CHEMICAL ENGINEERING THERMODYNAMICS II (0905323)
08.FLASH CALCULATION USING RAOULT'S LAW

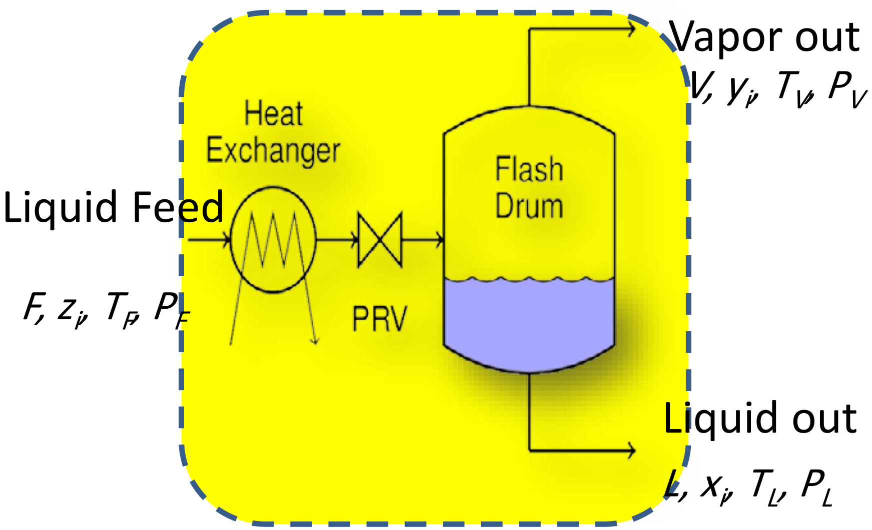
ALI KH. AL-MATAR (aalmatar@ju.edu.jo)

Chemical Engineering Department
University of Jordan
Amman 11942, Jordan

Outline

- Flash Concept and Types
- Flash Calculations
- Deriving Equations for Isothermal Flash
- The Rachford-Rice (RR) Equation
- Bubble and Dew Calculations Using RR
- Solving the Rachford-Rice (RR) Equation
- Algorithm for Isothermal Flash

Flash Concept and Types



- T_V, P_V Isothermal Flash
- V/F=0, P_L Bubble-Point Temperature
- V/F=1, P_V Dew-Point Temperature
- V/F=0, T_L Bubble-Point Pressure
- V/F=1, T_V Dew-Point Pressure
- Q=0, P_V Adiabatic Flash
- Q, P_V Nonadiabatic flash

Variables: there are 3C+10 variables: F, V, L, $\{T, P\}_3$, Q, $\{x_i, y_i, z_i\}_C$ and C+5 degrees of freedom.

Specify the C+3 variables F, z_i, T_F, P_F and **two additional variables**

Flash Calculations

- Flash calculations are a combination of material and energy balances, and equilibrium relations.
- In this course we are interested in isothermal flash which will avoid using energy balances.
- The flash problem is posed as:
  - **Given**: feed composition and flow rate.
  - **Feed** flow rate is assumed to be unity as a basis.
  - **Wanted**: $\{x_i\}$, $\{y_i\}$, and vapor (V) and liquid (L) flow rates.

Deriving Equations for Isothermal Flash

- Overall Material balance (MB)

$$L + V = 1$$

- Species balance

$$z_i = x_i L + y_i V \quad , i = 1, \cdots, C$$

- Eliminate L from the two balance equations to obtain

$$z_i = x_i (1 - V) + y_i V , \quad i = 1, \cdots, C$$

Combine MB and Equilibrium Relationships

- Introduce the distribution coefficient $K_i = y_i / x_i$

$$K_i = \frac{y_i}{x_i} = \frac{P_i^{vap}}{P}, \quad i = 1, \cdots, C$$

$$y_i = \frac{z_i K_i}{1 + V(K_i - 1)}, \quad \text{or} \quad x_i = \frac{z_i}{1 + V(K_i - 1)}, \quad i = 1, \cdots, C$$

