04-CHEM-A1, PROCESS BALANCES and CHEMICAL THERMODYNAMICS

DECEMBER 2016

Three Hours Duration

NOTES:

1) If doubt exists as to the interpretation of any question, you are urged to submit a clear statement of any assumptions made along with the answer paper.

2) Property data required to solve a given problem are provided in the problem statement or are available in the recommended texts. If you are unable to locate the required data, do not let this prevent you from solving the rest of the problem. Even in the absence of property data, you still have the opportunity to provide a solution methodology.

3) This is an open-book exam.

4) Any non-communicating calculator is permitted.

5) The examination is in two parts – Part A (Questions 1 to 3): Process Balances
Part B (Questions 4 to 6): Chemical Thermodynamics

6) Answer **TWO** questions from Part A and **TWO** questions from Part B.

7) **FOUR** questions constitute a complete paper.

8) Each question is of equal value.

PART A: PROCESS MASS and ENERGY BALANCES

1) Soda ash (Na_2CO_3) is manufactured by the decomposition of sodium bicarbonate ($NaHCO_3$). Other products of the decomposition reaction include carbon dioxide and water vapor. In an experimental investigation, wet sodium bicarbonate containing 8% water is premixed with recycled dry soda ash in order to reduce the water content to 5% before reintroducing into the calciner. The calciner is fed with 2000 kg/hr of wet sodium bicarbonate.

Determine the following:

a) Quantity of soda ash produced per hour of the final product.

b) Quantity of off gases produced per hour.

c) Mole ratio of carbon dioxide to water vapor in the off gases.

d) Quantity of soda ash recycled per hour of the final product.

2) Wood containing 45.9% carbon, 23.1% oxygen, 5.1% ash, and the rest containing moisture and hydrogen is burnt in a furnace. An Orsat analysis of the flue gas during a run shows 14.8% carbon dioxide, 1.66% carbon monoxide, 3.46% oxygen and 80.08% nitrogen.

Determine the following:

a) Complete analysis of the wood used.

b) Ratio of fuel to air by weight.

c) Percentage of excess air used.

d) Composition of the flue gas.

3) Obtain an empirical equation for calculating the heat of reaction at any temperature T for the following reaction:

$$CO\ (g) + 2H_2\ (g) \rightarrow CH_3OH\ (g)$$

The standard heat of reaction (ΔH^o_R) is - 21.59 kcal/mol, and the specific heat capacity (C^o_p) is given by the equation

$$C^o_p = a + bT + cT^2 + dT^3 \qquad \text{in kcal/mol.K}$$

Component	**a**	**b x 10³**	**c x 10⁶**	**d x 10⁹**
CO	29.03	- 2.82	11.64	- 4.71
H_2	28.61	1.02	- 0.15	0.77
CH_3OH	21.14	70.84	25.87	- 28.50

PART B: CHEMICAL THERMODYNAMICS

4) Calculate the fugacity of liquid hydrogen chloride at 277.4 K and 13.61 atm.

DATA: Vapor pressure of pure HCl at 277.4 K = 28.81 atm
Critical temperature of HCl = 324.68 K
Critical pressure of HCl = 81.5 atm

5) Consider the following methanol synthesis reversible gas-phase reaction:

$$CO\ (g) + 2H_2\ (g) \rightarrow CH_3OH\ (g)$$

At 298 K, the standard Gibbs free energy change of the reaction (ΔG^o) is - 25.2 kJ/mol and the standard enthalpy change of reaction (ΔH^o) is - 90.7 kJ/mol. We wish to know the ranges of temperatures and pressure for which the equilibrium conversion is at least 10% when the stoichiometric ratios of CO and H_2 are used. Show this favorable region on a pressure-temperature plot.

6) Experimental vapor-liquid equilibrium data for isopropanol-benzene binary system at 45 °C is given below:

Mole fraction of isopropanol in liquid	**Mole fraction of isopropanol in vapor**	**Vapor pressure of isopropanol,** in kPa
0.0000	0.0000	29.829
0.0472	0.1467	33.633
0.0980	0.2066	35.214
0.2047	0.2663	36.271
0.2960	0.2953	36.450
0.3862	0.3211	36.292
0.4753	0.3463	35.928
0.5504	0.3962	35.319
0.6198	0.3951	34.577
0.7096	0.4378	33.023
0.8073	0.5107	30.282
0.9120	0.6658	25.235
0.9655	0.8252	21.305
1.0000	1.0000	18.138

a) Plot the dew point and bubble point curves versus mole fraction isopropanol.

b) Calculate and plot partial vapor pressures of isopropanol and benzene versus mole fraction of isopropanol.

b) Calculate and plot the natural log of activity coefficient ($\ln \gamma$) of isopropanol and benzene versus mole fraction of isopropanol in liquid (X_1).

d) Calculate and plot the $G^E/(X_1 X_2 R T)$ versus mole fraction of isopropanol in liquid (X_1). Here X_2 is the mole fraction of benzene in liquid, R is the Universal gas constant and T is the temperature.

