## **CHFEN 3553 Chemical Reaction Engineering**

February 11, 2005; 12:55 PM – 1:45 PM Total – 100 points

1. Write down the concentration of B for the elementary, gas-phase reversible reaction  $A+2B \Leftrightarrow 2C$ . The feed contains one mole of A and three moles of B. Write down the rate of reaction in terms of reactant and product concentrations, the forward rate constant, k and the equilibrium constant  $K_c$ .

10 points

$$\Theta_{B} = \frac{C_{B0}}{C_{A0}} = 3$$

$$\partial = -1; \ y_{a0} = 0.25; \ \varepsilon = -0.25$$

$$C_{B} = \frac{C_{A0}(3 - 2X)}{(1 - 0.25X)}$$

$$-r_{A} = k(C_{A}C_{B}^{2} - \frac{C_{C}^{2}}{K_{C}})$$

2. The rate constant for a second-order reaction at 300 K is 2.5 and the activation energy is 20,000 J/mole. What are the units of the rate constant? At what temperature would the rate be triple (of the rate at 300K) for this reaction?

12 points

Units of rate are 
$$\frac{lit}{mol - min}$$

$$\ln \frac{k_2}{k_1} = -\frac{E}{R} \left( \frac{1}{T_2} - \frac{1}{T_1} \right)$$

$$\ln(3) = -\frac{20000}{8.314} \left( \frac{1}{T_2} - \frac{1}{300} \right)$$

$$T_2 = 347.63 \text{ K}$$

3. A first-order, irreversible liquid-phase reaction is taking place in a CSTR and 50% conversion is obtained. If two more CSTRs of the same size are placed downstream, what is the final conversion?

15 points

$$X = 1 - \frac{1}{1 + \tau k}$$

$$X = 0.5$$

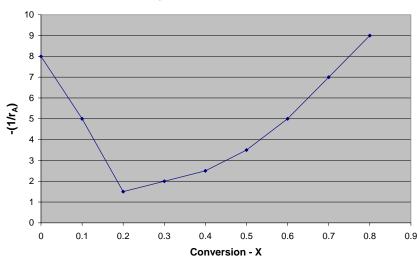
$$\tau k = 1$$

$$X = 1 - \frac{1}{(1 + \tau k)^3} = 1 - 0.125 = 0.875$$

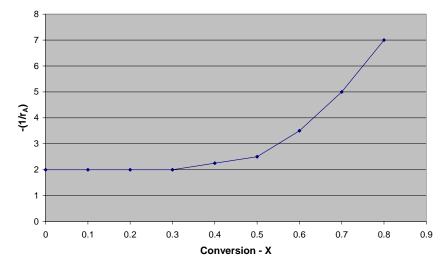
4. In the hippopotamus, digestion occurs as an autocatalytic reaction in the stomach followed by a catalytic reaction in the intestines. This system can be modeled as a series of CSTR-PFR. The volumetric flow rate of food intake into the system can be assumed to be 100 liters/day, at a concentration of 7.5 mol/liter. The volume of the stomach (modeled as CSTR) is 450 liters. Reciprocal rates (in moles/liter-day) for the two types of reactions are provided below. If the total conversion of 50% is observed, what is the volume of the intestines?

23 points

## Autocatalytic reaction in the stomach



## Catalytic reaction in the intestines



$$F_{A0} = 100 \cdot 7.5 = 750 \text{ mol/day}$$

$$\frac{V}{F_{A0}} = \frac{450}{750} = 0.6 \frac{\text{lit-day}}{\text{mol}} = \text{Area}$$

By inspection of the autocatalytic plot, X = 0.3

Area = 
$$0.3 \cdot 2 = 0.6$$

For a conversion of 0.5 in the intestines (catalytic reaction)

Area = 
$$\frac{(2+2.5)}{2}(0.5-0.3) = 0.45 = \frac{V_{\text{int}}}{F_{40}}$$

$$V_{\text{int}} = 0.45 \cdot 750 = 337.5 \text{ liters}$$

5. A first-order, gas-phase reaction is taking place in a recycle reactor. Starting with the design equation of the recycle reactor, obtain an integrated expression (an algebraic equation) that relates the residence time in the reactor to conversion and the volume change parameter. Use the integration result given below or the integration tables in the Appendix of your text.

$$\int \frac{(1+\varepsilon X)}{(1-X)} dX = \varepsilon (1-X) - (1+\varepsilon) \ln(1-X)$$

A reaction  $A \rightarrow 2B$  is taking place in a recycle reactor. If 67% (two-thirds) of the exit stream from the reactor (stream labeled 2 on the class diagram) is recycled, what is the residence time in the reactor for a conversion of 80%? The rate constant is 0.5 s<sup>-1</sup>.

25 points

$$\frac{V}{F_0} = (R+1) \int_{\frac{R}{R+1}X_f}^{X_f} \frac{dX}{-r} 
-r = kC = \frac{kC_{A0}(1-X)}{(1+\varepsilon X)} 
\frac{kVC_0}{(R+1)F_0} = \int_{\frac{R}{R+1}X_f}^{X_f} \frac{(1+\varepsilon X)dX}{(1-X)} = \varepsilon(1-X) - (1+\varepsilon)\ln(1-X) \updownarrow_{\frac{R}{R+1}X_f}^{X_f} 
\frac{k\tau}{(R+1)} = (1+\varepsilon)\ln\frac{R+1-RX_f}{(R+1)(1-X_f)} - \frac{\varepsilon X_f}{(R+1)}$$

$$\frac{R}{R+1} = \frac{2}{3}, R = 2, X_f = 0.8$$
  
 $\varepsilon = 1, k = 0.5s^{-1}$   
 $\tau = 8.56s$