- The vapor and liquid phase mole fractions must sum to unity, from which

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

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

The Rachford-Rice (RR) Equation

- Solution of any of the two last equations is dependent on the correct value of *V* i.e., the fraction of the feed that is vaporized.
- A more convenient way of solving is to take the difference between the F_y *and* F_x to obtain the Rachford-Rice equation:

$$F = F_y - F_x = \sum_{i=1}^{C} \frac{z_i (K_i - 1)}{1 + V (K_i - 1)} = 0$$

- This becomes convenient using the Newton-Raphson method due to the **monotonic** behavior of the derivative of this function.

$$\frac{dF}{dV} = -\sum_{i=1}^{C} \frac{z_i (K_i - 1)^2}{[1 + V (K_i - 1)]^2}$$

Bubble and Dew Calculations Using RR

- Bubble point ($V = 0$)

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

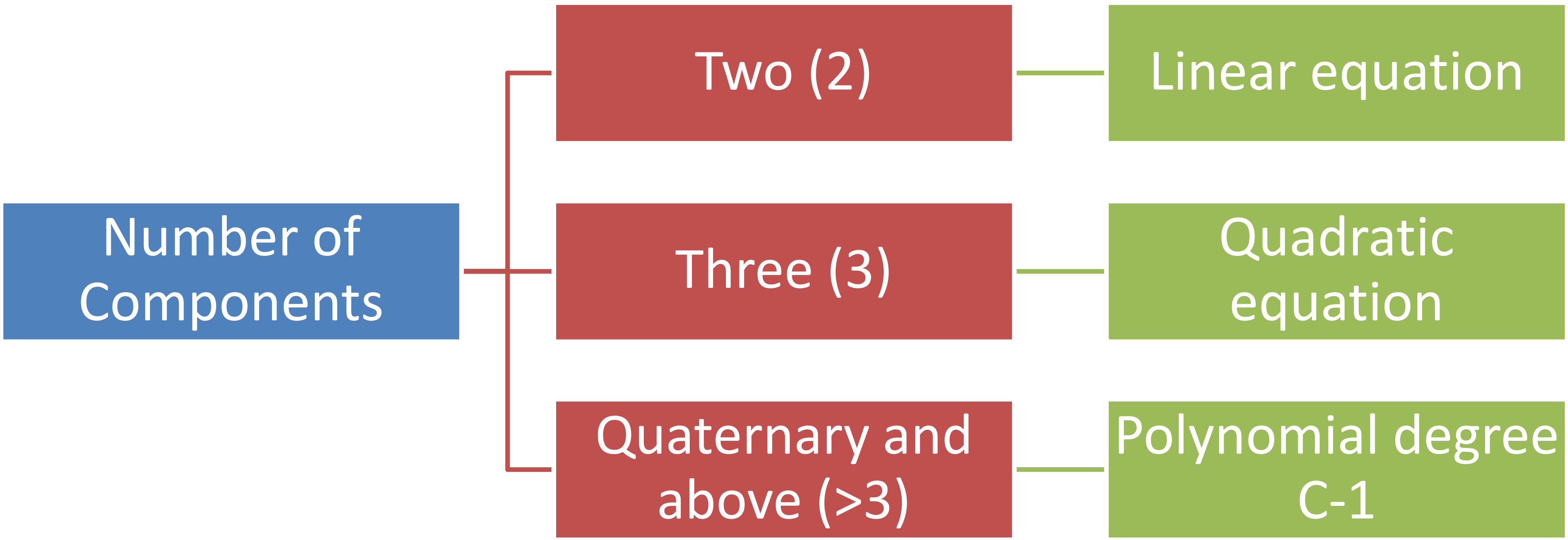
$$\Rightarrow \sum_{i=1}^{C} z_i K_i = 1$$

- Dew point ($V = 1$)

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

$$\Rightarrow \sum_{i=1}^{C} \frac{z_i}{K_i} = 1$$

Solving the Rachford-Rice (RR) Equation



A good initial guess for *V* is 0.5 since it is bracketed between 0 and 1!

