CHFEN 3553 Chemical Reaction Engineering

March 9, 2005; 12:55 PM – 1:45 PM - Solutions
Total – 100 points

1. A liquid-phase reaction $A + 2B \rightarrow C$ is taking place in a semi-batch reactor. The reaction is begun with 84 moles of A in the reactor. The initial reactor volume is 50 liters. B is added at a volumetric rate of 2 lit/min and a concentration of 10 mol/lit. The reaction is assumed to be zero order with respect to both A and B. The rate constant k is $0.125 \dfrac{\text{mol}}{\text{lit-min}}$. How much time does it take to reach a conversion of 50% A. What is the concentration of B at this time?

   20 points

Semi-batch design equation:

$$-r_A V = N_{A0} \frac{dX}{dt}$$

$$V = V_0 + vt$$

$$k(V_0 + vt) = N_{A0} \frac{dX}{dt}$$

$$\int_0^t (V_0 + vt)dt = \frac{N_{A0}}{k} \int_0^X dX$$

$$V_0 t + \frac{vt^2}{2} = \frac{N_{A0}}{k} X$$

$$t^2 + 50t - 336 = 0$$

$$t = 6$$

$$C_A = \frac{N_{A0}(1-X)}{V_0 + vt} = \frac{84 \cdot 0.5}{50 + 12} = 0.6774 \frac{\text{mol}}{\text{lit}}$$

$$C_B = \frac{C_{B0}vt - 2N_{A0}X}{V_0 + vt} = \frac{10 \cdot 2 \cdot 6 - 2 \cdot 84 \cdot 0.5}{62} = 0.58 \frac{\text{mol}}{\text{lit}}$$

2. A series reaction $A \xrightarrow{\text{1st order}} B \xrightarrow{\text{Zero order}} C$ is taking place in a CSTR. Derive the concentrations of A, B and C as functions of residence time τ, the rate constants (k_1 and k_2) and the initial concentration of A (C_{A0}). Assume that the concentrations of B and C in the reactor entrance stream are zero.

   20 points

Composite rates

1

$$-r_A = k_1 C_A$$

$$r_B = k_1 C_A - k_2$$

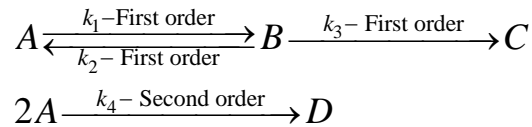$$\tau = \frac{C_{A0} - C_A}{-r_A} = \frac{C_{A0} - C_A}{k_1 C_A}$$

$$\frac{C_A}{C_{A0}} = \frac{1}{1 + k_1 \tau}$$

$$\tau = \frac{C_{B0} - C_B}{-r_B} = \frac{C_{B0} - C_B}{-k_1 C_A + k_2} = \frac{C_B}{k_1 C_A - k_2}$$

$$\frac{C_B}{\tau} = k_1 \frac{C_{A0}}{1 + k_1 \tau} - k_2$$

$$\boxed{\frac{C_B}{C_{A0}} = \frac{k_1 \tau}{1 + k_1 \tau} - \frac{k_2 \tau}{C_{A0}}}$$

3. Determine the composite rates of reaction for all of the species in the following reaction sequence.

$$A \underset{k_2-\text{ First order}}{\overset{k_1-\text{First order}}{\rightleftarrows}} B \xrightarrow{k_3-\text{ First order}} C$$

