Chemical Engineering Separations: A Handbook for Students

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Preface

Chemical Engineering Separations: A Handbook for Students is intended for use by undergraduate students who are taking a course in chemical engineering separations. The handbook assumes that students have taken one or two semesters of chemical engineering thermodynamics, one semester of heat and mass transfer, and one semester of computational methods for chemical engineering.

The purpose of this handbook is to introduce students to chemical engineering separations in a way that most closely aligns with what most entry-level chemical engineers will do in the workplace. Most newly hired chemical engineers will be responsible for monitoring and troubleshooting existing processes and proposing modifications to improve process performance. For this reason, we have written the handbook to emphasize how to optimize process conditions, how to retrofit an existing unit to meet a given separation objective while not exceeding operating capacity, or how to select the best existing or pre-fabricated unit to meet a separation objective while maintaining safe operation at a reasonable cost.

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1. Performance Metrics for Separation Processes

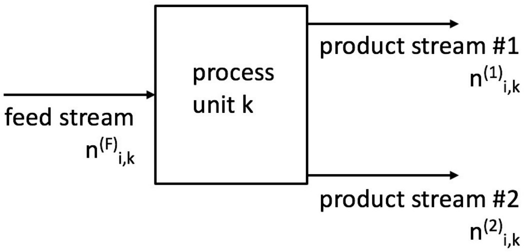
$n_{i,k}^{(F)}$ = mass or molar flow rate of species i entering separator k in feed stream (mass time^{-1} or mol time^{-1})

$n_{i,k}^{(1)}$ = mass or molar flow rate of species i leaving separator k in first product stream (mass time^{-1} or mol time^{-1})

$n_{i,k}^{(2)}$ = mass or molar flow rate of species i leaving separator k in second product stream (mass time^{-1} or mol time^{-1})

$\mathrm{SF}_{i,k}$ = split fraction for species i in separator k (dimensionless)

$\mathrm{SR}_{i,k}$ = split ratio for species i in separator k (dimensionless)

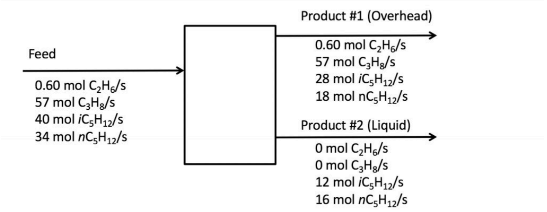


(1.1) $$\mathrm{SF}_{i,k} = n_{i,k}^{(1)}/n_{i,k}^{(F)}$$

(1.2) $$\mathrm{SR}_{i,k} = n_{i,k}^{(1)}/n_{i,k}^{(2)} = \mathrm{SF}_{i,k}/(1-\mathrm{SF}_{i,k})$$

Example

For the process below, compute the split fraction and the split ratio for iC_5H_{12}. Designate the overhead stream as product stream 1.



2. Mass Transfer in Gas-liquid Systems

In chemical separations, we can use thermodynamic models to predict the composition in each phase at equilibrium. For example, Raoult's Law describes the compositions of vapor and liquid phases at equilibrium. Mass transfer models help us understand how we can manipulate the process to reach equilibrium in a faster or more economical manner.

This chapter will briefly review fundamentals of mass transfer in gas-liquid systems because many of the separation processes in this handbook involve the movement of species between gas and liquid phases.

Diffusion-based Mass Transfer

J_{Az} = molar flux of A relative to the molar-average velocity of the mixture in the z direction

D_{AB} = mutual diffusion coefficient of A in B ($= D_{BA}$)

c_A = molar concentration of A

N_A= molar flux of species A

N = total molar flux

x_A= mole fraction of species A

c = total molar concentration

(1.1) $$J_{Az} = -D_{AB}\frac{dc_A}{dz}$$

(1.2) $$N_A = x_A N - cD_{AB}\frac{dx_A}{dz}$$

Falling Liquid Film with Gaseous Solute A Diffusing into Liquid B

Γ = liquid flow rate per unit width of film $= \rho\bar{u}_y r_H$ (mass length^{-1} time^{-1})

δ = film thickness (length)

η = metric used in selecting the appropriate equation for calculating k_c

μ = dynamic viscosity of the liquid (pressure time)

δ = density of the liquid (mass volume^{-1})

A = available area for mass transfer = $L * W$ (length^2)

c_A = concentration of species A in liquid B (mol volume^{-1})

c_{Ai} = concentration of species A in liquid B at the gas/liquid interface (mol volume^{-1})

c_{A0} = concentration of species A in liquid B when the liquid enters the enters (mol volume^{-1})

Δc_A = log mean concentration difference driving force (mol volume^{-1})

$\bar{c}_A$ = bulk concentration of species A in liquid B at any position y (mol volume^{-1})

$\bar{c}_{AL}$ = bulk concentration of species A in liquid B at any position $y = L$ (mol volume^{-1})

D_{AB} = diffusivity of solution A in liquid B (length^2 time^{-1})

g = gravitational constant (length time^{-2})

H_A = Henry's Law constant for solute A in our liquid at our system temperature (volume pressure mol^{-1})

$k_{c,\text{ ave}}$ = average mass transfer coefficient (length time^{-1})

L = film height (length)

n_A = molar flow rate of species A (mol time^{-1})

N_{Re} = Reynolds number (dimensionless)

N_{Sc} = Schmidt number (dimensionless)

$N_{\text{Pe, M}}$ = Peclet number for mass transfer (dimensionless)

P_A = partial pressure of species A in the gas phase (pressure)

r_H = flow cross section per wetted perimeter (length)

$\bar{u}_y$ = bulk velocity of the falling film in the y direction (length time^{-1})

W = film width (length)

Reynolds number for a falling film

(1.3) $$N_{\text{Re}} = \frac{\rho \bar{u}_y 4 r_H}{\mu} = \frac{4\Gamma}{\mu}$$

Rate

(1.4) $$n_A = \bar{u}_y \delta W (\bar{c}_{AL} - c_{A0})$$

(1.5) $$n_A = k_c A \Delta c_A$$

Film thickness

(1.6) $$\delta = \left(\frac{3\overline{u}_y \mu}{\rho g}\right)^{1/2} = \left(\frac{3\mu\Gamma}{\rho^2 g}\right)^{1/3}$$

Hydraulic radius for a falling film   Flow cross section: δW; wetted perimeter: W

(1.7) $$r_H = \frac{\delta W}{W} = \delta$$

Schmidt number

(1.8) $$N_{\mathrm{Sc}} = \frac{\mu}{\rho D_{AB}}$$

Peclet number for mass transfer

(1.9) $$N_{\mathrm{Pe,M}} = N_{\mathrm{Re}} N_{\mathrm{Sc}} = \frac{4\delta \overline{u}_y}{D_{AB}} = \frac{4\Gamma}{\rho D_{AB}}$$

Mass transfer coefficient $k_{c,\mathrm{ave}}$

(1.10) $$\eta = \frac{2D_{AB}L}{3\delta^2 \overline{u}_y} = \frac{8/3}{N_{\mathrm{Re}} N_{\mathrm{Sc}}(\delta/L)} = \frac{8/3}{(\delta/L) N_{\mathrm{Pe,M}}}$$

if $\eta < 0.001$,

(1.11) $$k_{c,\mathrm{ave}} = \left(\frac{6D_{AB}\Gamma}{\pi \delta \rho L}\right)^{1/2}$$

if $\eta > 0.1$,

(1.12) $$k_{c,\mathrm{ave}} = \left(\overline{u}_y \frac{\delta}{L}\right)(0.241 + 5.1213\eta)$$

if $\eta > 1$,

(1.13) $$k_{c,\mathrm{ave}} = 3.414 \frac{D_{AB}}{\delta}$$

Henry's Law, applies at the interface

(1.14) $$c_A = \frac{P_A}{H_A}$$

Log mean concentration difference

(1.15) $$\Delta c_A = (c_{A_i} - \bar{c}_A)_{\mathrm{LM}} = \frac{(c_{A_i} - c_{A_0}) - (c_{A_i} - \bar{c}_{A_L})}{\ln\left[(c_{A_i} - c_{A_0})/(c_{A_i} - \bar{c}_{A_L})\right]}$$

Example

10 mL/s of water at 25°C flows down a wall that is 1.0 m wide and 3.0 m high. This film is in contact with pure CO_2 at 1.0 atm, 25°C. Find the rate of absorption of CO_2 into the water (kmol/s).

- ρ_{H2O} = 998 kg/m^3
- μ_{H2O} = 8.90×10^{-4} Pa s
- $D_{\mathrm{CO2,H2O}}$ = 1.96×10^{-9} m^2/s
- $H_{\mathrm{CO2,H2O}}$ = 29.41 L atm mol^{-1}

Velocity and Concentration Boundary Layers for Laminar Horizontal Flow Across a Flat Plate

δ = thickness (height) of the velocity boundary layer (length)

δ_c = thickness (height) of the concentration boundary layer (length)

μ = fluid viscosity (pressure time) or (mass length-1 time-1)

ρ = fluid density (mass volume-1)

c_A = concentration of species A in fluid B at some point (x, z) (mol volume-1)

c_{A0} = initial concentration of species A in fluid B (mol volume-1)

c_{Ai} = concentration of species A in fluid B at the interface (mol volume-1)

D_{AB} = diffusivity of solute A in fluid B (length2 time-1)

$N_{\mathrm{Re,x}}$ = Reynolds number (dimensionless)

N_{Sc} = Schmidt number (dimensionless)

u_0 = free-stream velocity of the fluid in the x direction (length time-1)

u_x = fluid velocity in the x direction at some point (x, z) (length time-1)

x = horizontal distance from the leading edge of the flat plate (length)

z = vertical distance from the plate surface (length)

(2.1) $$\frac{\delta}{x} = \frac{4.96}{{N_{\text{Re,x}}}^{0.5}}$$

(2.2) $$N_{\text{Re,x}} = \frac{x u_0 \rho}{\mu}$$

(2.3) $$\frac{u_x}{u_0} = 1.5\left(\frac{z}{\delta}\right) - 0.5\left(\frac{z}{\delta}\right)^3$$

(2.4) $$\delta_c = \frac{\delta}{N_{\text{Sc}}^{1/3}}$$

(2.5) $$N_{\text{Sc}} = \frac{\mu}{\rho D_{AB}}$$

(2.6) $$\frac{(c_{A_i} - c_A)}{(c_{A_i} - c_{A_0})} = 1.5\left(\frac{z}{\delta_c}\right) - 0.5\left(\frac{z}{\delta_c}\right)^3$$

Example

Air at 100°C and 1.0 atm with a free-stream velocity of 5.0 m/s flows over a 3.0 m long flat plate made of naphthalene.

(a) At what horizontal position does flow become turbulent?

(b) What is the thickness of the velocity boundary layer at that point?

(c) What is the thickness of the concentration boundary layer at that point?

(d) What is the concentration of naphthalene in the air at this horizontal position and vertical position that is half of the height of the concentration boundary layer?

- μ_{air} = 2.15×10-5 kg m-1 s-1
- ρ_{air} = 0.0327 kmol m-3
- D_{AB} = 0.94×10-5 m2 s-1
- c_{Ai} = 4.3×10-3 kmol m-3

Film Theory and Overall Mass Transfer Coefficients

δ = thickness of the film in which $c_A \neq c_{Ab}$ (length)

c = total concentration of liquid B (mol volume^{-1})

c_{Ai} = concentration of species A in liquid B at the interface (mol volume^{-1})

c_{Ab} = bulk concentration of species A in liquid B (mol volume^{-1})

c_A^* = concentration of species A in liquid B at equilibrium with the bulk gas phase (mol volume^{-1})

D_{AB} = diffusivity of species A in liquid B (area time^{-1})

H'_A = Henry's Law constant for equation of the form $c_A = H'_A P_A$; (mol volume^{-1} pressure^{-1})

k_c = liquid-phase mass transfer coefficient, with respect to concentration driving force (length time^{-1})

K_G = overall mass transfer coefficient, with respect to pressure driving force (mol time^{-1} area^{-1} pressure^{-1})

K_L = overall mass transfer coefficient, with respect to concentration driving force (length time^{-1})

k_p = gas-phase mass transfer coefficient, pressure driving force (mol time^{-1} area^{-1} pressure^{-1})

N_A = molar flux (mol area^{-1} time^{-1})

$P_{Ab} = p_{Ab}$ = partial pressure of species A in the bulk gaseous phase (pressure)

P_A^* = partial pressure of species A in a gas at equilibrium with the bulk liquid phase (pressure) x_{Ai} = mole fraction of species A in liquid B at the interface

x_{Ab} = bulk mole fraction of species A in liquid B

Film Theory

$$N_A = \left(\frac{D_{AB}}{\delta}\right)(c_{Ai} - c_{Ab}) = \left(\frac{cD_{AB}}{\delta}\right)(x_{Ai} - x_{Ab}) \tag{3.1}$$

Example

SO_2 is absorbed from air into water using a packed absorption tower. At a specific location in the tower, we know that the pressure of SO_2 is 0.15 atm. Measurements of the gas composition above and below this location in the tower have told us that the flux of SO_2 into the water is 0.0270 kmol SO_2 m^{-2} hr^{-1}. We were able to sample the bulk liquid phase at this location and found that it contained 3.0×10^{-4} mol SO_2/mol. Assuming that this system fits film theory, find the thickness of the film.

- $D_{\mathrm{SO_2,H_2O}}$ = $1.7*10^{-9}$ m^2 s^{-1}
- $H_{\mathrm{SO_2,H_2O}}$ = 1.2 L atm mol^{-1}

Two-Film Theory, Overall Mass Transfer Coefficients, Gas/Liquid

(3.2) $$N_A = \left(P_{Ab}H'_A - c_{Ab}\right)\left(\frac{H'_A}{k_p} + \frac{1}{k_c}\right)^{-1}$$

(3.3) $$\frac{1}{K_L} = \frac{H'_A}{k_p} + \frac{1}{k_c}$$

(3.4) $$N_A = K_L(c^*_A - c_{Ab})$$

(3.5) $$N_A = (P_{Ab} - P^*_A)\left(\frac{1}{k_p} + \frac{1}{H'_A k_c}\right)^{-1}$$

(3.6) $$\frac{1}{K_G} = \frac{1}{k_p} + \frac{1}{H'_A k_c}$$

(3.7) $$N_A = K_G(P_{Ab} - P^*_A)$$

Example

We intend to use water to absorb SO_2 from air. The incoming air is at 50°C and 2.0 atm and contains 0.085 mol SO_2/mol. The incoming water, also at 50°C, already contains 0.0010 mol SO_2/mol.

(a) Which phase is most limiting to mass transfer?

(b) What is the expected initial flux value?

- k_c = 0.18 m hr^{-1}
- k_p = 0.040 kmol hr^{-1} m^{-2} kPa^{-1}
- H'_A (50°C) = 0.76 mol atm^{-1} L^{-1}

3. Liquid-liquid Extraction

Staged Liquid-Liquid Extraction and Hunter Nash Method

E_n = extract leaving stage n. This could refer to the mass of the stream or the composition of the stream.

F = solvent entering extractor stage 1. This could refer to the mass of the stream or the composition of the stream.

n = generic stage number

N = Final stage. This is where the fresh solvent S enters the system and the final raffinate R_N leaves the system.

M = Composition of the mixture representing the overall system. Points (F and S) and (E_1 and R_N) must be connected by a straight line that passes through point M. M will be located within the ternary phase diagram.

P = Operating point. P is determined by the intersection of the straight line connecting points (F, E_1) and the straight line connecting points (S, R_N). Every pair of passing streams must be connected by a straight line that passes through point P. P is expected to be located outside of the ternary phase diagram.

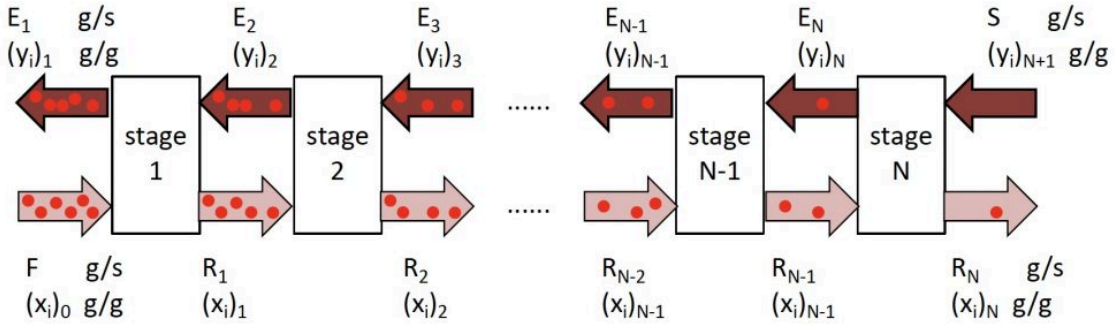
R_n = raffinate leaving stage n. This could refer to the mass of the stream or the composition of the stream.

S = solvent entering extractor stage N. This could refer to the mass of the stream or the composition of the stream.

S/F = mass ratio of solvent to feed

$(x_i)_n$ = Mass fraction of species i in the raffinate leaving stage n

$(y_i)_n$ = Mass fraction of species i in the extract leaving stage n



Process schematic for multistage liquid-liquid extraction.

Determining number of stages N when (1) feed rate; (2) feed composition; (3) incoming solvent rate; (4) incoming solvent composition; and (5) outgoing raffinate composition have been specified/selected.

1. Locate points F and S on the ternary phase diagram. Connect with a straight line.
2. Do a material balance to find the composition of one species in the overall mixture. Use this composition to locate point M along the straight line connection points F and S. Note the position of point M.
3. Locate point R_N on the ternary phase diagram. It will be on the equilibrium curve. Draw a straight line from R_N to M and extend to find the location of E_1 on the equilibrium curve.
4. On a fresh copy of the graph, with plenty of blank space on each side of the diagram, note the location of points F, S, and R_N (specified/selected) and E_1 (determined in step 3).
5. Draw a straight line between F and E_1. Extend to both sides of the diagram. Draw a second straight line between S and R_N. Note the intersection of these two lines and label as "P".
6. Determine the number of equilibrium stages required to achieve the desired separation with the selected solvent mass.

