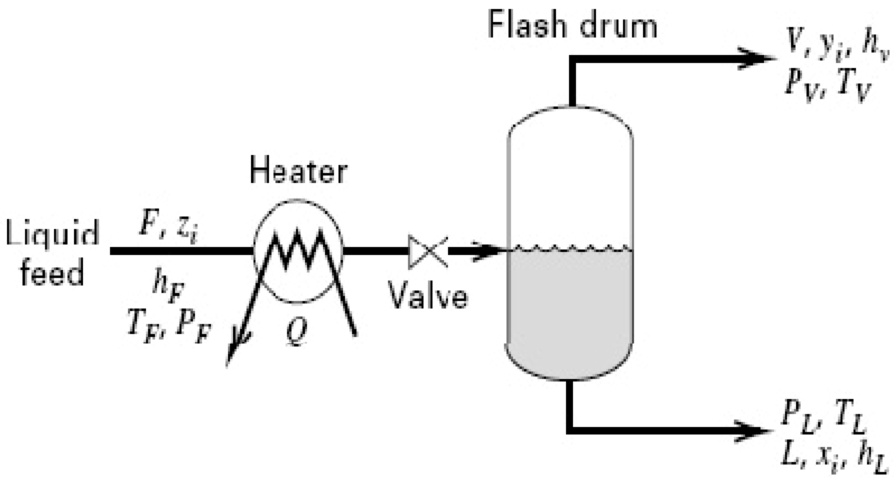
Lecture 6.
Single Equilibrium Stages (2)
[Ch. 4]

- Multicomponent Flash, Bubble-Point, and Dew-Point Calculations
  - Variables and equations in flash vaporization
  - Isothermal flash
  - Bubble and dew points
  - Adiabatic flash
- Ternary Liquid-Liquid Systems
  - Carrier A and solvent C mutually insoluble
  - Carrier A and solvent C partially soluble

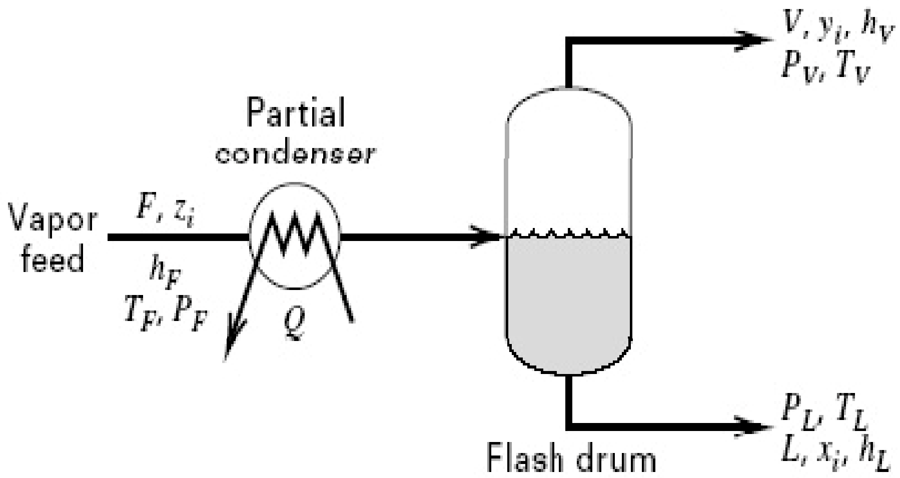
Flash Vaporization

- Flash : a single-equilibrium-stage distillation in which a feed is partially vaporized to give a vapor richer in the more-volatile components than the feed
- If the equipment is properly designed, the vapor and liquid leaving the flash drum are in equilibrium

