BIRLA INSTITUTE OF TECHNOLOGY AND SCIENCE, PILANI - HYDERABAD CAMPUS

FIRST SEMESTER 2022-2023

CHEMICAL ENGINEERING THERMODYNAMICS (CHE F213)

Date: 28 Dec 2022 Comprehensive Exam (Open Book) Duration: 150 min Maximum Marks: 65 M

Instructions:

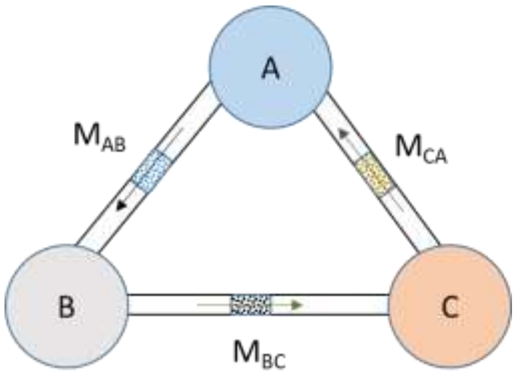
- All the questions are mandatory.
- State and take suitable assumptions, if required.

PART B

Q1) Three reactors (A, B and C) in an isolated chamber are initially charged as follows: Reactor A has pure ethane (C_2H_6), B has pure hydrogen (H_2) and C has pure ammonia (NH_3). All these three reactors are interconnected by a rigid, semipermeable membrane as shown below. These reactors have suitable catalysts so that the following reactions (R1 and R2) are always in equilibrium.

$$C_2H_{6(g)} \rightleftarrows C_2H_{4(g)} + H_{2(g)} \qquad \text{(R1)}$$

$$NH_{3(g)} \rightleftarrows 0.5\,N_{2(g)} + 1.5\,H_{2(g)} \qquad \text{(R2)}$$



Membrane M_{AB} is permeable only to C_2H_4, M_{BC} to H_2, and M_{CA} to N_2.

(a) Develop the conditions of restraint for total entropy using the fundamental property relation for open system.

Hint: Write fundamental property relation for each reactor and combine them to get total entropy.

(b) Considering extent of the reaction as ε_1 and ε_2 for reactions R1 and R2, write the change in number of moles of a component (dn_i^j, here i = C_2H_6, C_2H_4, H_2, N_2, and NH_3; j = Reactor A, B, and C) of in each compartment.

(c) As the overall system is isolated, the total entropy can be considered as zero. Combining the first and second law, develop generalized equilibrium criteria for temperatures and chemical potentials. **(3 + 6 + 3 = 12 M)**

Q2) Ten years ago, engineers at NASA's Jet Propulsion Lab celebrated the successful landing of its fourth robot (The Curiosity rover) on Mars. Curiosity rover has Sample Analysis at Mars (SAM) tool equipped with Gas Chromatograph and Mass Spectrometer to detect the atmospheric composition. A decade of the data obtained from SAM of Curiosity rover confirmed the average composition as, CO_2: N_2: O_2: CO: Ar: trace = 95: 2.6: 0.16: 0.06: 1.9: 0.28 (vol%).

(a) Find the average molecular weight by combining trace quantities with either N_2 or Ar.

(b) The mean surface temperature and pressure of the planet are minus 65°C (– 65 °C) and 650 Pa. Find the density of air on Mars using ideal gas law.

(c) Explain the procedure for finding the residual molar volume (V^R) and comment on ideal gas law validity.

(1 + 2 + 3 = 6 M)

Q3) NASA and Space-X are planning for human colonization on Mars. In order to do that Oxygen is essential and its availability is merely 0.16 vol% on Mars (Refer to the data in Q2). Extracting O_2 from Mars air is not feasible. Thus, scientists developed CO_2 reduction reactor (solid oxide fuel cells to be precise) to generate O_2 and pressurize the colonies with it. One of the CO_2 reduction reaction is, $CO_{2(g)} \rightleftharpoons CO_{(g)} + 0.5O_{2(g)}$. This reaction is feasible at 800°C and 1 bar. At these conditions all the components exist in ideal gas state.

(a) Find the heat of reaction, entropy and Gibbs energy change at 800°C and 1 bar.

(b) Calculate equilibrium constant (K).

(c) Calculate the equilibrium composition. **(8 + 4 + 6 = 18 M)**

Q4) The excess property of a binary solution at constant T and P is given as,

$M^E = 500x_1 + 1000x_2 + (50x_1 + 40x_2)x_1x_2$, J/mol of solution.

(a) Derive the expressions for partial molar excess properties ($\overline{M}_1^E$ and $\overline{M}_2^E$). Find $\overline{M}_1^E$ (in J/mol of component 1) and $\overline{M}_2^E$ (in J/mol of component 2) for a solution of $x_1 = 0.4$.

(b) Verify Gibbs/Duhem equation.

(c) Determine the partial molar property at infinite dilution. **(4 + 4 + 2 =10 M)**

Q5) Methanol is stored at 10 bar and 50°C.

(a) Calculate its vapor pressure using Antoine Equation.

(b) Find out the phase of methanol and its density or molar volume.

(c) Estimate its fugacity. **(1 + 2 + 4 = 7 M)**

Q6) The three suffix Margules parameters for acetone (1)-cyclohexane (2) at 25°C are $A_{12} = 2.0522$ and $A_{21} = 1.7201$. The Margules equations for the activity coefficients are,

$$\ln \gamma_1 = x_2^2\left[A_{12} + 2(A_{21} - A_{12})x_1\right]$$

$$\ln \gamma_2 = x_1^2\left[A_{21} + 2(A_{12} - A_{21})x_2\right]$$

(a) Find P, activity coefficients $\{\gamma_i\}$ and vapor phase compositions $\{y_i\}$ at $x_1 = 0.3$ and 25°C.

(b) Find the relative volatility in (a). Comment on the separation feasibility. **(5 + 1 = 6 M)**

Q7) Develop T-x,y plot on a graph sheet for benzene (1) and toluene (2) mixtures at 200 kPa. Make sure to have minimum 6 data points for each saturation line (bubble and dew lines). **(6 M)**

~~~ Wish you all the best ~~~