KATHMANDU UNIVERSITY
End Semester Examination
June/July, 2023

06 JUL 2023

Level : B.E.
Year : II
Time : 2 hrs. 30 mins

Course : CHEG 211
Semester : II
F.M. : 40

SECTION "B"

[4Q. × 5 = 20 marks]

Attempt *ALL* questions.

1. A steady flow adiabatic turbine (expander) accepts gas at 500 K and 6 bar and discharges at 371 K and 1.2 bar. Assuming ideal gas, determine actual work, ideal work, lost work and entropy generation rate. Take T_{surr} as 300 K and $C_p/R = 3.5$ [5]

2. For SO_2 at 600 K and 300 bar, determine good estimates of the fugacity coefficient, fugacity and G^R/RT. [5]

3. A liquid mixture of n-pentane and n-hexane containing 40 mol percent n-pentane is fed continuously to a flash separator operating at 121 °C and 552 kPa. Determine:
   a. The quantity of vapor and liquid obtained from the separator. [3]
   b. Compositions of both the vapor and the liquid leaving the separator. [2]

4. VLE data for a binary system at 35 C is given below.

P, kPa	x_1	y_1
85.265	0	0
80.481	0.0924	0.0416
72.422	0.2482	0.1314
65.096	0.3880	0.2457
56.833	0.5749	0.4564
51.62	0.7676	0.7176
50.455	0.8476	0.8238
49.72	0.9529	0.9502
49.624	1	1

   a. Determine the activity coefficients of both components at $x_1 = 0.2482$ and 0.8476. [2]
   b. Determine the bubble point pressure at $x_1 = 0.3880$ and the mole fraction composition of the first bubble. [2]
   c. Estimate the parameters for Margules equation. [1]

SECTION "C"

[2Q. × 10 = 20 marks]

Attempt *ALL* questions.

5. The excess Gibbs energy of the binary liquid mixture at T and P is given by:

$$\frac{G^E}{RT} = (-2.6x_1 - 1.8x_2)x_1x_2$$

   a. Find the expression for $\ln\gamma_1$ and $\ln\gamma_2$. [2]
   b. Show that the partial expressions obtained in part (a) when combined according to summability relation gives the expression for $\frac{G^E}{RT}$. [3]
   c. Show that the partial molar expressions satisfy the Gibbs Duhem equation. [3]
   d. Determine the numerical values of γ_1 and γ_2 at infinite dilutions. [2]

6. For the ammonia synthesis reaction

$$0.5N_2\,(g) + 1.5H_2\,(g) \rightarrow NH_3\,(g)$$

If the feed mixture of N_2 and H_2 are in stoichiometric proportions, and assuming $\Delta H_{rxn}{}^o$ is independent of temperature

a. Calculate the reaction coordinate at 1 bar and 298.15 K? [2]

b. At what temperature does the equilibrium mole fraction of NH_3 equal 0.5 for a pressure of 1 bar? [2]

c. At what temperature does the equilibrium mole fraction of NH_3 equal 0.5 for a pressure of 100 bar assuming the equilibrium mixture is an ideal gas? [2]

d. Calculate the equilibrium mole fraction of NH_3 at 500 K and 100 bar assuming the equilibrium mixture is an ideal solution of gases? [4]

Useful Equations and Tables:

$$\Delta S = \int_{T_1}^{T_2} \frac{C_p}{T} dT - nR\ln\frac{P_2}{P_1}$$

$$\Pi_i (y_i \emptyset_i)^{\upsilon_i} = \left(\frac{P}{P^0}\right)^{-\upsilon} K$$

$$y_i \emptyset_i P = x_i \gamma_i P_i^{sat}$$

$$\overline{M_1} = M + x_2 \frac{dM}{dx_1}$$

$$\overline{M_2} = M - x_1 \frac{dM}{dx_1}$$

For pure species:

$$\emptyset = (\emptyset^0)(\emptyset^1)^{\omega}$$

$$G^R = RT\ln\emptyset_i$$

$$\ln\left(\frac{K_2}{K_1}\right) = -\frac{\Delta H_{rxn}{}^o}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)$$

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

$$\ln\frac{K_2}{K_1} = -\frac{\Delta H^0_{rxn}}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)$$

Margule's equation:

$$\frac{G^E}{RT} = (A_{21}x_1 + A_{12}x_2)x_1x_2$$

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

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

$$\ln P^{sat}/\text{kPa} = A - \frac{B}{t/^\circ C + C}$$

Latent heat of vaporization at the normal boiling point (ΔH_n), and normal boiling point (t_n)