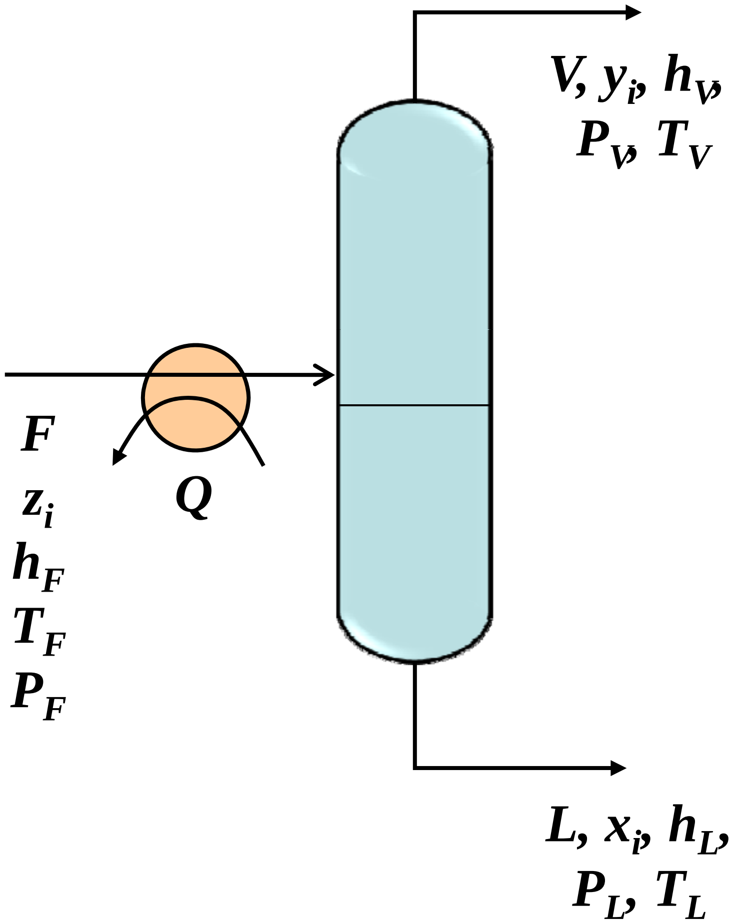
Flash vaporization



Partial condensation



Single–Stage Equilibrium Operation



- 3C + 10 variables

  F, V, L, z_i, y_i, x_i, T_F, T_V, T_L, P_F, P_V, P_L, Q

- 2C + 5 equations

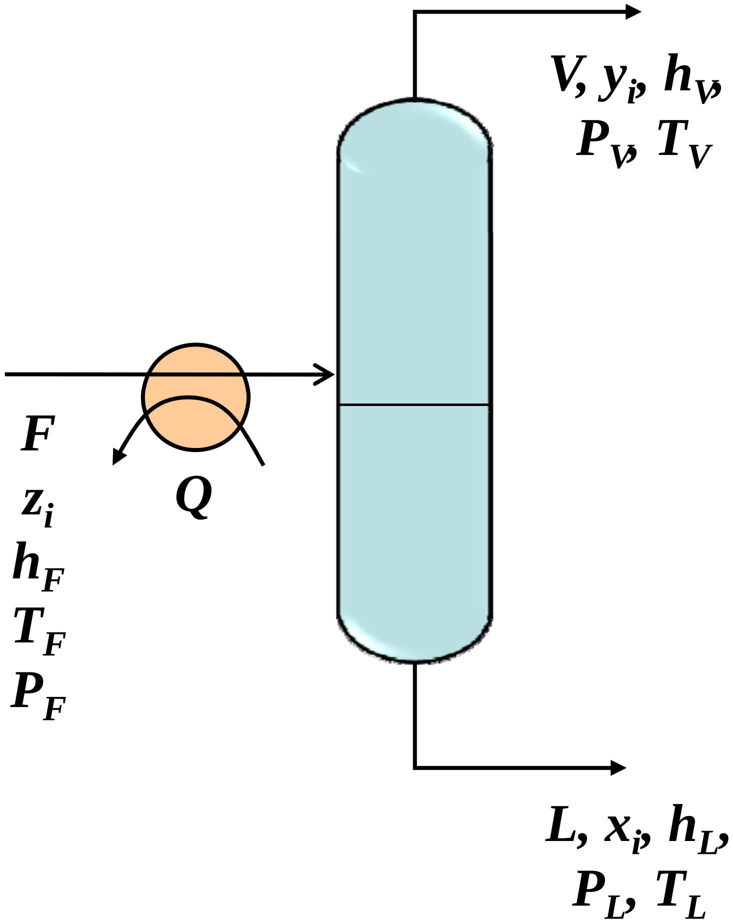
Equation		Number of Equations
(1) $P_V = P_L$	(mechanical equilibrium)	1
(2) $T_V = T_L$	(thermal equilibrium)	1
(3) $y_i = K_i x_i$	(phase equilibrium)	C
(4) $F z_i = V y_i + L x_i$	(component material balance)	C
(5) $F = V + L$	(total material balance)	1
(6) $h_F F + Q = h_V V + h_L L$	(energy balance)	1
(7) $\sum_i y_i - \sum_i x_i = 0$	(summations)	1
		$\mathscr{E} = 2C + 5$

$$K_i = K_i\{T_V, P_V, \mathbf{y}, \mathbf{x}\} \qquad h_F = h_F\{T_F, P_F, \mathbf{z}\}$$
$$h_V = h_V\{T_V, P_V, \mathbf{y}\} \qquad h_L = h_L\{T_L, P_L, \mathbf{x}\}$$

- C + 5 degrees of freedom

Common Sets of Specifications

- C + 3 feed variables (F, T_F, P_F, z_i) are known
  → 2 additional variables can be specified



• T_V, P_V	Isothermal flash
• V/F=0, P_L	Bubble-point T
• V/F=1, P_V	Dew-point T
• V/F=0, T_L	Bubble-point P
• V/F=1, T_V	Dew-point P
• Q=0, P_V	Adiabatic flash
• Q, P_V	Nonadiabatic flash
• V/F, P_V	Percent vaporization flash

Isothermal Flash (1)

- Isothermal flash calculation
  - When the equilibrium temperature T_V (or T_L) and the equilibrium pressure P_V (or P_L) are specified

    → 2C + 5 variables are determined from 2C + 5 equations
  - Not straightforward because of nonlinear equations
  - Use the Rachford-Rice procedure when K-values are independent of composition

Specified variables: $F, T_F, P_F, z_1, z_2, \ldots, z_C, T_V, P_V$

Steps

(1) $T_L = T_V$

(2) $P_L = P_V$

(3) Solve

$$f\{\Psi\} = \sum_{i=1}^{C} \frac{z_i(1-K_i)}{1+\Psi(K_i-1)} = 0$$

for $\Psi = V/F$, where $K_i = K_i\{T_V, P_V\}$.

