

CHEM E 435 Transport Process III

Separation Processes

| Types of Separations

| Separations by phase creation

Separation Operation	Feed Phase	Created Phase	Separating Agent
Partial condensation/vaporization	V and/or L	L or V	Heat transfer (ESA)
Flash vaporization	L	V	Pressure reduction
Distillation	V and/or L	V and L	Heat transfer (ESA) and sometimes shaft work (ESA)

| Separations by phase addition

Separation Operation	Feed Phase	Created Phase	Separating Agent
Absorption	V	L	Liquid absorbent (MSA)
Stripping	L	V	Stripping vapor (MSA)
Liquid-liquid extraction	L	L	Liquid solvent (MSA)
Adsorption	V or L	S	Solid adsorbent (MSA)

| Separations by barrier

Separation Operation	Feed Phase	Barrier	Separating Agent
Dialysis	L	Microporous membrane	Pressure (ESA)
Reverse osmosis	L	Microporous membrane	Pressure (ESA)
Gas permeation	Vapor	Nonporous membrane	Pressure (ESA)
Pervaporation	L	Nonporous membrane	Pressure and heat transfer (ESA)

| Separations by external field/gradient

- Centrifugation - pressure gradient
- Thermal diffusion - temperature gradient
- Electrolysis
- Electrodialysis - permeable membrane with fixed charge
- Electrophoresis - electric field
- Magnetophoresis - magnetic field
- Crystallization - solubility

Thermodynamics Review

Description	Equations
Equilibrium conditions	$T_1 = T_2$ $P_1 = P_2$ $\bar{f}_2 = \bar{f}_2$ $a_1 = a_2$
Fugacity	$\bar{f}_i = \bar{f}_i^\circ \exp\left(\frac{\mu_i}{RT}\right)$
Fugacity coefficient	$\phi_i = \frac{\bar{f}_i}{P}$
Partial fugacity coefficient	$\phi_i = \frac{\bar{f}_i}{x_i P}$
Activity	$a_i = \frac{\bar{f}_i}{\bar{f}_i^\circ}$
Activity coefficient	$\gamma_i = \frac{a_i}{x_i}$

| ***K*-values**

Description	Equations
<i>K</i> -value (vapor-liquid equilibrium ratio)	$K_i = \frac{y_i}{x_i}$
Distribution ratio (partition coefficient, liquid-liquid equilibrium ratio)	$K_{D_i} = \frac{x_i^\alpha}{x_i^\beta}$
Relative volatility	$\alpha_{i,j} = \frac{K_i}{K_j}$
Relative selectivity	$\beta_{i,j} = \frac{K_{D_i}}{K_{D_j}}$
Raoult's law ★ Ideal solution	$K_i = \frac{P_i^*}{P}$
Modified Raoult's law ★ Low pressure	$K_i = \gamma_{i,L} \frac{P_i^*}{P}$
Poynting correction ★ Moderate pressure	$K_i = \gamma_{i,L} \phi_{i,V}^{\text{sat}} \left(\frac{P_i^{\text{sat}}}{P} \right) \exp \left[\frac{1}{RT} \int_{P_i^{\text{sat}}}^P v_{i,L} dP \right]$
Henry's law ★ Dilute species	$K_i = \frac{H_i}{P}$

Mass Transfer and Diffusion

| Steady-state ordinary molecular diffusion (OMD)

Description	Equations
Fick's first law Molecular diffusion flux of species A	$J_A = -c D_{AB} \frac{dx_A}{dx} = -D_{AB} \frac{dc_A}{dz}$ $j_A = -\rho D_{AB} \frac{dw_A}{dz}$
Bulk flow flux	$N = N_A + N_B$

Description	Equations
Bulk flow flux of species A	$x_A N$
Molar flux of species A (definition)	$N_A = \frac{\dot{n}_A}{A}$
Molar flux of species A ★ No eddie diffusion flux	$N_A = \text{bulk flow flux} + \text{molecular diffusion flux}$ $N_A = x_A N - c D_{AB} \frac{dx_A}{dz}$
Total velocity of species A	$v_A = \frac{N_A}{c_A}$
Molar-average mixture velocity	$v_M = v_A x_A + v_B x_B$
Diffusion velocity of species A	$v_{D,A} = \frac{J_A}{c_A}$
Velocity relations	$v_A = v_M + v_{D,A}$

| Equimolar counter diffusion (EMD)

Description	Equations
Equimolar counter diffusion	$N_A = -N_B$
No bulk flow	$N = 0$
Molar flux of species A Molecular diffusion flux of species A	$N_A = J_A = -c D_{AB} \frac{\Delta x_A}{\Delta z}$
Concentration profile of species A	$c_A = c_{A0} - \frac{J_A z}{D_{AB}}$
Concentration profile of species B	$c_B = c_{B0} + \frac{J_A (z - L)}{D_{AB}}$

| Unimolecular diffusion (UMD)

Description	Equations
Stagnant B	$N_B = 0$
Molar flux of species A Bulk flow flux	$N = N_A$
Molar flux of species A	$N_A = \frac{c D_{AB}}{z - z_1} \ln \left(\frac{1 - x_A}{1 - x_{A,1}} \right)$
Molar flux of species A	$N_A = -\frac{c D_{AB}}{(1 - x_A)_{LM}} \frac{\Delta x_A}{\Delta z}$
Dilute A reduces UMD to EMD (no bulk flow)	$(1 - x_A)_{LM} \approx 1 \quad \text{if } x_A \rightarrow 0$
Log-mean	$x_{LM} = \frac{x_2 - x_1}{\ln(x_2/x_1)}$
Composition profile	$x_A(z) = 1 - (1 - x_A) \exp \left[\frac{N_A(z - z_1)}{c D_{AB}} \right]$
Molecular diffusion and bulk flow flux of species	$J_A = x_B N = -J_B$
Changing liquid level of A with stagnant B	$N_A = -\frac{c D_{AB}}{(1 - x_A)_{LM}} \frac{\Delta x_A}{z} = \frac{\rho_A}{\mathcal{M}_A} \frac{dz}{dt}$

| Diffusivity

| Diffusivity of gas mixtures

	Description	Equations
Fuller-Schettler-Giddings correlation	<ul style="list-style-type: none"> ★ Low pressure (0 - 10 atm) ★ D_{AB} [cm²/s] ★ P [atm], T [K] ★ \mathcal{M}_{AB} [g/mol] 	$D_{AB} = D_{BA} = \frac{0.00143T^{1.75}}{P\mathcal{M}_{AB}^{1/2} \left[(\sum_V)_A^{1/3} + (\sum_V)_B^{1/3} \right]^2}$
Effective molecular mass		$\mathcal{M}_{AB} = \frac{2}{\frac{1}{\mathcal{M}_A} + \frac{1}{\mathcal{M}_B}}$
Summation of atomic and structural diffusion volumes (Table 3.1)		\sum_V
Takahashi correlation	<ul style="list-style-type: none"> ★ High pressure (Figure 3.3) 	$\frac{D_{AB}P}{(D_{AB}P)_{\text{low } P}} = \text{const}$
Molar averaged reduced properties		$T_r = x_A T_{r,A} + x_B T_{r,B}$ $P_r = x_A P_{r,A} + x_B P_{r,B}$

