CBE 450 Chemical Reactor Fundamentals
Fall, 2009
Homework Assignment #8 Solutions

1. Nonisothermal CSTR – 1 irreversible reaction
Consider the irreversible reaction in a CSTR

A → 2B

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

$$r = kC_A$$

where the rate constant is given by

$$k = k_o \exp\left(-\frac{E_a}{RT}\right)$$

The activation energy for the forward reaction is 4000 J/mol. The rate constant prefactor for the forward reaction is 0.1 l/s. The heat capacities of A, B and the solvent are respectively 4.0, 7.0, and 3.0 J/mol/K. The heats of formation of A and B at a reference temperature of 298.15 K are respectively -1000.0 and -10000.0 J/mol. The inlet flowrate is 10 liters/s. The inlet temperature is 500 K. The inlet concentrations of A, B and S are 10.0, 0.0, and 30.0 mol/liter respectively. The volume of the reactor is 1000 liters. The reactor is well insulated. The initial temperature and concentrations in the reactor are the same as the inlet temperature and concentrations.

(a) Provide a plot of the transient behavior of the concentrations of A, B and S and the temperature. Explain the features.
(b) What are the steady-state temperature and conversion of A?

2. Nonisothermal CSTR – 2 sequential reactions
Consider the two sequential reactions in a CSTR

A + B → C
A + C → D

with elementary mechanism such that the rate of the first and second reaction respectively are

$$r_1 = k_1 C_A C_B \quad \text{and} \quad r_2 = k_2 C_A C_C$$

where the rate constants are given by

$$k_1 = k_{o,1} \exp\left(-\frac{E_{a,1}}{RT}\right) \quad \text{and} \quad k_2 = k_{o,2} \exp\left(-\frac{E_{a,2}}{RT}\right)$$

The activation energy for the first reaction is 5500 J/mol. The rate constant prefactor for the first reaction is 0.1 liter/mole/s. The activation energy for the second reaction is 3900 J/mol. The rate constant prefactor for the first reaction is 0.1 liter/mole/s. The heat capacities of A, B, C, D and S are respectively 4.0, 3.0, 6.0, 9.0, and 3.0 J/mol/K. The heats of formation of A, B, C and D at a reference temperature of 298.15 K are respectively -1.0, -6.0, -12.0 and -18.0 kJ/mol. The inlet flowrate is 5 liters/s. The inlet temperature is 600 K. The inlet concentrations of A, B, C, D and S are 10.0, 10.0, 0.0, 0.0, and 30.0 mol/liter respectively. The volume of the reactor is 1000 liters. The reactor is well insulated. The initial temperature and concentrations in the reactor are the same as the inlet temperature and concentrations.

(a) Provide a plot of the transient behavior of the concentrations of A, B, C, D and S and the temperature. Explain the features.
(b) What are the steady-state temperature and conversion of A?
(c) What are the steady state concentrations of C and D?

3. Nonisothermal PFR – 1 irreversible reaction
Consider the irreversible reaction in a PFR

$$A \rightarrow 2B$$

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

$$r = kC_A$$

where the rate constant is given by

$$k = k_o \exp\left(-\frac{E_a}{RT}\right)$$

The activation energy for the forward reaction is 4000 J/mol. The rate constant prefactor for the forward reaction is 0.1 l/s. The heat capacities of A, B and the solvent are respectively 4.0, 7.0, and 3.0 J/mol/K. The heats of formation of A and B at a reference temperature of 298.15 K are respectively -1000.0 and -10000.0 J/mol. The inlet flowrate is 10 liters/s. The inlet temperature is 500 K. The inlet concentrations of A, B and S are 10.0, 0.0, and 30.0 mol/liter respectively. The volume of the reactor is 1000 liters. The reactor is well insulated. The initial temperature and concentrations in the reactor are the same as the inlet temperature and concentrations.

(a) Provide a plot of the transient behavior of the concentrations of A, B and S and the temperature. Explain the features.
(b) What are the steady-state temperature and conversion of A?
(c) Compare this result with problem 1, in which the same reaction was carried out in a CSTR of the same volume. Explain the result.