– Stream R_N is in equilibrium with stream E_N. Follow the tie-lines from point R_N to E_N.

– Stream E_N passes stream R_{N-1}. Connect point E_N to operating point P with a straight line, mark the location of R_{N-1}.

– Stream R_{N-1} is in equilibrium with stream E_{N-1}. Follow the tie-lines from stream R_{N-1} to E_{N-1}.

– Stream E_{N-1} passes stream R_{N-2}. Connect E_{N-1} to operating point P with a straight line, mark the location of R_{N-2}.

– Continue in this manner until the extract composition has reached or passed E_1. Count the number of equilibrium stages.

Watch this two-part series of videos from LearnChemE that shows how to use the Hunter Nash method to find the number of equilibrium stages required for a liquid-liquid extraction process.

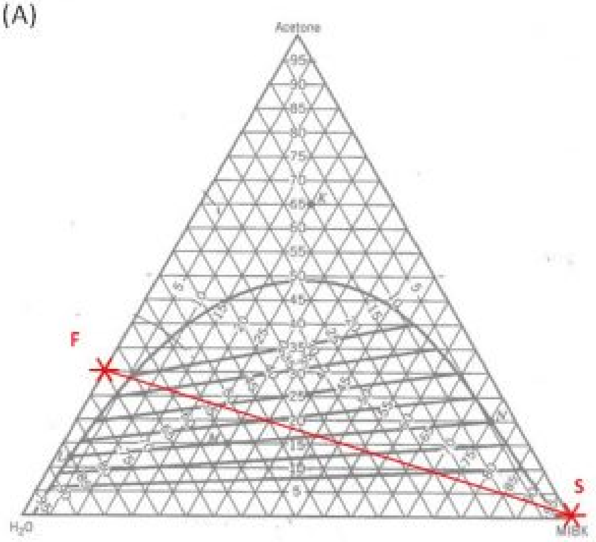
- Hunter Nash Method 1: Mixing and Operating Points (9:30)
- Hunter Nash Method 2: Number of Stages (6:30)

Example

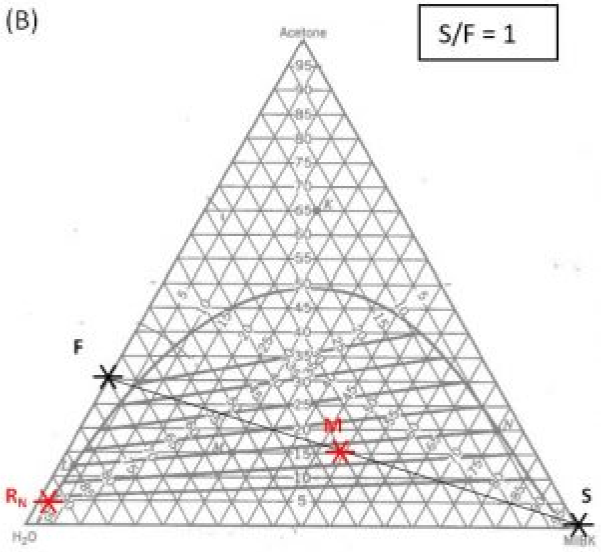
1000 kg/hr of a feed containing 30 wt% acetone, 70 wt% water. The solvent is pure MIBK. We intend that the raffinate contain no more than 5.0 wt% acetone. How many stages will be required for each proposed solvent to feed ratio in the table below?

$\mathbf{S/F}$	**S (kg/hr)**	$(\mathbf{x_A})_\mathbf{M}$	**target** $(\mathbf{y_A})_\mathbf{1}$	**N**
1.0				
2.0				
0.2				

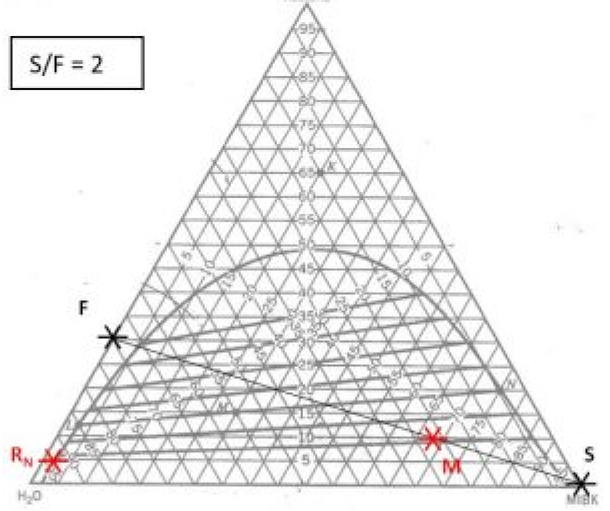
(A)



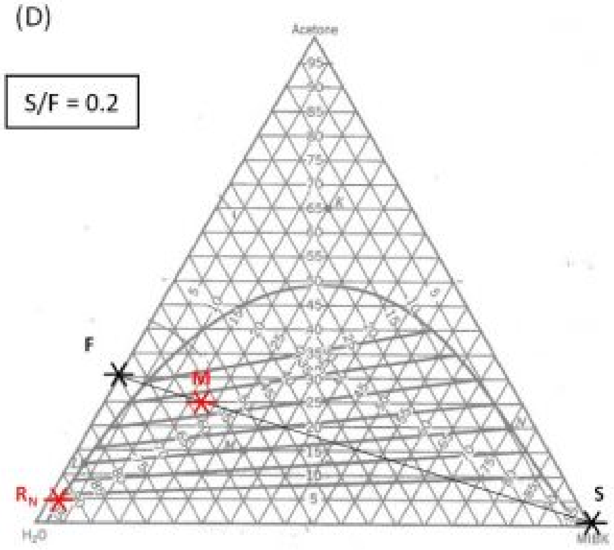
(B)

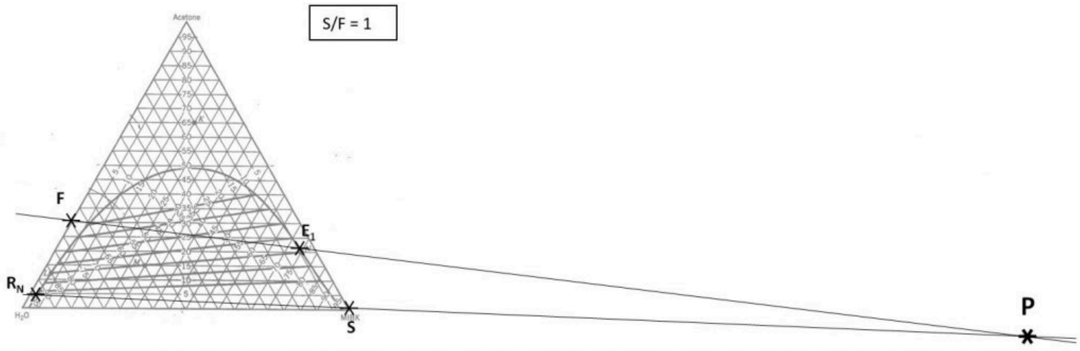


(C)


S/F = 2
Acetone
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
F
M
R_N
S
H_2O
MIBK

(D)


S/F = 0.2
Acetone
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
F
M
R_N
S
H_2O
MIBK


S/F = 1
Acetone
F
E_1
R_N
S
P
H_2O
MIBK

Hunter Nash Method for Finding Smin, Tank Sizing and Power Consumption for Mixer-Settler Units

Staged LLE: Hunter-Nash Method for Finding the Minimum Solvent to Feed Ratio

E_n = extract leaving stage n. This could refer to the mass of the stream or the composition of the stream.

F = solvent entering extractor stage 1. This could refer to the mass of the stream or the composition of the stream.

n = generic stage number

N = Final stage. This is where the fresh solvent S enters the system and the final raffinate R_N leaves the system.

M = Composition of the overall mixture. Points (F and S) and (E_1 and R_N) are connected by a straight line passing through M.

P = Operating point. Every pair of passing streams must be connected by a straight line that passes through P.

R_n = raffinate leaving stage n. This could refer to the mass of the stream or the composition of the stream.

S = solvent entering extractor stage N. This could refer to the mass of the stream or the composition of the stream.

S/F = mass ratio of solvent to feed

S_{min}/F = Minimum feasible mass ratio to achieve the desired separation, assuming the use of an infinite number of stages.

$(x_i)_n$ = Mass fraction of species i in the raffinate leaving stage n

$(y_i)_n$ = Mass fraction of species i in the extract leaving stage n

P_{min} = Point associated with the minimum feasible S/F for this feed, solvent and (raffinate or extract) composition. P_{min} is the intersection of the line connecting points (R_N, S) and the line that is an extension of the upper-most equilibrium tie-line.

Determining minimum feasible solvent mass ratio (S_{min}/F) when (1) feed composition; (2) incoming solvent composition; and (3) outgoing raffinate composition have been specified/selected.

1. Locate points S and R_N on the phase diagram. Connect with a straight line.
2. Extend the upper-most tie-line in a line that connects with the line connecting points (S and R_N). Label the intersection P_{min}.
3. Find point F on the diagram. Draw a line from P_{min} to F and extend to the other side of the

equilibrium curve. Label $E_1@S_{\text{min}}$.

4. On a fresh copy of the phase diagram, label points F, S, R_N and $E_1@S_{\text{min}}$. Draw one line connecting points S and F and another line connecting points $E_1@S_{\text{min}}$
5. and R_N. The intersection of these two lines is mixing point M. Note the composition of species i at this location.
6. Calculate

$$\frac{S_{\text{min}}}{F} = \frac{(x_i)_F - (x_i)_M}{(x_i)_M - (x_i)_S} \tag{5.1}$$

Example

We have a 1000 kg/hr feed that contains 30 wt% acetone and 70 wt% water. We want our raffinate to contain no more than 5.0 wt% acetone. What is the minimum mass of pure MIBK required?

Liquid-Liquid Extraction: Sizing Mixer-settler Units

Φ_C = volume fraction occupied by the continuous phase

Φ_D = volume fraction occupied by the dispersed phase

μ_C = viscosity of the continuous phase (mass time^{-1} length^{-1})

μ_D = viscosity of the dispersed phase (mass time^{-1} length^{-1})

μ_M = viscosity of the mixture (mass time^{-1} length^{-1})

ρ_C = density of the continuous phase (mass volume^{-1})

ρ_D = density of the dispersed phase (mass volume^{-1})

ρ_M = average density of the mixture (mass volume^{-1})

D_i = impeller diameter (length)

D_T = vessel diameter (length)

H = total height of mixer unit (length)

N = rate of impeller rotation (time^{-1})

N_{Po} = impeller power number, read from Fig 8-36 or Perry's 15-54 (below) based on value of N_{Re} (unitless)

$(N_{\text{Re}})_C$ = Reynold's number in the continuous phase = inertial force/viscous force (unitless)

P = agitator power (energy time^{-1})

Q_C = volumetric flowrate, continuous phase (volume time^{-1})

Q_D = volumetric flowrate, dispersed phase (volume time^{-1})

V = vessel volume (volume)

Tank and impeller sizing

(5.2) $$\text{residence time} = \frac{V}{Q_C + Q_D}$$

Geometry of a cylinder

(5.3) $$V = \frac{\pi D_T^2 H}{4}$$

General guidelines

(5.4) $$\frac{H}{D_T} = 1$$

(5.5) $$\frac{D_i}{D_T} = \frac{1}{3}$$

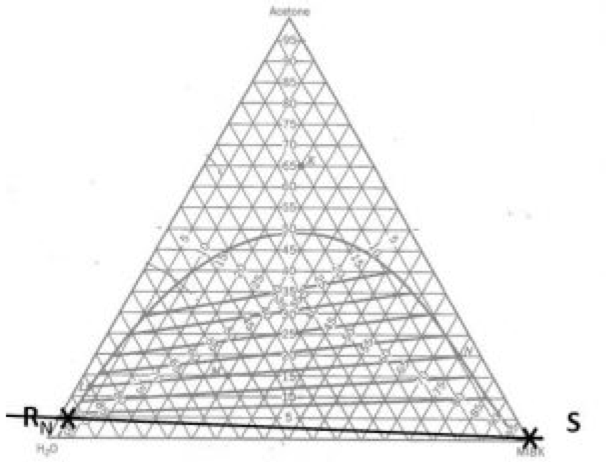
Impeller power consumption:

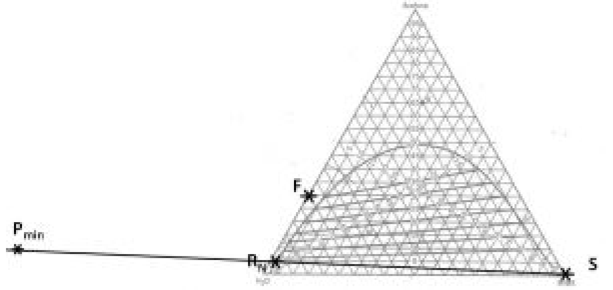
(5.6) $$P = N_{Po} N^3 D_i^5 \rho_m$$

(5.7) $$N_{Re} = \frac{D_i^2 N \rho_M}{\mu_M}$$

(5.8) $$\rho_M = \rho_C \Phi_C + \rho_D \Phi_D$$

(5.9) $$\mu_M = \frac{\mu_C}{\Phi_C} \left[1 + \frac{1.5 \mu_D \Phi_D}{\mu_C + \mu_D} \right]$$





Modeling Mass Transfer in Mixer-Settler Units

$\Delta\rho$ = density difference (absolute value) between the continuous and dispersed phases (mass volume^{-1})

ϕ_C = volume fraction occupied by the continuous phase

ϕ_D = volume fraction occupied by the dispersed phase

μ_C = viscosity of the continuous phase (mass time^{-1} length^{-1})

μ_D = viscosity of the dispersed phase (mass time^{-1} length^{-1})

μ_M = viscosity of the mixture (mass time^{-1} length^{-1})

ρ_C = density of the continuous phase (mass volume^{-1})

ρ_D = density of the dispersed phase (mass volume^{-1})

ρ_M = average density of the mixture (mass volume^{-1})

σ = interfacial tension between the continuous and dispersed phases
(mass time^{-2})

a = interfacial area between the two phases per unit volume (area volume^{-1})

$c_{D,\text{in}}$, $c_{D,\text{out}}$ = concentration of solute in the incoming or outgoing dispersed streams (mass volume^{-1})

c_D^* = concentration of solute in the dispersed phase if in equilibrium with the outgoing continuous phase (mass volume^{-1})

D_C = diffusivity of the solute in the continuous phase (area time^{-1})

D_D = diffusivity of the solute in the dispersed phase (area time^{-1})

D_i = impeller diameter (length)

D_T = vessel diameter (length)

d_{vs} = Sauter mean droplet diameter; actual drop size expected to range from $0.3d_{vs} - 3.0d_{vs}$ (length)

E_{MD} = Murphree dispersed-phase efficiency for extraction

g = gravitational constant (length time^{-2})

H = total height of mixer unit (length)

k_c = mass transfer coefficient of the solute in the continuous phase (length time^{-1})

k_D = mass transfer coefficient of the solute in the dispersed phase (length time^{-1})

K_{OD} = overall mass transfer coefficient, given on the basis of the dispersed phase (length time^{-1})

m = distribution coefficient of the solute, $\Delta c_C/\Delta c_D$ (unitless)

N = rate of impeller rotation (time^{-1})

$(N_{\text{Eo}})_C$ = Eotvos number = gravitational force/surface tension force (unitless)

$(N_{\text{Fr}})_C$ = Froude number in the continuous phase = inertial force/gravitational force (unitless)

N_{min} = minimum impeller rotation rate required for complete dispersion of one liquid into another

$(N_{\text{Re}})_C$ = Reynold's number in the continuous phase = inertial force/viscous force (unitless)

$(N_{\text{Sh}})_C$ = Sherwood number in the continuous phase = mass transfer rate/diffusion rate (unitless)

$(N_{\text{Sc}})_C$ = Schmidt number in the continuous phase = momentum/mass diffusivity (unitless)

$(N_{\text{We}})_C$ = Weber number = inertial force/surface tension (unitless)

Q_D = volumetric flowrate of the dispersed phase (volume time^{-1})

V = vessel volume (volume)

Calculating N_{min}

(6.1) $$\frac{N_{\text{min}}^2\rho_M D_i}{g\Delta\rho} = 1.03\left(\frac{D_T}{D_i}\right)^{2.76}(\phi_D)^{0.106}\left(\frac{\mu_M^2\sigma}{D_i^5\rho_M g^2(\Delta\rho)^2}\right)^{0.084}$$

(6.2) $$\rho_M = \rho_C\phi_C + \rho_D\phi_D$$

(6.3) $$\mu_M = \frac{\mu_C}{\phi_C}\left(1 + \frac{1.5\mu_D\phi_D}{\mu_C + \mu_D}\right)$$

Estimating Murphree efficiency for a proposed design

Sauter mean diameter

(6.4) $$\text{if} \quad N_{\text{We}} < 10,000,\ d_{vs} = 0.052 D_i (N_{\text{We}})^{-0.6} \exp(4\phi_D)$$

(6.5) $$\text{if} \quad N_{\text{We}} > 10,000,\ d_{vs} = 0.39 D_i (N_{\text{We}})^{-0.6}$$

(6.6) $$N_{\text{We}} = \frac{D_i^3 N^2 \rho_C}{\sigma}$$

mass transfer coefficient of the solute in each phase

(6.7) $$k_D = \frac{6.6 D_D}{d_{vs}}$$

(6.8) $$k_C = \frac{(N_{\text{Sh}})_C D_c}{d_{vs}}$$

(6.9) $$(N_{\text{Sh}})_C = 1.237 \times 10^{-5} (N_{\text{Sc}})_C^{1/3} (N_{\text{Re}})_C^{2/3} (\phi_D)^{-1/2} (N_{\text{Fr}})_C^{5/12} \left(\frac{D_i}{d_{vs}}\right)^2 \left(\frac{d_{vs}}{D_T}\right)^{1/2} (N_{\text{Eo}})_C^{5/4}$$

(6.10) $$(N_{\text{Sc}})_C = \frac{\mu_C}{\rho_C D_C}$$

(6.11) $$(N_{\text{Re}})_C = \frac{D_i^2 N \rho_C}{\mu_C}$$

(6.12) $$(N_{\text{Fr}})_C = \frac{D_i N^2}{g}$$

(6.13) $$(N_{\text{Eo}})_C = \frac{\rho_D d_{vs}^2 g}{\sigma}$$

Overall mass transfer coefficient for the solute

$$\frac{1}{K_{OD}} = \frac{1}{k_D} + \frac{1}{mk_C} \tag{6.14}$$

Murphree efficiency

$$E_{MD} = \frac{K_{OD}aV}{Q_D}\left(1 + \frac{K_{OD}aV}{Q_D}\right)^{-1} \tag{6.15}$$

$$a = \frac{6\phi_D}{d_{vs}} \tag{6.16}$$

Experimental assessment of efficiency

$$E_{MD} = \frac{c_{D,\text{in}} - c_{D,\text{out}}}{c_{D,\text{in}} - c_D^*} \tag{6.17}$$

Example

1000 kg/hr of 30 wt% acetone and 70 wt% water is to be extracted with 1000 kg/hr of pure MIBK. Assume that the extract is the continuous phase, a residence time of 5 minutes in the mixing vessel, standard sizing of the mixing vessel and impeller. Find the power consumption and Murphree efficiency if the system operates at N_{min}, controlled at the level of 1 rev/s. Ignore the contribution of the solute and the co-solvent to the physical properties of each phase.

