3140507: Chemical Engineering Thermodynamics – II

Tutorial 01:

Q.1:

Will it be possible to prepare 0.1 m³ of alcohol-water solution by mixing 0.03 m³ alcohol with 0.07 m³ pure water? If not possible, what volume should have been mixed in order to prepare a mixture of the same strength and of the required volume? Density of ethanol and water are 789 and 997 kg/m³ respectively. The partial molar volumes of ethanol and water at the desired compositions are: Ethanol = $53.6 \times 10^{-6} \text{ m}^3/\text{mol}$; water = $18 \times 10^{-6} \text{ m}^3/\text{mol}$.

Q.2:

At 300 K and 1 bar, the volumetric data for a liquid mixture of benzene and cyclohexane are represented by

$$V = 109.4 * 10^{-6} - 16.8 * 10^{-6} x_1 - 2.64 * 10^{-6} x_1^2,$$

where x_1 is the mole fraction of benzene and V has the units of m^3/mol . Find expressions for the partial molar volumes of benzene and cyclohexane.

Q.3:

If the molar density of a binary mixture is given by the empirical expression:

$$\rho = a_0 + a_1 x_1 + a_2 x_1^2$$

find the corresponding expressions for $\,\overline{V_1}\,$ and $\,\overline{V_2}\,$.

Q.4:

A 30 % by mole methanol-water solution is to be prepared. How many cubic meters of pure methanol (molar volume, $40.727 \times 10-6 \text{ m3/mol}$) and pure water (molar volume, $18.068 \times 10-6 \text{ m3/mole}$) are to be mixed to prepare 2 m3 of desired solution? The partial molar volumes of methanol and water in a 30 % solution are $38.632 \times 10-6 \text{ m3/mol}$ and $17.765 \times 10-6 \text{ m3/mol}$, respectively.

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Tutorial 02:

From the following compressibility-factor data for CO_2 at 423.15 K (150°C) prepare plots of the fugacity and fugacity coefficient of CO_2 vs. P for pressures up to 500 bar Compare results with those found from the generalized correlation represented by Eq

$$\phi = \exp\left[\frac{P_r}{T_r}(B^0 + \omega B^1)\right]$$

P (bar)	Z	
0	1	
10	0.985	
20	0.97	
40	0.942	
60	0.913	
80	0.885	
100	0.869	
200	0.765	
300	0.762	
400	0.824	
500	0.91	

$$\ln \phi_i = \int_0^P (Z_i - 1) \frac{dP}{P}$$

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Tutorial 03:

- 1. Calculate bubble point pressure for binary mixture of Benzene (1)/Toluene (2) at T= 400, 700 and 1000 K & x_1 =0.4. Draw P-x1y1 diagram at different T.
- 2. Then generate T-xy diagram at pressure P = 1, 10 and 100 atm.

Antoine equation:
$$\ln P = A - \frac{B}{T+C}$$
 where, P in kPa, T in K

A1=14.1603, **B1**=2948.78, **C1** = -44.5633

A2=14.2515, B2=3242.38, C2 = -47.1806

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Tutorial 04:

Q.1:

Estimate the values for the fugacity of 1-butane vapor at 473.15 K and 70 bar.

Data given: Tr = 1.127, Pr = 1.731 and $\omega = 0.191$

Q.2:

The saturation pressure of n-octane at 427.85 K is 215 Mpa. Estimate the fugacity of liquid n-octane at 427.85 K and 1 Mpa.

Data given:

For n-octane: $f_i^{sat} = 0.2368$ MPa and $v_i^L = 0.2003 \text{ x } 10^{-3} \text{ m}^3/\text{mol}$

Q.3:

Describe a graphical interpretation of following equations:

$$\overline{\mathbf{M}}_1 = \mathbf{M} + \mathbf{x}_2 \frac{\mathbf{d}\mathbf{M}}{\mathbf{d}\mathbf{x}_1} \qquad \qquad \overline{\mathbf{M}}_2 = \mathbf{M} - \mathbf{x}_1 \frac{\mathbf{d}\mathbf{M}}{\mathbf{d}\mathbf{x}_1}$$

Q.4:

At 25 0 C the density of a methanol (1) – water (2) solution at x₁ = 0.7779 is 825.959 kg/m³. Partial molar volume of water in this solution is 15.686 x 10⁻⁶ m³/mol. Determine the partial molar volume of methanol in the solution.

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Tutorial 05:

Q.1:

Ternary equimolar mixture is flashed at 110 °C to carry out 30 % vaporization. Determine equilibrium pressure, vapor and liquid composition.

