CBE 450 Chemical Reactor Fundamentals
Fall, 2009
Homework Assignment #1

1. Review of Mass Balances of Reacting Systems

Natural gas (assume pure methane) is being burned in air (assume 0.79 mol% N_2 and 0.21 mol% O_2). Assume complete combustion, which means that all of the natural gas is burned and is converted into carbon dioxide and water. Assume that the oxygen is provided in 100% excess. The flow rate of natural gas is 100 mol/s. The furnace operates at steady state.

(a) Draw a diagram with all input and output streams. Indicate known and unknown flowrates. Indicate known and unknown compositions.
(b) Determine the flowrate of air.
(c) Determine the flowrate and composition of the output gas using atomic balances.
(d) Determine the flowrate and composition of the output gas using molecular balances.

2. Molecular Description of Reaction Equilibrium

Consider, for example, the distribution of para-xylene, meta-xylene and ortho-xylene.
(a) For an ideal gas at a given temperature, what factors at the molecular level determine the equilibrium distribution of components?
(b) At a given temperature, will the mole faction of the component with the lowest enthalpy be greater or less than the mole fraction of the other components (all other things being equal)? Why?
(c) At a given temperature, will the mole faction of the component with the lowest entropy be greater or less than the mole fraction of the other components (all other things being equal)? Why?
(d) At a given temperature, will the mole faction of the component with the lowest free energy be greater or less than the mole fraction of the other components (all other things being equal)? Why?
(e) As the temperature is increased, will the mole fraction of the component with the lowest enthalpy increase or decrease (all other things being equal)? Why?
(f) As the temperature is increased, will the mole fraction of the component with the lowest entropy increase or decrease (all other things being equal)? Why?

3. Review Continuum Description of Reaction Equilibrium

Consider a batch reactor initially containing nitrogen and hydrogen gases. The volume of the batch reactor is 1 m^3. The initial pressure is 1 atm. The temperature is kept constant at 500 K. The initial mole fractions are 0.25 N_2 and 0.75 H_2. The relevant reaction is

$$\frac{1}{2}N_2 + \frac{3}{2}H_2 \rightarrow NH_3$$

The reference enthalpies of formation are at a reference temperature of 298.15 K

$$H_{f,N2} = 0\,kcal/mol$$

$$H_{f,H2} = 0\, kcal/mol$$
$$H_{f,NH3} = -10.96\ kcal/mol$$

The reference Gibbs free energies of formation are at a reference temperature of 298.15 K

$$G_{f,N2} = 0\, kcal/mol$$
$$G_{f,H2} = 0\, kcal/mol$$
$$G_{f,NH3} = -3.903\ kcal/mol$$

In this project, you may assume that the heat capacities are constant, given by

$$C_{p,N2} = 7.03\ cal/mol/K$$
$$C_{p,H2} = 6.92\ cal/mol/K$$
$$C_{p,NH3} = 9.31\ cal/mol/K$$

(a) What are the heats of formation at 500 K for each component?
(b) What are the free energies of formation at 500 K for each component. (You may assume that the heat of formation is constant in this part (b) calculation only.)
(c) Compute the heat of reaction and free energy of reaction at 500 K on a per mole basis of NH_3 produced.
(d) Compute the equilibrium coefficient of the reaction at 500 K.
(e) Compute the equilibrium mole fractions of each component at 500 K.