- MIBK
    - density = 802 kg m^{-3}
    - viscosity = 0.58 cP
    - diffusivity with acetone at 25°C = 2.90×10^{-9} m^2 s^{-1}
- Water
    - density = 1000 kg m^{-3}
    - viscosity = 0.895 cP
    - diffusivity with acetone at 25°C = 1.16×10^{-9} m^2 s^{-1}
- The interfacial tension of water and MIBK at 25°C = 0.0157 kg s^{-2}. Use the ternary phase diagram to find m.

Liquid-Liquid Extraction Columns

$\Delta\rho$ = density difference (absolute value) between the continuous and dispersed phases (mass volume$^{-1)}$

μ_C = viscosity of the continuous phase (mass time^{-1} length^{-1})

ρ_C = density of the continuous phase (mass volume^{-1})

ρ_D = density of the dispersed phase (mass volume^{-1})

σ = interfacial tension between the continuous and dispersed phases
(mass time^{-2})

D_T = column diameter (length)

H = total height of column (length)

HETS = height of equilibrium transfer stage (length)

m_C^* = mass flowrate of the entering continuous phase (mass time^{-1})

m_D^* = mass flowrate of the entering dispersed phase (mass time^{-1})

N = required number of equilibrium stages

u_0 = characteristic rise velocity of a droplet of the dispersed phase (length time^{-1})

U_i = superficial velocity of phase i (C = continuous, downward; D = dispersed, upward) (length time^{-1})

V_i^* = volumetric flowrate of phase i (volume time^{-1})

(7.1) $$U_i = \frac{4V_i^*}{\pi D_T^2}$$

definition of superficial velocity

(7.2) $$\frac{U_D}{U_C} = \frac{m_D^*}{m_C^*}\left(\frac{\rho_C}{\rho_D}\right)$$

(7.3) $$(U_D + U_C)_{\text{actual}} = 0.50(U_D + U_C)_f$$

for operation at 50% of flooding

(7.4) $$u_0 = \frac{0.01\sigma\Delta\rho}{\mu_C\rho_C}$$

for rotating-disk columns, D_T = 8 to 42 inches, with one aqueous phase

$$D_T = \left(\frac{4m_D^*}{\rho_D U_D \pi}\right)^{0.5} = \left(\frac{4m_C^*}{\rho_C U_C \pi}\right)^{0.5} \tag{7.5}$$

$$H = \text{HETS} * N \tag{7.6}$$

Example

1000 kg/hr of 30 wt% acetone and 70 wt% water is to be extracted with 1000 kg/hr of pure MIBK in a 2-stage column process. Assume that the extract is the dispersed phase. Ignoring the contribution of the solute and the co-solvent to the physical properties of each phase, find the required column diameter and height.

- MIBK
  - density = 802 kg m^{-3}
  - viscosity = 0.58 cP
- Water
  - density = 1000 kg m^{-3}
  - viscosity = 0.895 cP
- The interfacial tension of water and MIBK at 25°C = 0.0157 kg s^{-2}.

4. Absorption and Stripping

Overview of Absorption and Stripping Processes

ϕ_A = fraction not absorbed (unitless)

ϕ_S = fraction not stripped (unitless)

A = absorption factor (unitless)

K = equilibrium constant, (mole fraction in gas)/(mole fraction in liquid)

L = total liquid flow rate (mol time^{-1})

V = total gas flow rate (mol time^{-1})

S = stripping factor (unitless)

x (lowercase) = mol fraction of solute in liquid phase (mol solute/mol total liquid)

X (uppercase) = mol ratio of solute in liquid phase (mol solute/mol solvent)

y (lowercase) = mol fraction of solute in gas phase (mol solute/mol total vapor)

Y (uppercase) = mol ratio of solute in gas phase (mol solute/mol gaseous carrier)

(8.1) $$A = \frac{(L/V)}{K}$$

(8.2) $$S = \frac{K}{(L/V)} = \frac{1}{A}$$

Example

K for acetone in an air/water system is 2.0. We intend to absorb 90% of the acetone entering in the gaseous phase into the liquid phase. How many theoretical stages would be required for (L/V) = 1, (L/V) = 2, and (L/V) = 10?

Finding mole ratio from mole fraction:

(8.3) $$Y=\frac{y}{1-y}$$

(8.4) $$X=\frac{x}{1-x}$$

Finding mole fraction from mole ratio:

(8.5) $$y=\frac{Y}{1+Y}$$

(8.6) $$x=\frac{X}{1+X}$$

Graphical Method to Find Equilibrium Stages for Absorption Columns

K = equilibrium constant, (mole fraction in gas)/(mole fraction in liquid)

L = liquid flow rate (mol time^{-1})

L' = liquid flow rate on a solute-free basis (mol time^{-1})

N = total number of stages. For an absorption column, N is the bottom stage. For a stripping column, N is the top stage.

n = generic stage number

V = gas flow rate (mol total time^{-1})

V' = gas flow rate on a solute-free basis (mol gaseous carrier time^{-1})

x = mole fraction of solute in liquid phase (mol solute/mol total liquid)

X = mole ratio of solute in liquid phase (mol solute/mol liquid absorbent)

X_0 = mole ratio of solute/absorbent in liquid entering the top of the absorption column

X_N = mole ratio of solute/absorbent in liquid leaving the bottom of the absorption column

y = mole fraction of solute in gas phase (mol solute/mol total gas)

Y = mole ratio of solute in gas phase (mol solute/mol gaseous carrier)

Y_1 = mole ratio of solute/gaseous carrier in gas leaving the top of the absorption column

Y_{N+1} = mole ratio of solute/gaseous carrier in gas entering the bottom of the absorption column

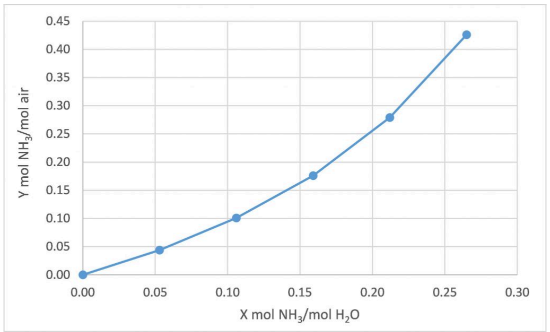
Operating line for absorption column:

$$Y_{n+1} = X_n \left(\frac{L'}{V'}\right) + Y_1 - X_0 \left(\frac{L'}{V'}\right) \tag{9.1}$$

Watch a video from LearnChemE that demonstrates how to determine the number of equilibrium stages required for an absorption column when given inlet and outlet specifications: Absorption of a Dilute Species (10:43): https://youtu.be/BoPKngZZwVI

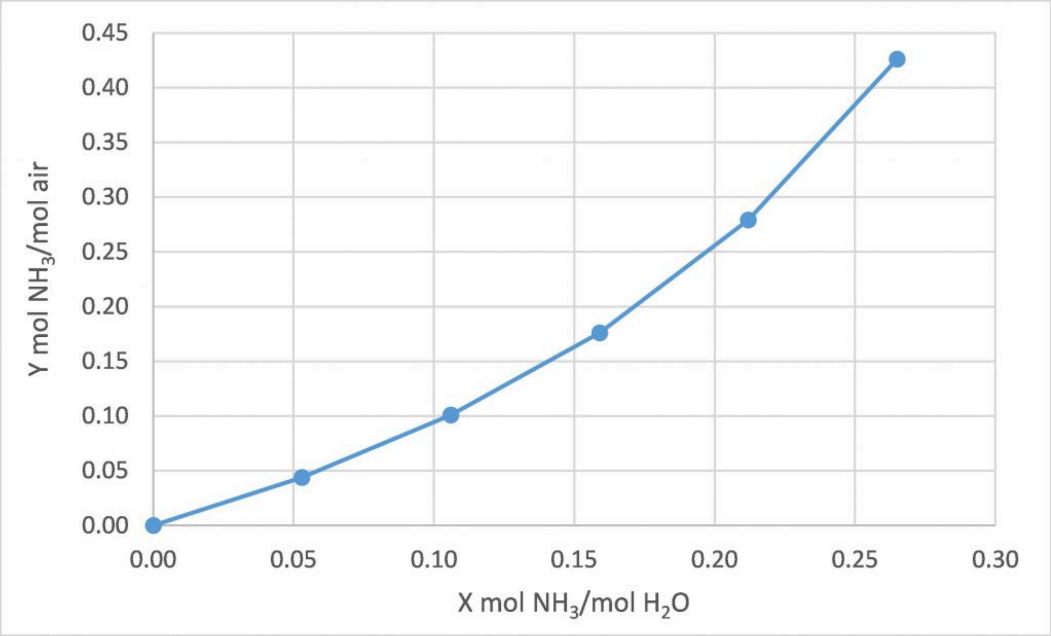
Example

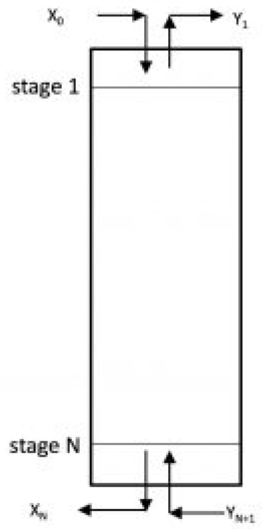
The following equilibrium data is available for water, ammonia, and air at 20°C.



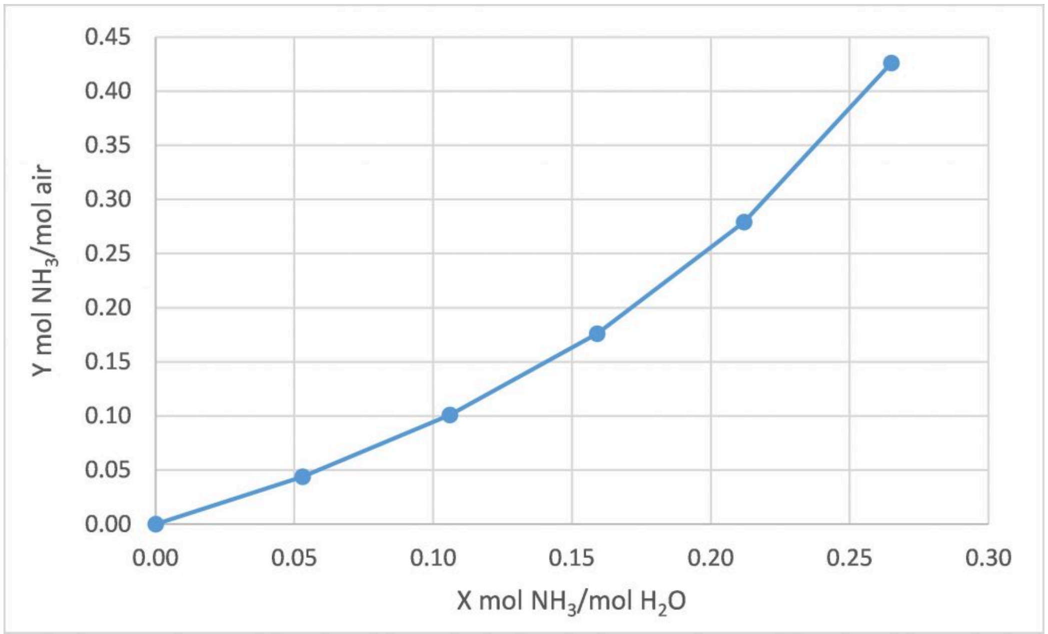
We intend to use fresh water to absorb the ammonia from a stream of air containing 28.5 mol% ammonia, with both streams at 20°C. We intend to absorb 80% of the incoming ammonia. How many equilibrium stages are required for each of the following design cases?

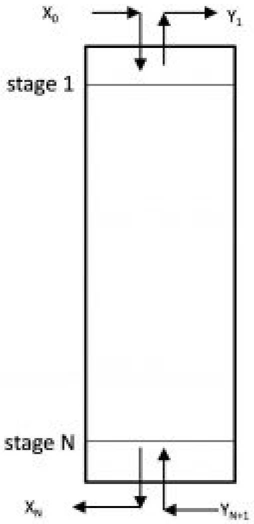
(a) L'/V' = 1.0


0.45
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
Y mol NH$_3$/mol air
0.00
0.05
0.10
0.15
0.20
0.25
0.30
X mol NH$_3$/mol H$_2$O

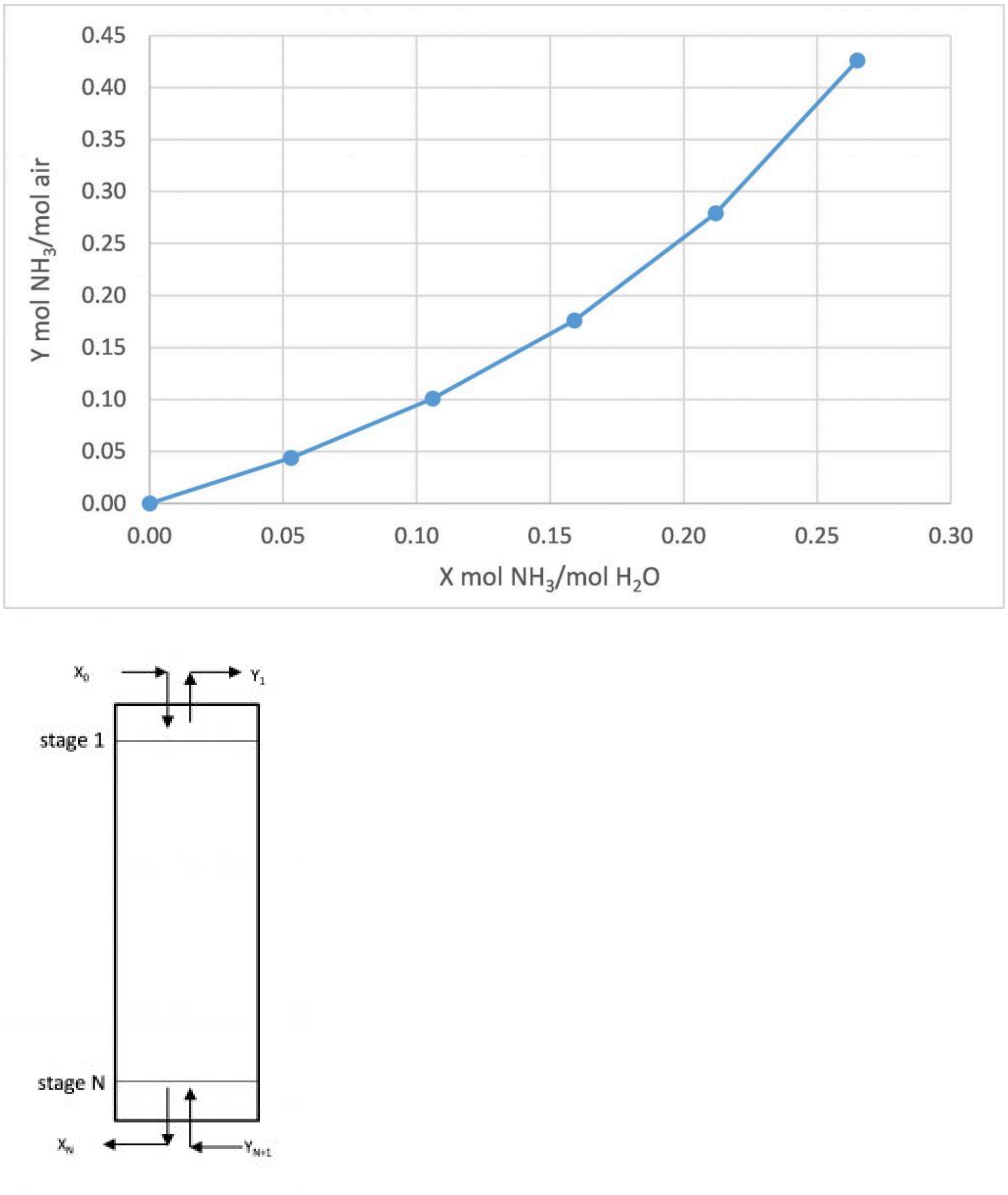

X$_0$
Y$_1$
stage 1
stage N
X$_N$
Y$_{N+1}$

(b) L'/V' = 1.6


Y mol NH$_3$/mol air
X mol NH$_3$/mol H$_2$O
0.45
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
0.00
0.05
0.10
0.15
0.20
0.25
0.30