(4) $V = F\Psi$

(5) $x_i = \dfrac{z_i}{1+\Psi(K_i-1)}$

(6) $y_i = \dfrac{z_i K_i}{1+\Psi(K_i-1)} = x_i K_i$

(7) $L = F - V$

(8) $Q = h_V V + h_L L - h_F F$

Isothermal Flash (2)

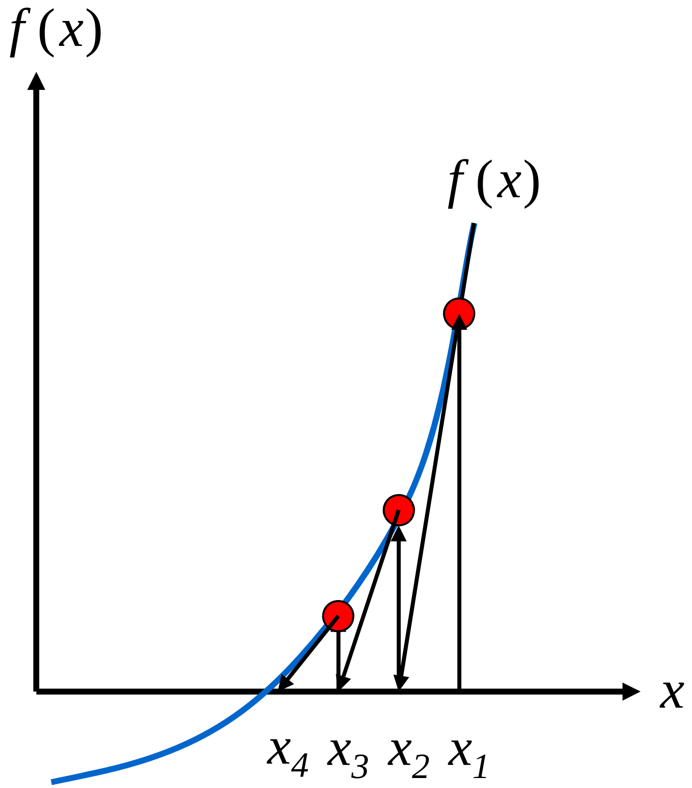
$$f\{\Psi\} = \sum_{i=1}^{C} \frac{z_i(1-K_i)}{1+\Psi(K_i-1)} = 0$$

- Solve iteratively by guessing values of Ψ between 0 and 1 until the function f{Ψ} = 0
- Newton's method

$$\Psi^{(k+1)} = \Psi^{(k)} - \frac{f\{\Psi^{(k)}\}}{f'\{\Psi^{(k)}\}}$$

$$f'\{\Psi^{(k)}\} = \sum_{i=1}^{C} \frac{z_i(1-K_i)^2}{\left[1+\Psi^{(k)}(K_i-1)\right]^2}$$

$$\left|\Psi^{(k+1)} - \Psi^{(k)}\right| / \Psi^{(k)} < \varepsilon\,(=0.0001)$$



Bubble and Dew Points (1)

$$f\{\Psi\} = \sum_{i=1}^{C} \frac{z_i(1-K_i)}{1+\Psi(K_i-1)} = 0$$

- At the bubble point, Ψ = 0 and f{0} = 0

$$f\{0\} = \sum_i z_i(1-K_i) = \sum_i z_i - \sum_i z_i K_i = 0 \quad \rightarrow \quad \boxed{\sum_i z_i K_i = 1}$$

- At the due point, Ψ = 1 and f{1} = 0

$$f\{1\} = \sum_i \frac{z_i(1-K_i)}{K_i} = \sum_i \frac{z_i}{K_i} - \sum_i z_i = 0 \quad \rightarrow \quad \boxed{\sum_i \frac{z_i}{K_i} = 1}$$

- For a given feed composition, z_i, the above equation can be used to find T for a specified P or to find P for a specified T

Bubble and Dew Points (2)

- How to determine K-values ?

(1) Plots of K-values for a specific T and P

(2) Equations for vapor-liquid equilibria

- Raoult's law $K_i = P_i^{sat} / P$
- Modified Raoult's law $K_i = \gamma_i P_i^{sat} / P$

(3) Iterative calculations

$$f\{P\} = \sum_i^C z_i K_i - 1 \qquad\qquad f\{P\} = \sum_i^C \frac{z_i}{K_i} - 1$$

⇓ Method of false position

$$P^{(k+2)} = P^{(k+1)} - f\{P^{(k+1)}\} / \left[\frac{f\{P^{(k+1)}\} - f\{P^{(k)}\}}{P^{(k+1)} - P^{(k)}} \right]$$

Adiabatic (Q=0) Flash

Start with guessed value of T_V

(wide-boiling mixtures)

Specified variables: F, T_F, P_F, $z_1, z_2, \ldots, z_C$, Q, P_V

Steps

Outer-loop

(1) $T_L = T_V$

(2) $P_L = P_V$

(3) Solve

$$f\{\Psi\} = \sum_{i=1}^{C} \frac{z_i(1-K_i)}{1+\Psi(K_i-1)} = 0$$

for $\Psi = V/F$, where $K_i = K_i\{T_V, P_V\}$.

