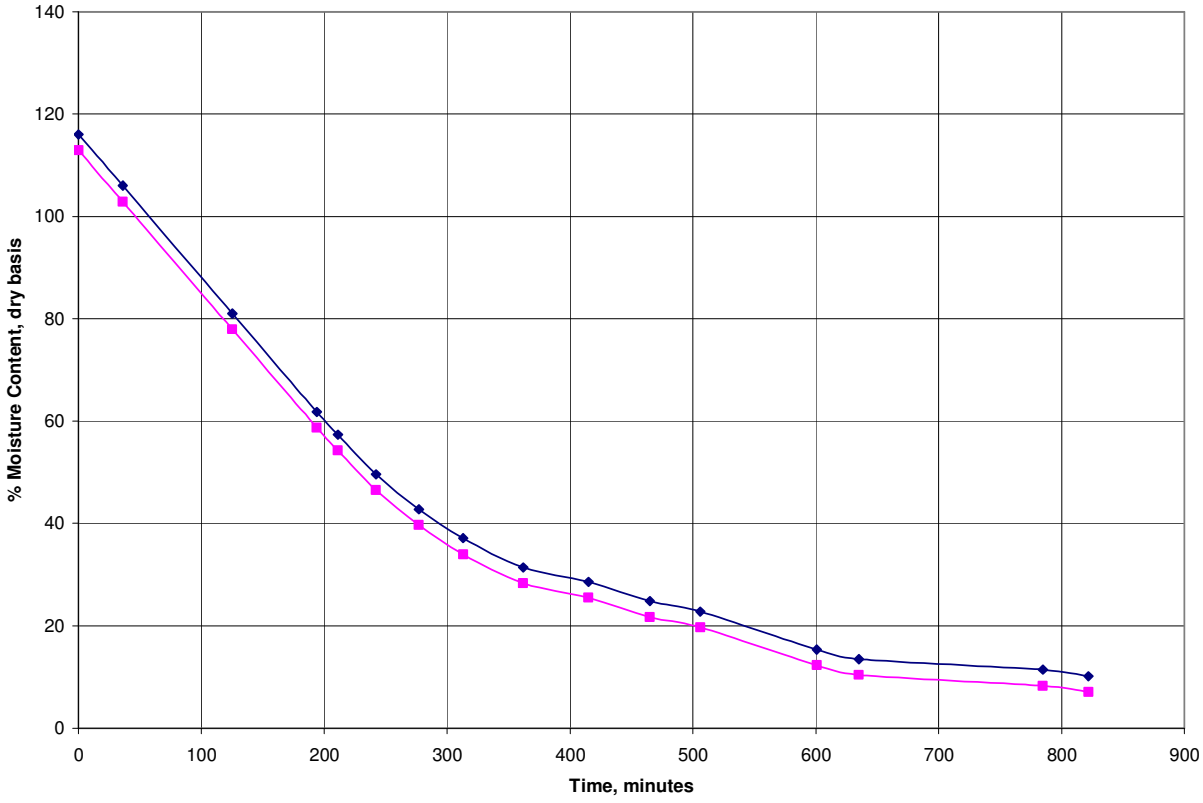
Subject: Tunnel drying of a wet solid on trays with drying by crossflow of air from both sides.

Given: Trays measuring 1.5 m long by 1.2 m wide by 25 cm deep. Initial total moisture content = 116 wt% dry basis and final average total moisture content = 10 wt% dry basis. Air is at 90°F, 1 atm, and a relative humidity of 15%. By interpolation of given data, equilibrium moisture content = 3.1 wt% dry basis. Drying-time data plotted below.

Assumptions: Critical moisture content is independent of drying conditions. Drying rate is proportional to the difference between dry-bulb and wet-bulb temperatures of the air.

Find: Drying time for 110 to 10 wt% dry basis using air at 125°F and 20% relative humidity.

Analysis: The following is a spreadsheet plot of the drying-time data for air at 90°F and an RH of 15% starting from 116% total moisture. Two lines are shown. The upper line is the total and the bottom line is the free moisture content = total – 3.1%.



From this plot, the critical free-moisture content, X_c = approximately 57.4 – 3.1 = 54.3 wt% dry basis at 211 minutes. During the constant-rate drying period, using the given drying-rate data,

The rate of drying = (1.16 – 0.574)/211 = 0.00278 lb H_2O/lb dry solid – min

Exercise 18.31 continued

In the constant-rate period, $R_c = \dfrac{h\left(T_g - T_w\right)}{\Delta H_w^{\text{vap}}}$ in lb H_2O/ft^2 of drying surface – min

For the test data with air at 90°F, 1 atm, and RH of 15%, from Fig. 18.17, T_w = 60°F.
From the steam tables, ΔH_w^{vap} = 1206.6 Btu/lb

For the new conditions with air at 125°F, 1 atm, and RH of 20%, T_w = 85°F
From the steam tables, ΔH_w^{vap} = 1045.8 Btu/lb

Therefore, the drying time for the constant-rate period for the new conditions, by ratio using the above expression for the rate of drying is, using total moisture content differences:

$$t_c = 211\left(\frac{90-60}{125-85}\right)\left(\frac{1045.8}{1206.6}\right)\left(\frac{110-57.4}{116-57.4}\right) = 123 \text{ min}$$

In the falling-rate period, since there is little change in the final moisture content between the test conditions and the new conditions, since both terminate at a total moisture content of approximately 10 wt%, ratio on rates using the temperature differences and the heat of vaporization. For the test data, t_f = 822 – 211 = 611 minutes.