X_0
Y_1
stage 1
stage N
X_N
Y_{N+1}

(c) L'/V'= 2.0



Determining the Minimum Ratio for Absorbent to Gas Flow Rates and a Mathematical Approach for Finding the Number of Equilibrium Stages

K = equilibrium constant, (mole fraction solute in gas)/(mole fraction solute in liquid)

L' = liquid flow rate on a solute-free basis (mol liquid absorbent time^{-1})

n = generic equilibrium stage

N = bottom equilibrium stage for an absorption column

V' = gas flow rate on a solute-free basis (mol gaseous carrier time^{-1})

$(L'/V')_{\text{min}}$ = relative molar flowrates of solute-free absorbent and solute-free carrier gas at which an infinite number of equilibrium stages is required in order to achieve the desired separation

x = mole fraction of solute in liquid phase (mol solute/mol total liquid)

X = mole ratio of solute in liquid phase (mol solute/mol liquid absorbent)

X_0 = mole ratio of solute/absorbent in liquid entering the top of the absorption column

X_N = mole ratio of solute/absorbent in liquid leaving the bottom of the absorption column

y = mole fraction of solute in gas phase (mol solute/mol total gas)

Y = mole ratio of solute in gas phase (mol solute/mol gaseous carrier)

Y_1 = mole ratio of solute/gaseous carrier in gas leaving the top of the absorption column

Y_{N+1} = mole ratio of solute/gaseous carrier in gas entering the bottom of the absorption column

Equilibrium:

(10.1) $$K_n = \frac{y_n}{x_n} = \frac{Y_n/(1+Y_n)}{X_n/(1+X_n)}$$

Operating line:

(10.2) $$Y_{n+1} = X_n\left(\frac{L'}{V'}\right) + Y_1 - X_0\left(\frac{L'}{V'}\right)$$

when X ~ x and Y ~ y,

(10.3) $$\left(\frac{L'}{V'}\right)_{\text{min}} = \frac{y_{N+1} - y_1}{\frac{y_{N+1}}{K_N} - x_0}$$

when X ~ x, Y ~ y and x_0 = 0

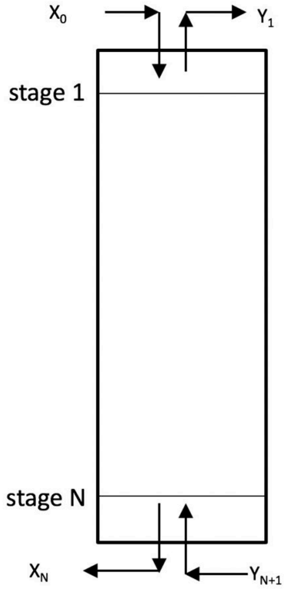
(10.4) $$\left(\frac{L'}{V'}\right)_{\text{min}} = K_N\left(1 - \frac{y_1}{y_{N+1}}\right)$$

Example

180 kmol/hr of off-gas from a fermentation unit contains 98 mol% CO_2 and 2 mol% ethanol. We would like to recover 97% of this ethanol and have proposed the use of a staged absorption column with water as the absorbent. The incoming water contains no ethanol and is at 30°C. The incoming gaseous stream is at 30°C, 110 kPa. Assume there is no absorption of CO_2 into the water. The activity coefficient at infinite dilution for ethanol in water at 30°C is 6.0 and P^{sat} is 10.5 kPa. Thus, $K = \gamma_i P_i^{sat}/P = 0.57$.

(a) What is $(L'/V')_{\text{min}}$?

(b) How many equilibrium stages are required if we operate at 1.5*$(L'/V')_{\text{min}}$?



Stage Efficiency and Column Height

λ = inverse absorption factor (unitless)

μ_L = liquid-phase viscosity (mass $time^{-1}$ $length^{-1}$)

ρ_L = liquid-phase density (mass $volume^{-1}$)

a = vapor-liquid interfacial area per volume of combined gas/liquid on the tray (area $volume^{-1}$)=($length^{-1}$)

A_b = portion of the column cross-sectional area dedicated to mixing of the gas/liquid (area)

D_T = column diameter (length)

E_{MV} = Murphree efficiency, calculated on the basis of the vapor phase composition

E_O = overall stage efficiency

K = equilibrium constant (gas-phase composition/liquid-phase composition)

K_G = overall gas mass-transfer coefficient, partial pressure driving force (mol time^{-1} area^{-1} pressure^{-1})

L = molar flow rate of liquid phase (mol time^{-1})

M_L = molecular weight of the liquid phase

N_a = actual number of stages required to achieve the desired separation

N_{OG} = number of overall gas phase mass transfer units

N_t = number of theoretical stages required to achieve the desired separation

P = pressure (force area^{-1})

T = temperature (temperature)

V = molar flow rate of gaseous phase (mol time^{-1})

$x_{i,n}$ = the actual mole fraction of species i in the liquid leaving stage n and entering stage n+1

y_i = the mole fraction of species i in a gas at some fixed point in the column

$y_{i,n+1}$ = the actual mole fraction of species i in the gas leaving stage n+1 and entering stage n

$y_{i,n}$ = the actual mole fraction of species i in the gas leaving stage n and entering stage n-1

$y^*_{i,n}$ = the mole fraction of species i in the gas leaving stage n if it had reached equilibrium with the liquid leaving that stage, where the liquid phase composition is $x_{i,n}$

Z_f = height of combined gas and liquid holdup on the tray (length)

(11.1) $$E_O = \frac{N_t}{N_a}$$

(11.2) $$E_O = 19.2 - 57.8\log_{10}\mu_L \quad 0.2 < \mu_L < 1.6\text{ cP}, \mu_L \text{ must be in cP}$$

0.2 < μ_L < 1.6 cP, μ_L must be in cP

(11.3)

$$\log_{10} E_O = 1.597 - 0.199\log_{10}\left(\frac{KM_L\mu_L}{\rho_L}\right) - 0.0896\left[\log_{10}\left(\frac{KM_L\mu_L}{\rho_L}\right)\right]^2$$

Eq 11.3 is applicable for this range of conditions: μ_L must be in cP, ρ_L must be in lb ft^{-3}; restricted to D_T = 2 in – 9 ft, average P = 14.7 – 485 psi, average T = 60 – 138°F, E_O = 0.65% – 69%

Example

For our CO$_2$/ethanol/water system, we found that for 97% removal of the ethanol using water as the absorbent and operating at 30°C, 110 kPa, with K = 0.57 and $(L'/V')_{\text{actual}}$ = $(L'/V')_{\text{min}}$ = 0.828, 7 theoretical stages required. How many actual stages are needed, according to equations 11.2 and 11.3?

- μ_L = 0.89 cP
- M_L = 18 lb/lb-mole
- ρ_L = 62.5 lb ft^{-3}

$$E_O = \frac{\log_{10}\left[1 + E_{MV}(\lambda - 1)\right]}{\log_{10}\lambda} \tag{11.4}$$

$$\lambda = \frac{KV}{L} \tag{11.5}$$

$$E_{MV} = \frac{y_{i,n+1} - y_{i,n}}{y_{i,n+1} - y^*_{i,n}} = 1 - \exp(-N_{OG}) \tag{11.6}$$

$$N_{OG} = \frac{K_G a P Z_f}{(V/A_b)} \tag{11.7}$$

Staged Column Height and Diameter

ρ_L = liquid-phase density (mass volume^{-1})

ρ_V = vapor-phase density (mass volume^{-1})

σ = liquid-phase surface tension (force length^{-1})

A = total column cross-sectional area (area)

A_a = active tray area (non downcomer) (area)

A_h = area of the tray open to vapor (area)

A_d = column cross-sectional area dedicated to downcomers (area)

D_T = column diameter (length)

f = fraction of flooding operation; usually we use 0.80

F_{LV} = internal variable, relating the kinetic energy of the liquid and gas streams (unitless)

L = molar flowrate of the liquid stream (mol time^{-1})

M_V = molecular weight of the gaseous stream

M_L = molecular weight of the liquid stream

U_f = Vapor velocity that is sufficient to suspend liquid droplets. Vapor velocity greater than U_f can be associated with entrainment flooding (length time^{-1})

V = molar flowrate of the gaseous stream (mol time^{-1})

**Note that many of the parameters can have different values for different stages in the column. Use an appropriate average value and document and justify your assumptions.*

(12.1) $$D_T = \left[\frac{4VM_V}{fU_f\pi(1-A_d/A)\rho_V}\right]^{0.5}$$

(12.2) $$F_{LV} = \frac{LM_L}{VM_V}\left(\frac{\rho_V}{\rho_L}\right)^{0.5}$$

Where A_d/A is estimated as follows

if $F_{LV} \leq 0.1,$

(12.3) $$A_d/A \sim 0.1$$

if $0.1 \leq F_{LV} \leq 1.0,$

(12.4) $$A_d/A \sim 0.1 + (F_{LV} - 0.1)/9$$

if $F_{LV} \geq 1.0,$

(12.5) $$A_d/A \sim 0.2$$

Example

180 kmol/hr of fermentation off-gas containing 98 mol% CO_2 and 2 mol% ethanol is to be fed to a staged absorption tower that operates at 30°C, 110 kPa. Fresh water will be supplied to this column at a ratio of $1.5 * (L'/V')_{\text{min}}$= 154 kmol/hr and we intend to have a sufficient number of stages so that 97% of the ethanol will be recovered. Ignore the contribution of the solute to the physical properties of the carrier streams and assume a vapor flooding velocity of 3.12 m/s.

Graphical and Mathematical Determination of Vapor Phase Flooding Velocity

ρ_L = liquid-phase density (mass volume^{-1})

ρ_V = vapor-phase density (mass volume^{-1})

σ = liquid surface tension (dyne cm^{-1})

A_a = active tray area for contact between the gas and liquid phases (area)

A_h = area of the holes (area)

C = Souders and Brown capacity parameter, also known as vapor velocity factor (ft/s)

C_1 = internal parameter for calculation of $C_{\text{S,ult}}$ (m s^{-1})

C_2 = internal parameter for calculation of $C_{\text{S,ult}}$ (m s^{-1})

C_D = liquid droplet drag coefficient

C_F = entrainment flooding capacity, from Figure 6.23 (ft/s)

$C_{\text{S,ult}}$ = ultimate capacity parameter (m s^{-1})

d_p = liquid droplet diameter (length)

F_F = foaming factor (unitless)

F_{HA} = internal variable based on plate-specific value of A_h/A_a (unitless)

F_{LV} = internal variable, relating the kinetic energy of the liquid and gas streams (unitless)

F_{ST} = surface tension factor (unitless)

F = internal parameter for calculation of $C_{\text{S,ult}}$

g = gravitational constant (length time^{-2})

L_S = superficial liquid velocity (length time^{-1})

U_f = superficial vapor velocity at flooding (length time^{-1})

U_S = superficial vapor velocity (length time^{-1})

$U_{\mathrm{S,ult}}$ = superficial vapor velocity at which the vapor velocity exceeds the liquid droplet settling velocity (m s^{-1})

Graphical Determination of Superficial Vapor Velocity at Flooding

(13.1) $$U_f = C\left(\frac{\rho_L - \rho_V}{\rho_V}\right)^{0.5}$$

(13.2) $$C = \left(\frac{4d_P g}{3C_D}\right)^{0.5}$$

we will use

(13.3) $$C = F_{ST}F_F F_{HA} C_F$$

(13.4) $$F_{ST} = (\sigma/20)^{0.2}$$

σ must be in dyne/cm

if $A_h/A_a > 0.10$ F_{HA} = 1.0

(13.5) $$F_{HA} = 1.0$$

if $0.06 < A_h/A_a < 0.1$ $F_{HA} = 5(A_h/A_a) + 0.5$

(13.6) $$F_{HA} = 5(A_h/A_a) + 0.5$$

C_F is from Fig 6.23, needs F_{LV} and tray spacing

Mathematical Determination of Superficial Vapor Velocity at Flooding

(13.7) $$U_f = U_{\text{S,ult}} = C_{\text{S,ult}} \left(\frac{\rho_L - \rho_V}{\rho_V} \right)^{0.5}$$

$C_{\text{S,ult}} = C_1 \text{ or } C_2$, whichever value is smaller

(13.8) $$C_1 = 0.445(1-F) \left[\frac{\sigma}{\rho_L - \rho_V} \right]^{0.25} - 1.4L_S$$

(13.9) $$C_2 = 0.356(1-F) \left[\frac{\sigma}{\rho_L - \rho_V} \right]^{0.25}$$

(13.10) $$F = \left(1 + 1.4 \left[\frac{\rho_L - \rho_V}{\rho_V} \right]^{0.5} \right)^{-1}$$

for equations 13.8, 13.9, and 13.10, densities must be in kg/m3 and surface tension must be in dyne/cm

(13.11) $$L_S = U_S \frac{LM_L}{\rho_L} \left(\frac{VM_V}{\rho_V} \right)^{-1}$$

*true in all conditions, not just flooding

Example

180 kmol/hr of fermentation off-gas containing 98 mol% CO_2 and 2 mol% ethanol is to be fed to a staged absorption tower that operates at 30°C, 110 kPa. Fresh water will be supplied to this column at a ratio of $1.5 * (L'/V')_{\text{min}}$ = 154 kmol/hr and we intend to have a sufficient number of stages so that 97% of the ethanol will be recovered. Assume a foaming factor of 0.90, trays that have an $A_h/A_a > 0.10$ and a surface tension of 70 dyne/cm and ignore the contribution of the solute to the physical properties of the carrier streams. Assume a tray spacing of 24 inches. What is U_f according to

(a) the graphical method

(b) ultimate superficial velocity computational method?

Staged Column Pressure Drop

ϕ_e = height of clear liquid/height of froth (unitless)

ρ_L = liquid-phase density (mass volume^{-1})

ρ_V = vapor-phase density (mass volume^{-1})

σ = liquid surface tension (dyne cm^{-1})

A_a = active tray area, hosting interaction between the gas and liquid phases (area)

A_d = downcomer area, hosting liquid handling (area)

A_h = total area of the holes on each tray (area)

C_0 = tray-specific parameter, generally between 0.68 and 0.85

C_l = internal parameter in calculation of h𝔏

$D_{B(\text{max})}$ = maximum bubble size (length). We will use maximum hole diameter D_H.

D_T = column diameter (length)

g = gravitational constant (length time^{-2})

h_d = pressure drop due to movement of the gas through tray perforations (inches of our liquid)

h_l = pressure drop due to movement of the gas through the liquid hold-up (inches of our liquid)

h_σ = pressure drop due to movement of the gas through the liquid surface (inches of our liquid)

h_t = total pressure drop for a single actual tray (inches of our liquid)

h_w = weir height (inches)

K_S = capacity parameter (ft s^{-1})

L_w = weir length (inches)

q_L = liquid flow rate across the tray (gal min^{-1})

u_0 = velocity of the vapor phase through the holes in the tray (ft s^{-1})

U_a = superficial vapor velocity, calculated based on the active bubbling area (ft s^{-1})

(14.1) $$h_t = h_d + h_l + h_\sigma$$

(14.2) $$h_d = 0.186 \left(\frac{u_0^2}{C_0^2}\right)\left(\frac{\rho_V}{\rho_L}\right)$$

(14.3) $$h_l = \phi_e \left[h_w + C_l \left(\frac{q_L}{L_w \phi_e}\right)^{2/3}\right]$$

(14.4) $$\phi_e = \exp(-4.257 K_S^{0.91})$$

(14.5) $$K_S = U_a \left(\frac{\rho_V}{\rho_L - \rho_V}\right)^{0.5}$$

(14.6) $$A_a = (A - 2A_d)$$

(14.7) $$L_w = 0.73 D_T$$

(14.8) $$C_l = 0.362 + 0.317 \exp(-3.5 h_w)$$

h_w, L_w *must be in inches,* q_L *must be in gal/min,* K_S *must be ft/s*

(14.9) $$h_\sigma = \frac{6\sigma}{g \rho_L D_{B(\max)}}$$

To prevent weeping, maintain

(14.10) $$h_d + h_\sigma > h_l$$

Example

180 kmol/hr of CO_2 containing 2 mol% ethanol and 154 kmol/hr of fresh water are fed to a column with a diameter of 0.80m. The weirs have a height of 2.0 inches, the sieve tray holes have a diameter of 3/16″, C_0 = 0.73. Ten percent (10%) of the column cross-sectional area is occupied by the downcomers and 10% of the active column area is occupied by the sieve tray holes. What is the pressure drop per tray?