Inner-loop

(4) $V = F\Psi$

(5) $x_i = \dfrac{z_i}{1+\Psi(K_i-1)}$

(6) $y_i = \dfrac{z_i K_i}{1+\Psi(K_i-1)} = x_i K_i$

(7) $L = F - V$

(8) $f\{T_V\} = \Psi h_V + (1-\Psi)h_L - h_F = 0$ Satisfy ?

Start with guessed value of Ψ

(close-boiling mixtures)

Specified variables: F, T_F, P_F, $z_1, z_2, \ldots, z_C$, Q, P_V

Steps

Outer-loop

Guess Ψ

(3) Solve

$$f\{T_V\} = \sum_{i=1}^{C} \frac{z_i(1-K_i)}{1+\Psi(K_i-1)} = 0$$

for $\Psi = V/F$, where $K_i = K_i\{T_V, P_V\}$.

Inner-loop

(4) $V = F\Psi$

(5) $x_i = \dfrac{z_i}{1+\Psi(K_i-1)}$

(6) $y_i = \dfrac{z_i K_i}{1+\Psi(K_i-1)} = x_i K_i$

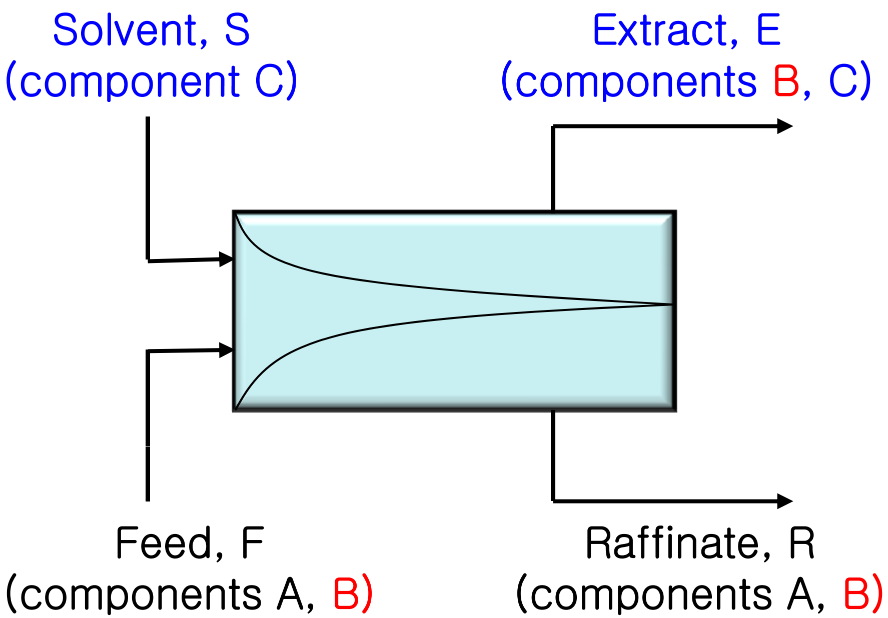
(7) $L = F - V$

(8) $f\{\Psi\} = \Psi h_V + (1-\Psi)h_L - h_F = 0$ Satisfy ?

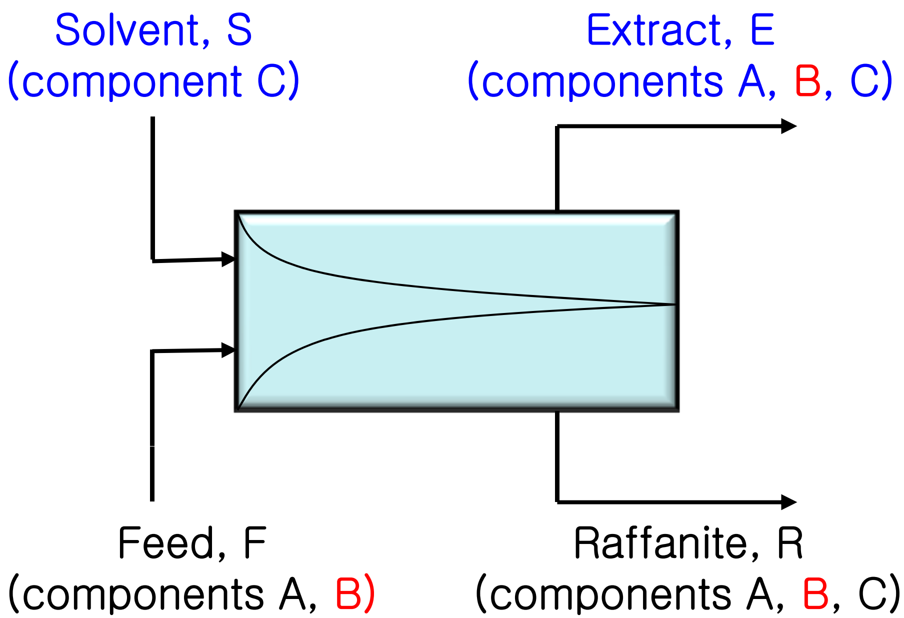
Ternary Liquid–Liquid Systems

- Ternary mixtures that undergo phase splitting to form two separate liquid phases : using solubility difference
- Extract : the exiting liquid phase that contains the solvent and the extracted solute
- Raffinate : the exiting liquid phase that contains the carrier, A, and the portion of the solute, B, that is not extracted

