BIRLA INSTITUTE OF TECHNOLOGY & SCIENCE, PILANI

Chemical Engineering Thermodynamics (CHE F213), Comprehensive Examination

Date – 21/12/2022 Part - A (Close Book) Maximum Marks 60

1. Starting with the mathematical definition of partial molar property, derive the following:
   Summability equation relating mixture molar property and partial molar properties of its constituents
   The Gibbs-Duhem equation [**5+3**]
2. What is Gibb's theorem? Apply Gibb's theorem to derive expressions for entropy change and Gibbs energy change of mixing for ideal gas as a function of composition. [**3+4+4**]
3. 5 kg of oxygen and 2 kg of hydrogen are mixed at 1 atm and 25^0C. Estimate the entropy change and Gibbs energy change of mixing (in SI units) assuming ideal behaviour. [**4+4**]
4. Vapor pressure expressions for three components in a ternary mixture are given as below:

$$lnP_1^{sat} = 14.3916 - \frac{2795.82}{T + 230}$$

$$lnP_2^{sat} = 14.2724 - \frac{2945.27}{T + 224}$$

$$lnP_3^{sat} = 14.2043 - \frac{2972.64}{T + 209}$$

   In the above equations T is in ^{0}C and P^{sat} is in kPa. Assuming that the system follows Rault's law, calculate total pressure (P), y_1, y_2 and y_3 at T = 75^0C and x_1 = 0.3 and x_2 = 0.4. x_i and y_i are mole fraction of component i in the liquid and vapor phase respectively. [**5+3**]

5. A pure gas obeys the two term virial equation of state $\frac{PV}{RT} = 1 + \frac{BP}{RT}$. The value of the second virial coefficient B = 1×10^{-4} m^3/mol. Determine the residual Gibbs energy and fugacity of this gas at 1000 kPa and 300 K. [**4+3**]
6. For a given binary system at constant temperature and pressure, the molar volume (in m3/mol) is given by $V = 30x_A + 20x_B + x_Ax_B(15x_A - 7x_B)$ where x_A and x_B are the mole fractions of component A and B respectively. Compute the volume change of mixing at x_A = 0.5. [**6**]
7. Carbon monoxide reacts with hydrogen sulphide at a constant temperature of 800 K and 2 bar as given below:

$$CO + H_2S \Leftrightarrow COS + H_2$$

   The standard Gibbs free energy of the reaction at 800 K is 22972.3 J/mol. All reactants and products can be assumed as ideal gases. If initially 1 mol of CO and 4 mol of H_2S are present, determine the extent of reaction at equilibrium. [**12**]

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1. A binary mixture of acetone/1,3 Butadiene has acetone mole fraction of 0.28. compute volume and residual Gibbs energy of this mixture. [**30**]

2. The activity coefficients in a binary mixture of acetaldehyde(1)/methanol(2) are given by $ln\gamma_1 = 0.64x_2^2$ and $ln\gamma_2 = 0.64x_1^2$. If this mixture forms an azeotrope at 320 K, compute the azeotropic composition. [**15**]

3. Consider the reaction $C_2H_5OH(g) + (1/2)O_2(g) \rightarrow CH_3CHO\ (g)+H_2O\ (g)$.

   The reaction reaches equilibrium at 600^0C and 1 bar. Assuming that the standard heat of this reaction is independent of temperature, Compute the value of equilibrium constant at 600^0C and 1 bar. [**15**]