$$2A \xrightarrow{k_4-\text{ Second order}} D$$

16 points

$$-r_{1A} = k_1 \left(C_A - \frac{C_B}{K_1} \right) + k_4 C_A^2$$

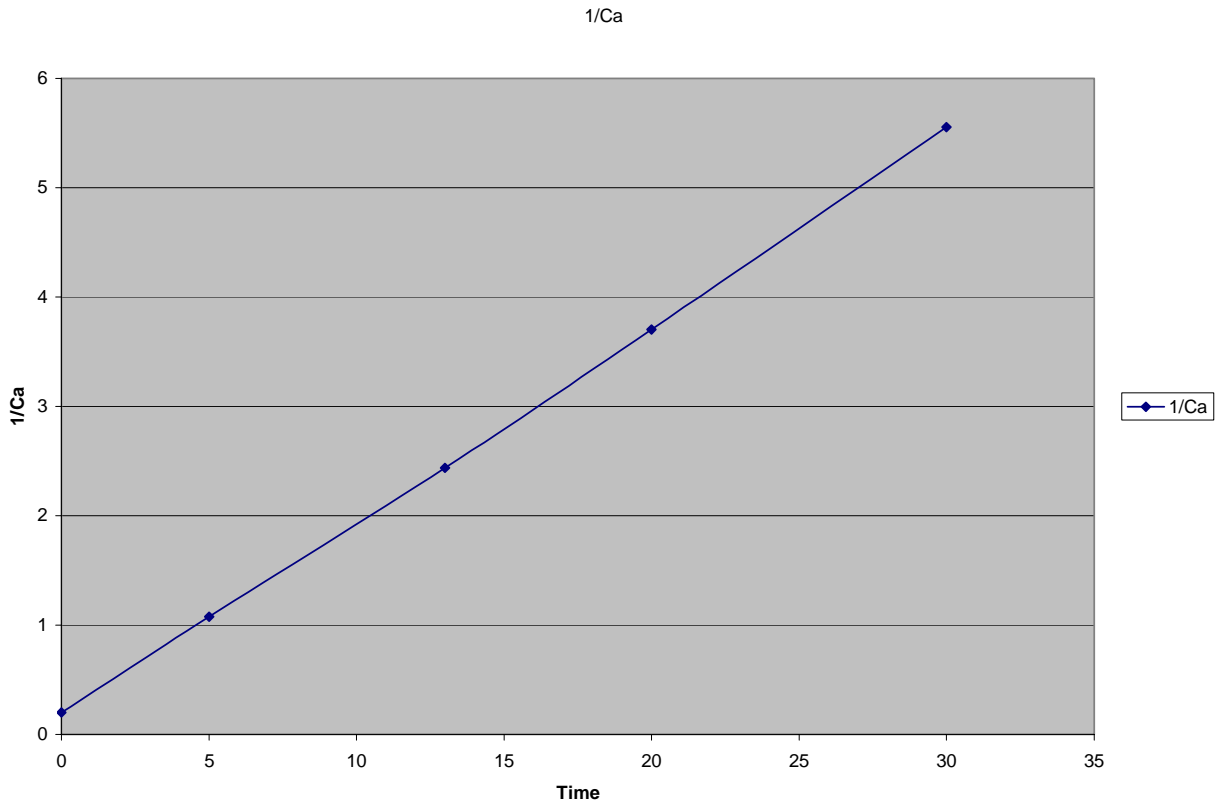$$r_B = k_1 \left(C_A - \frac{C_B}{K_1} \right) - k_3 C_B$$

$$r_C = k_3 C_B$$

$$r_D = \frac{1}{2} k_4 C_A^2$$

4. Measured concentrations in a constant-volume batch reactor are tabulated. Determine the order of the reaction and the rate constant.
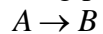
t (mins)	0	5	13	20	30
Ca (mol/lit)	5	0.93	0.41	0.27	0.18

22 points

1/Ca

Assume second order (n=2); slope=k=0.179

5. The following first-order reaction is taking place in a PBR.
$$A \rightarrow B$$
The reaction rate and the rate constant are given by:

$$-r_A^{'} = kp_A \quad \frac{\text{mol}}{\text{kg cat-h}}$$

$$k = 0.75 \frac{\text{mol}}{\text{atm-kg cat-h}}$$

A is fed to the reactor with 50% inerts at 327^0C and 1 atmosphere. Feed rate of A is 37.5 moles/h. The pressure drop parameter $\alpha = 0.0045\,\text{kg}^{-1}$. Obtain an expression that relates the conversion in the reactor to the weight of the catalyst used. State your assumptions. What conversion can you obtain with 100 kg of the catalyst?

22 points

$$-r_A^{'} = kp_A = kC_A RT$$

$$\varepsilon = 0$$

$$C_A = C_{A0}(1-X)y = C_{A0}(1-X)(1-\alpha W)^{1/2}$$

$$F_{A0}\frac{dX}{dW} = -r_A^{'} = kRT \cdot y_{A0}\frac{P_0}{R\cancel{T}}(1-X)(1-\alpha W)^{1/2}$$

$$\frac{dX}{dW} = \frac{kP_{A0}}{F_{A0}}(1-X)(1-\alpha W)^{1/2}$$

$$\int_0^X \frac{dX}{(1-X)} = \frac{kP_{A0}}{F_{A0}}\int_0^W (1-\alpha W)^{1/2}\, dW$$

$$-\ln(1-X) = \frac{kP_{A0}}{F_{A0}}\frac{2}{3\alpha}\left[1-(1-\alpha W)^{3/2}\right]$$

X=0.584 for the given parameters.