Therefore to get to 10.2 wt%, $t_f = 611\left(\dfrac{90-60}{125-85}\right)\left(\dfrac{1045.8}{1206.6}\right) = 397 \text{ min}$

From the above plot, it might take an additional 10 min to go from 10.2 to 10.0 wt %. Therefore, take t_f = 397 + 10 = 407 min. The total drying time = t_c + t_f = 123 + 407 = 530 min.

Exercise 18.32

Subject: Drying time for a piece of hemlock wood

Given: Hemlock wood measuring 15.15 x 14.8 x 0.75 cm is to be dried at the two large faces from an initial total moisture content of 90% to a final average total moisture content of 10%, both dry basis. Drying is in the liquid-diffusion-controlled falling-rate period with a diffusivity of 1.7×10^{-6} cm^2/s.

Assumptions: Equilibrium moisture content with bone-dry air is zero.

Find: Drying time if bone-dry air is used.

Analysis: Fig. 3.9 applies, but the coordinates are off the chart. Therefore, use (2) of Example 18.13, provided that N_{Fo} for mass transfer > 0.1

$$E_{\text{avg}} = \text{average unaccomplished free-moisture change} = \frac{X_{\text{avg}} - X^*}{X_o - X^*} = \frac{0.10 - 0}{0.90 - 0} = 0.111$$

$$N_{\text{Fo}_M} = \frac{D_{\text{AB}} t}{a^2} = \frac{1.7 \times 10^{-6} \left(t \text{ in s}\right)}{\left(0.75/2\right)^2} = 1.2 \times 10^{-5} \left(t \text{ in s}\right)$$

From (2) of Example 18.13, $\ln\left(\dfrac{X_{\text{avg}} - X^*}{X_o - X^*}\right) = \ln\left(\dfrac{8}{\pi^2}\right) - \dfrac{\pi^2}{4} N_{\text{Fo}_M}$

Therfore, $\ln\left(0.111\right) = -2.197 = -0.210 - 2.467 N_{\text{Fo}_M}$ Solving, $N_{\text{Fo}_M} = 0.805 > 0.1$

Therefore, $0.805 = 1.2 \times 10^{-5} \left(t \text{ in s}\right)$ and solving, t = 67,100 s or 18.6 h

Exercise 18.33

Subject: Mode of drying in the falling-rate period for hemlock wood

Given: A piece of hemlock wood measuring 15.15 x 14.8 x 0.75 cm, for which drying takes place only from the two largest faces. Air at 25°C is passed over the surfaces at 3.7 m/s. Drying-time data are plotted below starting at an average total moisture content of 127 wt% dry basis and finishing at an infinite time of 6.6 wt% dry basis.

Assumptions: Air is at 1 atm and a wet-bulb temperature of 17°C.

Find: Whether Case 1 or Case 2 applied for the falling-rate period. If Case 1 applies, determine from the data the effective diffusivity. If Case 2 applies, determine:

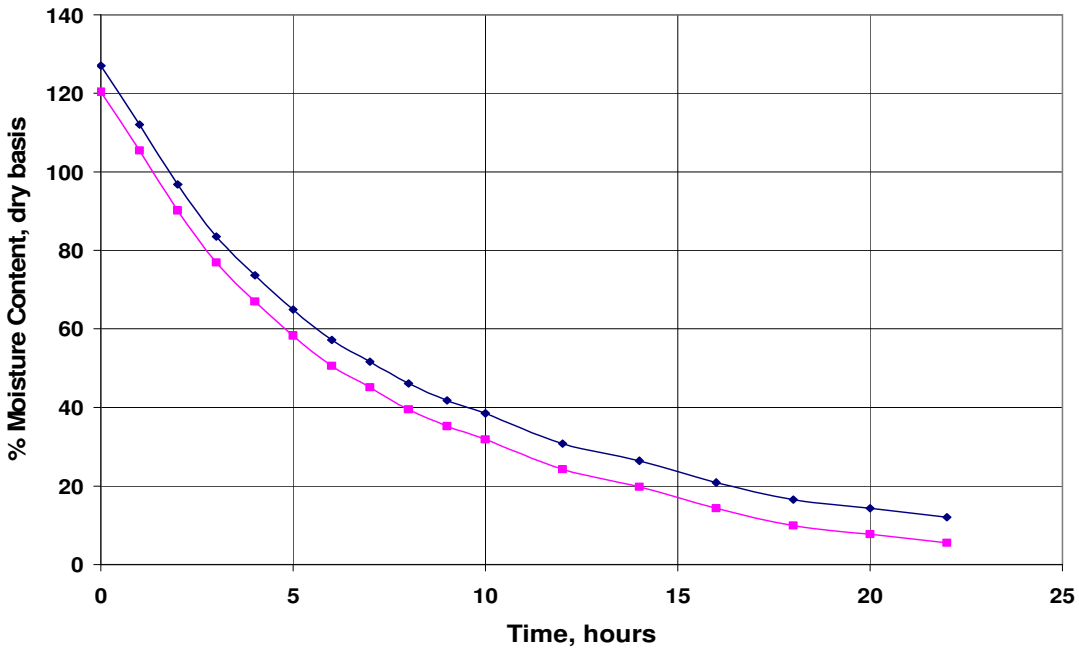
(a) Drying rate in g/h-cm^2 for the constant-rate period assuming a dry density of 0.5 g/cm^3 and no shrinkage.

(b) Critical moisture content.

