Table of Contents

Chapter 10 . . . 1
Problem 10.1 . . . 1
Problem 10.2 . . . 3
Problem 10.9 . . . 3
Problem 10.17 . . . 5

Chapter 10

Problem 10.1

Assuming the validity of Raoult's law, do the following calculations for the benzene(1)/toluene(2) system:

(a) Given $x_1 = 0.33$ and $T = 100$ °C, find y_1 and P.

(b) Given $y_1 = 0.33$ and $T = 100$ °C, find x_1 and P.

(c) Given $x_1 = 0.33$ and $P = 120$ kPa, find y_1 and T.

(d) Given $y_1 = 0.33$ and $P = 120$ kPa, find x_1 and T.

(e) Given $T = 105$ °C and $P = 120$ kPa find x_1 and y_1.

(f) For part (e), if the *overall* mole fraction of benzene is $z_1 = 0.33$, what molar fraction of the two-phase system is vapor?

(g) Why is Raoult's law likely to be an excellent VLE model for this system at the stated (or computed) conditions?

Solution:

$$\begin{aligned} A_1 &= 13.7819 & A_2 &= 13.9320 \\ B_1 &= 2726.81 & B_2 &= 3056.96 \\ C_1 &= 217.572 & C_2 &= 217.625 \end{aligned}$$

(a) $x_1 = 0.33$ and $T = 100$ °C, find P and y_1

$$\ln P_i^{\text{sat}}/\text{kPa} = A_i - \frac{B_i}{t/°\text{C} + C_i}$$

$$P_1^{\text{sat}} = 180.45 \text{ kPa}$$

$$P_2^{\text{sat}} = 74.26 \text{ kPa}$$

$$P = P_1^{\text{sat}} x_1 + P_2^{\text{sat}}(1 - x_1)$$

$$\boxed{P = 109.30 \text{ kPa}}$$

$$y_1 = \frac{x_1 P_1^{\text{sat}}}{P}$$

$$\boxed{y_1 = 0.5448}$$

(b) $y_1 = 0.33$ and $T = 100$ °C, find x_1 and P

$$x_1 = \frac{y_1 P}{P_1^{\text{sat}}}$$
$$P = y_1 P + P_2^{\text{sat}} \left(1 - \frac{y_1 P}{P_1^{\text{sat}}}\right)$$

$$\boxed{\begin{array}{c} P = 92.156 \text{ kPa} \\ x_1 = 0.169 \end{array}}$$

(c) $x_1 = 0.33$ and $P = 120$ kPa, find y_1 and T

$$x_1 \cdot \exp\left(A_1 - \frac{B_1}{T + C_1}\right) + x_2 \cdot \exp\left(A_2 - \frac{B_2}{T + C_2}\right) = P$$
$$P_1^{\text{sat}} = A_1 - \frac{B_1}{T + C_1}$$
$$y_1 = \frac{x_1 P_1^{\text{sat}}}{P}$$

$$\boxed{\begin{array}{c} T = 103.307 \text{ °C} \\ y_1 = 0.542 \end{array}}$$

(d) $y_1 = 0.33$ and $P = 120$ kPa, find x_1 and T

$$P = x_1 P_1^{\text{sat}} + (1 - x_1) P_2^{\text{sat}}$$
$$x_1 = \frac{y_1 P}{P_1^{\text{sat}}} P = y_1 P + (1 - \frac{y_1 P}{P_1^{\text{sat}}}) P_2^{\text{sat}}$$
$$P_i^{\text{sat}} = A_i - \frac{B_i}{T + C_i}$$

$$\boxed{\begin{array}{c} T = 109.13 \text{ °C} \\ x_1 = 0.1726 \end{array}}$$

(e) $T = 105$ °C, $P = 120$ kPa, find x_1, y_1

$$P = y_1 P + \left(1 - \frac{y_1 P}{P_1^{\text{sat}}}\right) P_2^{\text{sat}}$$
$$P_i^{\text{sat}} = A_i - \frac{B_i}{T + C_i} x_i = \frac{y_i P}{P_i^{\text{sat}}}$$

$$\boxed{\begin{array}{c} y_1 = 0.4840 \\ x_1 = 0.2818 \end{array}}$$

(f) $z_1 = 0.33$, find $\mathcal{V}$

$$z_1 = \frac{\mathcal{L}x_1 + \mathcal{V}y_1}{\mathcal{L} + \mathcal{V}}$$

Basis: $\mathcal{L} + \mathcal{V} = 1$ mol

$$z_1 = \mathcal{L}x_1 + (1 - \mathcal{L})y_1$$
$$\mathcal{L} = 0.7616$$
$$\boxed{V = 0.2384}$$

(g) Benzene and toluene are two very similar compounds on top of being non-polar, minimizing chemical interactions.

Problem 10.2

Assuming Raoult's law to be valid, prepare a $P-x-y$ diagram for a temperature of 90 °C and a $t-x-y$ diagram for a pressure of 90 kPa for one of the following systems:

(a) Benzene(1)/ethylbenzene(2);

(b) 1-Chlorobutane(1)/chlorobenzene(2).

