Chapter 8 Assignment
(Answers are in parenthesis)

1. Calculate the standard Gibbs free energy change and the equilibrium constant at 298K for the following reaction: $C_2H_5OH(g) + (1/2)O_2(g) \rightarrow CH_3CHO(g) + H_2O(g)$. **[– 188.9kJ; 1.4x10^{38}]**

2. Assuming that ΔH^o is constant in the temperature range 298 – 800 K, estimate the equilibrium constant at 800 K for the reaction of Problem 1. **[4.3x10^{14}]**

3. Ethanol can be produced according to the reaction: $C_2H_4(g) + H_2O(g) \rightarrow C_2H_5OH(g)$
If an equimolar mixture of ethylene and water vapor is fed to a reactor which is maintained at 1000 K and 1 bar determine the degree of conversion, assuming that the reaction mixture behaves like an ideal solution. Assume the following ideal gas specific heat data: $C_p^{ig} = a + bT + cT^2 + dT^3 + eT^{-2}$ (J/mol); T(K) **[0.5]**

Species	a	bx10^3	cx10^6	dx10^9	ex10^{-5}
C_2H_4	20.691	205.346	– 99.793	18.825	-
H_2O	4.196	154.565	– 81.076	16.813	-
C_2H_5OH	28.850	12.055	-	-	1.006

4. Calculate the degree of conversion and the composition of the reaction mixture if $N_2(g)$ and $H_2(g)$ are fed in the mole ratio of 1:5 at 800 K and 100 bar for the synthesis of ammonia. Assume that equilibrium is established and the reaction mixture behaves like an ideal gas. $C_p^{ig} = a + bT + cT^2 + dT^3 + eT^{-2}$ (J/mol); T(K) **[0.2356]**

Species	a	bx10^3	cx10^6	dx10^9	ex10^{-5}
N_2	20.270	4.930	-	-	0.333
H_2	27.012	3.509	-	-	0.690
NH_3	29.747	25.108	-	-	– 1.546

5. Calculate the degree of conversion if the feed to an ammonia synthesis reactor is a mixture of $N_2(g)$, $H_2(g)$ and $NH_3(g)$ in the mole ratio 1:3:0.1 at 800 K and 100 bar. Assume that the reaction mixture behaves like an ideal gas. **[0.1235]**

6. The following two independent reactions occur in the steam cracking of methane at 1000 K and 1 bar: $CH_4(g) + H_2O(g) \rightarrow CO(g) + 3H_2(g)$; and $CO(g) + H_2O(g) \rightarrow CO_2(g) + H_2(g)$. Assuming ideal gas behaviour determine the equilibrium composition of the gas leaving the reactor if an equimolar mixture of CH_4 and H_2O is fed to the reactor, and that at 1000K, the equilibrium constants for the two reactions are 30 and 1.5 respectively. **[$\varepsilon_1 = 0.8$; $\varepsilon_2 = 0.06$]**

7. Consider the following reaction: $Fe(s) + H_2O(g) \rightarrow FeO(s) + H_2(g)$. Assuming that equilibrium is achieved, determine the fraction of H_2O which decomposes at 1000°C. The equilibrium constant for the reaction at 1000°C is 1.6. **[61.5%]**

8. Show that:

$$\left(\frac{\partial \varepsilon_e}{\partial T}\right)_P = \frac{K_y}{RT^2}\frac{d\varepsilon_e}{dK_y}\Delta H^0 \quad \text{and} \quad \left(\frac{\partial \varepsilon_e}{\partial P}\right)_T = \frac{K_y}{P}\frac{d\varepsilon_e}{dK_y}(-\nu)$$

9. The gas stream from a sulfur burner is composed of 15-mol-% SO_2, 20-mol-% O_2, and 65-mol-% N_2. This gas stream at 1 bar and 480°C enters a catalytic converter, where the SO_2 is further oxidized to SO_3. Assuming that the reaction reaches equilibrium, how much heat must be removed from the converter to maintain isothermal conditions? Base your answer on 1 mol of entering gas. **[Ans: ε_e = 0.1455, Q = – 14314 J/mol]**

10. For the cracking reaction:$C_3H_8(g) \rightarrow C_2H_4(g) + CH_4(g)$; the equilibrium conversion is negligible at 300 K, but becomes appreciable at temperatures above 500 K. For a pressure of 1 bar, determine (a) The fractional conversion of propane at 625 K. (b) The temperature at which the fractional conversion is 85%. **[Ans: ε_e = 0.777, T = 647K]**

11. The following isomerization reaction occurs in the liquid phase: A → B; where A and B are miscible liquids for which: $G^E / RT = 0.1x_Ax_B$. (a) If ΔG^o_{298} = –1000 J/mol, what is the equilibrium composition of the mixture at 298°K? **[x_A = 0.3955]** (b) What is the answer for 'a' if one assumes that A and B form an ideal solution? **[x_A = 0.4005].**

12. Feed gas to a methanol synthesis reactor is: 75-mol-% H_2, 15-mol-% CO, 5-mol-% CO_2, and 5-mol-% N_2. The system comes to equilibrium at 550 K and 100 bar with respect to the following reactions: $2H_2(g) + CO(g) \rightarrow CH_3OH(g)$; and $H_2(g) + CO_2(g) \rightarrow CO(g) + H_2O(g)$. Assuming ideal gases, determine the composition of the equilibrium mixture. **[Ans: $K_1 = 6.749\text{x}10^{-4}$; $K_2 = 1.726\text{x}10^{-2}$; ε_1 = 0.1186; $\varepsilon_2 = 8.8812\text{x}10^{-3}$].**