(c) Predicted parabolic-moisture-content profile at the beginning of the falling-rate period.

(d) Effective diffusivity during the falling-rate period.

Analysis: Assume that the equilibrium-moisture content is that measured at infinite time. Thus, it is 6.6 wt% dry basis. Now find out if Case 1 or Case 2 applies by plotting moisture content against time with a spreadsheet.



From this plot, it is seen that the falling-rate period is preceded by a constant-rate period of w 2 h ours. Therefore, Case 2 applies.

Exercise 18.33 continued

(b) From the plot, the constant-rate period extends for 2 hours to X_c = 96.8 wt% dry basis.

(a) The drying rate in the constant-rate period = (127 – 96.8)/[(100)2] = 0.151 lb H_2O/lb dry wood-h. Convert this to g/h-cm^2.

Volume of one piece of wood = (15.15)(14.8)(0.75) = 168 cm^3
Mass of dry wood in one piece = 0.5(168) = 84 g
Area of 2 large faces = 2(15.15)(14.8) = 448 cm^2
Rate of drying in constant-rate period = 0.151 g H_2O/g dry wood-h
or 0.15(84) = 12.6 g H_2O/h-piece of wood
Therefore, R_c = 12.6/448 = 0.0281 g H_2O/h-cm^2

(d) Estimate the effective diffusivity from a rearrangement of (18-62).

From the given data, $X_c = 0.968$, $X^* = 0.066$, $X_{avg} = 0.121$ at t = 22 h
t_c = 2 h, therefore, t_f = 22 – 2 = 20 h or 72,000 s

$$D_{AB} = \frac{a^2}{3t_f}\ln\left[\frac{X_c - X^*}{X_{avg} - X^*}\right] = \frac{0.375^2}{3(72{,}000)}\ln\left[\frac{0.968-0.066}{0.121-0.066}\right] = 1.8\times10^{-6}\ \text{cm}^2/\text{s}$$

(c) Now check the Fourier number for mass transfer to see if moisture profile is parabolic at t_c.

$$N_{Fo_M}\ \text{at}\ t_c = \frac{D_{AB}t_c}{a^2} = \frac{\left(1.8\times10^{-6}\right)\left[2(3600)\right]}{(0.375)^2} = 0.092$$

which is less than 0.5. Therefore, profile is not parabolic.

Exercise 18.34

Subject: Falling-rate equations for drying.

Given: Solid undergoing drying in the falling-rate period either by liquid diffusion or capillary movement.

Find: Derive governing equations. Outline an experimental procedure for determining which mechanism prevails.

Analysis:

Case of Liquid diffusion controlling in falling-rate period:

From (3) in Example 18.13, which is a simplification of (18-49) when N_{Fo_M} <0.1,

$$N_{\mathrm{Fo}_M} = \frac{D_{\mathrm{AB}}t}{a^2} = \frac{4}{\pi^2}\ln\left[\frac{8}{\pi^2}\left(\frac{X_o - X^*}{X_{\mathrm{avg}} - X^*}\right)\right] \tag{1}$$

From (18-32), the rate of drying in terms of average moisture content is

$$R = -\frac{m_s}{A}\left(\frac{dX_{\mathrm{avg}}}{dt}\right) \tag{2}$$

Rearranging (1),

$$X_{\mathrm{avg}} = X^* + \frac{8\left(X_o - X^*\right)}{\pi^2}\exp\left(-\frac{\pi^2 D_{\mathrm{AB}}t}{4a^2}\right) \tag{3}$$

Taking the derivative of (3) with respect to t gives

$$\frac{dX_{\mathrm{avg}}}{dt} = \frac{8\left(X_o - X^*\right)}{\pi^2}\left(-\frac{\pi^2 D_{\mathrm{AB}}t}{4a^2}\right)\exp\left(-\frac{\pi^2 D_{\mathrm{AB}}t}{4a^2}\right) = \left(X_{\mathrm{avg}} - X^*\right)\left(-\frac{\pi^2 D_{\mathrm{AB}}t}{4a^2}\right) \tag{4}$$

Comparing (2) and (4), it is seen that the rate of drying varies inversely as the square of a, which is the thickness of the solid.

Case of capillary flow controlling in falling-rate period:

Capillary flow will be laminar. From (14-2), the rate of laminar flow is inversely proportional to the distance in the direction of flow, which is the thickness of the solid.

To determine experimentally which case applies, use solids of different thickness.

Exercise 18.35

Subject: Cross-circulation tray drying in the constant-rate drying period.

Given: Wet solid in a tray subject to heat transfer by convection to the bottom of the tray, in addition to the usual heat convection from the hot air to the surface of the wet solid.

Find: Derive the governing equation and show that the temperature of the surface of the wet solid will be higher than the wet-bulb temperature of the hot air used to dry the solid. In addition, determine the effect of radiation from the bottom of the tray to a tray below.

Assumption: Neglect the conduction resistance of the tray bottom and heat transfer to the sides of the trays.

Analysis: This situation is discussed in the reference: Shepherd, C.B, C. Hadlock, and R.C. Brewer, *Ind. Eng. Chem.*, **30**, 388-397 (1938), which develops the theory and provides experimental data on the drying of wet sand that supports the theory. Their results clearly show that when heat is transferred also to the bottom of the tray, the temperature at the surface of the wet solid is higher than the wet-bulb temperature by a few degrees, thus reducing slightly the temperature driving force for heat transfer from the hot air to the wet surface of the solid. However, the overall heat-transfer coefficient for heating from both the top and bottom is increased considerably. The result is a significantly higher drying rate.