Components A and C mutually insoluble



Components A and C partially soluble



Components A and C mutually Insoluble

- Solute material balance

$$X_B^{(F)} F_A = X_B^{(E)} S + X_B^{(R)} F_A$$

$$K'_{D_B} = X_B^{(E)} / X_B^{(R)} \quad \rightarrow \quad X_B^{(E)} = K'_{D_B} X_B^{(R)}$$

X_B: ratio of mass (or moles) of solute B, to mass (or moles) of the other component in F, R, or E

K'_{D_B}: distribution coefficient defined in terms of mass or mole ratios

$$X_B^{(R)} = \frac{X_B^{(F)} F_A}{F_A + K'_{D_B} S}$$

- Extraction factor, E_B

$$E_B = K'_{D_B} S / F_A$$

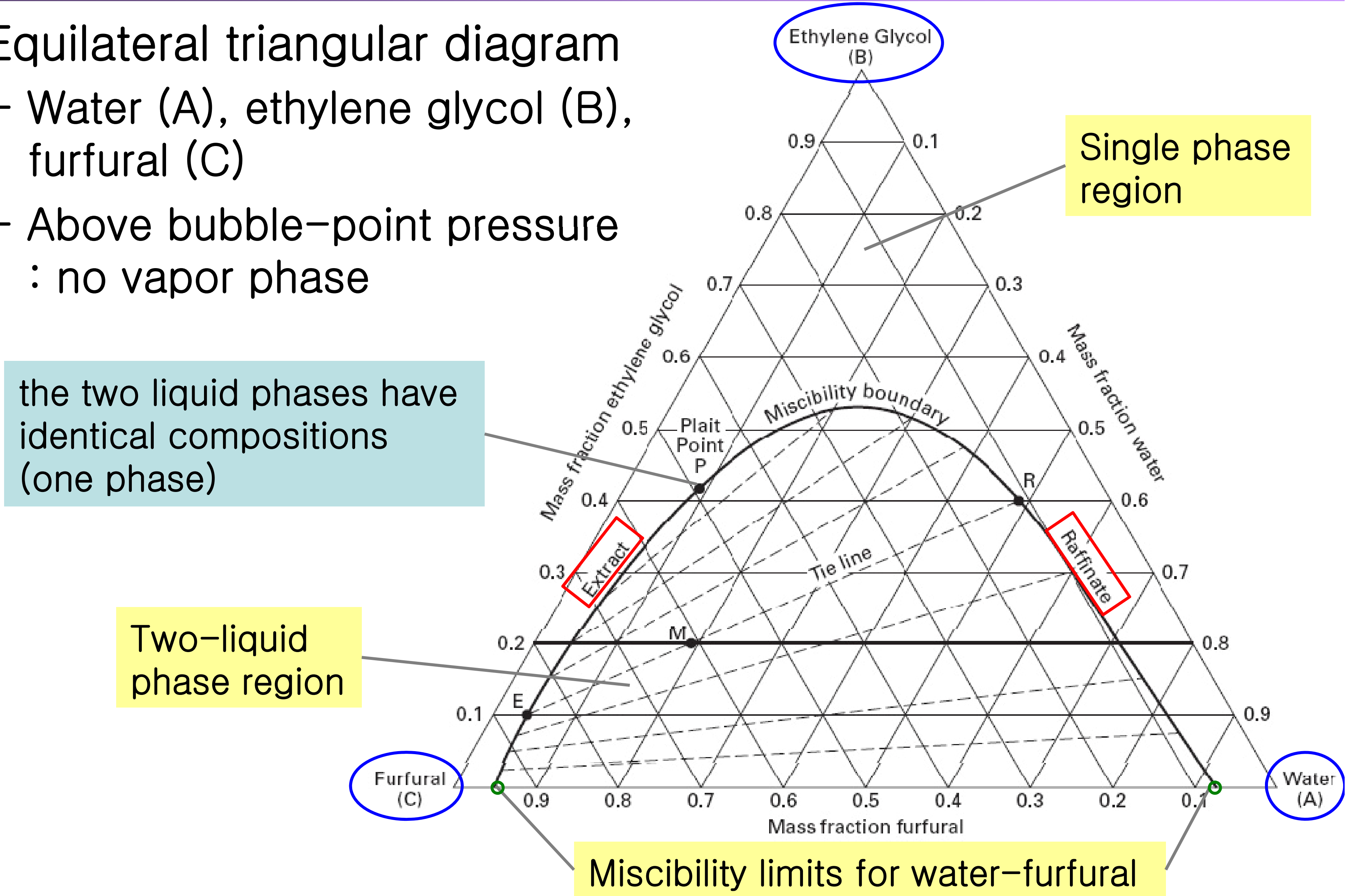
E↑ : (the extent to which the solute is extracted) ↑