Data Given:

At 110 °C:

$$\begin{split} P_1{}^{sat} &= 224 \text{ kPa} \\ P_2{}^{sat} &= 98.6 \text{ kPa} \\ P_3{}^{sat} &= 48 \text{ kPa} \end{split}$$

Q.2:

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 V of the vapor formed. Assume that Raoult's law applies.

- (a) T = 383.15 K, P = 90 kPa.
- (b) T = 383.15 K, P = 100 kPa.
- (c) T = 383.15 K, P = 110 kPa.
- (d) T = 383.15 K, P = 120 kPa.

Q.3:

For a perticular binary system, the activity coefficients are adequately represented by following equations:

$$\ln \gamma_1 = 0.6 \, \mathrm{x}_2^2$$
 and $\ln \gamma_2 = 0.6 \, \mathrm{x}_1^2$

The saturation pressures of the components at 80 °C are given by P1sat = 900 mmHg and P2sat = 600 mmHg. Is it possible for the system to exhibit azeotropy at 80 C? If yes, calculate azeotropic pressure and composition.

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Tutorial 06:

Q.1:

Water (1) – hydrazine (2) system forms an azeotrope containing 58.5% (mol) hydrazine at 393 K and 101.3 kPa. Calculate the equilibrium vapour composition for a solution containing 20% (mol) hydrazine. The relative volatility of water with reference to hydrazine is 1.6 and may be assumed to remain constant in the temperature range involved. The vapour pressure of hydrazine at 393 K is 124.76 kPa.

Q.2:

Using van Laar constants and the vapour pressures of the pure substances how would you prove whether a given binary system forms an azeotrope or not?

Q.3:

From vapour–liquid equilibrium measurements for ethanol–benzene system at 318 K and 40.25 kPa it is found that the vapour in equilibrium with a liquid containing 38.4% (mol) benzene contained 56.6% (mol) benzene. The system forms an azeotrope at 318 K. At this temperature, the vapour pressures of ethanol and benzene are 22.9 and 29.6 kPa respectively. Determine the composition and total pressure of the azeotrope. Assume that van Laar equation is applicable for the system.

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Tutorial 07:

Q.1:

Using the criterion of phase equilibrium, show that the change in entropy during phase changes can be calculated from the latent heat of phase change and the absolute temperature as $\Delta S = \Delta H/T$.

Q.2:

Using van Laar constants and the vapour pressures of the pure substances how would you prove whether a given binary system forms an azeotrope or not?

Q.3:

The following results were obtained by experimental VLE measurements on the system, ethanol (1)-benzene (2) at 101.3 kPa. Test whether the data are thermodynamically consistent or not.

<i>x</i> ₁	0.003	0.449	0.700	0.900	
<i>y</i> 1	0.432	0.449	0.520	0.719	
, kPa	65.31	63.98	66.64	81.31	
, kPa	68.64	68.64	69.31	72.24	

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Tutorial 08:

Q.1:

Develop expressions for the mole fractions of reacting species as functions of the reaction coordinate for: (a) A system initially containing 2 mol NH_3 and 5 mol O_2 and undergoing the reaction:

$$4\mathrm{NH}_3(g) + 5\mathrm{O}_2(g) \rightarrow 4\mathrm{NO}(g) + 6\mathrm{H}_2\mathrm{O}(g)$$

(b) A system initially containing 3 mol H_2S and 5 mol O_2 and undergoing the reaction:

$$2\mathrm{H}_2\mathrm{S}(g) + 3\mathrm{O}_2(g) \to 2\mathrm{H}_2\mathrm{O}(g) + 2\mathrm{SO}_2(g)$$

(c) A system initially containing 3 mol NO_2 , 4 mol NH_3 , and 1 mol N_2 and undergoing the reaction:

$$6\text{NO}_2(g) + 8\text{NH}_3(g) \rightarrow 7\text{N}_2(g) + 12\text{H}_2\text{O}(g)$$

Q.2:

A system initially containing 2 mol C_2H_4 and 3 mol O_2 undergoes the reactions:

$$C_2H_4(g) + \frac{1}{2}O_2(g) \rightarrow \langle (CH_2)_2 \rangle O(g)$$

$$C_2H_4(g) + 3O_2(g) \rightarrow 2CO_2(g) + 2H_2O(g)$$

Develop expressions for the mole fractions of the reacting species as functions of the reaction coordinates for the two reactions.

Q.3:

A system formed initially of $2 \mod CO_2$, $5 \mod H_2$, and $1 \mod CO$ undergoes the reactions:

$$CO_2(g) + 3H_2(g) \rightarrow CH_3OH(g) + H_2O(g)$$

$$CO_2(g) + H_2(g) \rightarrow CO(g) + H_2O(g)$$

Develop expressions for the mole fractions of the reacting species as functions of the reaction coordinates for the two reactions.