From Eqs. (18-34) and (18-35), the drying-rate flux in the constant-rate drying period, R_c, in the absence of heat-transfer to the tray bottom and radiation to the wet surface of the solid is:

$$R_c = \frac{h\left(T_g - T_v\right)}{\Delta H_v^{\text{vap}}} = M_{\text{dry air}} k_y \left(\mathcal{H}_v - \mathcal{H}_d\right) \tag{1}$$

where, here, the subscript v refers to the wet-bulb temperature, w.

Assuming the area for heat transfer to the top and bottom of the tray is the same, then, if convection to the uninsulated bottom of the tray is taken into account, with subsequent conduction through the tray thickness and the wet solid, then h in (1) is replaced by an overall coefficient:

$$U = h_{c,t} + \frac{1}{\dfrac{1}{h_{c,b}} + \dfrac{t_t}{k_t} + \dfrac{t_{ws}}{k_{ws}}} \tag{2}$$

Assume that $h_{c,t}$ at the top = $h_{c,b}$ at the bottom = h_c. Assume that the thermal resistance of the metal tray thickness, t_t / k_t , is negligible compared to the thermal resistance of the wet solid, t_{ws} / k_{ws} , where t is thickness and k is thermal conductivity. Then (2) becomes:

Exercise 18.35 (continued)

$$U = h_c + \frac{1}{\frac{1}{h_c} + \frac{t_{ws}}{k_{ws}}} \tag{3}$$

Now U in (3) is greater than h in (1). Therefore, the ratio $U / (k_y C_s M_B) > h / (k_y C_s M_B)$, the psychrometric ratio, and the temperature of the evaporating moisture will be higher than the wet-bulb temperature of the hot air, thus reducing the temperature driving force.

If we also account for radiation from the bottom of a tray to the tray below, the overall heat transfer coefficient for heat transfer to the tray below will be even higher than U, because an additional term for a radiation coefficient will be added to the right-hand side of (3). Therefore, the temperature of the evaporating moisture will be further increased.

Exercise 18.36

Subject: Tunnel drying of raw cotton.

Given: Dry 30 lb/h of raw cotton (dry basis) at 70°F and a moisture content of 100% (dry basis) in a tunnel dryer with a countercurrent flow of 1,800 lb/h of air (dry basis) entering at 200°F, 1 atm, and a relative humidity of 10%. The cotton will exit at 150°F with a moisture content of 10% (dry basis). Specific heat of dry cotton = 0.35 Btu/lb-°F.

Assumptions: Adiabatic drying conditions. Specific heat of dry air = 0.24 Btu/ lb- °F. Specific heat of steam = 0.45 Btu/lb-°F.

Find: (a) The rate of evaporation of moisture.
(b) The outlet temperature of the air.
(c) The rate of heat transfer.

Analysis:

(a) The rate of evaporation of moisture = 30(1.00 – 0.10) = 27 lb/h

(b) The air must supply sensible heat and latent heat. Assume that moisture evaporation occurs at the wet-bulb temperature of the air. From Figure 18.17, this is 117°F. Therefore, heat the wet cotton from 70°F to 117°F, evaporate the 27 lb/h of moisture at 117°F, heat (or cool) the evaporated moisture to the final gas temperature, and heat the final partially dry cotton to 150°F.

Let the final temperature of the air = T_{go}. From the steam tables, the heat of vaporization of water at 117°F = 1027.5 Btu/lb. Also, the humidity of the air from Figure 18.17 = 0.0528 lb H_2O/lb dry air.

Q transferred from the air to the wet, evaporating cotton = Q =
30(0.35)(150 – 70) + 27(1)(117 – 70) + 27(1027.5) + 3(1)(150 – 117) + 27(0.45)(T_{go} – 117) =
29,950 + 12.15(T_{go} – 117) = 28,530 + 12.15 T_{go} Btu/h

Q lost by the air = Q = [1,800(0.24) + 1,800(0.0528)(0.45)](200 - T_{go}) =
474.8(200 - T_{go}) = 94,960 – 474.8 T_{go} Btu/h

Q transferred from the air to the wet, evaporating cotton = Q lost by the air
Therefore, 28,530 + 12.15 T_{go} = 94,960 – 474.8 T_{go}
Solving, T_{go} = 136.4°F

(c) The rate of heat transfer = Q lost by the air = 94,960 – 474.8(136.4) = 30,200 Btu/h

Exercise 18.37

Subject: Spray drying of an aqueous coffee solution.

Given: A 25 wt% aqueous solution of coffee at 70°F. Air enters at 450°F and 1 atm with a humidity of 0.01 lb H_2O/lb dry air. Final moisture content of the coffee solution is to be 5 wt% on the dry basis. Air exits at 200°F.

Assumptions: Specific heat of coffee (solid or in solution) = 0.3 Btu/lb-°F. Dried coffee and heating air exit at the same temperature.

Find: (a) The air rate in lb dry air/lb coffee solution.
(b) The temperature of evaporation.
(c) The heat-transfer rate in Btu/lb coffee solution.

Analysis:

Take as a basis: 100 lb of coffee solution containing 25 lb of coffee and 75 lb of water.
Therefore, the amount of water evaporated = 75 – 25(0.05) = 73.75 lb

(b) From a high-temperature humidity chart in Perry's Handbook, T_w is approximately 120°F. From the steam tables, the heat of vaporization of water at 120°F = 1025.8°F.

