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## Chapter 10

### Problem 10.1

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

- Given  $x_1 = 0.33$  and  $T = 100^\circ\text{C}$ , find  $y_1$  and  $P$ .
- Given  $y_1 = 0.33$  and  $T = 100^\circ\text{C}$ , find  $x_1$  and  $P$ .
- Given  $x_1 = 0.33$  and  $P = 120\text{ kPa}$ , find  $y_1$  and  $T$ .
- Given  $y_1 = 0.33$  and  $P = 120\text{ kPa}$ , find  $x_1$  and  $T$ .
- Given  $T = 105^\circ\text{C}$  and  $P = 120\text{ kPa}$  find  $x_1$  and  $y_1$ .
- 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?
- Why is Raoult's law likely to be an excellent VLE model for this system at the stated (or computed) conditions?

**Solution:**

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

- $x_1 = 0.33$  and  $T = 100^\circ\text{C}$ , find  $P$  and  $y_1$

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

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

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

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

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

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

$$\boxed{y_1 = 0.5448}$$

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

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

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

$P = 92.156 \text{ kPa}$ $x_1 = 0.169$
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(c)  $x_1 = 0.33$  and  $P = 120$  kPa, find  $y_1$  and  $T$

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

$$P_1^{\text{sat}} = A_1 - \frac{B_1}{T + C_1}$$

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

$T = 103.307$ °C $y_1 = 0.542$
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(d)  $y_1 = 0.33$  and  $P = 120$  kPa, find  $x_1$  and  $T$

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

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

$$P_i^{\text{sat}} = A_i - \frac{B_i}{T + C_i}$$

$T = 109.13$ °C $x_1 = 0.1726$
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(e)  $T = 105$  °C,  $P = 120$  kPa, find  $x_1, y_1$

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

$$P_i^{\text{sat}} = A_i - \frac{B_i}{T + C_i} x_i = \frac{y_i P}{P_i^{\text{sat}}}$$

$y_1 = 0.4840$ $x_1 = 0.2818$
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(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:**

$$B_1 = 2773.78$$

$$B_2 = 3279.47$$

### 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.

- (a)  $T = 110$  °C,  $P = 90$  kPa

(b)  $T = 110\text{ }^{\circ}\text{C}$ ,  $P = 100\text{ kPa}$

(c)  $T = 110\text{ }^{\circ}\text{C}$ ,  $P = 110\text{ kPa}$

(d)  $T = 110\text{ }^{\circ}\text{C}$ ,  $P = 120\text{ kPa}$

**Solution:**

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

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

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

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

$$x_i = \frac{y_i P_i^{\text{sat}}}{P}$$

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

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

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

### Problem 10.17

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

$$\ln \gamma_1 = 0.95x_2^2 \ln \gamma_2 = 0.95x_1^2$$

$$P_1^{\text{sat}} = 79.80\text{ kPa} P_2^{\text{sat}} = 40.50\text{ kPa}$$

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)

$$P = x_1\gamma_1P_1^{\text{sat}} + x_2\gamma_2P_2^{\text{sat}}$$

$$P = 47.971 \text{ kPa}$$

$$y_1 = 0.196$$