The Periodic Table of the Elements

- Alkali metals
- Alkaline earth metals
- Transition metals
- Other metals
- Metalloids (semi-metal)
- Nonmetals
- Halogens
- Noble gases

Element name → Mercury
Atomic # → 80
Symbol → Hg
Avg. Mass → 200.59

1	2		3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
Hydrogen 1 H 1.01																		Helium 2 He 4.00
Lithium 3 Li 6.94	Beryllium 4 Be 9.01												Boron 5 B 10.81	Carbon 6 C 12.01	Nitrogen 7 N 14.01	Oxygen 8 O 16.00	Fluorine 9 F 19.00	Neon 10 Ne 20.18
Sodium 11 Na 22.99	Magnesium 12 Mg 24.31												Aluminum 13 Al 26.98	Silicon 14 Si 28.09	Phosphorus 15 P 30.97	Sulfur 16 S 32.07	Chlorine 17 Cl 35.45	Argon 18 Ar 39.95
Potassium 19 K 39.10	Calcium 20 Ca 40.08		Scandium 21 Sc 44.96	Titanium 22 Ti 47.88	Vanadium 23 V 50.94	Chromium 24 Cr 52.00	Manganese 25 Mn 54.94	Iron 26 Fe 55.85	Cobalt 27 Co 58.93	Nickel 28 Ni 58.69	Copper 29 Cu 63.55	Zinc 30 Zn 65.39	Gallium 31 Ga 69.72	Germanium 32 Ge 72.61	Arsenic 33 As 74.92	Selenium 34 Se 78.96	Bromine 35 Br 79.90	Krypton 36 Kr 83.80
Rubidium 37 Rb 85.47	Strontium 38 Sr 87.62		Yttrium 39 Y 88.91	Zirconium 40 Zr 91.22	Niobium 41 Nb 92.91	Molybdenum 42 Mo 95.94	Technetium 43 Tc (98)	Ruthenium 44 Ru 101.07	Rhodium 45 Rh 102.91	Palladium 46 Pd 106.42	Silver 47 Ag 107.87	Cadmium 48 Cd 112.41	Indium 49 In 114.82	Tin 50 Sn 118.71	Antimony 51 Sb 121.76	Tellurium 52 Te 127.60	Iodine 53 I 126.90	Xenon 54 Xe 131.29
Cesium 55 Cs 132.91	Barium 56 Ba 137.33	57-70 *	Lutetium 71 Lu 174.97	Hafnium 72 Hf 178.49	Tantalum 73 Ta 180.95	Tungsten 74 W 183.84	Rhenium 75 Re 186.21	Osmium 76 Os 190.23	Iridium 77 Ir 192.22	Platinum 78 Pt 195.08	Gold 79 Au 196.97	Mercury 80 Hg 200.59	Thallium 81 Tl 204.38	Lead 82 Pb 207.20	Bismuth 83 Bi 208.98	Polonium 84 Po (209)	Astatine 85 At (210)	Radon 86 Rn (222)
Francium 87 Fr (223)	Radium 88 Ra (226)	89-102 **	Lawrencium 103 Lr (262)	Rutherfordium 104 Rf (267)	Dubnium 105 Db (268)	Seaborgium 106 Sg (271)	Bohrium 107 Bh (272)	Hassium 108 Hs (270)	Meitnerium 109 Mt (276)	Darmstadtium 110 Ds (281)	Roentgenium 111 Rg (280)	Copernicium 112 Cn (285)	Ununtrium 113 Uut (284)	Ununquadium 114 Uuq (289)	Ununpentium 115 Uup (288)	Ununhexium 116 Uuh (293)	Ununseptium 117 Uus (294?)	Ununoctium 118 Uuo (294)

*lanthanides	Lanthanum 57 La 138.91	Cerium 58 Ce 140.12	Praseodymium 59 Pr 140.91	Neodymium 60 Nd 144.24	Promethium 61 Pm (145)	Samarium 62 Sm 150.36	Europium 63 Eu 151.97	Gadolinium 64 Gd 157.25	Terbium 65 Tb 158.93	Dysprosium 66 Dy 162.50	Holmium 67 Ho 164.93	Erbium 68 Er 167.26	Thulium 69 Tm 168.93	Ytterbium 70 Yb 173.04
**actinides	Actinium 89 Ac (227)	Thorium 90 Th 232.04	Protactinium 91 Pa 231.04	Uranium 92 U 238.03	Neptunium 93 Np (237)	Plutonium 94 Pu (244)	Americium 95 Am (243)	Curium 96 Cm (247)	Berkelium 97 Bk (247)	Californium 98 Cf (251)	Einsteinium 99 Es (252)	Fermium 100 Fm (257)	Mendelevium 101 Md (258)	Nobelium 102 No (259)