(a) Q transferred from the air to the evaporating coffee solution = Q = 25(0.30)(200 – 70) + 75(1)(120 – 70) + 73.75(1025.8) +1.25(1)(200 – 120) + 73.75(0.45)(200 – 120) = 83,200 Btu

Q lost by the air = Q = 83,200 = $m_{\text{dry air}}$ (0.24 + 0.45 $\mathcal{H}$)(450 – 200)
Solving, $m_{\text{dry air}}$ = 1,360 lb
Therefore, the dry air rate for 100 lb of coffee solution = 1,360/100 = 13.6 lb

(c) The heat transfer rate = 83,200/100 = 832 Btu/lb coffee solution

Exercise 18.38

Subject: Flash drying of wet, pulverized clay particles.

Given: 7,000 lb/h of wet, pulverized clay particles at 15°C and 1 atm with 27 wt% moisture (dry basis). Dry clay to a moisture content of 5 wt% (dry basis) with an exit temperature at the air wet-bulb temperature of 50°C. Cocurrent air enters at 525°C and exits at 75°C.

Assumptions: Specific heat of dry clay = 0.3 Btu/lb-°F. Adiabatic drying conditions. Neglect moisture content of the entering air.

Find: (a) The flow rate of air in lb/h (dry basis).
(b) The rate of evaporation of moisture.
(c) The heat-transfer rate in Btu/h.

Analysis:

Heat of vaporization at 50°C = 122°F = 1024.6 Btu/lb

(b) mass flow rate of clay = 7000/1.27 = 5,512 lb/h
mass flow rate of entering moisture in the clay = 7,000 – 5,512 = 1,488 lb/h
moisture evaporated in dryer = 1,488 – 5,512(0.05) = 1,212 lb/h

(c) Q to the feed for sensible and latent heat = 5,512(0.3)[(50 – 15)1.8] + 1,488(1)[(50 – 15)1.8] + 1,212[(1024.6) + (0.45)[(75 – 15)1.8] = 1,499,000 Btu/h

(a) Q from the air = 1,499,000 = m_{air} (0.25)[525 – 75)1.8]
Solving, m_{air} = 7,400 lb air/h

Exercise 18.39

Subject: Drying of isophthalic acid crystals in an indirect-heat, steam-tube, rotary dryer.

Given: 5,000 lb/h of wet, isophthalic acid crystals at 30°C and 1 atm with 30 wt% moisture (wet basis) to be dried to a moisture content of 2 wt% (wet basis). Evaporation takes place at 100°C, which is also the crystals exit temperature. Dryer uses condensing steam at 25 psig (barometer = 15 psia). Specific heat of isophthalic acid = 0.2 cal/g-°C.

Assumptions: Adiabatic dryer. Heating steam enters as a saturated vapor and leaves as a saturated liquid.

Find: (a) The rate of evaporation.
(b) The rate of heat transfer.
(c) The flow rate of steam.

Analysis:

(a) mass flow rate of isophthalic acid = 5,000(0.70) = 3,500 lb/h
mass flow rate of entering moisture = 5,000 – 3,500 = 1,500 lb/h
mass flow rate of moisture in exiting crystals = 3,500(0.02/0.98) = 71.4 lb/h
rate of evaporation = 1,500 – 71.4 = 1,429 lb/h

(b) Evaporation at 100°C = 212°F. From steam tables, heat of vaporization = 970.3 Btu/lb
Rate of heat transfer =
3,500(0.2)[(100 – 30)1.8] + 1,500(1)[(100 – 30)1.8] + 1,429(970.3) = 1,664,000 Btu/h

(c) From steam tables, heat of vaporization at 25 + 15 = 40 psia = 933.7 Btu/lb
Flow rate of heating steam = 1,664,000/933.7 = 1,782 lb/h

Exercise 18.40

Subject: Drying of extruded filter cake of calcium carbonate with a through-circulation belt dryer having 3 zones.

Given: Calcium carbonate extruded into cylindrical pieces of 1/4-inch diameter and 1/2-inch length with an initial moisture content of 30% (dry basis) and a critical moisture content of 10% (dry basis). Belt dryer is 6-ft wide with three drying zones of 8-ft long each, running with a belt speed, S, of 1 ft/min (0.00508 m/s). Carbonate bed height on the belt is 2-inches with an external porosity of 50%. Air at 170°F (76.7°C) and 10% relative humidity flows through the bed at a superficial velocity, u_s,of 2 m/s, upward in the first and third zones and downward in the zone 2.

Assumptions: Negligible preheat period. Constant-rate drying at the wet-bulb temperature of the entering air.

Find: Moisture content distribution with height at the end of each zone and the final average moisture content.

Analysis: This exercise is exactly the same as Example 18.18 except that three zones of 8-ft length each are used instead of two zones of 12-ft length each. Thus, the following preliminary calculations from Example 18.18 apply here:

Entering air has a wet-bulb temperature of 110.2°F = 37.8°C = T_w
Entering air has a humidity of 0.0265 lb H_2O/lb dry air
Heat of vaporization of water at 110.2°F = 2413 kJ/kg = ΔH_w^{vap}
Particle area /volume = a = 395 m^2/m^3
Convective heat-transfer coefficient = 0.188 kJ/s-m^2-K = h
Specific heat to the air = 1.09 kJ/kg-K = $(C_P)_g$
Density of the air = 0.942 kg/m^3 = ρ_g
Bed cross-sectional area = 0.0929 m^2
Volumetric flow rate of solid particles = 0.0283 m^3/min
Dry density of calcium carbonate = 1500 kg/m^2 = $(\rho_b)_{ds}$
Mass flow rate of calcium carbonate = 42.5 kg/min = 0.708 kg/s (dry basis)
Solve this exercise using SI units, but with temperature in °C and time in sec