| Diffusivity of nonelectrolyte liquid mixtures

	Description	Equations
Stoke-Einstein equation	<ul style="list-style-type: none"> ★ Infinite dilution 	$(D_{AB})_\infty = \frac{RT}{6\pi\mu_B R_A N_A} \propto \frac{T}{\mu_B R_A}$
Wilke-Chang equation	<ul style="list-style-type: none"> ★ Low pressure (0 - 10 atm) ★ D_{AB} [cm²/s] ★ μ_B [cP], T [K] ★ \mathcal{M}_{AB} [g/mol] ★ v_A [cm³/mol] 	$(D_{AB})_\infty = 7.4 \times 10^{-8} \frac{(\phi_B \mathcal{M}_B)^{1/2} T}{\mu_B v_A^{0.6}}$
Hayduk-Minhas correlation (Modified Wilke-Chang equation)		$(D_{AB})_\infty = 13/3 \times 10^{-8} \frac{T^{1.47} \mu_B^\varepsilon}{v_A^{0.71}}$ $\varepsilon = \frac{10.2}{v_A} - 0.791$

| Film theory for mass transfer at fluid-fluid interface

| Single film theory

	Description	Equations
Concentration and mole fraction		$c_A = x_A c$
Mass transfer coefficient (no bulk flow)		$k_c = \frac{D_{AB}}{\delta}$
Mass transfer coefficient (with bulk flow)		$k'_c = \frac{D_{AB}}{\delta(1 - x_A)_{\text{LM}}}$
Molar flux of species A	<ul style="list-style-type: none"> ★ Interface (i), bulk (b) 	$N_A = \pm k_c(c_{A,i} - c_{A,b})$ $N_A = \pm k'_c(c_{A,i} - c_{A,b})$
Film thickness		$\delta = \frac{D_{AB}}{k_c} = \frac{D_{AB}}{k'_c(1 - x_A)_{\text{LM}}}$

| Mass transfer coefficient and driving force

Driving Force	Mass Transfer Coefficient	Equations
Concentration (liquid)	$k_c \text{ [m/s]}$	$N_A = \pm k_c(c_{A,i} - c_{A,b})$
Pressure (vapor)	$k_p \text{ [mol/m}^2 \cdot \text{s} \cdot \text{Pa]}$	$N_A = \pm k_p(P_{A,i} - P_{A,b})$
Mole fraction (liquid)	$k_x \text{ [mol/m}^2 \cdot \text{s}]$	$N_A = \pm k_x(x_{A,i} - x_{A,b})$
Mole fraction (vapor)	$k_y \text{ [mol/m}^2 \cdot \text{s}]$	$N_A = \pm k_y(y_{A,i} - y_{A,b})$

Description	Equations
Liquid phase coefficient conversion	$k_x = k_c c = k_c \frac{\rho_L}{\mathcal{M}_L}$
Vapor phase coefficient conversion	$k_y = k_p P = (k_c)_g c = (k_c)_g \frac{P}{RT} = (k_c)_g \frac{\rho_G}{\mathcal{M}_G}$
Liquid phase bulk flow correction	$k' = \frac{k}{(1 - x_A)_{LM}}$
Gas phase bulk flow correction	$k' = \frac{k}{(1 - y_A)_{LM}}$

| Two-film theory

Based on	Overall Mass Transfer Coefficient	Equations	Fictitious properties
Liquid phase	$\frac{1}{K_L} = \frac{H_A}{k_p} + \frac{1}{k_c}$	$N_A = \pm K_L(c_A^* - c_{A,b})$	$c_A^* = P_{A,b} H_A$
Gas phase	$\frac{1}{K_G} = \frac{1}{k_p} + \frac{1}{H_A k_c}$	$N_A = \pm K_G(P_{A,b} - P_A^*)$	$P_A^* = \frac{c_{A,b}}{H_A}$
Liquid phase mole fraction	$\frac{1}{K_x} = \frac{1}{K_a k_y} + \frac{1}{k_x}$	$N_A = \pm K_y(y_{A,b} - y_A^*)$	$y_A^* = x_{A,b} K_A$
Gas phase mole fraction	$\frac{1}{K_y} = \frac{1}{k_y} + \frac{K_A}{k_x}$	$N_A = \pm K_x(x_A^* - x_{A,b})$	$x_A^* = \frac{y_{A,b}}{K_A}$

Single Equilibrium Stages

| Degrees of freedom

Description	Equations
Gibbs' phase rule	DOF = component – phase + 2
Degree of freedom	DOF = # intensive variables – # independent eqns
Azeotrope	$x_i = y_i$
q -line	$y_H = \left[\frac{(V/F) - 1}{(V/F)} \right] x_H + \left[\frac{1}{(V/F)} \right] z_H$

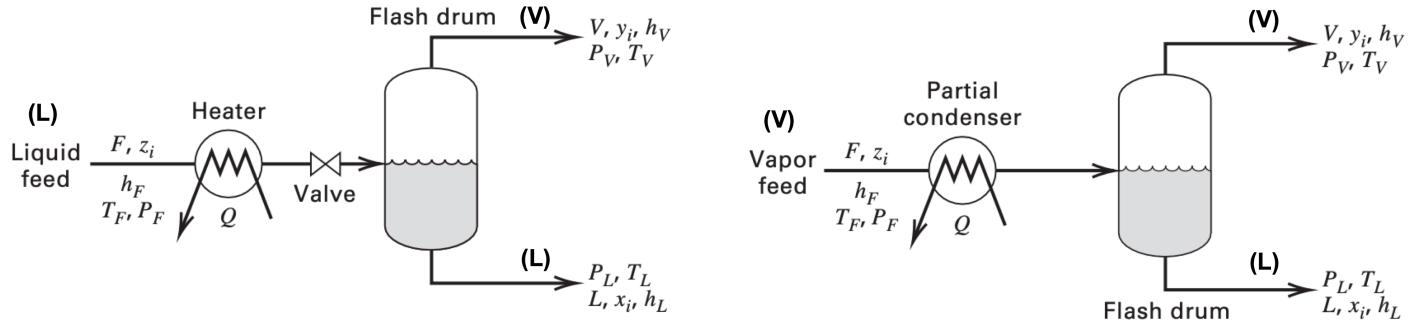
| Rachford-Rice algorithm for isothermal flash calculation

ⓘ Symbol Conventions

- Molar flow rates
 - F - Feed
 - V - Output vapor
 - L - Output liquid
- Molar fraction of component i

- x_i - In the liquid
- y_i - In the vapor
- z_i - Overall

Description	Equations
Road map	Known - K_i, z_i, F Solve - $\Psi \rightarrow V \rightarrow L \rightarrow x_i, y_i \rightarrow Q$
Vapor-to feed ratio	$\Psi \equiv \frac{V}{F}$
Objective function ★ Derived from $\sum y_i - \sum x_i = 0$	$f(\Psi) = \sum_i \frac{z_i(1 - K_i)}{[1 + \Psi(K_i - 1)]} = 0$
Derivative of objective function	$f'(\Psi) = \sum_i \frac{z_i(1 - K_i)^2}{[1 + \Psi(K_i - 1)]^2}$
Newton's method for root finding	$\Psi_{n+1} = \Psi_n - \frac{f(\Psi_n)}{f'(\Psi_n)}$
Vapor molar flow rate	$V = \Psi F$
Liquid molar flow rate	$L = F - V$
Vapor mole fraction	$x_i = \frac{z_i}{1 + \Psi(K_i - 1)}$
Liquid mole fraction	$y_i = \frac{z_i K_i}{1 + \Psi(K_i - 1)}$
Heat	$Q = h_V V + h_L L - h_F F$



