Assignment 10

Due April 12, 2006

Do not submit this assignment. This is for practice. Solutions will be posted on April 12.

1. The gas-phase reaction $A \rightarrow \dfrac{B}{2}$ is taking place in a PFR. Pure A enters the reactor at a pressure of 4 atmospheres and 350 K. The heat of reaction which can be assumed to be independent of temperature is -27 kJ/mol of A. Specific heat of A is 30 J/mol-K. The rate constant at 350 K is 0.2 s^{-1} and the activation energy is 18 kJ/mol. The volumetric flow rate is 10 liters/s. When the conversion of A is plotted versus the reactor volume, the following plot is obtained. Determine the temperature and concentration of A in the reactor at the mid-point (V=50) and at the exit of the reactor (V=100).
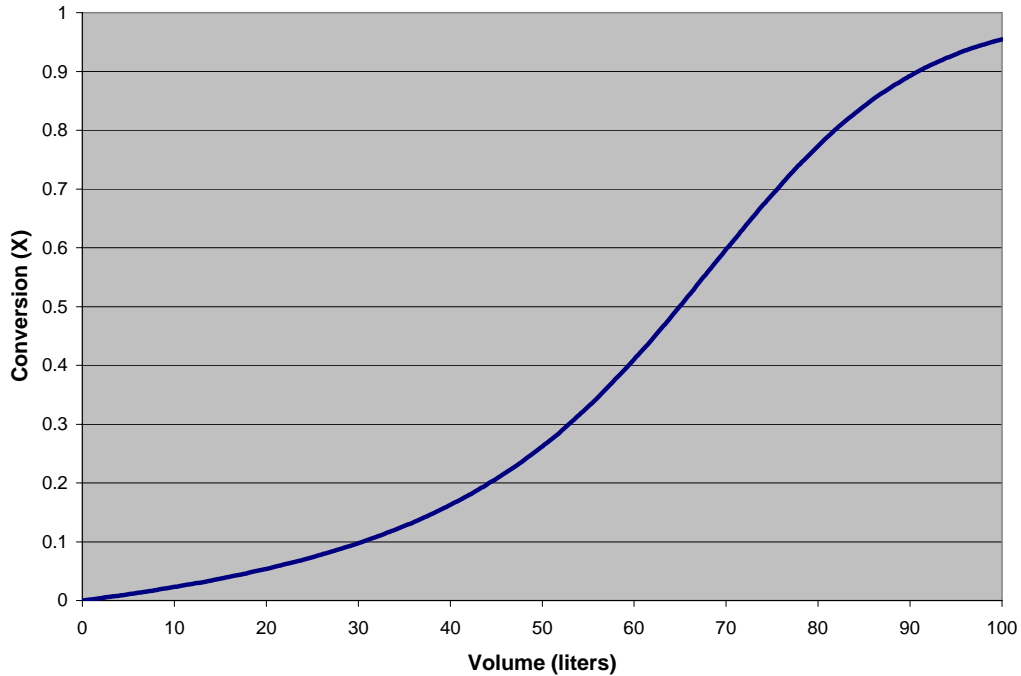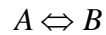

2. The following liquid-phase consecutive reaction is taking place in a constant volume batch reactor.

$$A \xrightarrow{\ k_1\ } B \xrightarrow{\ k_2\ } C$$
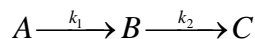
The first reaction is first order and the second reaction is zero order. Derive expressions for the concentrations of A, B and C as functions of time.

3. A first-order reversible liquid phase reaction is carried out in a CSTR at 427^0C, with the initial concentration of A being equal to 2 mol/liter.
$$A \Leftrightarrow B$$
Following parameters are given:
$$C_{pA} = 40 \text{ J/mol K}; \ C_{pB} = 40 \text{ J/mol K}; \ \Delta H_{300\,K} = -80 \text{ kJ/mol}$$
$$K(@\ 27^0 C) = 2 \times 10^9; \ k_f (@\ 327^0 C) = 1 \text{hr}^{-1}; \ E = 30,000 \text{ J/mole}$$
Determine the residence time in the reactor for 80% of the ***equilibrium conversion***.