Zone 1: H = 2 in = 0.0508 m, L_1 = 8 ft = 2.44 m
From (18-74), gas temperature leaving Zone 1 is

$$T_{go} = 37.8 + (76.7 - 37.8)\exp\left[-\frac{0.188(395)(0.0508)}{0.942(1.09)(2)}\right] = 50^{\circ}C$$

The moisture-content distribution is given by (18-75). Applying this equation at the end of Zone 1 gives the following, where x is distance along the bed, which equals 8 ft = 2.44 m and z is the height measured from the bottom of the bed for upward flow of air.

Exercise 18.40 (continued)

$$X_1\{L_1,z\}=0.30\left[1-\frac{2.44(0.188)(395)(76.7-37.8)}{0.00508(2413)(1500)}\exp\left(-\frac{0.188(395)z}{0.942(1.09)(2)}\right)\right]$$

Using a spreadsheet, the following results are obtained:

***z*, m**	***X*, %**
0.0000	18.5
0.0127	22.7
0.0254	25.4
0.0381	27.1
0.0508	28.2

Zone 2: Use (18-78), with x measured at L_1 and height given by $(H - z)$, because of downward flow from $z = H$ to $z = 0$. Thus,

$$X_2\{L_2,z\}=X_1\{L_1,z\}\left[1-\frac{L_2 ha\left(T_{gi}-T_w\right)}{S\Delta H_w^{\text{vap}}\left(\rho_b\right)_{ds}}\exp\left(-\frac{ha(H-z)}{\rho_g\left(C_P\right)_g u_s}\right)\right] \qquad (1)$$

where L_2 = length of zone 2 = 2.44 m and, again, z is measured from the bottom of the bed.
Using a spreadsheet, the following results are obtained:

***z*, m**	***X*, %**
0.0000	17.4
0.0127	20.5
0.0254	21.5
0.0381	20.5
0.0508	17.4

Zone 3: Use (18-78), with x measured at L_2 and height given by z because of upward flow from $z. = H$ to $z = 0$. Thus, using an equation similar to (1), but with X_3 in terms of X_2.
Using a spreadsheet, the following results are obtained:

***z*, m**	***X*, %**
0.0000	10.7
0.0127	15.6
0.0254	18.2
0.0381	18.6
0.0508	16.3

The final average moisture content is obtained from integrating the values of X at the end of zone 3 with (18-76), which gives X_{avg} = 16.5% or 0.165 lbH_2O/lb dry solid, which is greater than the critical moisture content so that drying is in the constant-rate period as assumed.

Exercise 18.41

Subject: Drying of extruded filter cake of calcium carbonate with a through-circulation belt dryer having 2 zones.

Given: Calcium carbonate extruded into cylindrical pieces of 3/8-inch diameter and 1/2-inch length with an initial moisture content of 30% (dry basis) and a critical moisture content of 10% (dry basis). Belt dryer is 6-ft wide with two drying zones of 12-ft long each, running with a belt speed, *S*, of 1 ft/min (0.00508 m/s). Carbonate bed height on the belt is 2-inches with an external porosity of 50%. Air at 170°F (76.7°C) and 10% relative humidity flows through the bed at a superficial velocity, u_s,of 2 m/s, upward in the first zone and downward in zone 2.

Assumptions: Negligible preheat period. Constant-rate drying at the wet-bulb temperature of the entering air.

Find: Moisture content distribution with height at the end of each zone and the final average moisture content.

Analysis: This exercise is exactly the same as Example 18.18 except that the diameter of the extrusion is 3/8 inch instead of 2/8 inch. Thus, the following preliminary calculations from Example 18.18 apply here:

Entering air has a wet-bulb temperature of 110.2°F = 37.8°C = T_w

Entering air has a humidity of 0.0265 lb H_2O/lb dry air

Heat of vaporization of water at 110.2°F = 2413 kJ/kg = ΔH_w^{vap}

Specific heat to the air = 1.09 kJ/kg-K = $\left(C_P\right)_g$

Density of the air = 0.942 kg/m^3 = ρ_g

Bed cross-sectional area = 0,0929 m^2

Dry density of calcium carbonate = 1500 kg/m^2 = $\left(\rho_b\right)_{ds}$

Preliminary calculations:

First, calculate the effective particle diameter, d_p, the diameter of a sphere having the same particle surface area, with D = 3/8 inch, L = 4/8

$$\pi d_p^3 = 2\frac{\pi D^2}{4} + \pi DL$$

Solving, d_p = 0.506 inch = 0.013 m

Now, compute the heat-transfer coefficient from Table 18.6. Need to calculate the bed Reynolds number to determine whether (3) or (4) applies. Using data in Example 18.8,

$$N_{\text{Re}} = (0.013)(1.96)/2\text{x}10^{-5} = 1{,}274$$

Therefore, (3) in Table 18.6 applies:

$$h = 0.151\left(14{,}300/2\right)^{0.59}/\left(0.013\right)^{0.41} = 168 \text{ J/s-m}^2\text{-K} \text{ or } 0.168 \text{ kJ/s-m}^2\text{-K}$$

Now compute the extrusion surface area per volume of bed.