A better initial guess is to use

$$V^{(0)} = \frac{P_B - P}{P_B - P_D}$$

Binary System in Rachford-Rice Equation

$$\frac{z_1(K_1-1)}{1+V(K_1-1)}+\frac{z_2(K_2-1)}{1+V(K_2-1)}=0$$

$$z_1(K_1-1)\left(1+V(K_2-1)\right)+z_2(K_2-1)\left(1+V(K_1-1)\right)=0$$

$$z_1(K_1-1)+z_1V(K_1-1)(K_2-1)+z_2(K_2-1)+z_2V(K_2-1)(K_1-1)=0$$

$$V\left[z_1(K_1-1)(K_2-1)+z_2(K_2-1)(K_1-1)\right]=-z_2(K_2-1)-z_1(K_1-1)$$

$$V=-\frac{z_2(K_2-1)+z_1(K_1-1)}{\left[(K_1-1)(K_2-1)\right]}$$

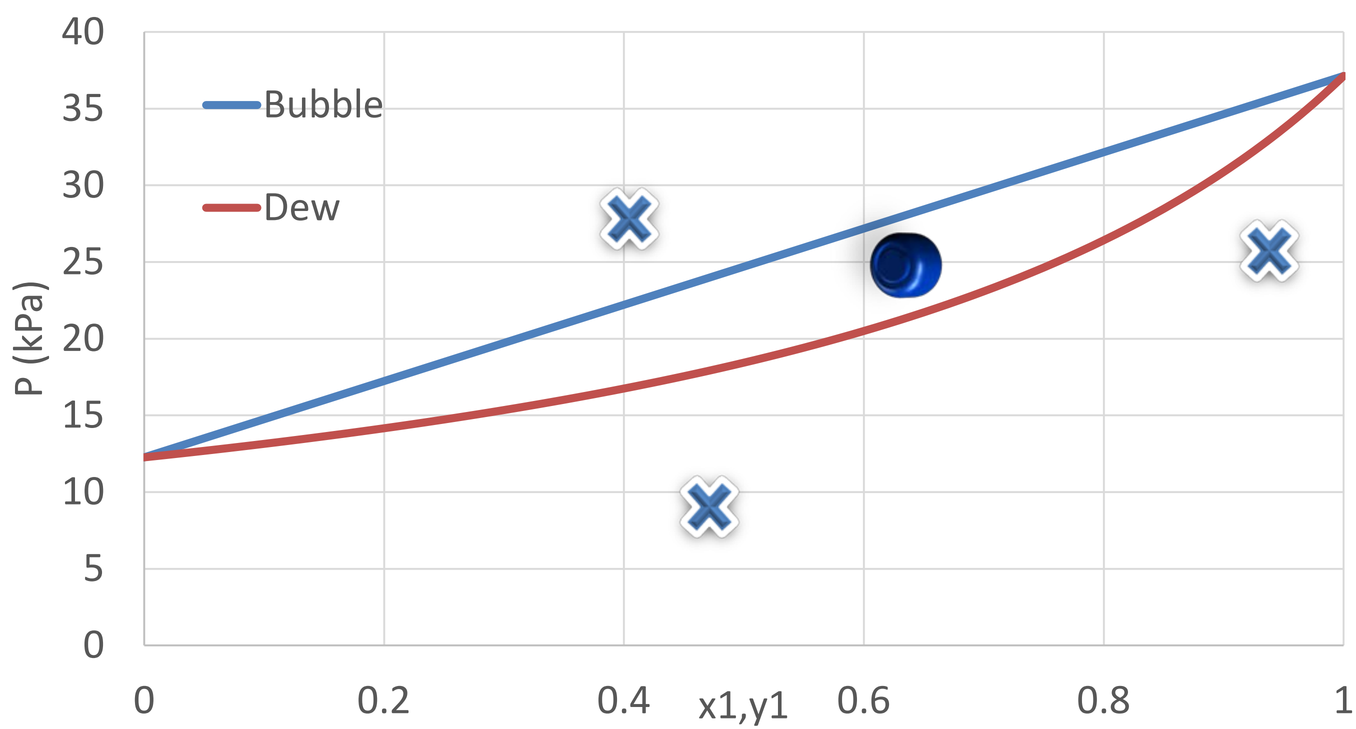
Quiz

- Show that for a ternary system the RR equation reduces to a quadratic equation that can be solved using the discriminator method for V.
- Derive a general expression for any arbitrary number of components using the RR equation.
  - Hint you are going to get summations and products.