4. The following reaction goes to 80% completion in a CSTR. A and B are fed to the reactor at rates of
2 mol/s and 3 mol/s respectively at a temperature of 37^0C. Specific heats (in J/mol-K) of A, B, C and D are 200, 150, 220 and 180 respectively.

$$A + B \rightarrow C + D$$
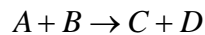
The reactor is jacketed by water at a temperature of 20^0C. The overall heat transfer coefficient has been estimated at 300 J/(m^2.s.K), while the heat transfer area is 0.75 m^2. Mixing is ensured through an agitator, which contributes a work of 12 KW to the reactor. The heat of reaction is -30,000 J/mole of A at 300 K. Calculate the steady state temperature in the reactor.

5. A first-order, reversible reaction $A \leftrightarrow B$ is taking place adiabatically. The equilibrium constant at 400 K is 3 and the heat of reaction, which can be assumed constant is –50 kJ/mole. Pure A with a specific heat of 100 J/mole-K (which is the same as that of B) enters the reactor at 300 K. The equilibrium conversion as a function of temperature is plotted in the figure shown below.
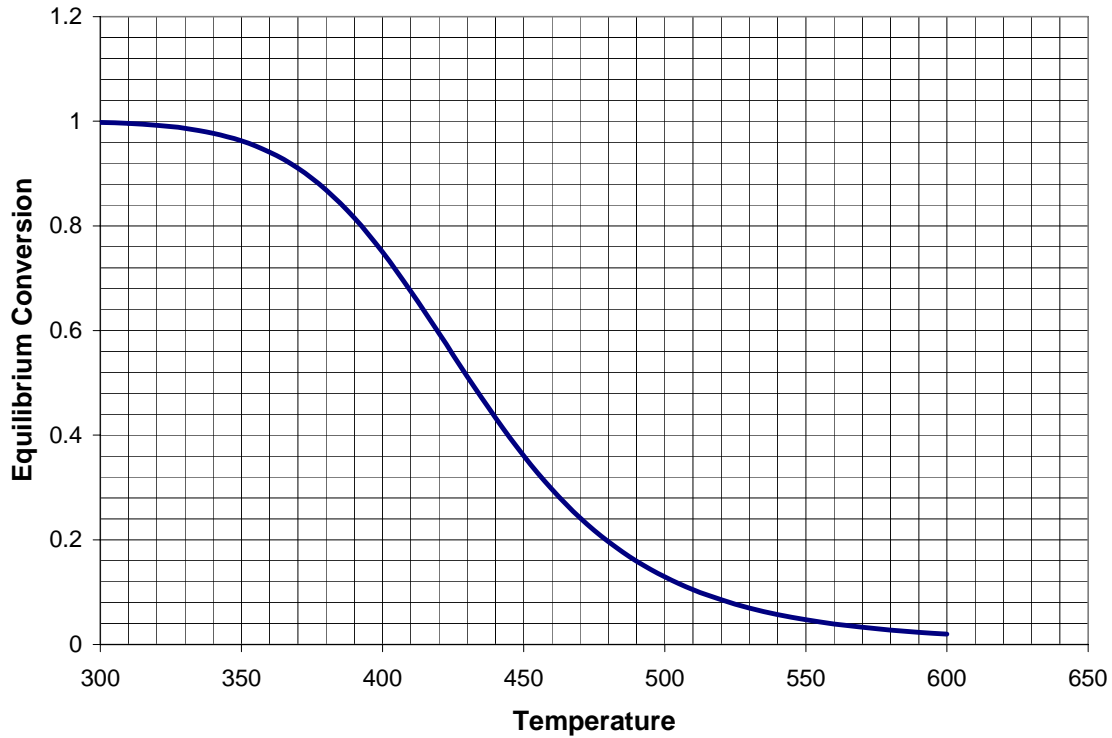
a. Show the equations that were used for constructing the plot shown.