Volume of one extrusion = $\pi D^2 L/4$ = 3.14(0.375)^2(0.5)/4 = 0.0552 in^3 = 9.05x10^{-7} m^3

Surface area for one extrusion = $\pi[DL + 2(D)^2/4]$ = 3.14[0.375(0.5) + (0.375)^2/2] =

0.81 in^2 = 0.000522 m^2

Exercise 18.41 (continued)

For an external porosity of 0.5, $a = 0.000522(0.5)/9.05\text{x}10^{-7} = 288\ \text{m}^2/\text{m}^3$

Solve this exercise using SI units, but with temperature in $^{\text{o}}$C and time in sec

Zone 1: $H = 2$ in $= 0.0508$ m, $L_1 = 12$ ft $= 3.66$ m

From (18-74), gas temperature leaving Zone 1 is

$$T_{go} = 37.8 + (76.7 - 37.8)\exp\left[-\frac{0.168(288)(0.0508)}{0.942(1.09)(2)}\right] = 49.6^{\text{o}}\text{C}$$

The moisture-content distribution is given by (18-75). Applying this equation at the end of Zone 1 gives the following, where x is distance along the bed, which equals 8 ft = 2.44 m and z is the height measured from the bottom of the bed for upward flow of air.

$$X_1\{L_1, z\} = 0.30\left[1 - \frac{3.66(0.168)(288)(76.7 - 37.8)}{0.00508(2413)(1500)}\exp\left(-\frac{0.168(288)z}{0.942(1.09)(2)}\right)\right]$$

Using a spreadsheet, the following results are obtained:

***z*, m**	***X*, %**
0.0000	18.8
0.0127	21.7
0.0254	23.8
0.0381	25.4
0.0508	26.6

Zone 2: Use (18-78), with x measured at L_1 and height given by $(H - z)$, because of downward flow from $z = H$ to $z = 0$. Thus,

$$X_2\{L_2, z\} = X_1\{L_1, z\}\left[1 - \frac{L_2 ha(T_{gi} - T_w)}{S\Delta H_w^{\text{vap}}(\rho_b)_{ds}}\exp\left(-\frac{ha(H - z)}{\rho_g (C_P)_g u_s}\right)\right] \qquad (1)$$

where L_2 = length of zone 2 = 3.66 m and, again, z is measured from the bottom of the bed.

Using a spreadsheet, the following results are obtained:

***z*, m**	***X*, %**
0.0000	16.6
0.0127	18.4
0.0254	18.9
0.0381	18.4
0.0508	16.6

The final average moisture content is obtained from integrating the values of X at the end of zone 3 with (18-76), which gives $X_{\text{avg}} = 18.1\%$ or 0.181 lbH_2O/lb dry solid, which is greater than the value of 15.5% for Example 18.18 because, here, the extrusions are larger in diameter giving smaller values of a and h.

Exercise 18.42

Subject: Drying of titanium dioxide particles in a direct-heat, countercurrent-flow, rotary dryer.

Given: TiO_2 particles at 70°F and 1 atm, with a moisture content of 30% (dry basis) to be dried to a moisture content of 2% (dry basis). Available rotary dryer with a 6-ft diameter and 60-ft length. Hot air at 400°F with a humidity of 0.015 lb/lb dry air. Air mass velocity through dryer at 500 lb/h-ft^2 will prevent serious dusting. For the TiO_2 particles, true density = 240 lb/ft^3 and specific heat = 0.165 Btu/lb-°F.

Assumptions: Particles are non-porous. Adiabatic operation. Drying is in the constant-rate period at the entering air wet-bulb temperature.

Find: (a) A reasonable production rate of TiO_2 on the dry basis.
(b) Heat-transfer rate.
(c) A reasonable air rate (dry basis) in lb/h.
(d) Reasonable values for exit air and exit solids temperatures.

Analysis:

Preliminary calculations:

Dryer cross-sectional area = $\pi D^2/4 = 3.14(6)^2/4 = 28.3$ ft^2

From a high-temperature humidity chart in Perry's Handbook, wet-bulb temperature = 115°F = solids drying temperature.

(c) Air rate = 500(28.3) = 14,200 lb/h (take this as dry air)

(a) Heat of vaporization at 115°F = 1028.7 Btu/lb.

Heat-transfer rate, Btu/lb dry TiO_2 = 0.165(115 – 70) + 0.30(1)(115 – 70) + (0.30 – 0.02)(1028.7) + (0.30 – 0.02)(0.45)(T_{go} – 115) = 295 + 0.126 T_{go}

To obtain a reasonable value for T_{go}, use the N_T concept of Example 18.17, with an intermediate value of $N_T = 2$. From (1) of Example 18.17,

$$N_T = \ln\left[\frac{T_{gi} - T_w}{T_{go} - T_w}\right], \text{ which rearranges to}$$

$$T_{go} = T_w + (T_{gi} - T_w)\exp(-N_T) = 115 + (400 - 115)\exp(-2) = 154^\circ\text{F}$$

Therefore, Q = 295 + 0.126(154) = 315 Btu/lb dry TiO_2

Energy balance with the air, letting m_s = lb/h of dry TiO_2,

315 m_s = 14,200(0.24)(400 – 154) + 0.015(14,200)(0.45)(400 – 154) = 862,000 Btu/h

Solving, production rate of TiO_2 (dry basis) = 2,730 lb/h

(b) Q = heat-transfer rate = 315(2,730) = 860,000 Btu/h

(d) Exit temperatures are 115°F for the solids and 154°F for the air

Exercise 18.43

Subject: Drying of spherical, polymer beads in a fluidized-bed dryer.