Flash Vaporization

Partial Condensation

Flash operations of flash vaporization and partial condensation. (*Separation Process Principles with Applications Using Process Simulators 4e* by Seader p93, Figures 4.8, 4.9.)

| Bubble and dew point calculations

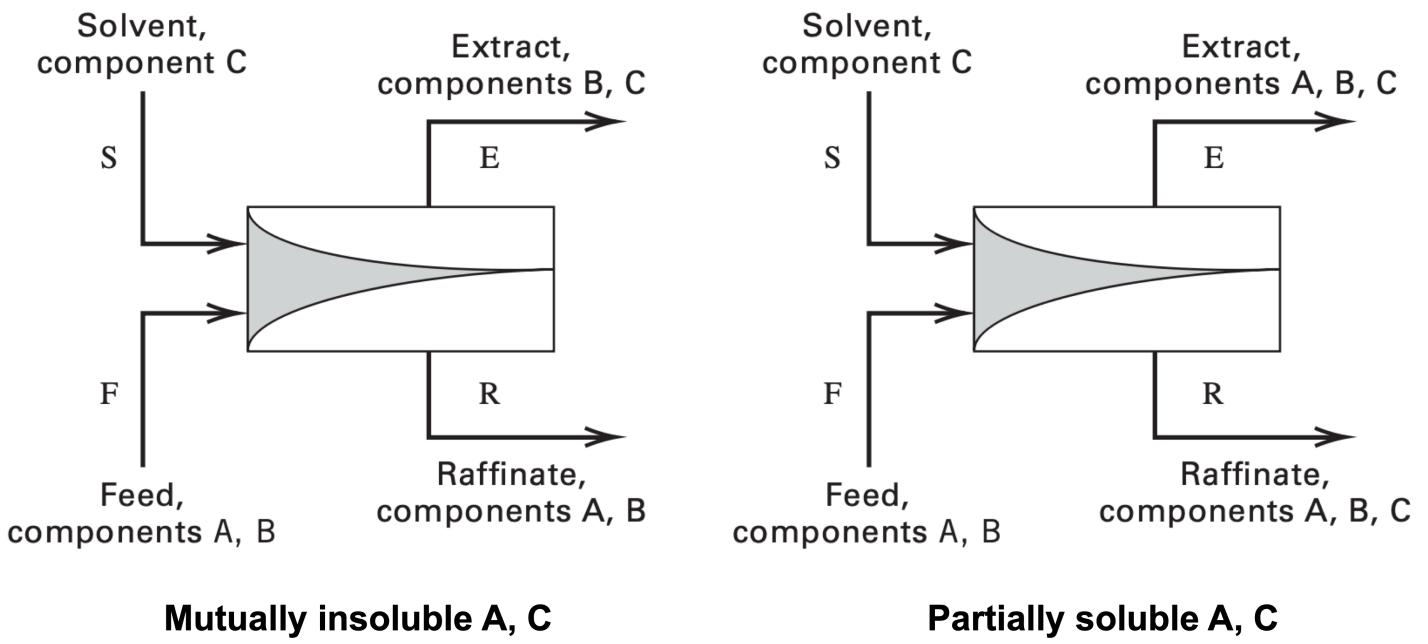
Description	Equations
Bubble point	$\Psi = 0$ $\sum z_i K_i = 1$ $\sum \frac{y_i}{P_i^*(T)} = \frac{1}{P}$
Dew point	$\Psi = 1$ $\sum \frac{z_i}{K_i} = 1$ $\sum x_i P_i^*(T) = P$

| Ternary liquid-liquid extraction

Symbol Conventions

- Components
 - A - Carrier (feed solvent)
 - B - Solute
 - C - Solvent
- Mass flow rates
 - F - Feed
 - S - Solvent
 - E - Extract (Majority of solvent C carrier extracted solute B)
 - R - Raffinate
- Mass fraction of component i
 - x_i - In the liquid
 - y_i - In the vapor
 - z_i - Overall
- Mass ratio of component i
 - X_i - In the liquid
 - Y_i - In the vapor

Description	Equations	
Mass fraction	$x_i = \frac{m_i}{m}$	
Mass ratio	$X_i = \frac{m_i}{m - m_i}$	
Conversion between mass fraction and ratio	$X_i = \frac{x_i}{1 - x_i}$ $x_i = \frac{X_i}{1 - X_i}$	
Solute balance ★ Solvent A, Solute B ★ Feed F, Solvent S, Extract E, Raffinate R	$F_B = E_B + R_B$ $X_{F,B}F_A = Y_{E,B}S + X_{R,B}F_A$ $X_{F,B}F_A = K'_{D_B}X_{R,B}S + X_{R,B}F_A$ $X_{R,B} = \frac{X_{F,B}F_A}{F_A + K'_{D_B}S}$	$Y_{E,B} = K'_{D_B}X_{R,B}$
Extraction factor of solute B	$\mathcal{E} = \frac{K'_{D_B}S}{F_A}$	
Fraction of solute B unextracted	$\frac{X_{R,B}}{X_{F,B}} = \frac{1}{1 + \mathcal{E}}$	