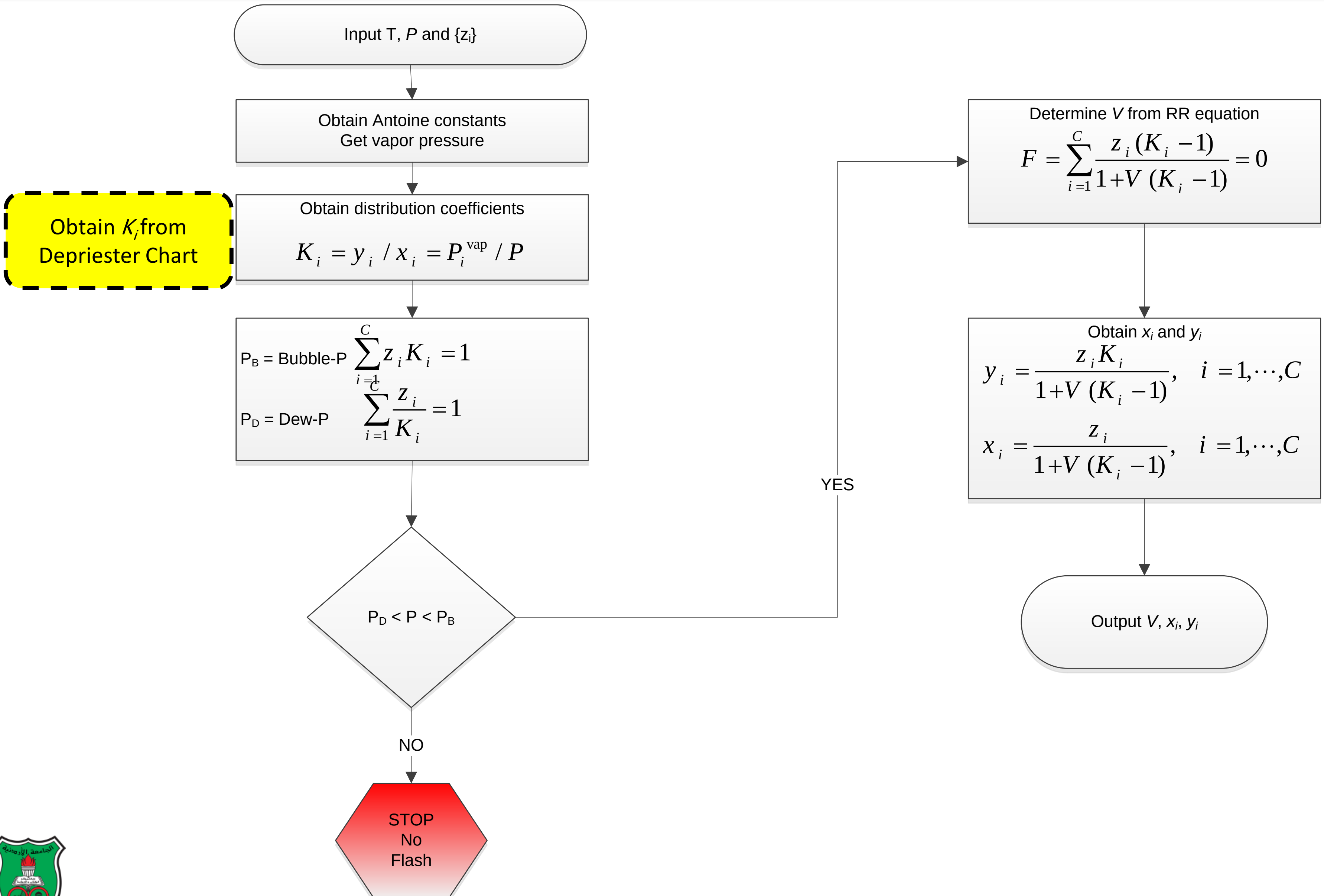
Precautions and Tricks

- Carry a Bubble-P and a Dew-P calculation to check that the given pressure is indeed within the two phase region

