CBE 450 Chemical Reactor Fundamentals
Fall, 2009
Homework Assignment #7

1. Nonisothermal Batch Reactor

Consider the reversible reaction

$$2A \leftrightarrow B$$

with elementary mechanism such that the rate of the forward reaction is

$$r_1 = k_1 C_A^{\ 2}$$

and the reverse reaction is

$$r_2 = k_2 C_B$$

where the rate constants are given by

$$k_1 = k_{o,1} \exp\left(-\frac{E_{a,1}}{RT} \right)$$

and

$$k_2 = k_{o,2} \exp\left(-\frac{E_{a,2}}{RT} \right)$$

The activation energy for the forward reaction is 5000 J/mol. The rate constant prefactor for the forward reaction is 0.001 liter/mol/s. The heat of reaction for the forward reaction is -12 kJ/mol. The rate constant prefactor for the reverse reaction is 0.001 1/s. The reaction occurs in a solvent, S. The heat capacities of A, B and the solvent are respectively 4, 7, and 3.5 J/mol/K. The initial concentration in the batch reactor for A, B and S are 10, 0 and 30 mol/liter. The initial temperature is 300 K. The reactor is well insulated.

(a) What are the temperature and conversion of A at 1 hr?
(b) Provide a plot of the transient behavior of the concentrations of A, B and S and the temperature. Explain the features.
(c) Make a plot or table of conversion after 1 hr vs heat of reaction for the forward reaction with at least three points (all of which are exothermic). Explain the behavior.

2. Nonisothermal Batch Reactor

Consider the system of irreversible reactions

A → B
A → C
A + B → D

with elementary mechanism such that the rate of the forward reaction is

$$r_1 = k_1 C_A, \qquad r_2 = k_2 C_A, \qquad \text{and} \qquad r_3 = k_3 C_A C_B$$

All reactions have an Arrhenius dependence on temperature

$$k_j = k_{o,j} \exp\left(-\frac{E_{a,j}}{RT} \right)$$

where the reaction properties are given in the table below

reaction	k_o (1/s or liter/mol/s)	E_a (J/mol)	heat of reaction (kJ/mol)
1	1.0	4000	0
2	1.0	3000	0
3	1.0	2000	-20

The reaction occurs in a solvent, S. The heat capacities of A, B, C, D and the solvent are respectively 4.0, 3.0, 5.0, 6.0, and 4.0 J/mol/K. The initial concentration in the batch reactor for A, B, C, D and S are 10, 0, 0, 0 and 40 mol/liter. The initial temperature is 300 K. The reactor is well insulated.

(a) What are the steady state temperature and concentrations of each component?
(b) What operating condition could you change if you want to form a higher ratio of C to D? Demonstrate.