Mutually insoluble A, C

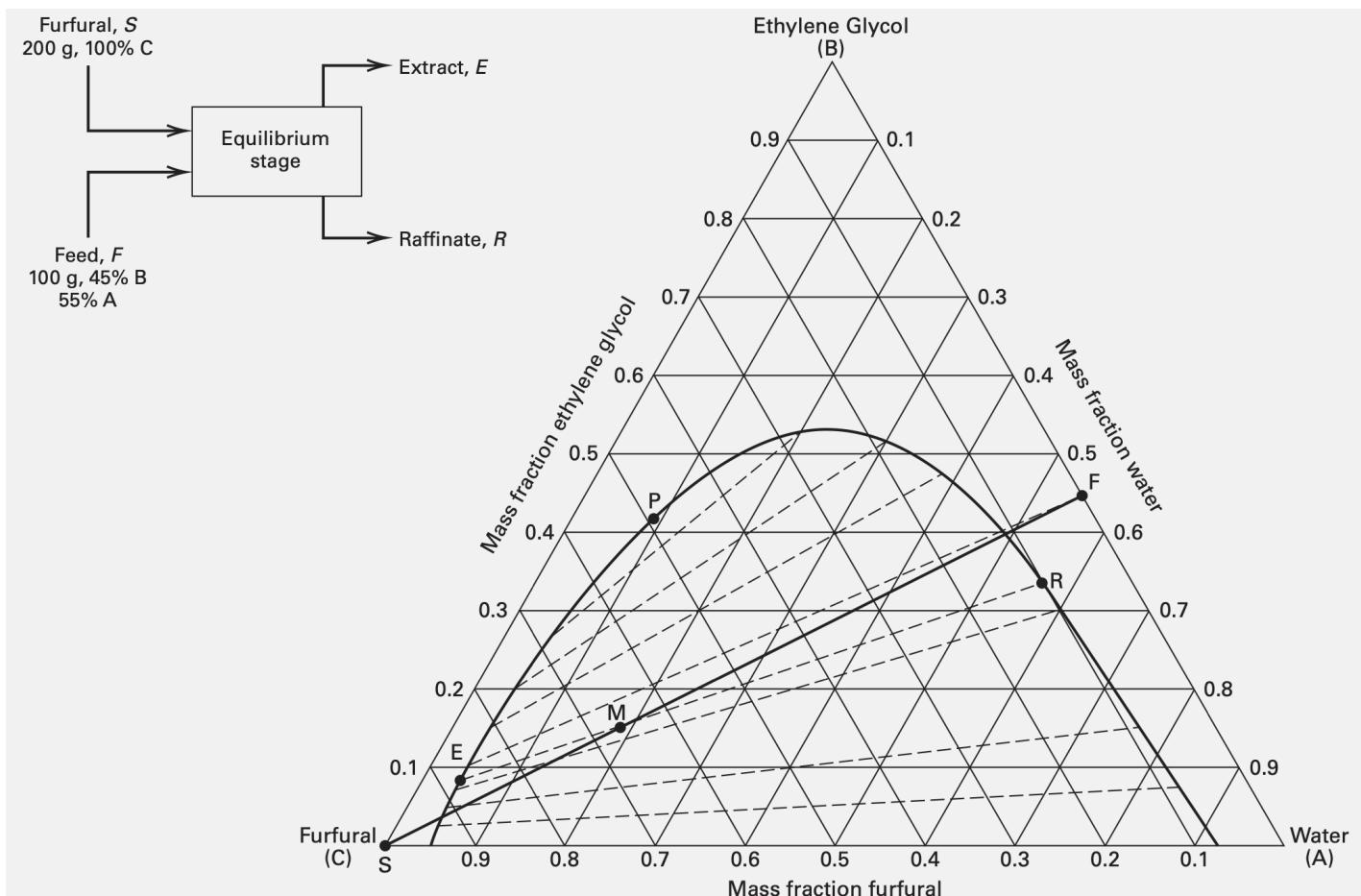
Partially soluble A, C

Liquid-liquid extraction of ternary mixture. (*Separation Process Principles with Applications Using Process Simulators 4e* by Seader p98, Figure 4.12.)

| Ternary phase diagram

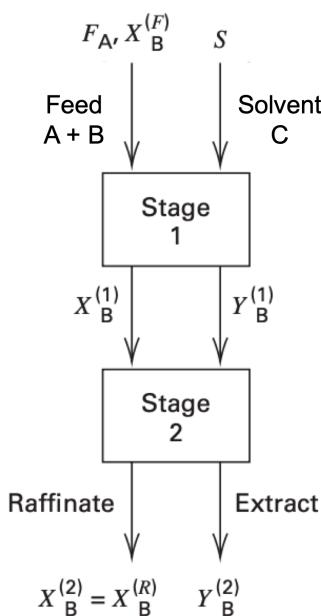
General principles are the same for different types of ternary phase diagrams. Here, algorithm for using **equilateral** ternary phase diagrams is presented.

- Identify chemical species at the apexes: feed solvent (A), feed solute (B), and pure solvent (S)
 - Apexes are pure components
 - Lines parallel to the apex are used to read values
 - Label each side of the triangle according to the apex
- Identify compositions of entering streams: feed (F) and solvent (S)
 - Assume feed only contains A and B, and solvent is pure S
 - Calculate composition of mixture (M) with component balances
 - $x_{M,A} = \frac{x_{F,A}F}{F+S}$, $x_{M,B} = \frac{x_{F,B}F}{F+S}$, $x_{M,C} = \frac{S}{F+S}$
- Interpolate tie line on the ternary phase diagram
- Identify compositions of exiting streams: extract (E) and raffinate (R)
 - E and R lies on the intersection of tie line and miscibility boundary (binodal) curve
 - E has a larger S component than R (extracted component is dissolved in solvent), being closer to point S
- Identify plait point (P)
 - P lies between E and R on the miscibility boundary curve
 - P is the point where E and R merge together and tie line collapses to a point
- Determine flow rate ratio with inverse level rule
 - $\frac{E}{F+S} = \frac{E}{E+R} = \frac{MR}{ER}$, $\frac{E}{R} = \frac{MR}{ME}$

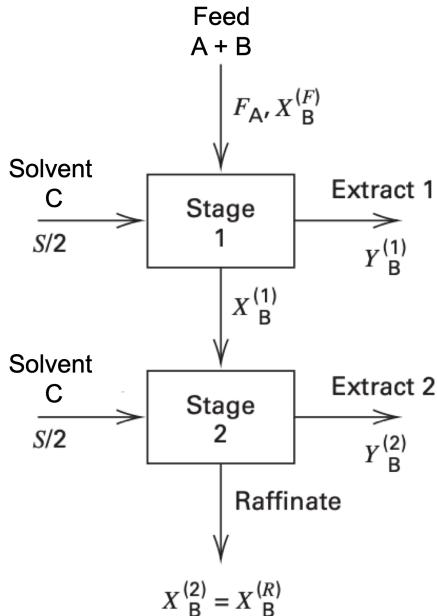


Multistage Cascades

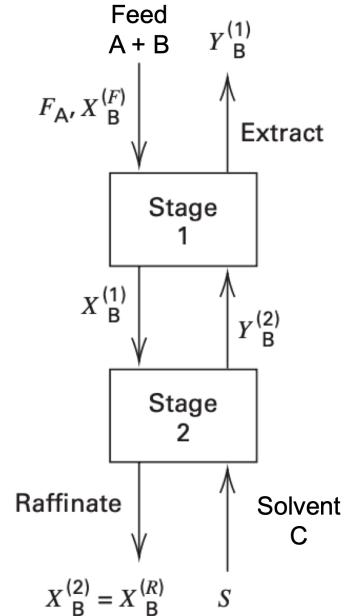
Configuration	Fraction of solute B unextracted
Single stage	$\frac{X_{R,B}}{X_{F,B}} = \frac{1}{1 + \mathcal{E}}$
Cocurrent cascade (N stages)	$\frac{X_{N,B}}{X_{F,B}} = \frac{1}{1 + \mathcal{E}}$
Crosscurrent cascade (N stages)	$\frac{X_{N,B}}{X_{F,B}} = \frac{1}{(1 + \mathcal{E}/N)^N}$
Crosscurrent cascade (∞ stages)	$\frac{X_{\infty,B}}{X_{F,B}} = \frac{1}{\exp(\mathcal{E})}$
Countercurrent cascade (N stages)	$\frac{X_{R,B}}{X_{F,B}} = \left[\sum_{n=0}^N \mathcal{E}^n \right]^{-1} = \frac{\mathcal{E} - 1}{\mathcal{E}^{N+1} - 1}$
Countercurrent cascade (∞ stages)	$\begin{cases} \frac{X_{\infty,B}}{X_{F,B}} = 0, & \mathcal{E} \in [1, \infty) \\ \frac{X_{\infty,B}}{X_{F,B}} = 1 - \mathcal{E}, & \mathcal{E} \in (-\infty, 1) \end{cases}$