$$P_{\text{dew}} < P < P_{\text{bubble}}$$



Algorithm for Isothermal Flash



Example

- An equimolar mixture of benzene and toluene at 370 K and 1 bar is to be fed to a flash drum.
  I. Determine the vapor fraction of the feed. If the total flowrate is 10000 mole/h determine the vapor flowrate.
  II. Determine the compositions of the vapor and liquid streams exiting the flash drum.
  III. Is Raoult's law a good model for such system?
  IV. Would you recommend ordinary distillation to separate these two components?

Solution using Excel

Example

- A mixture containing benzene, toluene, and m-xylene at 400 K and 1.5 bar is to be fed to a flash drum. The composition is $z_i = \{0.4, 0.2, 0.4\}$.
  I. Determine the vapor fraction of the feed.
  II. Determine the compositions of the vapor and liquid streams exiting the flash drum.
  III. Is Raoult's law a good model for such system?
  IV. Would you recommend ordinary distillation to separate these two components?

Solution using Excel

Solution

	zi	P*i	Ki	Ki-1	zi(Ki-1)	zi(Ki-1)/(1+V*(Ki-1))	xi	yi
Benzene	0.4	3.5231	2.3487	1.3487	0.5395	0.2954	0.2190	0.5144
Toluene	0.2	1.5723	1.0482	0.0482	0.0096	0.0094	0.1943	0.2036
m-xylene	0.4	0.7208	0.4806	-0.5194	-0.2078	-0.3048	0.5867	0.2819
					sum	0.0000	1.0000	1.0000

PB	2.0120
PD	1.2568
PB-P/(PB-PD)	0.6780
V	0.6127

Example

- A 100-kmol/h feed consisting of 10, 20, 30, and 40 mol% of propane (3), n-butane (4), n-pentane (5), and n-hexane (6), respectively, enters a distillation column at 689.5 kPa and 366.5K. Assuming equilibrium, what fraction of the feed enters as liquid, and what are the liquid and vapor compositions?

At flash conditions, from Figure 2.4, $K_3 = 4.2$, $K_4 = 1.75$, $K_5 = 0.74$, $K_6 = 0.34$, independent of compositions. Because some K-values are greater than 1 and some less than 1, it is necessary first to compute values of $f\{0\}$ and $f\{1\}$ for Eq. (3) in Table 4.4 to see if the mixture is between the bubble and dew points.

$$f\{0\} = \frac{0.1(1-4.2)}{1} + \frac{0.2(1-1.75)}{1} + \frac{0.3(1-0.74)}{1} + \frac{0.4(1-0.34)}{1} = -0.128$$

Since $f\{0\}$ is not more than zero, the mixture is above the bubble point. Now compute $f\{1\}$:

$$f\{1\} = \frac{0.1(1-4.2)}{1+(4.2-1)} + \frac{0.2(1-1.75)}{1+(1.75-1)} + \frac{0.3(1-0.74)}{1+(0.74-1)} + \frac{0.4(1-0.34)}{1+(0.34-1)} = 0.720$$

Since $f\{1\}$ is not less than zero, the mixture is below the dew point. Therefore, the mixture is part vapor. Using the Rachford–Rice pro-

$$0 = \frac{0.1(1-4.2)}{1+\Psi(4.2-1)} + \frac{0.2(1-1.75)}{1+\Psi(1.75-1)} + \frac{0.3(1-0.74)}{1+\Psi(0.74-1)} + \frac{0.4(1-0.34)}{1+\Psi(0.34-1)}$$