Name	Formula	Parameters for Antoine Eqn. A†	B	C	Temp. Range °C	ΔH_n kJ/mol	t_n °C
Acetone	C_3H_6O	14.3145	2756.22	228.060	−26—77	29.10	56.2
Acetic acid	$C_2H_4O_2$	15.0717	3580.80	224.650	24—142	23.70	117.9
Acetonitrile*	C_2H_3N	14.8950	3413.10	250.523	−27—81	30.19	81.6
Benzene	C_6H_6	13.7819	2726.81	217.572	6—104	30.72	80.0
iso-Butane	C_4H_{10}	13.8254	2181.79	248.870	−83—7	21.30	−11.9
n-Butane	C_4H_{10}	13.6608	2154.70	238.789	−73—19	22.44	−0.5
1-Butanol	$C_4H_{10}O$	15.3144	3212.43	182.739	37—138	43.29	117.6
2-Butanol*	$C_4H_{10}O$	15.1989	3026.03	186.500	25—120	40.75	99.5
iso-Butanol	$C_4H_{10}O$	14.6047	2740.95	166.670	30—128	41.82	107.8
tert-Butanol	$C_4H_{10}O$	14.8445	2658.29	177.650	10—101	39.07	82.3
Carbon tetrachloride	CCl_4	14.0572	2914.23	232.148	−14—101	29.82	76.6
Chlorobenzene	C_6H_5Cl	13.8635	3174.78	211.700	29—159	35.19	131.7
1-Chlorobutane	C_4H_9Cl	13.7965	2723.73	218.265	−17—79	30.39	78.5
Chloroform	$CHCl_3$	13.7324	2548.74	218.552	−23—84	29.24	61.1
Cyclohexane	C_6H_{12}	13.6568	2723.44	220.618	9—105	29.97	80.7
Cyclopentane	C_5H_{10}	13.9727	2653.90	234.510	−35—71	27.30	49.2
n-Decane	$C_{10}H_{22}$	13.9748	3442.76	193.858	65—203	38.75	174.1
Dichloromethane	CH_2Cl_2	13.9891	2463.93	223.240	−38—60	28.06	39.7
Diethyl ether	$C_4H_{10}O$	14.0735	2511.29	231.200	−43—55	26.52	34.4
1,4-Dioxane	$C_4H_8O_2$	15.0967	3579.78	240.337	20—105	34.16	101.3
n-Eicosane	$C_{20}H_{42}$	14.4575	4680.46	132.100	208—379	57.49	[illegible]3.6
Ethanol	C_2H_6O	16.8958	3795.17	230.918	3—96	38.56	78.2
Ethylbenzene	C_8H_{10}	13.9726	3259.93	212.300	33—163	35.57	136.2
Ethylene glycol*	$C_2H_6O_2$	15.7567	4187.46	178.650	100—222	50.73	197.3
n-Heptane	C_7H_{16}	13.8622	2910.26	216.432	4—123	31.77	98.4
n-Hexane	C_6H_{14}	13.8193	2696.04	224.317	−19—92	28.85	68.7
Methanol	CH_4O	16.5785	3638.27	239.500	−11—83	35.21	64.7

Chemical species		State (Note 2)	$\Delta H^\circ_{f_{298}}$ (Note 1)	$\Delta G^\circ_{f_{298}}$ (Note 1)
Miscellaneous inorganics:				
Ammonia	NH_3	(*g*)	−46,110	−16,400
Ammonia	NH_3	(*aq*)		−26,500
Calcium carbide	CaC_2	(*s*)	−59,800	−64,900
Calcium carbonate	$CaCO_3$	(*s*)	−1,206,920	−1,128,790
Calcium chloride	$CaCl_2$	(*s*)	−795,800	−748,100
Calcium chloride	$CaCl_2$	(*aq*)		−8,101,900
Calcium chloride	$CaCl_2{\cdot}6H_2O$	(*s*)	−2,607,900	
Calcium hydroxide	$Ca(OH)_2$	(*s*)	−986,090	−898,490
Calcium hydroxide	$Ca(OH)_2$	(*aq*)		−868,070
Calcium oxide	CaO	(*s*)	−635,090	−604,030
Carbon dioxide	CO_2	(*g*)	−393,509	−394,359
Carbon monoxide	CO	(*g*)	−110,525	−137,169