Staged Column Mass Transfer

ϕ_e = height of clear liquid/height of froth (unitless); equation 14.4 from Lecture 2.2 Staged Column Pressure Drop

ρ_L = density of the liquid phase (mass volume^{-1})

ρ_V = density of the vapor phase (mass volume^{-1})

a = interfacial gas-liquid area per unit volume of combined gas and liquid hold up (area/volume = length^{-1})

$\bar{a}$ = interfacial gas-liquid area per unit volume of equivalent clear liquid (area/volume = length^{-1})

A_a = active tray area, hosting interaction between the gas and liquid phases (area)

A_b = active bubbling area of the tray (area)

D_L = diffusivity of the solute in the liquid phase (cm^2 s^{-1})

D_V = diffusivity of the solute in the vapor phase (cm^2 s^{-1})

E_{MV} = Murphree efficiency of a stage, based on the vapor phase

f = fractional value representing proximity to flooding value, based on U_a instead of U_f (unitless)

F = F-factor [(kg/m)$^{0.5}$s^{-1}]

h_l = pressure drop due to movement of the gas through the liquid hold-up, from Lecture 2.2 Staged Column Pressure Drop (pressure)

k_G = gas-phase mass transfer coefficient (length time^{-1})

k_L = liquid-phase mass transfer coefficient (length time^{-1})

K = equilibrium constant for our system (y/x)

K_G = overall mass transfer coefficient, based on partial-pressure driving force (time^{-1})

L = molar flow rate of the liquid phase (mol time^{-1})

M_L = molecular weight of the liquid phase (mass mole^{-1})

N_G = number of transfer units in the gas phase

N_L = number of transfer units in the liquid phase

N_{OG} = number of overall mass transfer units, expressed on a gas-phase basis

P = pressure of the gas phase (pressure)

q_L = liquid volumetric flow rate across the tray (volume time^{-1})

$\bar{t}_G$ = average gas residence time in the froth (time)

$\bar{t}_L$ = average liquid residence time in the froth (time)

U_a = superficial vapor velocity, calculated based on the active bubbling area (length time^{-1})

U_f = superficial vapor velocity at flooding, found by Souders and Brown or superficial velocity method, Lecture 2.1 Graphical and mathematical determination of vapor phase flooding velocity (length time^{-1})

V = molar flow rate of the gas phase (mole time^{-1})

$y_{i,n+1}$ = composition (mole fraction) of the gas entering stage n from stage $n+1$

$y_{i,n}$ = composition (mole fraction) of the gas leaving stage n

$y^*_{i,n}$ = composition (mole fraction) of the gas leaving stage n if it had reached equilibrium with the liquid leaving stage n

Z_f = height of combined gas and liquid hold up (length)

Refer to Lecture 1.13 Stage Efficiency and Column Height for the first part of this topic

(15.1) $$E_{MV} = \frac{y_{i,n+1} - y_{i,n}}{y_{i,n+1} - y^*_{i,n}} = 1 - \exp(N_{OG})$$

(15.2) $$N_{OG} = \frac{K_G a P Z_f}{(V/A_b)}$$

(15.3) $$\frac{1}{N_{OG}} = \frac{1}{N_G} + \frac{(KV/L)}{N_L}$$

(15.4) $$N_G = \frac{k_G a P Z_f}{(V/A_b)}$$

(15.5) $$N_G = k_G \bar{a} \bar{t}_G$$

$$N_L = \frac{k_L a \rho_L Z_f}{(LM_L/A_b)} \quad (15.6)$$

$$N_L = k_L \bar{a} \bar{t}_L \quad (15.7)$$

$$\bar{t}_G = \frac{(1-\phi_e)h_l}{\phi_e U_a} \quad (15.8)$$

$$\bar{t}_L = \frac{h_l A_a}{q_L} \quad (15.9)$$

$$k_G \bar{a} = \frac{1030 D_V^{0.5}(f - 0.842 f^2)}{h_l^{0.5}} \quad (15.10)$$

$$f = U_a/U_f \quad (15.11)$$

$$k_L \bar{a} = 78.8 D_L^{0.5}(F + 0.425) \quad (15.12)$$

$$F = U_a \rho_V^{0.5} \quad (15.13)$$

In equations 15.12 and 15.13, D_V and D_L must be in cm^2/s, h_l must be in cm, F must be in (kg/m)$^{0.5}$s^{-1}

Example

180 kmol/hr of CO_2 containing 2 mol% ethanol is fed to an absorption column. 154 kmol/hr of fresh water is used as the liquid absorbent. The column has a diameter of 0.80m, weir height of 2.0 inches, 3/16” hole diameter, C_0 = 0.73, 10% of the column area is occupied by downcomers, 10% of the active area is occupied by sieve tray holes. Based on mass transfer principles, what is the expected Murphree efficiency of each stage? Ignore the contribution of the solute.

At the proposed operating conditions, the diffusivity of ethanol in CO_2 is 7.85×10^{-2} cm^2 s^{-1} and the diffusivity of ethanol in liquid water is 1.81×10^{-5} cm^2 s^{-1}

Packed Columns

ϵ = packing void fraction (volume volume^{-1}), tabulated value

ρ_V = density of the vapor phase (mass volume^{-1})

ρ_L = density of the liquid phase (mass volume^{-1})

A = absorption factor (unitless)

a = specific surface area of the selected packing (area volume^{-1}), tabulated value

a_h = specific hydraulic area of the selected packing (area volume^{-1})

C_h = dimensionless holdup parameter, tabulated value

D_T = packed bed diameter (length)

f = target value of fraction of flooding; for packed columns we typically use 0.5 – 0.7

h_L = volume of liquid per unit volume of packed bed (volume volume^{-1})

H_{OG} = overall height of a gas transfer unit (length) – will be discussed in Lecture 2.7 Packed Bed HOG

K = equilibrium constant for our system at our operating condition

$K_y a$ = overall mass transfer coefficient in gas-phase mole fraction units (mole time^{-1} volume^{-1})

L = liquid phase molar flow rate (mole time^{-1})

l_T = depth of packed bed (length)

M_V = vapor phase molecular weight

$N_{\mathrm{Fr},L}$ = Froude number for the liquid phase, inertial force/gravitational force (unitless)

N_{OG} = number of overall gas-phase mass transfer units

$N_{\mathrm{Re},L}$ = Reynolds number for the liquid phase, inertial force/viscous force (unitless)

S = cross-sectional area of the packed bed (area)

u_L = liquid-phase superficial velocity through the packed bed (length time^{-1})

$u_{V,f}$ = superficial gas velocity at flooding (length time^{-1})

V = vapor phase molar flow rate (mole time^{-1})

x_{in} = mole fraction of the solute in the entering liquid

y_{in} = mole fraction of the solute in the entering vapor

y_{out} = mole fraction of the solute in the exiting vapor

Packed Bed Diameter Sizing

$$D_T = \left(\frac{4VM_V}{f u_{V,f} \pi \rho_V} \right)^{0.5} \tag{16.1}$$

Depth of Packing Required

(16.2) $$l_T = H_{OG}N_{OG}$$

(16.3) $$H_{OG} = \frac{V}{K_y a S}$$

(16.4) $$N_{OG} = \left(\frac{A}{A-1}\right)\ln\left[\left(\frac{A-1}{A}\right)\left(\frac{y_{in}-Kx_{in}}{y_{out}-Kx_{in}}+\frac{1}{A}\right)\right]$$

(16.5) $$A = \frac{(L/V)}{K}$$

Example

180 kmol/hr of a fermentation off-gas stream (98 mol% CO_2, 2 mol% ethanol) is fed to a packed absorption column. We aim to recover 97% of the incoming ethanol using 154 kmol/hr of fresh water. If H_{OG} = 2.0 ft, what is the required depth of packed bed? K = 0.57.

Liquid Hold-up in a Packed Bed, Operating in Pre-loading Region

(16.6) $$h_L = \left(\frac{12N_{\mathrm{Fr},L}}{N_{\mathrm{Re},L}}\right)^{1/3}\left(\frac{a_h}{a}\right)^{2/3}$$

(16.7) $$N_{\mathrm{Fr},L} = \frac{u_L^2 a}{g}$$

(16.8) $$N_{\mathrm{Re},L} = \frac{u_L \rho_L}{a\mu_L}$$

if $N_{\mathrm{Re},L} < 5$

(16.9) $$\frac{a_h}{a} = C_h N_{\mathrm{Re},L}^{0.15} N_{\mathrm{Fr},L}^{0.1}$$

if $N_{\mathrm{Re},L} \geq 5$

(16.10) $$\frac{a_h}{a} = 0.85 C_h N_{\text{Re},L}^{0.25} N_{\text{Fr},L}^{0.1}$$

Example

For our CO_2/water/ethanol system, we have proposed to use 50-mm metal Hiflow rings as our packing material and a column diameter that results in a superficial liquid velocity of 0.01 m/s. Find the specific liquid holdup and specific volume available for the gas for this proposed design. Ignore the contribution of the solute.

Parameters for 50mm Hiflow Metal Rings: a = 92.3 m^2/m^3, C_h = 0.876, ϵ = 0.977 m^3/m^3

- V = 180 kmol/hr
- L = 154 kmol/hr
- ρ_L = 1000 kg/m^3
- μ_L = 8.9×10^{-4} kg s^{-1} m^{-1}

Packed Bed Pressure Drop by the Graphical Method

ϵ = packing void fraction (volume $volume^{-1}$), tabulated value

μ_L = viscosity of the liquid phase (mass $time^{-1}$ $length^{-1}$)

$\rho_{H_2O,L}$ = density of liquid water (mass $volume^{-1}$)

ρ_L = density of the liquid phase (mass $volume^{-1}$)

ρ_V = density of the vapor phase (mass $volume^{-1}$)

F_{LV} = internal variable (unitless)

F_P = packing factor (area $volume^{-1}$), tabulated value

L = liquid phase flow rate (mole $time^{-1}$)

M_L = liquid phase molecular weight

M_V = vapor phase molecular weight

u_L = liquid-phase superficial velocity through the packed bed (length $time^{-1}$)

u_V = superficial gas velocity (length $time^{-1}$)

$u_{V,f}$ = superficial gas velocity at flooding (length $time^{-1}$)

V = vapor phase molar flow rate (mole time^{-1})

Y = internal variable for the GPDC method, y-axis value of Figure 6-35 (unitless)

Generalized Pressure Drop Correlation (GPDC) for Finding Flooding Velocity

$$F_{LV} = \left(\frac{LM_L}{VM_V}\right)\left(\frac{\rho_V}{\rho_L}\right)^{0.5} \tag{17.1}$$

$$Y = \left(\frac{u_V^2 F_P}{g}\right)\left(\frac{\rho_V}{\rho_{H_2O,L}}\right) f[\rho_V] f[\mu_L] \tag{17.2}$$

Example

180 kmol/hr of CO_2 containing 2.0 mol% ethanol is fed to a packed column operating at 30°C and 110 kPa. 97% of the ethanol is to be removed via the addition of 154 kmol/hr of fresh water. The packed column contains 1" ceramic Raschig rings.

Find:

(a) the superficial gas velocity associated with flooding

(b) the necessary column diameter if we operate at 70% of flooding

(c) the pressure drop per foot of packing. Ignore the contribution of the solute to the magnitude and physical properties of each phase.

For 1" ceramic Raschig rings: F_p = 179 ft^2/ft^3

Packed Bed Pressure Drop by the Mathematical Method

ϵ = packing void fraction (volume volume^{-1}), tabulated value

ΔP = actual pressure drop across a packed bed during operation at your condition (pressure)
ΔP_0 = pressure drop across your packed bed during dry operation (pressure)
ξ_l = internal parameter for pressure drop calculation at the loading point (unitless)
μ_L = viscosity of the liquid (mass time^{-1} length^{-1})
μ_V= viscosity of the vapor phase (mass time^{-1} length^{-1})
ρ_L = density of the liquid phase (mass volume-1)
ρ_V = density of the vapor phase (mass volume^{-1})
Ψ_0 = resistance coefficient of dry packing (unitless)
Ψ_l= internal parameter for pressure drop calculation at the loading point (unitless)

a = specific surface area of the selected packing (area volume^{-1}), tabulated value
C = internal parameter for pressure drop calculation at the loading point (unitless)
C_p = packing parameter, tabulated value
C_s = packing parameter (unitless)
D_p = effective packing diameter (length)
D_T = packed bed diameter (length)
g = gravitational constant (length time^{-2})
h_L = liquid hold-up (volume volume^{-1})
K_W = wall factor (unitless)
L = liquid phase molar flow rate (mole time^{-1})
l_T = depth of packed bed (length)
M_V = vapor phase molecular weight
M_L = liquid phase molecular weight
$N_{\mathrm{Fr},L}$ = Froude number, inertial force/gravitational force (unitless)
$N_{\mathrm{Re},V}$ = Reynold's number of the vapor phase, inertial force/viscous force (unitless)
n_s = internal parameter for pressure drop calculation at the loading point (unitless)
u_L = liquid phase superficial velocity (length time^{-1})
$u_{L,l}$ = liquid phase superficial velocity at the loading point (length time^{-1})
u_V= vapor phase superficial velocity (length time^{-1})
$u_{V,f}$ = vapor phase superficial velocity at the flooding point (length time^{-1})

$u_{V,l}$ = vapor phase superficial velocity at the loading point (length time^{-1})

V = vapor phase molar flow rate (mole time^{-1})

(18.1) $$\left(\frac{\Delta P}{\Delta P_0}\right)=\left(\frac{\epsilon}{\epsilon-h_L}\right)^{(3/2)} exp\left(\frac{13,300N_{\mathrm{Fr},L}^{0.5}}{a^{1.5}}\right)$$

(18.2) $$N_{\mathrm{Fr},L}=\frac{u_L^2 a}{g}$$

(18.3) $$\frac{\Delta P_0}{l_T}=\Psi_0\left(\frac{a}{\epsilon^3}\right)\left(\frac{u_V^2\rho_V}{2}\right)\left(\frac{1}{K_W}\right)$$

(18.4) $$\Psi_0=C_P\left(\frac{64}{N_{\mathrm{Re},V}}+\frac{1.8}{N_{\mathrm{Re},V}^{0.08}}\right)$$

(18.5) $$N_{\mathrm{Re},V}=\frac{u_V D_P \rho_V K_W}{(1-\epsilon)\mu_V}$$

(18.6) $$D_P=6\left(\frac{1-\epsilon}{a}\right)$$

(18.7) $$\frac{1}{K_W}=1+\frac{2}{3}\left(\frac{1}{1-\epsilon}\right)\left(\frac{D_P}{D_T}\right)$$

**at any operating condition:* $u_L=u_V\left(\frac{LM_L}{\rho_L}\right)\left(\frac{\rho_V}{VM_V}\right)$

Vapor flooding velocity

(18.8) $$u_{V,f}=\frac{u_{V,l}}{0.7}$$

At the loading point:

(18.9) $$u_{V,l}=\left(\frac{g}{\Psi_l}\right)^{1/2}\left[\frac{\epsilon}{a^{1/6}}-a^{0.5}\xi_l^{1/3}\right]\xi_l^{1/6}\left(\frac{\rho_L}{\rho_V}\right)^{1/2}$$

$$\Psi_l = \frac{g}{C^2}\left[F_{LV}\left(\frac{\mu_L}{\mu_V}\right)^{0.4}\right]^{-2n_s}$$ (18.10)

$$F_{LV} = \left(\frac{LM_L}{VM_V}\right)\left(\frac{\rho_V}{\rho_L}\right)^{0.5}$$ (18.11)

If $F_{LV} \leq 0.4$, liquid is disperse, $C = C_S, n_S = -0.326$

If $F_{LV} > 0.4$, liquid is continuous, $C = 0.695\left(\frac{\mu_L}{\mu_V}\right)^{0.1588} C_S, n_S = -0.723$

$$\xi_l = 12\frac{\mu_L u_{L,l}}{g\rho_L}$$ (18.12)

Example

180 kmol/hr of CO_2 containing 2.0 mol% ethanol and 154 kmol/hr fresh liquid water are fed to a packed column containing 1” ceramic Raschig rings. Find (a) superficial gas velocity at flooding; (b) column diameter, if we intend to operate at 70% of the flooding velocity; (c) pressure drop per foot of packing at loading point.

Determining the Overall Height of a Gas-liquid Transfer Unit for a Packed Column

ϵ = packing void fraction (volume volume^{-1}), tabulated value

μ_V = viscosity of the vapor phase (mass time^{-1} length^{-1})

ρ_L = density of the liquid phase (mass volume^{-1})

ρ_V = density of the vapor phase (mass volume^{-1})

σ = surface tension of the liquid phase (force length^{-1})

a = specific surface area of the selected packing (area volume^{-1}), tabulated value

a_{Ph} = specific area of the gas/liquid interface (area volume^{-1})

C_V = packing parameter, tabulated value

C_L = packing parameter, tabulated value

D_G = diffusivity of the solute in the gas phase (length^2 time^{-1})

d_h = packing hydraulic diameter (length)

D_L = diffusivity of the solute in the liquid phase (length^2 time^{-1})

g = gravitational constant (length time^{-2})

H_G = height of gas-phase transfer unit, with partial pressure driving force (length)

h_L = liquid hold-up (volume volume^{-1})

H_L = height of liquid-phase transfer unit, with mole fraction driving force (length)

H_{OG} = overall height of gas/liquid transfer unit, on a gas phase basis (length)

K = equilibrium constant for our species in our selected operating condition

L = liquid phase molar flow rate (mole time^{-1})

$N_{\mathrm{Fr}_L,h}$ = Froude number of the liquid phase with the hydraulic diameter as the characteristic length (unitless)

$N_{\mathrm{Re}_L,h}$ = Reynold's number of the liquid phase, hydraulic diameter as the characteristic length (unitless)

N_{Re_V} = Reynold's number of the vapor phase, inertial force/viscous force (unitless)

N_{Sc_V} = Schmidt number of the vapor phase (unitless)

$N_{\mathrm{We}_L,h}$ = Weber number of the liquid phase with the hydraulic diameter as the characteristic length (unitless)

u_L = liquid phase superficial velocity (length time^{-1})

u_V = vapor phase superficial velocity (length time^{-1})

V = vapor phase molar flow rate (mole time^{-1})

(19.1)
$$H_{OG} = H_G + \left(\frac{KV}{L}\right) H_L$$

(19.2)
$$H_G = \frac{1}{C_V}(\epsilon - h_L)^{0.5}\left(\frac{4\epsilon}{a^4}\right)^{0.5}\left(\frac{1}{N_{\mathrm{Re}_V}}\right)^{0.75}\left(\frac{1}{N_{\mathrm{Sc}_V}}\right)^{1/3}\left(\frac{u_V a}{D_G a_{Ph}}\right)$$

(19.3)
$$N_{\mathrm{Re}_V} = \frac{u_V \rho_V}{a \mu_V}$$

(19.4)
$$N_{\mathrm{Sc}_V} = \frac{\mu_V}{\rho_V D_G}$$

$$\frac{a_{Ph}}{a} = \frac{1.5N_{\mathrm{We},L,h}^{0.75}}{(ad_h)^{0.5}N_{\mathrm{Re}_L,h}^{0.2}N_{\mathrm{Fr}_L,h}^{0.45}} \tag{19.5}$$

$$d_h = \frac{4\epsilon}{a} \tag{19.6}$$

$$N_{\mathrm{Re}_L,h} = \frac{u_L d_h \rho_L}{\mu_L} \tag{19.7}$$

$$N_{\mathrm{We}_L,h} = \frac{u_L^2 \rho_L d_h}{\sigma} \tag{19.8}$$

$$N_{\mathrm{Fr}_L,h} = \frac{u_L^2}{g d_h} \tag{19.9}$$

$$H_L = \frac{1}{C_L}\left(\frac{1}{12}\right)^{1/6}\left[\frac{4h_L\epsilon}{D_L a u_L}\right]^{0.5}\left(\frac{u_L}{a}\right)\left(\frac{a}{a_{Ph}}\right) \tag{19.10}$$

Example

180 kmol/hr of CO_2 containing 2.0 mol% ethanol and 154 kmol/hr liquid water are fed to a packed column with diameter of 1.1m containing 1” (25mm) ceramic Raschig rings, with a pressure drop of 1.1 kPa/m. Find the necessary column height and total pressure drop if we aim to recover 97% of the incoming solute and the column is operated at the loading point. Ignore the contribution of the solute.

