

NB:

1. Question No. 1 is compulsory.
2. Attempt any three questions out of remaining five questions.
3. Assumptions made should be clearly stated. All relevant data has been provided at the end of questions.
4. Illustrate answers with sketch wherever required.

1.

a Fill in the blanks 10

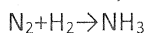
- i. At equilibrium the entropy of an isolated system _____.
- ii. For a reversible reaction the Gibbs Energy is _____ at equilibrium.
- iii. For a system obeying Henry's law the product of the Henry's constant and the mole fraction of a component is equal to _____ of the component in vapour phase.
- iv. For an ideal gas mixture the total pressure is equal to the sum of _____.
- v. When an ideal gas is mixed the entropy of mixing at constant temperature and pressure is _____.

b 10

- i. For an ideal solution the activity coefficient is
 - a. 1.
 - b. Greater than 1.
 - c. Less than 1.
 - d. Depends on the solution.
- ii. When the VLE of a mixture exhibits positive deviation from Raoult's law at constant temperature
 - a. The actual pressures exceed those predicted by Raoult's law.
 - b. The actual pressure is less than that predicted by Raoult's Law.
 - c. The actual and the ideal pressures are the same.
 - d. None of the choices.
- iii. A constant temperature VLE mixture shows negative deviation from Raoult's law, its azeotropic mixture will form
 - a. Maximum boiling azeotrope
 - b. Minimum Boiling azeotrope
 - c. Cannot be predicted
 - d. none of the choices.
- iv. The fugacity coefficient for an ideal gas mixture is
 - a. 1.
 - b. greater than 1.
 - c. less than 1.
 - d. depends on temperature and pressure.
- v. For a minimum boiling azeotrope the boiling temperature of the azeotrope
 - a. is less than the low boiler and the high boiler.
 - b. less than the low boiler.
 - c. Higher than the high boiler.
 - d. Higher than the low boiler and the high boiler.

2

- a. Ammonia is produced by Habers Process by the reaction 10



The reaction is carried out in gas phase. The Feed and the exit conditions of the reactors are given below. It is assumed that the mixture behaves as ideal gas and the products leave at equilibrium. Calculate the flowrate and the composition of the exit stream of the reactor.

Mole Fraction	Inlet	Outlet
N ₂	0.24	To be calculated
H ₂	0.70	To be calculated
Ar	0.01	To be calculated
CH ₄	0.04	To be calculated
NH ₃	0.01	To be calculated
Total Flow kmol/s	3.274	To be calculated
Temp K	284	650
Press	100 bar	100 bar

The equilibrium constant for the reaction is

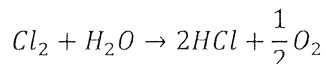
$$\log K_a = -2.691122 \log T - 5.519265 \times 10^{-5} T + 1.848863 \times 10^{-7} T^2 + \frac{2001.6}{T} + 2.6899$$

,where T is in K .

- b. Calculate the heat to be removed from the reactor 10

3

In a manufacturing process HCl is manufactured via the following reaction:



This gas phase reaction is carried out at 200°C with saturated steam at 200°C and chlorine at 200°C entering the reactor with ratio of 3 mol of steam per mol of chlorine gas.

- a. If the reaction is 100% complete and the products leave the reactor at 200°C, how much heat must be added or removed for every kg mol of HCl obtained? (note:heat of solution cannot be neglected) 10
- b. The gas stream leaving the reactor is to be cooled and the steam and HCl condensed so that leaving the cooler will be an aqueous solution of HCl and pure oxygen stream each at 25°C. How much heat must be removed from the cooler per kg mol of HCl produced in the reactor? 10

4

- a. A system of n-pentane(1)/n-heptane(2) obeys Raoult's Law. For this system find the fraction that is liquid, x_1 and y_1 at 60°C and 115 kPa when the overall composition of the system is equimolar. 10
- b. The boiling point estimation of n-octane is done by Joback group contribution method. The formula for this is $T_b(K) = 198 + \sum_i \vartheta_i \Delta T_b$ where ϑ_i is the number of groups and ΔT_b is the boiling point contribution. Find the boiling point of n-octane given that the boiling point contribution of non ring CH₃ group, non ring CH₂ group, are 23.58 and 22.88, respectively. 10

5

- a. An ideal ammonia absorption refrigeration system is used to cool an enclosure to -15°C. Heat is available in the generator at 110°C. Cooling water is available at 30°C. Assuming that cooling and heating are done isothermally, 10

in all the exchangers, calculate the COP. The COP of absorption refrigeration system is given by $COP = \frac{T_R}{T_2 - T_R} \times \frac{T_1 - T_2}{T_1}$. T_R is the temperature of the evaporator, T_1 is the temperature of the generator, T_2 is the temperature of the Absorber/Condenser. For 1T refrigeration, what is the heat supplied in the generator, and heat to be removed from the absorber, if the heat removed from the condenser is 3 kW. Take 1 T refrigeration as 3.5 kW

- b At 30°C infinite dilution activity coefficients for a binary vle system of diethylether(1)/chloroform(2) are $\gamma_1^\infty = 0.71, \gamma_2^\infty = 0.57$. The vapour pressures are $P_1^{sat} = 33.73 \text{ kPa}, P_2^{sat} = 86.59 \text{ kPa}$. The activity coefficients can be modelled using two parameter Margules equation. Prepare a P-x-y table for six equidistant points, between $x_1 = 0, 1$. No graph required 10

6 20

- a Prove that the fugacity of a liquid is equal to that of vapour at equilibrium
 b With a neat diagram explain the Vapor Absorption Refrigeration System
 c Write the equation of non-ideal vapour liquid equilibrium. Show that it is equal to Raoult's law as a special case. What is the special case?
 d Derive the equation $\ln\left(\frac{K}{K_1}\right) = -\frac{\Delta H_{Reaction}}{R}\left(\frac{1}{T} - \frac{1}{T_1}\right)$

Thermodynamic Data:

Heats of formation at 25°C in kJ/mol

Compound	ΔH_f^{298} kJ/mol
H_2O	-242.0 (g) -286.0 (l)
HCl	-92.37 (g)
NH_3	-46.22 (g)
CO	-110.6 (g)
CO_2	-393.8 (g)

Heat of solution

1 mol of HCl in 1 mol of water -45.61 kJ/ mol of HCl.

Specific heat of gases

c_p cal/gmol.K, T(K)

$$c_p = a + bT + cT^2 + dT^3$$

Compound	a	$b \times 10^2$	$c \times 10^5$	$d \times 10^9$
Cl_2	6.8214	0.57095	-0.5107	1.547
H_2O	7.7	0.04594	0.2521	-0.8587
HCl	7.244	-0.1820	0.3170	-1.036
O_2	6.085	0.3631	-0.1709	0.3133
NH_3	6.5846	0.61251	0.23663	-1.5981
H_2	6.952	-0.04967	0.09563	-0.2079
N_2	6.903	-0.03753	0.1930	-0.6861
CO	6.726	0.04001	0.1283	-0.5307
CO_2	5.316	1.4285	-0.8362	1.784
Ar	Same as Nitrogen			
CH_4	4.750	1.2	0.3030	-2.630

Antoine constants

Equation

$$\ln P^{sat}(\text{kPa}) = \frac{B}{t(^{\circ}C) + C}$$

Comp	A	B	C
n-pentane	13.8183	2477.07	233.21
n-heptane	13.8587	2911.32	216.64