$$X_B^{(R)} / X_B^{(F)} = \frac{1}{1 + E_B}$$

: fraction of B that is not extracted

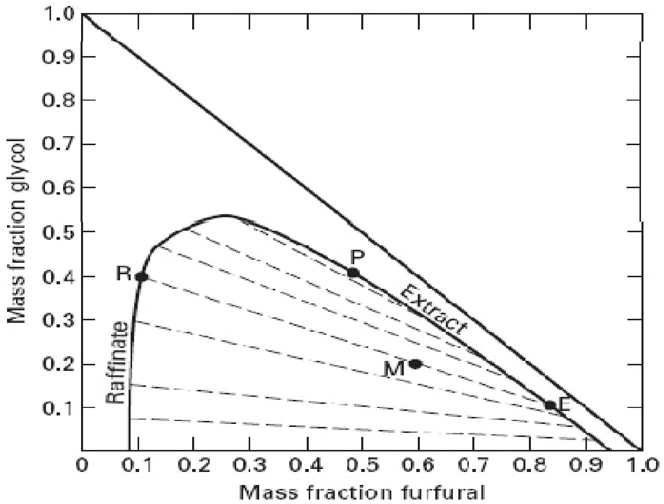
Components A and C Partially Soluble

- Equilateral triangular diagram
  - Water (A), ethylene glycol (B), furfural (C)
  - Above bubble-point pressure : no vapor phase

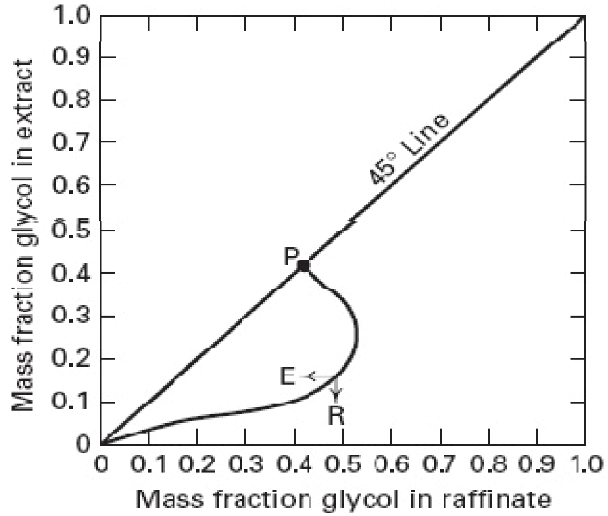


Other Liquid–Liquid Equilibrium Diagrams

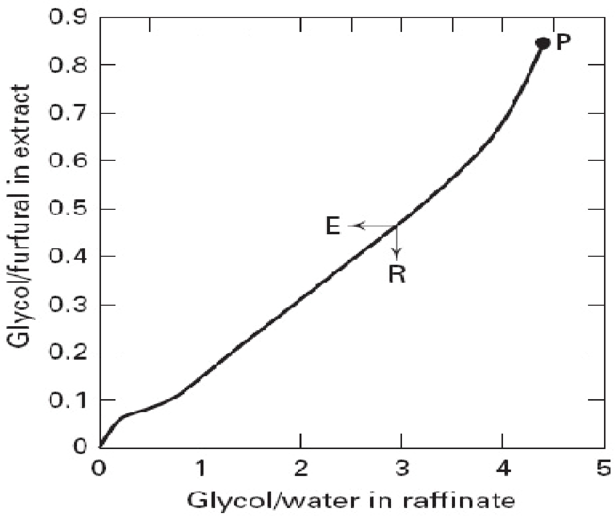
Right triangular diagram



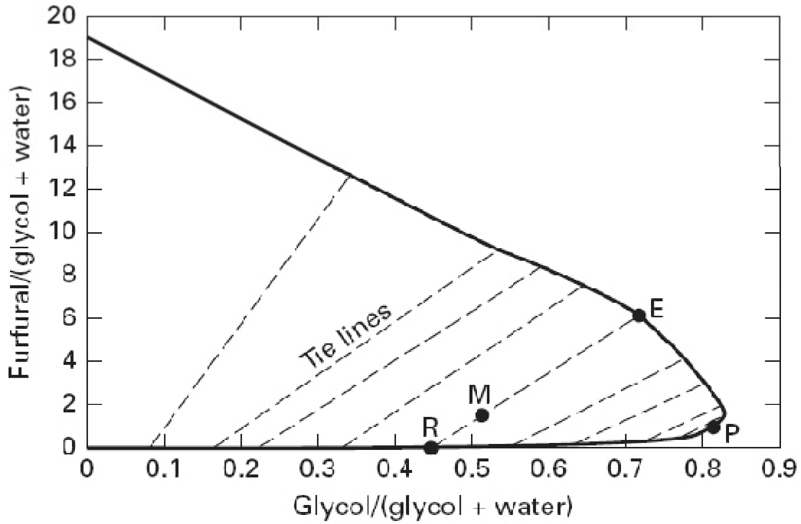
Equilibrium solute diagram in mass fractions



