CBE 450 Chemical Reactor Fundamentals
Fall, 2009
Homework Assignment #9

Consider the two sequential reactions

A + B → C
A + C → D

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

$$r_1 = k_1 C_A C_B$$

and the reverse reaction is

$$r_2 = k_2 C_A C_C$$

where the rate constants are given by

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

and

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

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 4.0 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.

1. Jacketed Batch Reactor

This reaction takes place in a jacketed batch reactor. The initial concentration is 300 K. The initial concentrations of A, B, C, D and S are 10.0, 4.0, 0.0, 0.0, and 40.0 mol/liter respectively. The volume of the reactor is 1000 liters. The surface area of the reactor is 1.5 m^2.

The jacket has a volume of 0.5 m^3. The overall heat transfer coefficient from the reactor to the jacket is 1500.0 J/s/m^2/K. The heat capacity of the coolant is 4.184 J/mol/K and the concentration is 55.6 mol/liter. The flowrate of coolant is 10 liters/s. The inlet temperature of the coolant is 273.15. The initial temperature of the coolant is the same as the inlet temperature.

(a) Provide a plot of the transient behavior of the concentrations of A, B, C, D and S and the temperature for a period of 1000 sec. Explain the features.
(b) What are the reactor and jacket temperatures, conversion of A and concentrations of C and D at the end of this time period?

2. Jacketed CSTR

This reaction takes place in a jacketed CSTR. The inlet concentration is 300 K. The inlet concentrations of A, B, C, D and S are 10.0, 4.0, 0.0, 0.0, and 40.0 mol/liter respectively. The initial conditions within the CSTR are the same as the inlet conditions. The inlet flowrate is 1 liter/s. The volume of the reactor is 1000 liters. The surface area of the reactor is 1.5 m^2.

The jacket has a volume of 0.5 m^3. The overall heat transfer coefficient from the reactor to the jacket is 1500.0 J/s/m^2/K. The heat capacity of the coolant is 4.184 J/mol/K and the concentration is 55.6 mol/liter. The flowrate of coolant is 10 liters/s. The inlet temperature of the coolant is 273.15. The initial temperature of the coolant is the same as the inlet temperature.

(a) Provide a plot of the transient behavior of the concentrations of A, B, C, D and S and the temperatures for a period of X sec. Explain the features.
(b) What are the reactor and jacket temperatures, conversion of A and concentrations of C and D at steady state?

3. Jacketed PFR

This reaction takes place in a jacketed CSTR. The inlet concentration is 300 K. The inlet concentrations of A, B, C, D and S are 10.0, 4.0, 0.0, 0.0, and 30.0 mol/liter respectively. The initial conditions within the CSTR are the same as the inlet conditions. The inlet flowrate is 1 liter/s. The volume of the reactor is 1000 liters. The reactor is circular with diameter 0.1 m.

The jacket is a cylindrical shell of diameter 0.2 m around the reactor. It is of the same length as the reactor. The overall heat transfer coefficient from the reactor to the jacket is 1500.0 J/s/m^2/K. The heat capacity of the coolant is 4.184 J/mol/K and the concentration is 55.6 mol/liter. The flowrate of coolant is 10 liters/s and is co-current. The inlet temperature of the coolant is 273.15. The initial temperature of the coolant is the same as the inlet temperature.

(a) Provide a plot of the steady state profiles of the concentrations of A, B, C, D and S and the temperatures. Explain the features.
(b) What are the reactor and jacket temperatures, conversion of A and concentrations of C and D at the exit of the reactor?