Packing properties: a=190 m^2/m^3, ϵ=0.680, C_h = 0.577, C_P = 1.329, C_L = 1.361, C_V = 0.412, c_s = 2.454

- Diffusivity of ethanol in CO_2 at 30°C D_G = 7.85×10^{-2} cm^2/s
- Diffusivity of ethanol in water at 30°C D_L = 1.81×10^{-5} cm^2/s
- ρ_L = 1000 kg/m^3
- ρ_V = 1.92 kg/m^3
- σ_L = 70 dyne/cm
- μ_L = 8.9×10^{-4} kg $m^{-1}s^{-1}$
- μ_V = 1.53×10^{-5} kg $m^{-1}s^{-1}$

5. Distillation

Introduction to Distillation

B = mass or molar flow rate of the bottoms stream leaving the systems (mass time^{-1} or mole time^{-1})

D = mass or molar flow rate of the distillate stream leaving the system (mass time^{-1} or mole time^{-1})

F = mass or molar flow rate of the feed stream entering the system (mass time^{-1} or mole time^{-1})

L = mass or molar flow rate of the liquid reflux returned to the column from the condenser (mass time^{-1} or mole time^{-1}); also generic flow rate of the liquid phase in the rectifying section

$\overline{L}$ = mass or molar flow rate of the liquid leaving the bottom of the column and entering the reboiler (mass time^{-1} or mole time^{-1}); also generic flow rate of the liquid phase in the stripping section

n = generic stage number, stage 1 is at the top of the column

R = reflux ratio

V = mass or molar flow rate of vapor leaving the top of the column and entering the condenser (mass time^{-1} or mole time^{-1}); also generic flow rate of the vapor phase in the rectifying section

$\overline{V}$ = mass or molar flow rate of the gaseous boilup returned to the column from the reboiler (mass time^{-1} or mole time^{-1}); also generic flow rate of the vapor phase in the stripping section

x = mass or mole fraction of the light key in a liquid stream

x_B = mass or mole fraction of the light key in the bottoms stream

x_D = mass or mole fraction of the light key in the distillate stream

x_n = mass or mole fraction of the light key in the liquid leaving stage n

y = mass or mole fraction of the light key in vapor stream

y_n = mass or mole fraction of the light key in the vapor leaving stage n

z_F = mass or mole fraction of the light key in the feed stream

Overall material balance

(20.1) $F = D + B$

Material balance on light key

(20.2) $Fz_F = x_D D + x_B B$

Combination of material balances in Equations 20.1 and 20.2

(20.3) $$D = F\left(\frac{z_F - x_B}{x_D - x_B}\right)$$

(20.4) $$R = \frac{L}{D}$$

(20.5) $$V_B = \frac{\overline{V}}{B}$$

Material balance on stages $1 - n$, the rectifying section of the column

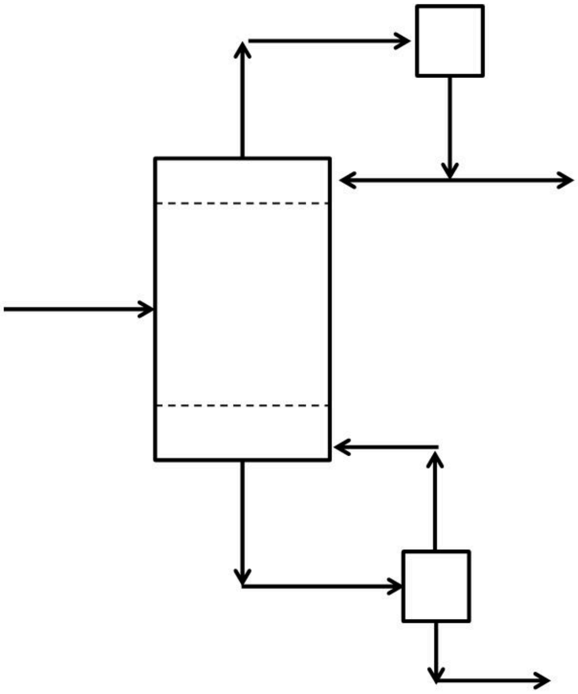
(20.6) $$y_{n+1} = \left(\frac{L}{V}\right)x_n + y_1 - \left(\frac{L}{V}\right)x_0$$

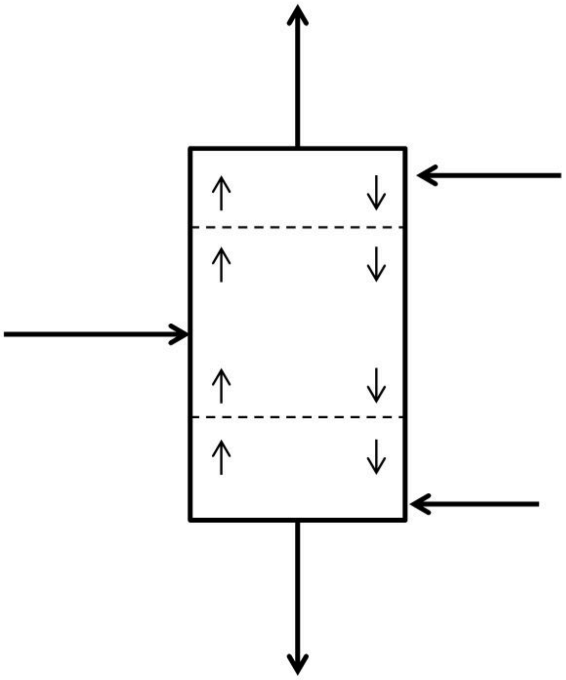
Rectifying section operating line

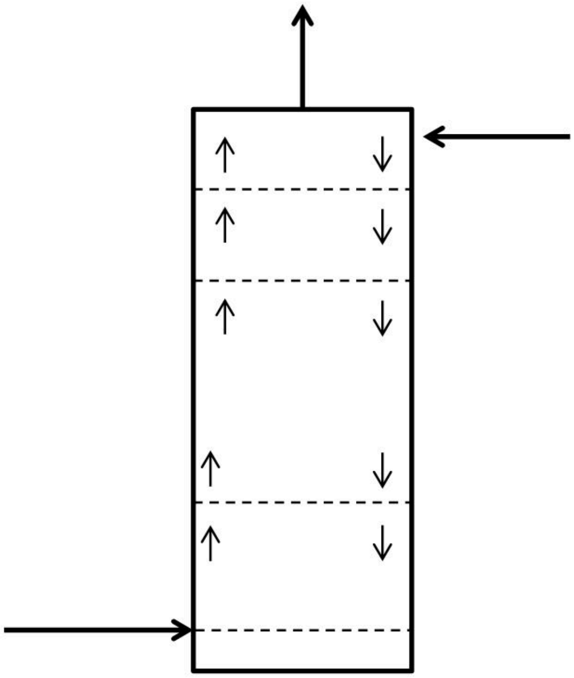
(20.7) $$y_{n+1} = \left(\frac{R}{R+1}\right)x_n + \left(\frac{x_D}{R+1}\right)$$

Stripping section operating line

(20.8) $$y_{n+1} = \left(\frac{V_B+1}{V_B}\right)x_n - \left(\frac{x_B}{V_B}\right)$$







McCabe-Thiele Method for Finding N and Feed Stage Location

ΔH^{vap} = enthalpy change of vaporization of the feed stream at the column operating pressure (energy mole^{-1})

C_{P_L} = heat capacity of the liquid feed stream (energy mole^{-1} temperature^{-1})

C_{P_V} = heat capacity of the vapor feed stream (energy mole^{-1} temperature^{-1})

F = molar flow rate of the feed stream entering the system (mole time^{-1})

L = molar flow rate of the liquid phase in the rectifying section (mole time^{-1})

$\overline{L}$ = molar flow rate of the liquid phase in the stripping section (mole time^{-1})

L_F = molar flow rate of the liquid portion of the feed stream (mole time^{-1})

n = generic stage number, stage 1 is at the top of the column

q = metric that reflects the physical state of the feed stream (unitless)

R = reflux ratio

T_b = bubble-point temperature of the feed stream at the column operating pressure (temperature)

T_d = dew-point temperature of the feed stream at the column operating pressure (temperature)

T_F = temperature of the feed stream (temperature)

V = molar flow rate of the vapor phase in the rectifying section (mole time^{-1})

$\overline{V}$ = molar flow rate of the vapor phase in the stripping section (mole time^{-1})

V_F = molar flow rate of the vapor portion of the feed stream (mole time^{-1})

x_B = mole fraction of the light key in the bottoms stream

x_D = mole fraction of the light key in the distillate stream

x_n = mole fraction of the light key in the liquid leaving stage

z_F = mole fraction of the light key in the feed stream

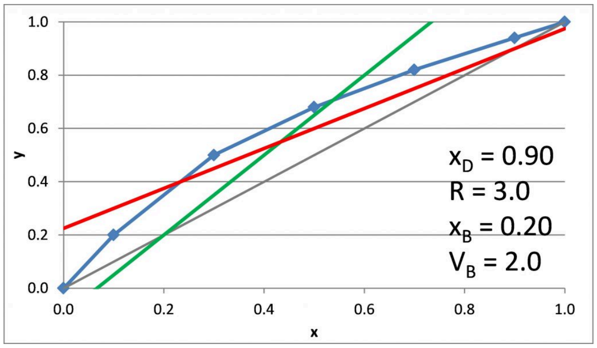
Finding the Theoretical Number of Stages from known Reflux Ratio, Boilup Ratio, Distillate Composition and Bottoms Composition

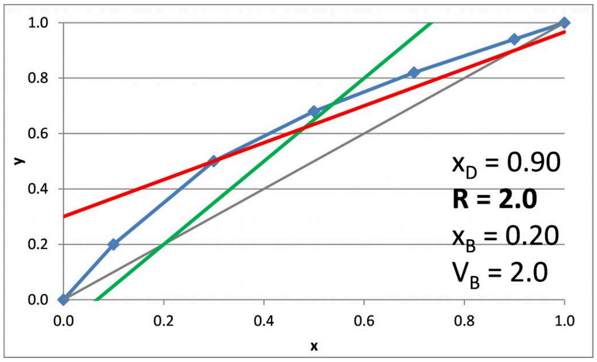
Rectifying section operating line

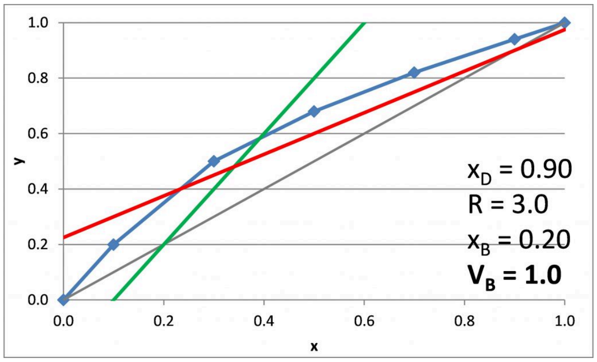
$$y_{n+1} = \left(\frac{R}{R+1}\right) x_n + \left(\frac{1}{R+1}\right) x_D \tag{21.1}$$

Stripping section operating line

$$y_{n+1} = \left(\frac{V_B+1}{V_B}\right) x_n - \left(\frac{1}{V_B}\right) x_B \tag{21.2}$$







Plotting the q-line

(21.3) $$F = L_F + V_F$$

(21.4) $$q = \frac{(\overline{L} - L)}{F} = 1 + (\frac{\overline{V} - V}{F})$$

For sub-cooled liquid, q > 1

(21.5) $$q = 1 + \frac{C_{P_L}(T_b - T_F)}{\Delta H^{\text{vap}}}$$

For a saturated liquid,

(21.6) $$q = 1$$

For a mixture of liquid and vapor, 0 < q < 1

(21.7) $$q = \frac{L_F}{F}$$

For a saturated vapor, q = 0

(21.8) $$q = 0$$

For sub-heated vapor, q < 0

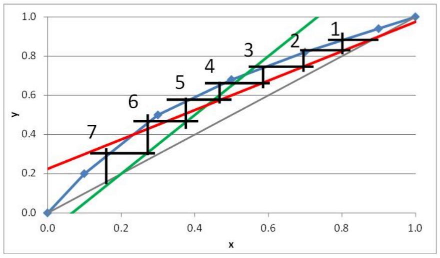
$$q = \frac{C_{P_V}(T_d - T_F)}{\Delta H^{\text{vap}}} \tag{21.9}$$

q-line

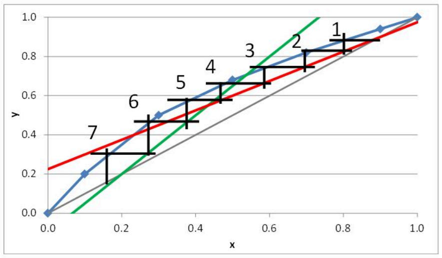
$$y = \left(\frac{q}{q-1}\right)x - \left(\frac{1}{q-1}\right)z_F \tag{21.10}$$

Watch this two-part video series from LearnChemE that demonstrates how to use the McCabe-Thiele graphical method to determine the number of equilibrium stages needed to meet a specified separation objective: McCabe-Thiele Graphical Method Example Part 1 (8:21): https://youtu.be/Cv4KjY2BJTA and McCabe-Thiele Graphical Method Example Part 2 (6:35): https://youtu.be/eIJk5uXmBRc

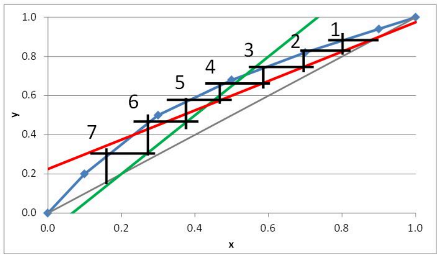
Watch this video from LearnChemE for a conceptual demonstration of how to relate stepping off stages to distillation column design: McCabe-Thiele Stepping Off Stages (7:02): https://youtu.be/rlg-ptQMAsg



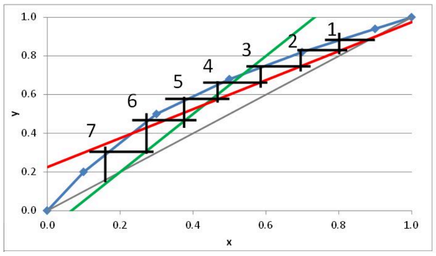
$x_D = 0.90$,
R = 3.0,
$x_B = 0.20$,
$V_B = 2.0$,
7 stages
q = 0,
$z_F = 0.50$
→ feed at stage
_____



$x_D = 0.90$,
R = 3.0,
$x_B = 0.20$,
$V_B = 2.0$,
7 stages
q = 1,
$z_F = 0.50$
→ feed at stage
_____



$x_D = 0.90$,
R = 3.0,
$x_B = 0.20$,
$V_B = 2.0$,
7 stages
q = 3,
$z_F = 0.50$
→ feed at stage
_____



x_D = 0.90,
R = 3.0,
x_B = 0.20,
V_B = 2.0,
7 stages
q = -3,
z_F = 0.50
→ feed at stage
_____

McCabe-Thiele Method for Finding the Minimum Number of Stages, the Minimum Reflux Ratio, and the Minimum Boilup Ratio

α = relative volatility of the light key and the heavy key at a given temperature (unitless)

α_F = relative volatility of the light key and the heavy key at the feed temperature (unitless)

γ_{HK} = activity coefficient of the heavy key; can be a function of x and/or T; 1 for an ideal solution (unitless)

γ_{LK} = activity coefficient of the light key; can be a function of x and/or T; 1 for an ideal solution (unitless)

B = molar flow rate of the bottoms leaving the system (mol time^{-1})

D = molar flow rate of the distillate leaving the system (mol time^{-1})

F = molar flow rate of the feed stream (mol time^{-1})

L = molar flow rate of liquid within the rectifying section, assumed constant in McCabe-Thiele model (mol time^{-1})

$\overline{L}$ = molar flow rate of liquid within the stripping section, assumed constant in McCabe-Thiele model (mol time^{-1})

$N_{t,\text{min}}$ = minimum required number of theoretical stages for a given combination of equilibrium data, x_D and x_B

P_{HK}^{sat} = saturated vapor pressure of the heavy key at a given temperature, i.e. by Antoine equation (pressure)

P_{LK}^{sat} = saturated vapor pressure of the light key at a given temperature, i.e. by Antoine equation (pressure)

q = metric that indicates that physical state of the feed stream, i.e. q = 1 for saturated liquid (unitless)

R = reflux ratio = L/D (unitless)