Equilibrium solute diagram in mass ratios



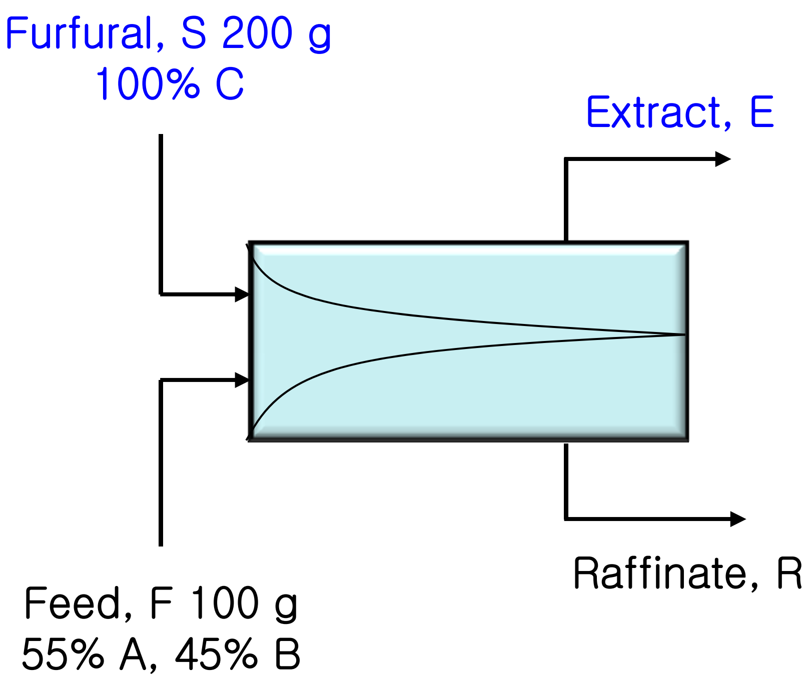
Janecke diagram



[Example] Water–Glycol–Furfural Equilibrium (1)

A 45% by weight glycol (B)–55% water (A) solution is contacted with twice its weight of pure furfural solvent (C) at 25℃ and 101 kPa.

Determine the composition of the equilibrium extract and raffinate phases produced.



- Basis : 100 g of feed
- Overall material balance

  $F + S = E + R$

[Example] Water–Glycol–Furfural Equilibrium (2)

Locate the feed (F) and solvent (S) compositions

Define M, the mixing point
M = F + S = E + R

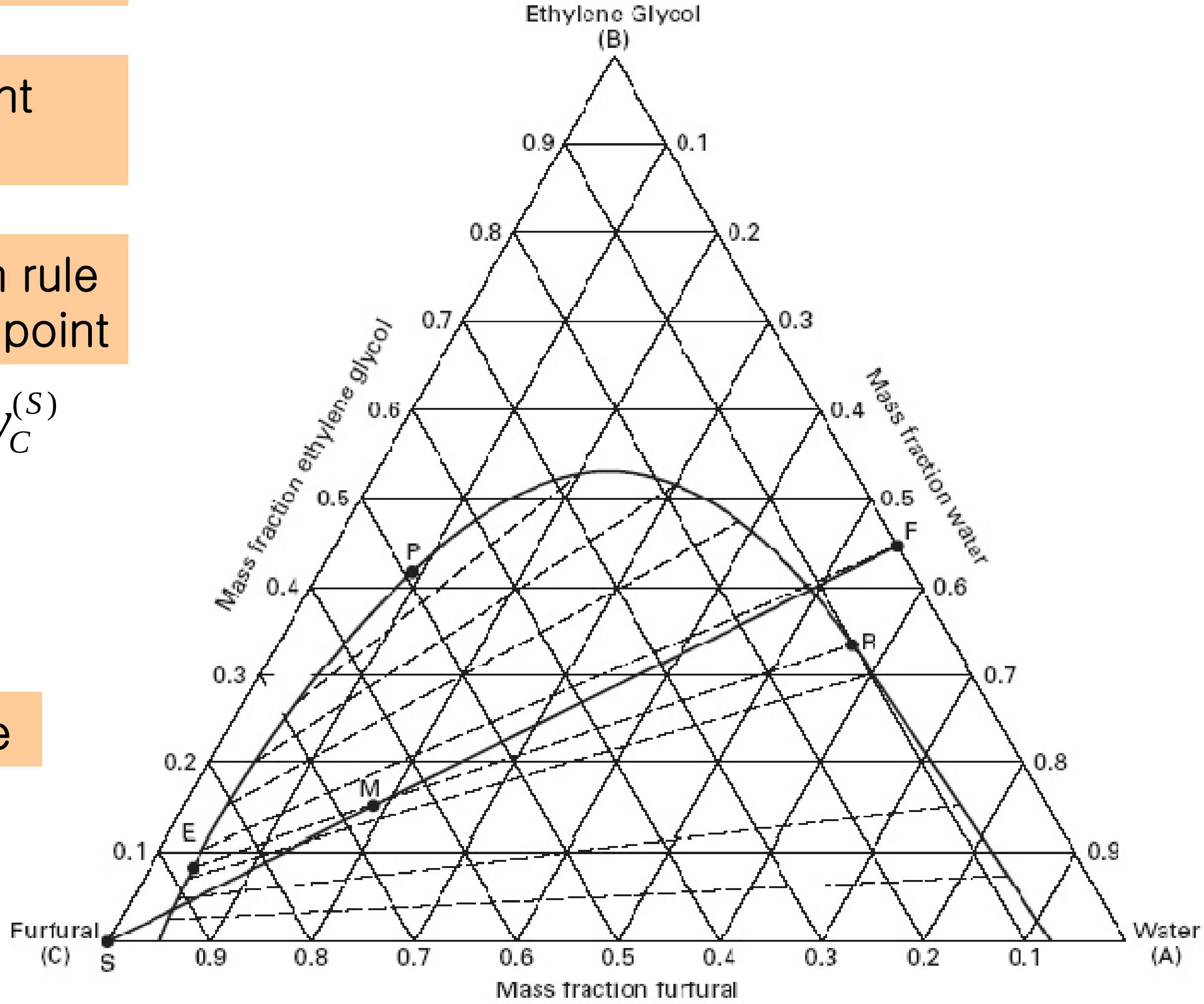
Apply the inverse-lever-arm rule (or mass balance) to find M point