Solving this equation by Newton's method using an initial guess for Ψ of 0.50 gives the following iteration history:

k	$\Psi^{(k)}$	$f\{\Psi^{(k)}\}$	$f'\{\Psi^{(k)}\}$	$\Psi^{(k+1)}$	$\left\lvert \frac{\Psi^{(k+1)} - \Psi^{(k)}}{\Psi^{(k)}} \right\rvert$
1	0.5000	0.2515	0.6259	0.0982	0.8037
2	0.0982	−0.0209	0.9111	0.1211	0.2335
3	0.1211	−0.0007	0.8539	0.1219	0.0065
4	0.1219	0.0000	0.8521	0.1219	0.0000

Convergence is rapid, giving $\Psi = V/F = 0.1219$. From Eq. (4) of Table 4.4, the vapor flow rate is $0.1219(100) = 12.19$ kmol/h, and the liquid flow rate from Eq. (7) is $(100 - 12.19) = 87.81$ kmol/h. Liquid and vapor compositions from Eqs. (5) and (6) are

	x	y
Propane	0.0719	0.3021
n-Butane	0.1833	0.3207
n-Pentane	0.3098	0.2293
n-Hexane	0.4350	0.1479
Sum	1.0000	1.0000

A plot of $f\{\Psi\}$ as a function of Ψ is shown in Figure 4.10.

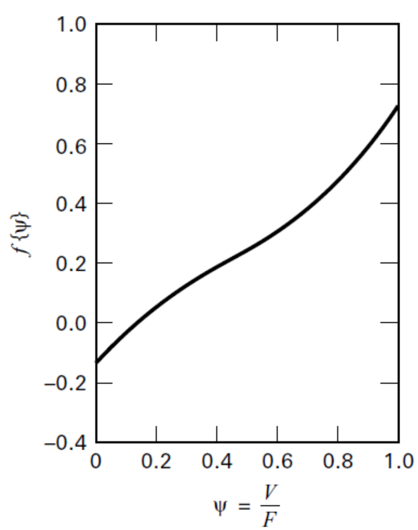
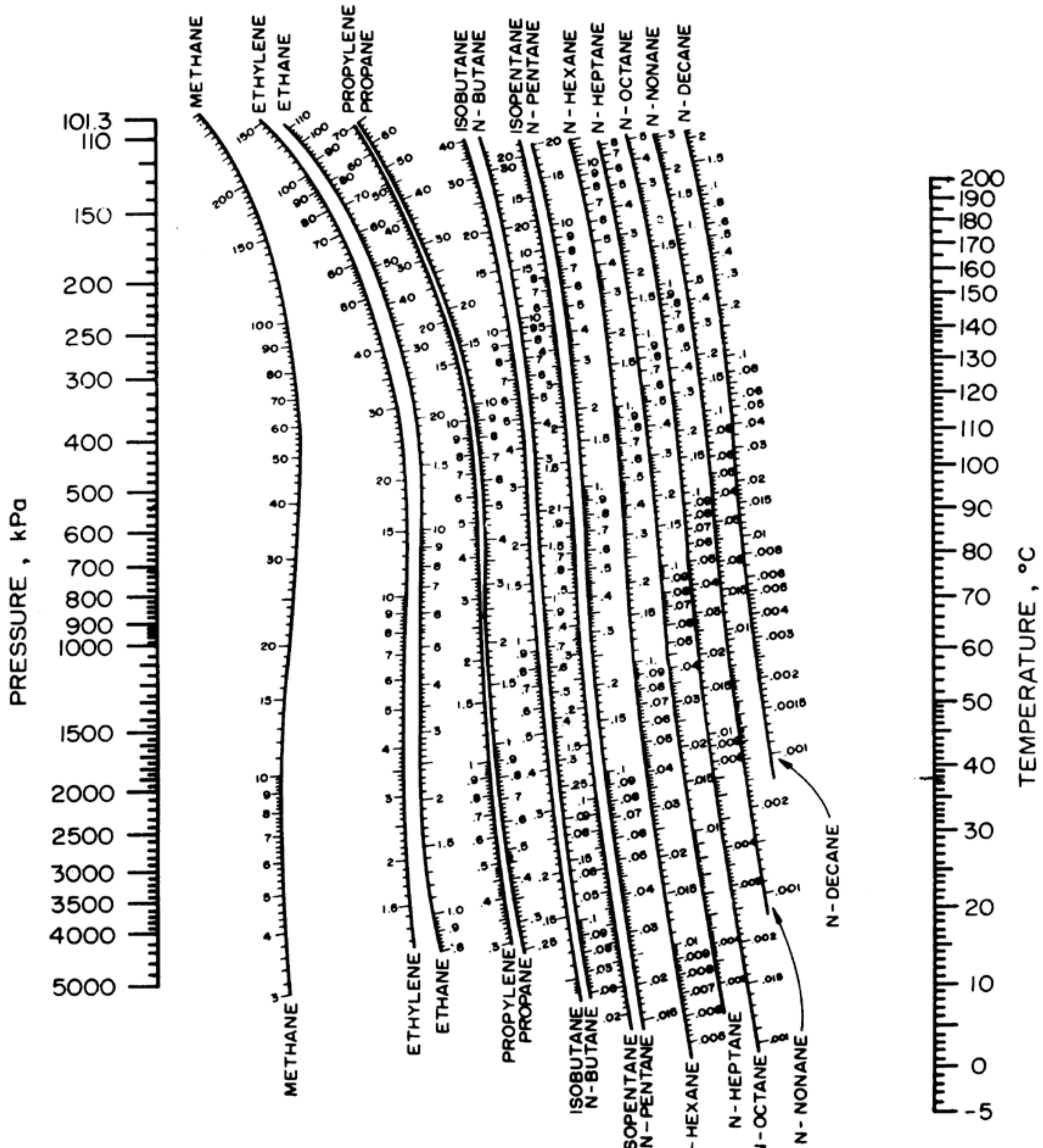