R_{min} = reflux ratio that requires an infinite number of stages in the rectifying section (unitless)

V = molar flow rate of vapor within the rectifying section, assumed constant in McCabe-Thiele model (mol time^{-1})

$\overline{V}$ = molar flow rate of vapor within the stripping section, assumed constant in McCabe-Thiele model (mol time^{-1})

V_B = boilup ratio = $\overline{V}/B$

$V_{B,\text{min}}$ = boilup ratio that requires an infinite number of stages in the stripping section (unitless)

V_F = molar flow rate of the vapor component of the feed stream (mol time^{-1})

x_B = target mole fraction of the light key in the bottoms product

x_D = target mole fraction of the light key in the distillate product

x_{HK} = mole fraction of the heavy key in the liquid phase

x_{LK} = mole fraction of the light key in the liquid phase

y_{HK} = mole fraction of the heavy key in the vapor phase

y_{LK} = mole fraction of the light key in the vapor phase

z_F = mole fraction of the light key in the feed stream

(22.1)
$$R_{\text{min}} = \frac{(L/V)_{\text{min}}}{1-(L/V)_{\text{min}}}$$

$(L/V)_{\text{min}}$ = slope of the line that connects (x_D, x_D) to the intersection of the q-line and the equilibrium curve

(22.2)
$$\alpha = \frac{y_{LK}/y_{HK}}{x_{LK}/x_{HK}} = \frac{\gamma_{LK}P_{LK}^{\text{sat}}}{\gamma_{HK}P_{HK}^{\text{sat}}}$$

(22.3)
$$V_{B,\text{min}} = \frac{1}{(\overline{L}/\overline{V})_{\text{max}}-1}$$

$(\overline{L}/\overline{V})_{\text{min}}$ = slope of the line that connects (x_B, x_B) to the intersection of the q-line and the equilibrium curve

(22.4)
$$V_B = \frac{L+D-V_F}{B} = \frac{D(R+1)-V_F}{B}$$

when $q \leq 0, V_F = F$; when $0 < q < 1, V_F = (1-q)F$; when $q \geq 1, V_F = 0$

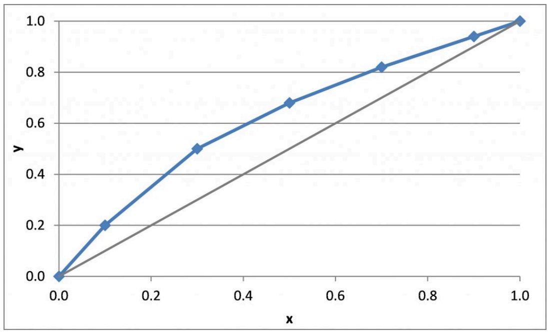
*we will use Eq 22.4 to calculate V_B as a function of our selected R

Example

$x_D = 0.80, q = 0, z_F = 0.25$

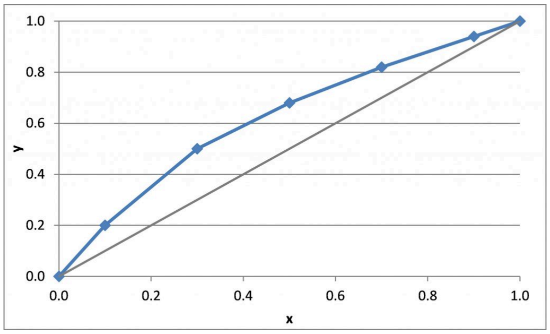
$(L/V)_{\text{min}}$ =

R_{min} =



Example

$$x_D = 0.90, x_B = 0.20$$
$$N_{t,\min} =$$



Distillation Energy Demand and Correlations for Efficiency

α = relative volatility of the light key and heavy key (unitless). For equation 23.2, this is evaluated at the average column temperature.

ΔH^{vap} = average heat of vaporization for the stream entering the condenser or reboiler (energy mole^{-1})

ΔH_S^{vap} = average heat of vaporization for the steam entering the reboiler (energy mole^{-1})

μ = liquid phase viscosity (cP). For eqs 23.1 and 23.2, this is the viscosity of the feed stream at the average column temperature.

B = bottoms flow rate (mole time^{-1})

$C_{P,\text{H}_2\text{O}}$ = heat capacity of liquid water (energy mole^{-1} temperature^{-1}) or (energy mass^{-1} temperature^{-1})

D = distillate flow rate (mole time^{-1})

E_O = stage efficiency (unitless)

L = liquid flow rate in the rectifying section (mole time^{-1})

$\overline{L}$ = liquid flow rate in the stripping section (mole time^{-1})

m_{cw} = flow rate of cooling water to condenser (mass time^{-1}) or (mole time^{-1})

m_s = flow rate of steam to reboiler (mass time^{-1}) or (mole time^{-1})

Q_C = energy demand (cooling) for the condenser (energy time^{-1})

Q_R = energy demand (heating) for the reboiler (energy time^{-1})

R = reflux ratio = L/D (unitless)

T_{in} = temperature of cooling water entering the condenser (temperature)

T_{out} = temperature of cooling water leaving the condenser (temperature)

V_B = boilup ratio = $\overline{V}/B$ (unitless)

V_F = molar flow rate of the vapor portion of the feed (mole time^{-1})

Correlations for Stage Efficiency

Drickamer and Bradford

(23.1) $$E_O = 13.3 - 68.8 \log_{10} \mu$$

> Restrictions on eq 23.1: $\mu = 0.066 - 0.355$ cP, $T = 157 - 420$°F, $P = 14.7 - 366$ psia, $E_O = 41 - 88$%

O’Connell

(23.2) $$E_O = \frac{50.3}{(\alpha\mu)^{0.226}}$$

> when $0.1 \leq \alpha\mu \leq 1$, adjust E_O calculated by 23.2 with correction factor from Table 7.5
>
> Restriction on eq 23.2: $\alpha = 1.16 - 20.5$

Condenser and Reboiler Energy Demand

total condenser

(23.3) $$Q_C = D(R+1)\Delta H^{\mathrm{vap}}$$

partial reboiler

(23.4) $$Q_R = BV_B\Delta H^{\mathrm{vap}}$$

for partially vaporized feed $(0 < q < 1)$ and total condenser

$$Q_R = Q_C \left[1 - \frac{V_F}{D(R+1)}\right] \tag{23.5}$$

$$m_{\text{cw}} = \frac{Q_C}{C_{P,\text{H}_2\text{O}}(T_{\text{out}} - T_{\text{in}})} \tag{23.6}$$

if using saturated steam for the reboiler

$$m_S = \frac{Q_R}{\Delta H_S^{\text{vap}}} \tag{23.7}$$

Distillation Packed Column Depth

HETP = height of equivalent theoretical plates

$H_{OG} = x$ (length)

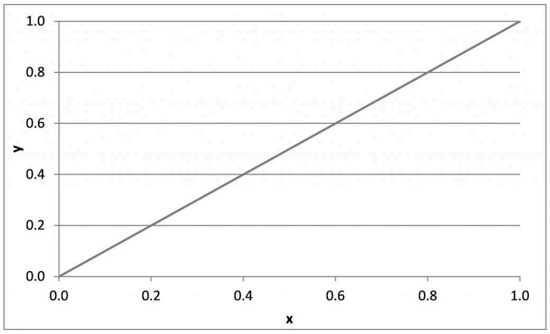
λ = local slope of equilibrium curve/local slope of operating line

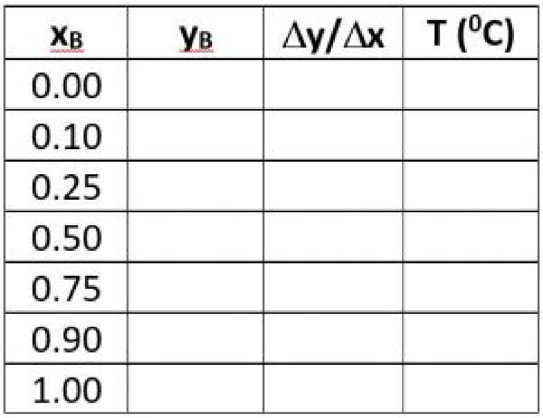
$$\text{HETP} = H_{OG} \frac{\ln \lambda}{\lambda - 1} \tag{24.1}$$

Example

We aim to distill benzene and toluene to a distillate that contains 95 mol% benzene and a bottoms stream that contains 95% toluene. The feed stream is 100 kmol/hr of an equimolar mixture with q = 0.50. We will be operating at 1.0 atm, R/R_{min} of 1.8 with a packed column containing 25-mm metal Bialecki rings. Assume operating at 70% of the flooding velocity. What depth of packing is needed to achieve this separation?

- For Antoine equation of the form $\log_{10} p^* = A - B/(T + C)$, where T is in °C and p^* is in mmHg
    - Benzene: $A = 6.89, B = 1204, C = 220$
    - Toluene: $A = 6.96, B = 1350, C = 220$
- 25-mm metal Bialecki rings: $a = 210, \epsilon = 0.956, C_h = 0.692, C_p = 0.891, C_l = 1.461, C_v = 0.331, C_s = 2.521$
- Toluene: $\text{MW} = 92.14, \rho_L = 0.87$ g/mL, $\mu_L = 0.590$ cP, $\sigma_L = 27.73$ dyne/cm
- Benzene: $\text{MW} = 78.11, \rho_L = 0.88$ g/mL, $\mu_L = 0.652$ cP, $\sigma_L = 28.88$ dyne/cm
- $D_L = 1.85 * 10^{-5}$ cm^2/s (Table 3.4, Seader)
- $D_V = 0.0565$ cm^2/s (estimated via eq 3-36, Seader)
- $\mu_V = 0.0133$ cP, estimated from online gas viscosity calculator (LMNO Engineering) as a function of T (94°C)





x_B	y_B	$\Delta y/\Delta x$	T (^{0}C)
0.00			
0.10			
0.25			
0.50			
0.75			
0.90			
1.00			

6. Membranes

Introduction to Membrane Processes and Modeling Porous Membranes

ΔP = pressure driving force across the membrane (pressure)

Δz = membrane thickness (length)

ϵ = membrane porosity; volume of pores per unit volume of membrane (unitless)

μ = permeate viscosity (cP) or (mass length^{-1} time^{-1})

ρ = fluid density (mass volume^{-1})

τ = membrane tortuosity factor (>1)

A_M = membrane cross-sectional area (area)

a_V = total pore surface area per volume of membrane solid material (area volume^{-1})

D = pore diameter (length)

d_H = hydraulic pore diameter (length)

J = permeate flux (vol area^{-1} time^{-1}) or (length time^{-1})

k = permeability of component i (length^2)

L = pore length

l_M = membrane thickness (length)

n = number of pores per unit of flow area (i.e. top down, not a cross-section) of membrane

N_i = molar flux through the membrane per unit area (mol time^{-1} area^{-1})

N_{Re} = Reynold's number (unitless)

P = pressure (pressure)

P_0 = pressure at the surface of the pore (pressure)

P_L = pressure at position L within the membrane pore (pressure)

P_{M_i} = permeability of the membrane to species i (length^2 time^{-1})

$\overline{P}_{M_i}$ = permeance of the membrane to species i (length time^{-1})

R_c = resistance of the filter cake (length^{-1})

R_i = resistance of component i (length^{-1})

R_m = resistance of the membrane (length^{-1})

t = time (time)

u = superficial velocity of the permeate (length time^{-1})

v = flow velocity (length time^{-1})

$V(t)$ = cumulative volume of permeate collected since the start of the filtration (volume)

z = direction of flux (length)

General Flux Equation

(25.1) $$N_i = \left(\frac{P_{M_i}}{l_M}\right) * [\text{driving force}] = \overline{P}_{M_i} * [\text{driving force}]$$

Dead-end Filtration

(25.2) $$J = \frac{1}{A_M}\frac{dV(t)}{dt} = \left(\frac{-k}{\mu}\right)\frac{dP}{dz}$$

(25.3) $$R_i = \frac{\Delta z_i}{k_i}$$

(25.4) $$u = J = \frac{\Delta P}{\mu(R_m + R_c)}$$

Modeling of Porous Membranes

Hagen-Poiseuille Law

(25.5) $$v = \frac{D^2}{32\mu L}(P_0 - P_L)$$

*eq 25.5 is restricted to $N_{\text{Re}} < 2100$, where $N_{\text{Re}} = Dv\rho/\mu$

(25.6) $$\epsilon = \frac{n\pi D^2}{4}$$

Ideal porous membrane: straight pores of uniform diameter

(25.7) $$N = v\rho\epsilon = \frac{D^2\rho\epsilon}{32\mu\, l_M}(P_0 - P_L) = \frac{n\pi D^4\rho}{128\mu\, l_M}(P_0 - P_L)$$

Compensation for tortuous pores and variation in pore diameter

(25.8) $$L = l_M\tau$$

(25.9) $$d_H = \frac{4\epsilon}{a_V(1-\epsilon)}$$

(25.10) $$N = \frac{\rho\epsilon^3(P_0 - P_L)}{2(1-\epsilon)^2\tau a_V^2\mu\, l_M}$$

Example

A membrane of thickness 0.003 cm will be used to filter room-temperature water. In order to justify the cost of the membrane, we need to filter 200 m^3 of water every day per m^2 of membrane purchased. We are able to maintain a pressure of 50 kPa on the permeate side. What pressure do we need to apply on the retentate side? Ignore any resistance from the retentate. Assume operation with an ideal porous membrane with a porosity of 35% and pore diameter of 0.2 µm.

Porous Membranes

α = internal parameter (length mass^{-1})

ΔP = pressure driving force across the membrane (pressure)

ΔP_{UL} = pressure across the membrane during the constant pressure segment of combined operation (pressure)

ϵ_c = filter cake porosity; volume of void space per unit volume of filter cake (unitless)

μ = permeate viscosity (cP) or (mass length^{-1} time^{-1})

ρ_c = filter cake density (mass volume^{-1})

A_c = surface area of the accumulated filter cake (area)

A_M = surface area of the membrane (area)

c_F = concentration of solid material per unit volume of feed (mass volume^{-1})

D_p = effective diameter of cake particles (length)

J = permeate flux (volume area^{-1} time^{-1}) or (length time^{-1})

K = internal parameter used in modeling constant pressure operation (volume^2 hr^{-1})

K_1 = internal parameter, function of effective particle diameter (length^{-2})

K_2 = parameter used in modeling combined constant flux/constant pressure operation, equals α (length mass^{-1})

l_c = thickness of accumulated filter cake (length)

R_c = resistance of the accumulating filter cake (length^{-1})

R_m = resistance of the membrane (length^{-1})

t = time (time)

t_{CF} = total time elapsed during the constant flux operation mode (time)

u = target permeate flux value (volume time^{-1})

$V(t)$ = cumulative volume of permeate collected since the start of the filtration (volume)

V_0 = internal parameter for modeling constant pressure operation (volume)

V_{CF} = total permeate collected during the constant flux operation mode (volume)

Resistance from Filter Cake

(26.1) $$R_c = \frac{150 l_c (1-\epsilon_c)^2}{D_P^2 \epsilon_c^3} = \frac{K_1 l_c (1-\epsilon)^2}{\epsilon_c^3}$$

(26.2) $$K_1 = \frac{150}{D_P^2}$$

for large, relatively flat membranes

$$R_c(t) = \frac{K_1(1-\epsilon_c)c_F V(t)}{\epsilon_c^3 \rho_c A_c} = \frac{\alpha c_F V(t)}{A_c} \tag{26.3}$$

An equation for the cake resistance, $R_c(t)$, for capillary or hollow fiber membranes given in Seader (14-22).

Operation with Constant Pressure (Flux Decreases with Time)

$$\frac{t}{V(t)} = \frac{V(t) + 2V_0}{K} \tag{26.4}$$

$$K = \frac{2A_c^2 \Delta P}{\alpha c_F \mu} \tag{26.5}$$

$$V_0 = \frac{R_m A_c}{\alpha c_F} \tag{26.6}$$

$$\alpha = \frac{K_1(1-\epsilon)}{\epsilon_c^3 \rho_c} \tag{26.7}$$

$$K_1 = \frac{150}{D_P^2} \tag{26.8}$$

Operation with Constant Flux (Applied Pressure Drop Increases with Time)

$$\Delta P(t) = \left(\frac{\alpha c_F \mu}{A_c^2}\right) u^2 t + \left(\frac{R_m \mu}{A_c}\right) u \tag{26.9}$$

Combined Operation: Constant Flux to Maximum Pressure Drop, Then Continue at Constant Pressure with Decreasing Flux

$$V(t) = \frac{-R_m A_M}{K_2 c_F} + [\left(\frac{A_M R_m}{K_2 c_F}\right)^2 + \frac{2A_M}{K_2 c_F}\left(R_m V_{CF} + \frac{0.5 K_2 c_F V_{CF}^2}{A_M} + \frac{A_M \Delta P_{UL}\left(t - t_{CF}\right)}{\mu}\right)]^{0.5} \tag{26.10}$$

$$J(t) = \frac{A_M \Delta P_{UL}}{K_2 c_F \mu}[\left(\frac{A_M R_M}{K_2 c_F}\right)^2 + \frac{2A_M}{K_2 c_F}\left(R_m V_{CF} + \frac{0.5 K_2 c_F V_{CF}^2}{A_M} + \frac{A_M \Delta P_{UL}\left(t - t_{CF}\right)}{\mu}\right)]^{-0.5} \tag{26.11}$$

$$K_2 = \alpha \tag{26.12}$$

Example

We aim to use a flat, porous membrane to filter milk. The membrane has a surface area of 17.3 cm^2; the membrane resistance and thickness are not known. The milk contains 4.3 kg/m^3 solids and has a viscosity of 0.001 Pa-s. We previously filtered this milk at an applied pressure drop of 20 psi and the following data was collected:

Time (hr)	0.5	1.0	1.5	2.0
Total volume collected (L)	0.31	0.40	0.53	0.61

1. How much filtered milk could be collected over a 12-hour period if we operate at $\Delta P = 20$ psi?
2. How much filtered milk could be collected over a 12-hour period if we operate at $\Delta P = 40$ psi?
3. If we operate in constant flux mode at 0.1 L/hr, how long will it take to reach our maximum allowable ΔP of 40 psi? How much permeate would be collected during this time?
4. If we operate in combined mode for 24 hours with a constant flux of 0.1 L/hr and maximum allowable pressure drop of 40 psi, how much permeate would be collected?