$$(F+S)w_C^{(M)} = Fw_C^{(F)} + Sw_C^{(S)}$$

$$\frac{F}{S} = \frac{w_C^{(S)} - w_C^{(M)}}{w_C^{(M)} - w_C^{(F)}} = \frac{\overline{SM}}{\overline{MF}}$$

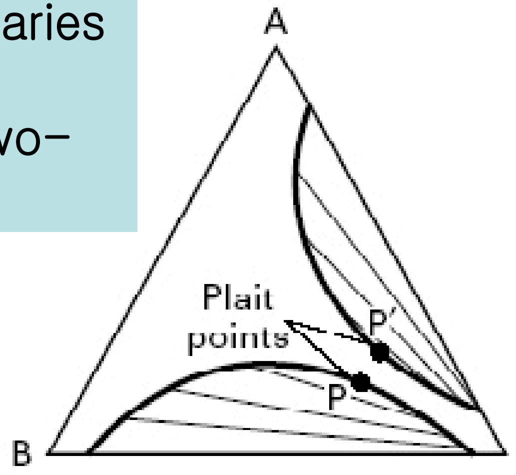
Find E and R along a tie line

Apply the inverse-lever-arm rule to find the amounts of E and R

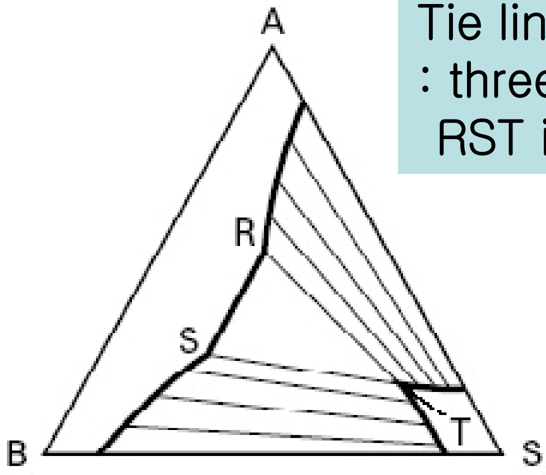


When Two Pairs of Components are Partially Soluble

Miscibility boundaries are separate
: two separate two-phase regions



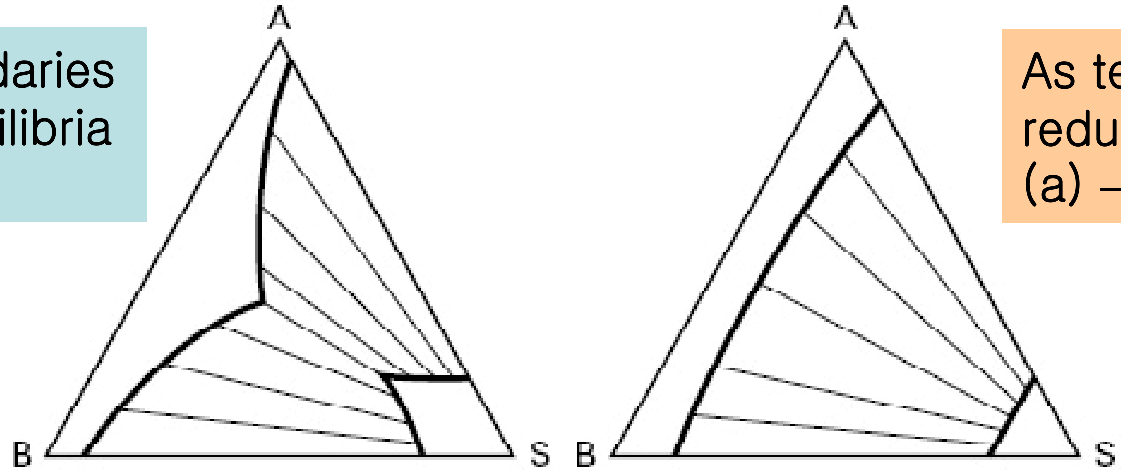
(a)



(c)

Tie lines do not merge
: three-phase region, RST is formed

Miscibility boundaries and tie-line equilibria merge



(b)

As temperature is reduced,
(a) → (b) → (c)