Given: 5,000 kg/h (dry basis) of 1-mm diameter spherical beads at 25°C with a moisture content of 80% (dry basis), to be dried to 10% (dry basis) with superheated steam entering at 250°C in a fluidized-bed dryer. Pressure in space above the bed = 1 atm. Use a fluidization velocity of twice the minimum. Bed expansion is expected to be about 20%. Solids and steam exit at 100°C. Before fluidization, bed void fraction = 0.47. For the dry polymer, specific heat = 1.15 kJ/kg-K and density = 1,500 kg/m^3. Drying will take place in the falling-rate period by diffusion. From experiment, 50% of moisture is evaporated in 150 s.

Assumptions: Adiabatic conditions.

Find: Dryer diameter, average bead residence time, and expanded bed height. Reasonable dryer size. Entering steam flow rate and heat-transfer rate.

Analysis:

Mass balance on the beads:

Solids (dry basis): 5,000 kg/h

Moisture in = 5,000(0.8) = 4,000 kg/h, Moisture out in solids =5,000(0.1) = 500 kg/h

Evaporation rate = 4,000 – 500 = 3,500 kg/h

In SI units, specific heat of liquid water = 4.184 kJ/kg-K and

heat of vaporization at 100°C = 2,255 kJ/kg

Heat transfer rate based on the beads = Q = 5,000(1.15)(100 – 25) +

4,000(4.184)(100 – 25) + 3,500 (2,255) = 9,580,000 kJ/h

Heat transfer rate based on the steam = 9,580,000 = m_g[(0.45)(4.184)](250 – 100)

Solving, m_g = 33,900 kg/h of superheated steam

Calculate minimum fluidization velocity from (18-87), using cgs units:

d_p = 1 mm = 0.1 cm

ρ_p = 1.5 g/cm^3

Use the ideal-gas law for gas density based on steam at 100°C

$$\rho_g = \frac{PM}{RT} = \frac{(1)(18.02)}{(82.06)(373)} = 0.00059 \text{ g/cm}^3$$

g = 980 cm/s^2

φ_s = 1.0 (spherical particles)

ε_b = 0.47

Take gas viscosity for steam at 100°C = 0.000123 g/cm-s

$$u_{mf} = \frac{(0.1)^2(1.5-0.00059)980}{150(0.000123)}\left(\frac{0.47^3(1)^2}{1-0.47}\right) = 156 \text{ cm/s}$$

Exercise 18.43 (continued)

Must check for turbulent-flow contribution.

Particle Reynolds number = $N_{\mathrm{Re},p} = \dfrac{d_p u_{mf} \rho_g}{\mu} = \dfrac{0.1(156)(0.00059)}{0.000123} = 74.8 > 20$

Therefore, there is a turbulent-flow contribution and we must solve (18-85) for u_{mf}.

$$\frac{\Delta P_b}{L_b} = (1-\varepsilon_b)(\rho_p - \rho_g)\, g = 150\frac{(1-\varepsilon_b)^2}{\varepsilon_b^3}\frac{\mu u_{mf}}{\varphi_s^2 d_p^2} + 1.75\frac{(1-\varepsilon_b)\rho_g u_{mf}^2}{\varepsilon_b^3 \varphi_s d_p}$$

$$(1-0.47)(1.5-0.00059)980 = 779 =$$

$$150\frac{(1-0.47)^2}{0.47^3}\frac{(0.000123)u_{mf}}{1^2(0.1)^2} + 1.75\frac{(1-0.47)(0.00059)u_{mf}^2}{(0.47)^3 1(0.1)} = 4.99\, u_{mf} + 0.0527\, u_{mf}^2$$

Solving, u_{mf} = the positive root of the quadratic equation = 83.1 cm/s (much lower)
Take $u_f = 2\, u_{mf} = 2(83.1) = 166$ cm/s
Calculate bed diameter by the continuity equation:

$$m_g = u_f A_b \rho_g = u_f \left(\frac{\pi D^2}{4}\right)\rho_g, \quad \text{therefore,}$$

$$D = \left[\frac{4m_g}{\pi u_f \rho_g}\right]^{0.5} = \left[\frac{4\left(\frac{33{,}900{,}000}{3{,}600}\right)}{3.14(166)(0.00059)}\right]^{0.5} = 350\ \text{cm} = 11.5\ \text{ft, which is a reasonable}$$

Now calculate the average particle residence time. From (18-62) for diffusion control,

t_f = Constant $\times \ln\left[\dfrac{X_o}{X_f}\right]$, assuming $X^* = 0$ and no constant-rate period

From the experimental data, Constant = $150/\ln\left[\dfrac{X_o}{X_f}\right] = 150/\ln(0.8/0.4) = 216$

Therefore, t_f to dry to 10% = 216 ln(0.8/0.1) = 450 s

For this time, have (5,000/3600)(450) = 625 kg dry solids in dryer.
Before fluidization, with a bed void fraction of 0.47 and a dry solids density = 1500 kg/m^3,
bed volume = (625/1500)/(1 – 0.47) = 0.786 m^3
With a 20% bed expansion, bed volume = 1.2(0.786) = 0.94 m^3 = 33.3 ft^3 = V_b

For a diameter of 11.5 ft, with $V_b = \pi D^2 H_b/4$, $H_b = 33.3(4)/[3.14(11.5)^2] = 0.32$ ft
This bed height is much too small for the diameter. Increase to at least 6 ft.