Cocurrent



Crosscurrent



Countercurrent

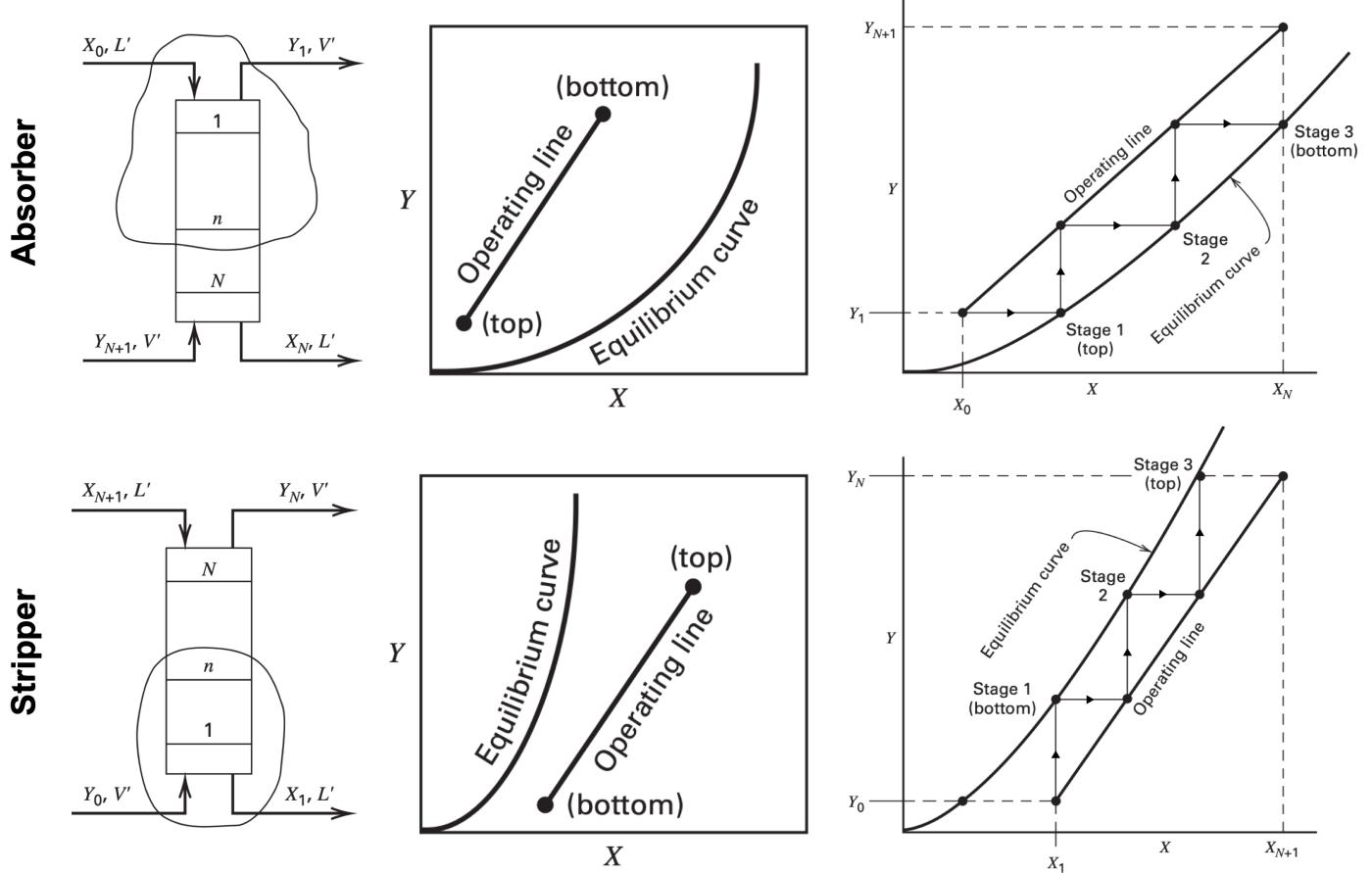
Multistage arrangements of cocurrent, crosscurrent, and countercurrent. (*Separation Process Principles with Applications Using Process Simulators 4e* by Seader p120, Figures 5.4.)

Absorption and Stripping

| Graphical method for trayed towers

Symbol Conventions

- Molar flow rates**
 - L - Total liquid feed
 - V - Total gas feed
 - L' - solute-free absorbent - constant at each stage
 - V' - solute-free gas (carrier gas) - constant at each stage
- Mole ratio of solute to solute-free absorbent**
 - X - In the liquid
 - Y - In the vapor



Equilibrium curve and operating lines of absorber and stripper. (*Separation Process Principles with Applications Using Process Simulators 4e* by Seader p144, 146, Figures 6.9, 6.12.)

- Construct the equilibrium curve from thermodynamics
 - $K_n = \frac{y_n}{x_n} = \frac{Y_n}{X_n} \frac{1 + X_n}{1 + Y_n} \implies Y_n = \frac{K_n X_n}{1 + X_n - K_n X_n}$
- Identify absorption and stripping process
 - Absorption - Use liquid to remove components from gas mixture
 - Stripping - Use gas to remove components from liquid mixture
- Construct operating line for ∞ stages for L'_{\min} or V'_{\min}
 - Absorption (L'_{\min})
 - Identify (liquid in, gas out) = (X_0, Y_1)
 - Identify (liquid out, gas in) = (X_N, Y_{N+1}) with minimum operating line intersects and ends at the equilibrium curve
 - Stripping (V'_{\min})
 - Identify (gas in, liquid out) = (X_1, Y_0)
 - Identify (liquid out, gas in) = (X_{N+1}, Y_N) with minimum operating line intersects and ends at the equilibrium curve
 - Slope of operating line = $\frac{L'}{V'}$
- Determine number of equilibrium stages for L' and V'
 - Absorption (L')
 - Construct operating line with point (liquid in, gas out) = (X_0, Y_1) and slope = $\frac{L'}{V'}$
 - From (X_0, Y_1) , draw horizontal line toward the equilibrium curve and vertical lines back to the operating line until it reaches (X_N, Y_{N+1})
 - Stripping (V')
 - Construct operating line with point (gas in, liquid out) = (X_1, Y_0) and slope = $\frac{L'}{V'}$
 - From (X_1, Y_0) , draw horizontal line toward the equilibrium curve and vertical lines back to the operating line until it reaches (X_{N+1}, Y_N)
 - The number of equilibrium stages is the number of intersections on the equilibrium curve
 - Interpolate number of stages if not exact

| Absorption

	Description	Equations
Absorption operating line		$Y_{n+1} = X_n \frac{L'}{V'} + Y_1 - X_0 \frac{L'}{V'}$
Absorbent flow rate		$L' = V' \frac{Y_{N+1} - Y_1}{X_N - X_0}$
Minimum absorbent flow rate (∞ stages)		$L'_{\min} = V' K_N \cdot (\text{fraction solute absorbed})$
Absorption factor		$\mathcal{A} = \frac{L}{KV}$

| Stripping

	Description	Equations
Stripping operating line		$Y_n = X_n \frac{L'}{V'} + Y_0 - X_1 \frac{L'}{V'}$
Stripping agent flow rate		$V' = L' \frac{X_N - X_1}{Y_N - Y_0}$
Minimum stripping agent flow rate (∞ stages)		$V'_{\min} = \frac{L'}{K_N} \cdot (\text{fraction solute stripped})$
Stripping factor		$\mathcal{S} = \frac{V}{L}$
Relating stripping factor and adsorption factor		$\mathcal{S} = \frac{1}{\mathcal{A}}$

| Stage efficiency and packed columns

	Description	Equations
Overall stage efficiency		$E_o = \frac{\# \text{ theoretical stages}}{\# \text{ actual stages}}$
Drickamer and Bradford correlation ★ Hydrocarbons, $\mu_L \in (0.2, 1.6)$ cP		$E_o[\%] = 19.2 - 57.8 \log(\mu_L)$
Height equivalent to a theoretical plate (HETP)		$\text{HETP} = \frac{l_T}{N_t} = \frac{\text{packed height}}{\# \text{ equiv eqm stages}}$
Packed height		$l_T = H_{OG} N_{OG}$
Overall height of a transfer unit (HTU)		$H_{OG} = \frac{V}{K_y a A_c}$
Overall number of transfer unit (NTU)		$N_{OG} = \int_{y_{\text{out}}}^{y_{\text{in}}} \frac{dy}{y - y^*}$
Overall volumetric mass transfer coefficient		$K_y a$