Nonporous Membranes Gas Permeation

$\alpha^*_{A,B}$ = ideal separation factor of species A and B (unitless)

$\alpha_{A,B}$ = actual separation factor of species A and B (unitless)

D_i = diffusivity of species i in the membrane (length^2 time^{-1})

H_i = Henry's Law coefficient of species i in the membrane (mol volume^{-1} pressure^{-1})

l_M = membrane thickness (length)

N_i = molar transmembrane flux of species i (mol area^{-1} time^{-1})

P_F = total pressure of the feed (pressure)

p_{i_0} = partial pressure of species i at the membrane on the feed side (pressure)

p_{i_F} = partial pressure of species i in the bulk feed (pressure)

p_{i_L} = partial pressure of species i at the membrane on the permeate side (pressure)

p_{i_P} = partial pressure of species i in the bulk permeate (pressure)

P_{M_i} = permeability of the membrane to species i (length^2 time^{-1})

$\overline{P}_{M_i}$ = permeance of the membrane to species i (length time^{-1})

P_P = total pressure of the permeate (pressure)

r = pressure ratio (unitless)

x_i = mole fraction of species i on the feed side

y_i = mole fraction of species i in the permeate

Gas through a non-porous membrane

$$N_i = \frac{H_i D_i}{l_M}(p_{i_0} - p_{i_L}) \tag{27.1}$$

if film resistance is negligible

$$N_i = \frac{H_i D_i}{l_M}(p_{i_F} - p_{i_P}) \tag{27.2}$$

(27.3) $$\alpha_{A,B}=\frac{y_A/x_A}{y_B/x_B}$$

(27.4) $$\alpha^*_{A,B}=\frac{H_AD_A}{H_BD_B}=\frac{P_{M_A}}{P_{M_B}}$$

(27.5) $$\alpha_{A,B}=\alpha^*_{A,B}\left[\frac{(x_B/y_B)-r\alpha_{A,B}}{(x_B/y_B)-r}\right]$$

(27.6) $$r=P_P/P_F$$

when A and B are the only components of the feed and permeate, so that

(27.7) $$x_A+x_B=y_A+y_B=1$$

(27.8) $$\alpha_{A,B}=\alpha^*_{A,B}\left[\frac{x_A(\alpha_{A,B}-1)+1-r\alpha_{A,B}}{x_A(\alpha_{A,B}-1)+1-r}\right]$$

Example

A certain membrane has an ideal separation factor of 5.12 for O_2 (A) and N_2 (B). It has been proposed to use this membrane to separate O_2 from air. If our feed pressure is 5.0 atm and our permeate pressure is maintained at 0.25 atm, what is the composition of our product gas?

Dialysis

$(\Delta c_i)_{\text{LM}}$ = log mean concentration difference (mol volume^{-1})

A_M = area of membrane cross-sectional to the flow path (area)

c_{i_F} = concentration of species i on the feed side of the membrane (mol volume^{-1})

c_{i_P} = concentration of species i on the permeate side of the membrane (mol volume^{-1})

c_{i_R} = concentration of species i in the retentate (mol volume^{-1})

$c_{I,\text{wash}}$ = concentration of species i in the wash solution (mol volume^{-1})

k_{i_F} = mass transfer coefficient of species i in the feed (length time^{-1})

k_{i_P} = mass transfer coefficient of species i in the permeate (length time^{-1})

K_i = overall mass transfer coefficient of species i (length time^{-1})

l_M = thickness of the membrane (length)

n_i = rate of mass transfer of species i (mol time^{-1})

P_{M_i} = permeability of the membrane to species i (length^2 time^{-1})

Transport across a small membrane segment

(28.1) $$dn_i = K_i(c_{i_F} - c_{i_P})dA_M$$

(28.2) $$\frac{1}{K_i} = \frac{1}{k_{i_F}} + \frac{l_M}{P_{M_i}} + \frac{1}{k_{i_P}}$$

(28.3) $$n_i = K_i A_M (\Delta c_i)_{\mathrm{LM}}$$

For counter-current operation:

(28.4) $$(\Delta c_i)_{\mathrm{LM}} = \frac{(c_{i_F} - c_{i_P}) - (c_{i_R} - c_{i,\mathrm{wash}})}{\ln\left[\frac{(c_{i_F} - c_{i_P})}{(c_{i_R} - c_{i,\mathrm{wash}})}\right]}$$

Water (solvent) transport number = water (solvent) flux / solute flux

Example

We aim to recover 30% of the H_2SO_4 from a 0.78 m^3/hr feed containing 300 kg/m^3 of H_2SO_4 and smaller amounts of $CuSO_4$ and $NiSO_4$. We have up to 1.0 m^3/hr of water available as a wash stream. The process is to run counter-current and at 25°C. The available membrane has an H_2SO_4 permeance of 0.025 cm/min, negligible permeance to the other sulfates, and a water transport number (mass) of +1.5. Previous experience suggests that $1/k_F + 1/k_P =$1/(0.020 cm/min). What is the required membrane area and the volumetric flowrate of the two streams exiting the dialysis unit?

Reverse Osmosis

ΔP = pressure drop across the membrane (pressure)

$\Delta \pi$ = osmotic pressure drop across the membrane (pressure)

γ_A^1 = activity coefficient of the solvent on the feed/retentate side (unitless)

Γ = concentration polarization factor (unitless)

μ = viscosity of the feed solution (cP)

π = osmotic pressure (pressure)

ρ = density of the feed solution (mass volume^{-1})

a = internal parameter used in estimating k_i (unitless)

b = internal parameter used in estimating k_i (unitless)

c_i^1 = concentration of species i in feed/permeate (mol volume^{-1})

$(c_{\text{salt}})_{\text{permeate}}$ = concentration of solute in the permeate (mol volume^{-1}) or (mass volume^{-1})

$(c_{\text{salt}})_{\text{feed}}$ = concentration of solute in the feed (mol volume^{-1}) or (mass volume^{-1})

d = internal parameter used in estimating k_i (unitless)

D = tube diameter (length)

d_H = hydraulic diameter (length)

D_i = diffusivity of species i in the indicated solvent (length^2 time^{-1})

h = height of flow channel (length)

k_i = mass transfer coefficient of species i (length time^{-1})

N_A = molar flux of solvent A through the membrane (mol area^{-1} time^{-1})

N_{Re} = Reynold's number of the feed/retentate (unitless)

N_{Sc} = Schmidt number of the feed/retentate (unitless)

R = universal gas constant (pressure volume mol^{-1} temperature^{-1}) or (energy mol temperature^{-1})

SP = salt (solute) passage number (unitless)

SR = salt (solute) rejection factor (unitless)

T = system temperature (temperature)

v = velocity of the feed (length time^{-1})

v_{A_L} = specific volume of the solvent (volume mol^{-1})

w = width of flow channel (length)

x_i^1 = mole fraction of species i on the feed/retentate side (unitless)

(29.1) $$\pi = \frac{-RT}{v_{A_L}} \ln\left(x_A^1 \gamma_A^1\right)$$

when $\gamma_A^1 \sim 1$ and $\ln(1 - x_B^1) \sim -x_B^1$ then

(29.2) $$\pi = \frac{RTx_B^1}{v_{A_L}}$$

if x_B is sufficiently small, then $x_B/v_{AL} = c_B$ and

(29.3) $$\pi \sim RTc_B^1$$

(29.4) $$N_A = \frac{P_{M_A}}{l_M}(\Delta P - \Delta\pi)$$

(29.5) $$k_i = \frac{aN_{\mathrm{Re}}^b N_{\mathrm{Sc}}^{0.33}(d_H/L)^d}{(d_H/D_i)}$$

(29.6) $$N_{\mathrm{Re}} = \frac{d_H v \rho}{\mu}$$

(29.7) $$N_{\mathrm{Sc}} = \frac{\mu}{\rho D_i}$$

for a circular tube, $d_H = D$

for a rectangular channel, $d_H = 2hw/(h+w)$

during turbulent flow $(N_{\mathrm{Re}} > 10{,}000)$ $a = 0.023, b = 0.8, d = 0$

during laminar flow, circular tube $(N_{\mathrm{Re}} < 2{,}100)$ $a = 1.86, b = 0.33, d = 0.33$

during laminar flow, rectangular channel $(N_{\mathrm{Re}} < 2{,}100)$ $a = 1.62, b = 0.33, d = 0.33$

(29.8) $$SP = \frac{(c_{\mathrm{salt}})_{\mathrm{permeate}}}{(c_{\mathrm{salt}})_{\mathrm{feed}}}$$

(29.9) $$SR = 1 - SP$$

(29.10) $$\Gamma = \frac{N_{\text{solvent}}(SR)}{k_{\text{solute}}}$$

Watch a video from LearnChemE that explains osmotic pressure: Osmotic Pressure Derivation (5:00).

Example

We intend to use reverse osmosis on a feed stream containing 1.8 wt% NaCl to produce water containing 0.05 wt% NaCl. The separation is to take place at 25°C with a feed side pressure of 1,000 psia and a permeate-side pressure of 50 psia. The proposed membrane has permeance of 1.1×10^{-5} g/cm^2-s-atm for water.

(a) Ignoring resistances to mass transfer, how much water can be produced per day per unit area of membrane?

(b) If k_{salt} = 0.005 cm/s, what is the concentration polarization factor?

Pervaporation

γ_i = activity coefficient of species i (unitless)

A_{12}, A_{21} = system-specific parameters for the van Laar model

l_M = membrane thickness (length)

P_i^{sat} = saturated vapor pressure of species i, function of temperature and Antoine equation coefficients (pressure)

P_{M_i} = permeability of the membrane to species i (length^2 time^{-1})

P_P = total pressure on permeate side (pressure)

x_i = mole fraction of species i on the feed/retentate side (unitless)

y_i = mole fraction of species i on the permeate side (unitless)

(30.1) $$N_i = \frac{P_{M_i}}{l_M}\left(\gamma_i x_i P_i^{\text{sat}} - y_i P_P\right)$$

van Laar model for activity coefficients, binary system

$$\ln\gamma_1 = \frac{A_{12}}{\left[1+\frac{x_1 A_{12}}{x_2 A_{21}}\right]^2}$$ (30.2)

$$\ln\gamma_2 = \frac{A_{21}}{\left[1+\frac{x_2 A_{21}}{x_1 A_{12}}\right]^2}$$ (30.3)

Example

We have obtained a potential pervaporation membrane and we aim to use it to separate ethanol and water. We tested this system at 60°C, a permeate pressure of 76 mmHg and a feed containing 8.8 wt% EtOH. Using 1.0 cm^2 of membrane, we collected 0.25 g/hr of permeate that was found to contain 10.0 wt% EtOH.

(a) What is the permeance of our membrane to ethanol and to water?

(b) What is the expected product composition and flowrate (g/hr) for a feed containing 10.0 wt% EtOH at 60°C with operation at a permeate pressure of 100 mmHg?

- $A_{EtOH,H2O}$ = 1.6276
- $A_{H2O,EtOH}$ = 0.9232
- P_{EtOH}^{sat}(60°C) = 352 mmHg
- P_{H2O}^{sat}(60°C) = 149 mmHg

7. Sorption and Chromatography

Adsorption, Ion Exchange, and Chromatography

c_i = concentration of species i in the mobile phase (mass volume^{-1}) or (mole volume^{-1})

k_i = empirical constant for species i for isotherms (units vary)

K_i = adsorption equilibrium constant for species i

n_i= internal parameter for isotherms (units vary)

p_i= partial pressure of species i (pressure)

q_i= amount of species i adsorbed per unit mass of adsorbent at equilibrium (mass mass^{-1}) or (mole mass^{-1})

q_{m_i} = amount of species i adsorbed per unit mass of adsorbent at maximum loading, where maximum loading corresponds to complete surface coverage (mass mass^{-1}) or (mole mass^{-1})

linear isotherm:

(31.1) $$q_i = k_i p_i$$

Freundlich isotherm:

(31.2) $$q_i = k_i p_i^{1/n_i}$$

Langmuir isotherm:

(31.3) $$q_i = \frac{K_i q_{m_i} p_i}{1 + K_i p_i}$$

chromatography equilibrium:

(31.4) $$K_i = \frac{q_i}{c_i}$$

Watch a video from LearnChemE for an explanation about the concept of adsorption: Adsorption Introduction (8:49)

Modeling Differential Chromatography

α_i = average partitioning of species i between the bulk fluid and sorbent (unitless)

ϵ_b = sorbent porosity, ranges from 0 to 1 (unitless)

$\epsilon_{p,i}^{*}$ = inclusion porosity, accounts for accessibility of sorbent pores to species i (unitless)

τ_f = sorbent tortuosity factor, usually approximately 1.4 (unitless)

ω_i = fraction of solute in the mobile phase, relative to sorbed solute, at equilibrium (unitless)

A = cross-sectional area of the column (area)

$c_{f,i}$ = concentration of species i in the mobile phase (mass volume^{-1}) or (mol volume^{-1})

$D_{e,i}$ = effective diffusivity of species i within the sorbent pores (length^{2} time^{-1})

E_i = coefficient that accounts for axial diffusion of species i and non-uniformities of flow (length^{2} time^{-1})

H_i = height of theoretical chromatographic plate for species i (length)

$k_{a,i}$ = kinetic rate constant of adsorption of species i to the sorbent (time^{-1})

$k_{c,i}$ = mass transfer coefficient of species i in the mobile phase (length time^{-1})

$k_{c,i,tot}$ = overall mass transfer coefficient of species i (length time^{-1})

$K_{d,i}$ = equilibrium distribution coefficient of species i between the mobile phase and sorbent (unitless)

L = length of column (length)

m_{0_i} = amount of solute i fed to column (mass) or (mol)

$R_{1,2}$ = resolution of species 1 and 2 in the proposed operating condition (unitless)

R_p = radius of sorbent particles (length)

s_i = variance of the Gaussian peak of the distribution of species i along the column length (time)

t = elapsed time since loading of the column (time)

$\bar{t}_i$ = mean residence time of species i in the column (time)

u = actual fluid velocity through the bed (length time^{-1})

u_s = superficial fluid velocity through the bed (length time^{-1})

z = position along the length of the column, in the direction of flow (length)

$z_{0,i}$ = mean position of species i along the length of the column as a function of time (length)

(32.1) $$z_{0,i}(t) = \omega_i u t$$

(32.2) $$\omega_i = \frac{1}{1 + \frac{1-\epsilon_b}{\epsilon_b \alpha_i}}$$

(32.3) $$\alpha_i = \frac{1}{\epsilon^*_{p,i}(1+K_{d,i})}$$

(32.4) $$u = u_s/\epsilon_b$$

(32.5) $$\bar{t}_i = \frac{L}{\omega_i u}$$

(32.6) $$c_{f,i}(z,t) = \frac{m_{0_i}\omega_i}{A\epsilon_b(2\pi H_i z_0)^{0.5}}\exp\left(\frac{-(z-z_0)^2}{2H_i z_0}\right)$$

(32.7) $$H_i = 2\left[\frac{E_i}{u} + \frac{\omega_i(1-\omega_i)R_p u}{3\alpha_i k_{ci,tot}}\right]$$

(32.8) $$N_{\mathrm{Pe},i} = N_{\mathrm{Re}}N_{\mathrm{Sc},i} = \frac{2R_p u\epsilon_b}{D_i}$$

if $N_{\mathrm{Pe},i} << 1$

(32.9) $$E_i = \frac{D_i}{\tau_f}$$

else

(32.10) $$E_i = \frac{2R_p u\epsilon_b}{N_{\mathrm{Pe},E,i}}$$

$N_{\mathrm{Pe},E,i}$ calculated by 15-61 or 15-62, Seader

(32.11) $$\frac{1}{k_{ci,tot}} = \frac{1}{k_{c,i}} + \frac{R_p}{5\epsilon^*_{p,i}D_{e,i}} + \frac{3}{R_p k_{a,i}\epsilon^*_{p,i}}\left[\frac{K_{d,i}}{1+K_{d,i}}\right]^2$$

(32.12) $$s_i^2 = \frac{\bar{t}_i H_i}{\omega_i u}$$

(32.13) $$R_{1,2} = \frac{\mathrm{abs}(\bar{t}_1 - \bar{t}_2)}{2(s_1+s_2)}$$

Example

1.0 g of species A is added to a chromatography column of cross-sectional area 1.0 m^2 and length 1.0 m. Mobile phase is added at a flowrate of 4.0×10^{-3} m^3/s. Species A has a mass transfer coefficient of 2.0×10^{-5} m/s in this solvent. The selected sorbent has a porosity of 0.40 m and average particle radius of 5.0×10^{-6} m. For species A in this sorbent, the inclusion porosity is 0.80, $K_d = 50$, $E = 2.0 \times 10^{-8}$ m^2/s, $k_a = 100$ s^{-1} and the effective diffusivity is 3.5×10^{-12} m^2/s.

(a) When is mean expected elution time for species A?

(b) Plot the concentration profile for species A at 0.05 m increments along the column length in 10-minute increments, until all of the solute has eluted.

(c) Find the variance of the peak for species A in the proposed operating condition.

(d) The column feed also contains 1.0 g of species B. Species B has a mass transfer coefficient of 1.0×10^{-5} m/s in the mobile phase, inclusion porosity of 0.50, $K_d = 60$, $E = 3.0 \times 10^{-8}$ m^2/s, effective diffusivity of 4×10^{-12} m^2/s and $k_a = 200$ s^{-1}. What is the resolution of these two species in the proposed operating condition?