Solution:

$$A_1 = 13.8594 B_1 = 2773.78 C_1 = 220.07$$
$$A_2 = 14.0045 B_2 = 3279.47 C_2 = 213.20$$

$$P_i^{\text{sat}} = A_i - \frac{B_i}{t + C}$$
$$P = x_1 P_1^{\text{sat}} + x_2 P_2^{\text{sat}}$$
$$y_1 = \frac{x_1 P_1^{\text{sat}}}{P}$$

Problem 10.9

A mixture containing equimolar amounts of benzene(1), toluene(2), and ethylbenzene(3) is flashed to conditions T and P. For one of the conditions following determine the equilibrium mole fractions x_i and $\{y_i\}$ of the liquid and vapor phases formed and the molar fraction $\mathcal{V}$ of the vapor formed. Assume that Raoult's law applies.

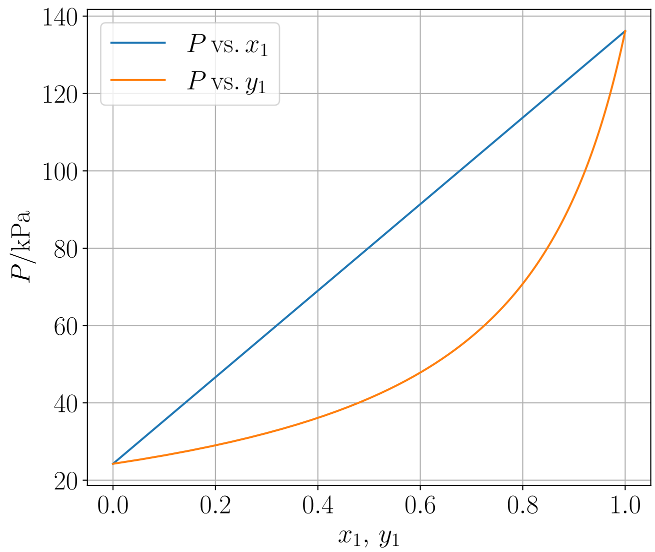

Figure 1: $P - x - y$ diagram of the system described in Problem 10.2.

(a) $T = 110$ °C, $P = 90$ kPa

(b) $T = 110$ °C, $P = 100$ kPa

(c) $T = 110$ °C, $P = 110$ kPa

(d) $T = 110$ °C, $P = 120$ kPa

Solution:

$$P_i^{\text{sat}} = \exp\left(A_i - \frac{B_i}{T + C_i}\right)$$

$$k_i = \frac{P_i^{\text{sat}}}{P}$$

$$1 = \sum_i \frac{z_i k_i}{1 + \mathcal{V}(k_i - 1)}$$

$$y_i = \frac{z_i k_i}{1 + \mathcal{V}(k_i - 1)}$$
$$x_i = \frac{y_i P_i^{\text{sat}}}{P}$$

$$\boxed{\mathcal{V} = 0.834, 0.573, 0.349, 0.143,}$$

$$\boxed{x = \begin{bmatrix} 0.143 \\ 0.306 \\ 0.551 \end{bmatrix}, \begin{bmatrix} 0.188 \\ 0.334 \\ 0.477 \end{bmatrix}, \begin{bmatrix} 0.239 \\ 0.345 \\ 0.416 \end{bmatrix}, \begin{bmatrix} 0.293 \\ 0.342 \\ 0.365 \end{bmatrix}}$$

$$\boxed{y = \begin{bmatrix} 0.371 \\ 0.339 \\ 0.290 \end{bmatrix}, \begin{bmatrix} 0.441 \\ 0.333 \\ 0.226 \end{bmatrix}, \begin{bmatrix} 0.509 \\ 0.312 \\ 0.179 \end{bmatrix}, \begin{bmatrix} 0.573 \\ 0.342 \\ 0.144 \end{bmatrix}}$$

Problem 10.17

For the system ethyl ethanoate(1)/n-heptane(2) at 343.15 K.

$$\ln \gamma_1 = 0.95 x_2^2 \ln \gamma_2 = 0.95 x_1^2$$
$$P_1^{\text{sat}} = 79.80 \text{ kPa} P_2^{\text{sat}} = 40.50 \text{ kPa}$$

Assuming the validity of Eq. 1

$$y_i P = \gamma_i x_i P_i^{\text{sat}} \tag{1}$$

(a) Make a BUBL P calculation for $T = 343.15$ K, $x_1 = 0.05$.

(b) Make a DEW P calculation for $T = 343.15$ K, $y_1 = 0.05$.

(c) What is the azeotrope composition and pressure at $T = 343.15$ K?

Solution:

(a)

$$P = x_1 \gamma_1 P_1^{\text{sat}} + x_2 \gamma_2 P_2^{\text{sat}}$$

$$\boxed{\begin{gathered} P = 47.971 \text{ kPa} \\ y_1 = 0.196 \end{gathered}}$$