Distillation of Binary Mixtures

| McCabe-Thiele graphical method for trayed towers

ⓘ Symbol Conventions

- Molar flow rates
 - F - Feed
 - D - Distillate
 - B - Bottoms

- L - Liquid in the rectifying section, Reflux
- V - Vapor in the rectifying section
- \bar{L} - Liquid in the stripping section
- \bar{V} - Vapor in the stripping section, Boilup
- Mole fraction of the light key component
 - x - In the liquid
 - y - In the vapor
 - x_D - In the distillate
 - x_B - In the bottoms
- Ratio
 - $\alpha_{1,2}$ - Relative volatility
 - R - Reflux ratio
 - V_B - Boilup ratio

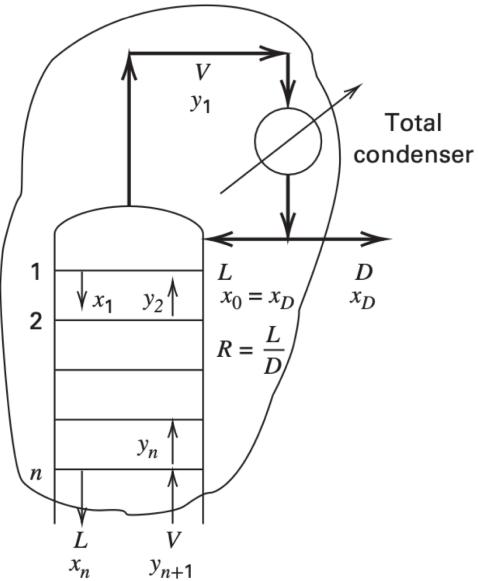
	Description	Equations
McCabe-Thiele assumptions		1. Equal and constant ΔH_{vap} 2. Negligible $C_P \Delta T$ and ΔH_{mix} 3. Insulated column $q = 0$ 4. No pressure drop $\Delta P = 0$
Constant molar overflow in rectifying section		$L_1 = L_i = L$ $V_1 = V_i = V$
Constant molar overflow in stripping section		$\bar{L}_1 = \bar{L}_i = \bar{L}$ $\bar{V}_1 = \bar{V}_i = \bar{V}$
Non-equal flow rate in rectifying and stripping sections		$L \neq \bar{L}$ $V \neq \bar{V}$
Reflux ratio		$R = \frac{L}{D}$
Boilup ratio		$V_B = \frac{\bar{V}}{B}$
Equilibrium curve		$y_1 = \frac{\alpha_{1,2}x_1}{1 + x_1(\alpha_{1,2} - 1)}$
Rectifying section operating line		$y = \left(\frac{R}{R+1} \right) x + \left(\frac{x_D}{R+1} \right)$
Stripping section operating line		$y = \left(\frac{V_B+1}{V_B} \right) x - \left(\frac{x_B}{V_B} \right)$
q -parameter		$\begin{cases} q > 1 & \text{subcooled liq} \\ q = 1 & \text{saturated liq (bubble pt)} \\ q \in (0, 1) & \text{liq + vap} \\ q = 0 & \text{saturated vap (dew pt)} \\ q < 0 & \text{superheated vap} \end{cases}$
q -parameter		$q = \frac{\bar{L} - L}{F} = 1 + \frac{\bar{V} - V}{F}$
q -line		$y = \left(\frac{q}{q-1} \right) x + \left(\frac{z_F}{q-1} \right)$