b. What is the maximum conversion that can be achieved, if the reactor is operated adiabatically.
c. If two adiabatic reactors are used, with inter-stage cooling, and if the first reactor exit stream is cooled to 350 K, what maximum conversion can be achieved in the second reactor? What would be the exit temperature from this second stage?
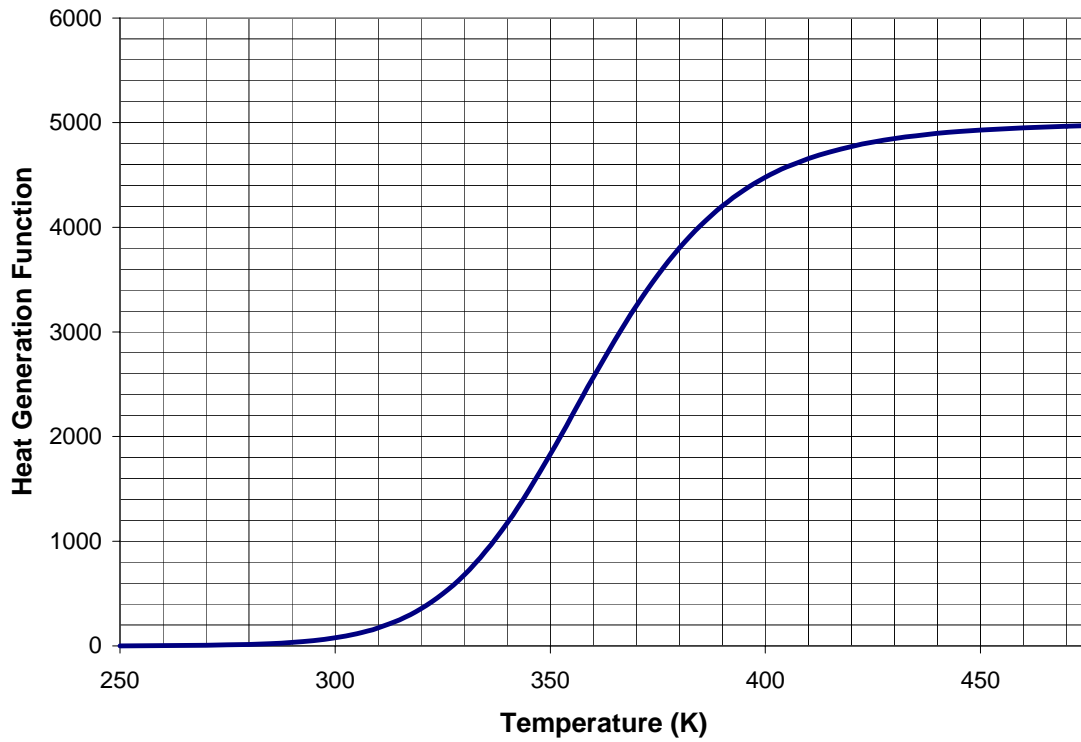
6.
A first-order irreversible liquid-phase reaction ($A \rightarrow B$) is taking place in a CSTR. Reactant A enters the reactor at 300 K at a concentration of 3 mol/liter. The reactor volume is 18 liters and flow rate of pure A is 0.06 liters/s. Other parameters are:

$$\Delta H_{Rx}^0 = -5000 \text{ cal/mole}, \tilde{C}_{pA} = \tilde{C}_{pB} = 30 \text{ cal/mole} \cdot \text{K}$$

$$k = \exp(15.32 - \frac{7550}{T}) \text{ s}^{-1}$$

The heat generated term given by $(-\Delta H_{Rx}^0 \cdot X)$ is plotted in the figure shown.

a. For the conditions given, determine the number of steady states, and the conversions and temperatures at these steady states.

b. What is the minimum incoming temperature at which multiple steady states are possible?

c. What is the maximum incoming temperature above which only one steady state occurs?