CBE 450 Chemical Reactor Fundamentals Fall, 2009 Homework Assignment #6

1. Reactors in Series

Consider the reaction

$$A + B \rightarrow C$$

with elementary mechanism such that the rate is

$$r = kC_A C_B$$

where the rate constants are given by

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

The temperature is 300 K. The activation energy for the reaction is 5000 J/mol. The rate constant prefactor for the reaction is 0.001 liter/mol/s. The feed flowrate is 2 liters/sec. The concentration of A in the feed stream is 10 mol/liter. The concentration of B in the feed stream is 15 mol/liter. The concentration of C in the feed stream is 0 mol/liter. Consider a CSTR of 100 liters and a PFR of 100 liters total volume.

(a) What is the net conversion of A if the reactors are placed in series with the CSTR first and PFR second?

(b) What is the net conversion of A if the reactors are placed in series with the PFR first and CSTR second?

2. Gas-Phase Batch Reactor

Consider the gas-phase reaction

$$A + B \rightarrow C$$

with elementary mechanism such that the rate is

$$r = kC_A C_B$$

where the rate constants are given by

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

The temperature is 500 K. The pressure is constant at 10 atm. The activation energy for the reaction is 5000 J/mol. The rate constant prefactor for the reaction is 0.001 m³/mol/s.. Consider a batch reactor of variable volume . The initial mole fraction of A is 0.6 and B is 0.4. The initial volume of the reactor is 10 m³.

- (a) Generate a plot of the concentration of A, B and C as a function of time.
- (b) What is the concentration of C after 100 sec?
- (c) What is the conversion of A after 100 sec?
- (d) What is the volume of the reactor after 100 sec?

3. Constant-Volume CSTRs with variable exit flowrate

Consider the gas-phase reaction

$$A + B \rightarrow C$$

with elementary mechanism such that the rate is

$$r = kC_A C_B$$

where the rate constants are given by

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

The temperature is 500 K and the pressure is 10 atm. The activation energy for the reaction is 5000 J/mol. The rate constant prefactor for the reaction is $1.0 \text{ m}^3/\text{mol/s}$. The feed flowrate is $1.0 \text{ m}^3/\text{sec}$. The inlet feed stream is 60% A and 40% B.

(a) What is the steady state conversion of A?

(b) Provide a plot of the exit flow-rate as a function of time from your initial conditions to steady state.

(c) What is the steady state exit flow-rate?