| Limiting conditions

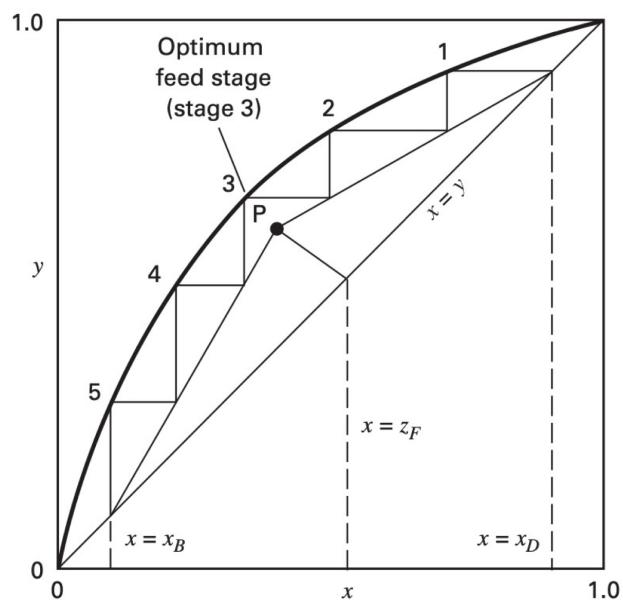
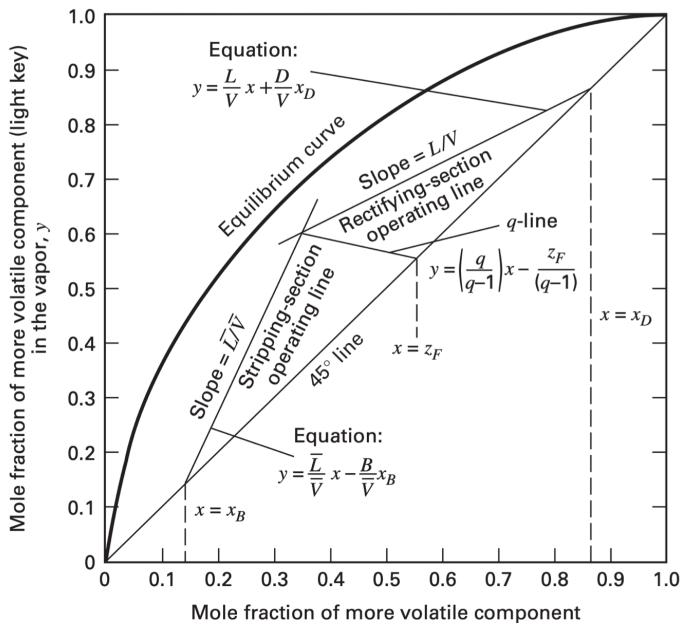
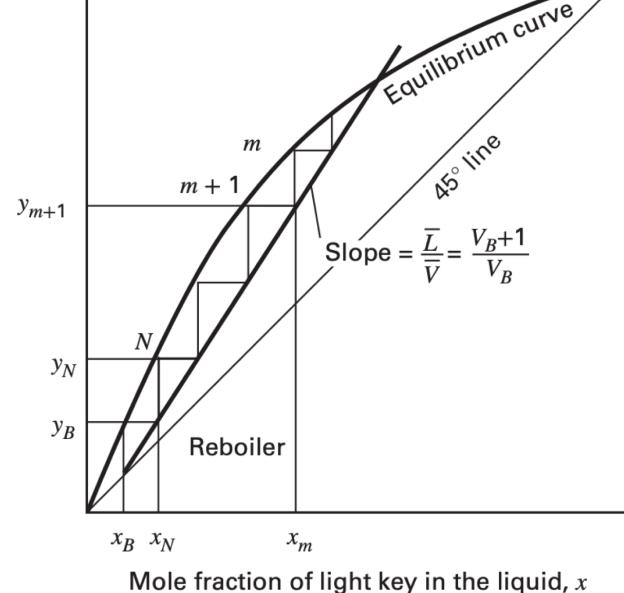
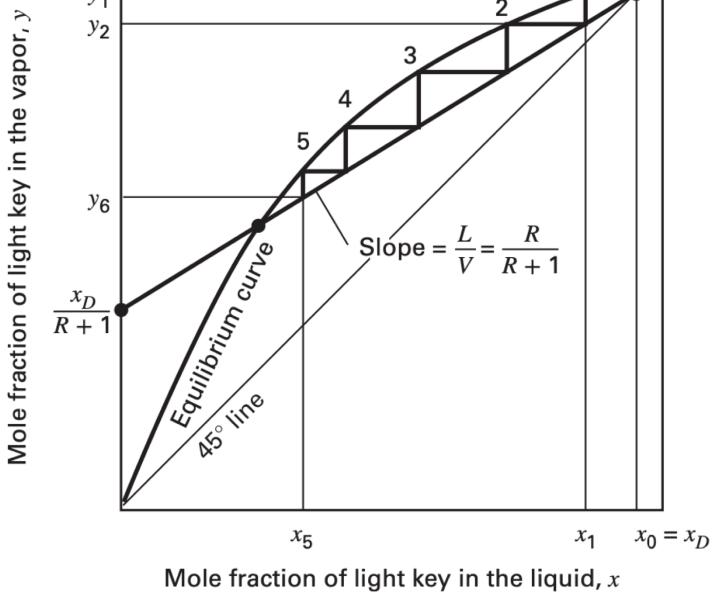
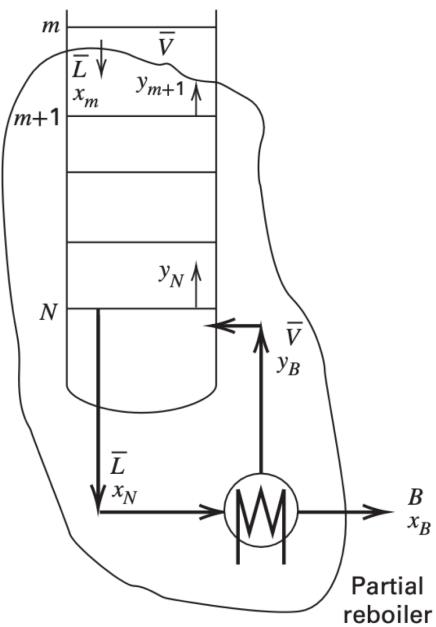
	Description	Equations
Total reflux (Useless)		$R_\infty = \infty$ $N_{\min} = 0$

Description	Equations
	$L = V$
	$D = B = 0$
	$R_{\min} = \frac{(L/V)_{\min}}{1 - (L/V)_{\min}}$
Minimum reflux	$N_{\infty} = \infty$
	$V_{B,\min} = \frac{1}{(\overline{L}/\overline{V})_{\min} - 1}$
	$x_D = 1, \quad x_B = 0$
Perfect separation	$R \geq R_{\min} \begin{cases} R_{\min} = \frac{1}{z_F(\alpha_{1,2} - 1)} & q = 1 \\ R_{\min} = \frac{\alpha_{1,2}}{z_F(\alpha_{1,2} - 1)} - 1 & q = 0 \end{cases}$

Rectifying Section



Stripping Section



(light key) in the liquid, x

Equilibrium curve and operating lines of rectifying and stripping sections of distillation column. Optimal feed stage is indicated by the transition between operating lines on the equilibrium curve. (*Separation Process Principles with Applications Using Process Simulators* 4e by Seader p195, 196, 197, 200, Figures 7.5, 7.6, 7.7, 7.10.)

Membrane Separations

Description	Equations
Transmembrane molar flux	$N_i = \frac{P_{M,i}}{l_M} \cdot (\text{driving force})$ $= \bar{P}_{M,i} \cdot (\text{driving force})$
Permeance	$\bar{P}_{M,i} = \frac{P_{M,i}}{l_M}$
Permeability	$P_{M,i} = \bar{P}_{M,i} l_M$
Selectivity	$S_{i,j} = \frac{P_{M,i}}{P_{M,j}}$
Gas permeability unit	1 barrer $= 10^{-10} \text{ cm}_\text{STP}^3 \cdot \text{cm}/(\text{cm}^2 \cdot \text{s} \cdot \text{cmHg})$ $= 3.35 \times 10^{-16} \text{ mol} \cdot \text{m}/(\text{m}^2 \cdot \text{s} \cdot \text{Pa})$ $= 5.58 \times 10^{-12} \text{ lbmol} \cdot \text{ft}/(\text{ft}^2 \cdot \text{h} \cdot \text{psi})$
Mole of gas in standard temperature and pressure (STP)	$1 \text{ mol} \sim 22.4 \text{ L}_\text{STP}$

| Transport through porous membranes

| Bulk flow

Description	Equations
Hagen-Poiseuille flow ★ Laminar flow $\text{Re} < 2100$	$v = \frac{D^2}{32\mu L}(P_0 - P_L)$
Pore number density	$n = \frac{n_\text{total}}{A_c} = \frac{\text{total } \# \text{ of pores}}{\text{membrane cross sectional area}}$
Porosity (void fraction) ★ Straight cylindrical pore	$\varepsilon = \frac{1}{4}n\pi D^2$
Bulk flow flux ★ Straight cylindrical pore	$N = v\rho\varepsilon$ $= \frac{\varepsilon\rho D^2}{32\mu l_M}(P_0 - P_L)$ $= \frac{n\pi\rho D^4}{128v l_M}(P_0 - P_L)$
Empirical hydraulic diameter	$d_H = \frac{4\varepsilon}{a_v}$
Specific surface area	$a_v = \frac{a}{1 - \varepsilon}$
Total pore surface area	$a = a_v(1 - \varepsilon)$
Tortuosity correction of membrane width	τl_M
Bulk flow flux ★ General pore	$N = \frac{\rho\varepsilon^2}{2(1 - \varepsilon)^2\tau a_v^2\mu l_M}(P_0 - P_L)$
Ergun equation	$\frac{P_0 - P_L}{l_M} = \frac{150\mu v_0(1 - \varepsilon)^2}{D_P^2\varepsilon^3} + \frac{1.75\rho v_0^2(1 - \varepsilon)}{D_P\varepsilon^3}$