Figure 4.10 Rachford–Rice function for Example 4.1.

Depriester Determination of K-Values



General Flash Approach

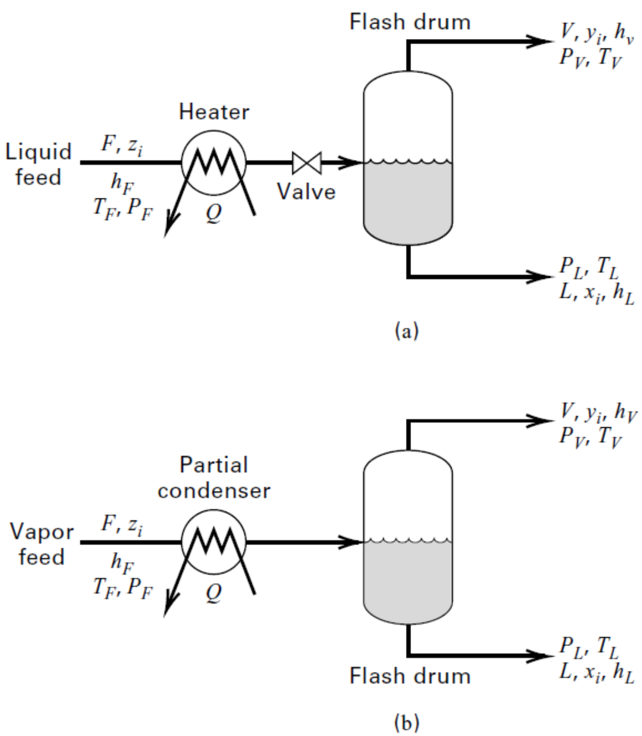


Figure 4.9 Continuous, single-stage equilibrium separations: (a) flash vaporization and (b) partial condensation.

Table 4.3 Equations for Single-Stage Flash Vaporization and Partial Condensation Operations. Feed mole fractions must sum to one.

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) $Fz_i = Vy_i + Lx_i$	(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
		$\mathscr{E} = 2C + 5$
$K_i = K_i\{T_V, P_V, \mathbf{y}, \mathbf{x}\}$	$h_F = h_F\ \{T_F, P_F, \mathbf{z}\}$	
$h_V = h_V\{T_V, P_V, \mathbf{y}\}$	$h_L = h_L\ \{T_L, P_L, \mathbf{x}\}$	

From Seader, Henley and Ruper, 3rd edition.