Description	Equations
Mean spherical particle diameter	$D_P = \frac{6}{a_v}$

| Liquid diffusion

Description	Equations
Concentration driving force	$\Delta c \neq 0$ $\Delta P = 0$
Transmembrane mass flux	$N_i = \frac{D_{e,i}}{l_M} (c_{i,0} - c_{i,L})$
Effective diffusivity	$D_{e,i} = \frac{\varepsilon D_i}{\tau} K_{r,i}$
Restrictive factor of solute	$K_r = \left[1 - \frac{d_m}{d_p} \right]^4$
Selectivity	$S_{i,j} = \frac{D_i K_{r,i}}{D_j K_{r,j}}$

| Gas diffusion

Description	Equations
Transmembrane molar flux ★ Ideal gas, uniform transmembrane T, P	$N_i = \frac{c_M}{P} \frac{D_{e,i}}{l_M} (P_{i,0} - P_{i,L})$ $= \frac{1}{RT} \frac{D_{e,i}}{l_M} (P_{i,0} - P_{i,L})$
Effective diffusivity	$D_{e,i} = \frac{\varepsilon}{\tau} \left[\frac{1}{(1/D_i) + (1/D_{K,i})} \right]$
Knudsen diffusivity of straight cylindrical pore ★ Kinetic theory of gas	$D_{K,i} [\text{cm/s}] = 4850 d_p [\text{cm}] \sqrt{\frac{T}{\mathcal{M}_i}} \frac{[\text{K}]}{[\text{g/mol}]}$
Selectivity of Knudsen diffusion ★ $D_i \gg D_{K,i}$ ★ $D_{e,i} \sim D_{K,i}$	$S_{i,j} = \frac{P_{M,i}}{P_{M,j}} = \sqrt{\frac{\mathcal{M}_j}{\mathcal{M}_i}}$

| Transport through nonporous (dense) membranes

| Solution-diffusion of liquid mixtures

Description	Equations
Thermodynamic equilibrium partition coefficient	$K_i = \frac{c_i}{c'_i}$
Transmembrane mass flux ★ Fick's law	$N_i = \frac{D_i}{l_M} (c_{i,0} - c_{i,L})$
Transmembrane mass flux ★ $K_{i,0} = K_{i,L} = K_i$	$N_i = \frac{K_i D_i}{l_M} (c'_{i,0} - c'_{i,L})$
Transmembrane mass flux ★ No mass transfer resistance in fluid boundary layers ★ $c'_{i,0} = c_{i,F}$ and $c'_{i,L} = c_{i,P}$	$N_i = \frac{K_i D_i}{l_M} (c_{i,F} - c_{i,P})$

| Solution-diffusion of gas mixtures

	Description	Equations
	Henry's constant	$H_i = \frac{c_i}{P_i}$
	Transmembrane mass flux ★ Fick's law	$N_i = \frac{D_i}{l_M} (c_{i,0} - c_{i,L})$
	Transmembrane mass flux ★ $H_{i,0} = H_{i,L} = H_i$	$N_i = \frac{H_i D_i}{l_M} (P_{i,0} - P_{i,L})$
★ No mass transfer resistance in external boundary layers ★ $P_{i,0} = P_{i,F}$ and $P_{i,L} = P_{i,P}$	Transmembrane mass flux	$N_i = \frac{H_i D_i}{l_M} (P_{i,F} - P_{i,P})$

| Separation factor

	Description	Equations
	Ideal separation factor	
★ Downstream permeate pressure negligible compared to upstream feed pressure ★ $x_{i,P} P_P \ll x_{i,F} P_F$ and $x_{j,P} P_P \ll x_{j,F} P_F$		$\alpha_{i,j}^* = \frac{H_i D_i}{H_j D_j} = \frac{P_{M,i}}{P_{M,j}}$
	Separation factor	$\alpha_{i,j} = \alpha_{i,j}^* \left[\frac{(x_{j,F}/x_{j,P}) - r\alpha_{i,j}}{(x_{j,F}/x_{j,P}) - r} \right]$
Cut (fraction of feed permeated)		$\theta = \frac{\dot{n}_P}{\dot{n}_F}$

| Summary of transport through membranes

Type of transport	Permselective	Membrane Type	Driving Force	Permeability
(L) Bulk flow	No	Macroporous	ΔP	$P_M = \frac{\rho \varepsilon^3}{2(1-\varepsilon)^2 \tau a_v^2 \mu}$
(L) Molecular diffusion	Yes	Microporous	Δc	$P_M = D_{e,i} = \frac{\varepsilon D_i K_{r,i}}{\tau}$
(G) Molecular diffusion ★ high P ★ $d_p > d_m$	Yes	Microporous	$\frac{\Delta P_i}{\Delta P = 0}$	$P_{M,i} = \frac{D_{e,i}}{RT}$
(G) Knudsen diffusion ★ low P ★ $d_p \sim d_m$	Yes	Microporous	$\frac{\Delta P_i}{\Delta P = 0}$	$P_{M,i} = \frac{D_{e,i}}{RT}$
(L) Solution diffusion	Yes	Nonporous (dense)	Δc	$P_{M,i} = K_i D_i$
(G) Solution diffusion	Yes	Nonporous (dense)	$\frac{\Delta P_i}{\Delta P = 0}$	$P_{M,i} = H_i D_i$

| Reverse osmosis

Description	Equations
Osmotic pressure ★ Equilibrium	$\Pi \equiv P_1 - P_{\text{H}_2\text{O}}$
Osmotic pressure of water	$\Pi_{\text{H}_2\text{O}} = 0$
Osmotic process	$P_1 - P_{\text{H}_2\text{O}} < \Pi$
Reverse osmotic process	$P_1 - P_{\text{H}_2\text{O}} > \Pi$
Osmotic pressure's thermodynamic derivation ★ Between pure water and solution ★ Solvent <i>A</i> , solute <i>B</i>	$\Pi = -\frac{RT}{v_A} \ln(x_A \gamma_A)$
Osmotic pressure ★ Ideal solution, dilute <i>B</i>	$\Pi = \frac{RTn_B}{v_A} = \frac{RTc_B}{M_B}$

| Seawater reverse osmosis

Description	Equations
Seawater as solution 1; salt as solute B	$A = \text{water} = \text{H}_2\text{O}$ $B = \text{salt} = \text{S}$
Molar mass	$\mathcal{M} = \frac{m}{n}$
Molarity (molar concentration)	$M = \frac{n}{V} = \frac{\text{wt\% S}}{100\% - \text{wt\% S}} \frac{\rho_{\text{H}_2\text{O}}}{\mathcal{M}_S}$
Seawater osmotic pressure correlation	$\Pi [\text{psia}] = 1.12T [\text{K}] \sum M_i [\text{mol/L}]$
Transmembrane molar flux of water (solvent A)	$N_{\text{H}_2\text{O}} = \frac{P_{M,\text{H}_2\text{O}}}{l_M} (\Delta P - \Delta \pi)$
Salt passage	$SP = \frac{c_{S,P}}{c_{S,F}}$
Salt rejection	$SR = 1 - SP$
Concentration polarization factor	$\Gamma \equiv \frac{c_{S,i} - c_{S,F}}{c_{S,F}} = \frac{N_{\text{H}_2\text{O}}(SR)}{k_S}$
Significant concentration polarization	$\Gamma > 0.2$