CHFEN 3553 Chemical Reaction Engineering

April 28, 2003; 1:00 PM – 3:00 PM

Answer all questions

1. A first-order reaction $A \rightarrow B$ is taking place in a recycle reactor. The initial concentration is 4 mol/liter, the reactor volume is 200 liters and the volumetric flow rate is 20 liters/s. For a recycle ratio of 5, a conversion of 60% is obtained. This configuration is to be replaced with a CSTR-PFR combination. A 50-liter CSTR is followed by a PFR of unknown volume. What volume of PFR is required is achieve the same conversion as in the recycle reactor?

17 points

Recycle Reactor

$$\frac{k\tau}{R+1} = \ln\left[\frac{C_{A0} + RC_{Af}}{(R+1)C_{Af}}\right]$$

$$C_{A0} = 4, X = 0.6, C_{Af} = 1.6, R = 5, \tau = 10$$

$$\frac{k\tau}{R+1} = \ln\left[\frac{C_{A0} + RC_{Af}}{(R+1)C_{Af}}\right] = \ln\left[\frac{4 + 5 \cdot 1.6}{(5+1) \cdot 1.6}\right] = 0.2231$$

$$k = 0.1339\,\text{s}^{-1}$$

CSTR first, $\tau_{cstr} = 50/20 = 2.5s$

$$X_1 = \frac{k\tau}{1+k\tau} = \frac{0.1339 \cdot 2.5}{1 + 0.1339 \cdot 2.5} = 0.2508$$

PFR following the CSTR

$$k\tau = \ln\frac{1-X_1}{1-X_2} = \ln\frac{1-0.2508}{1-0.6} = 0.6276$$

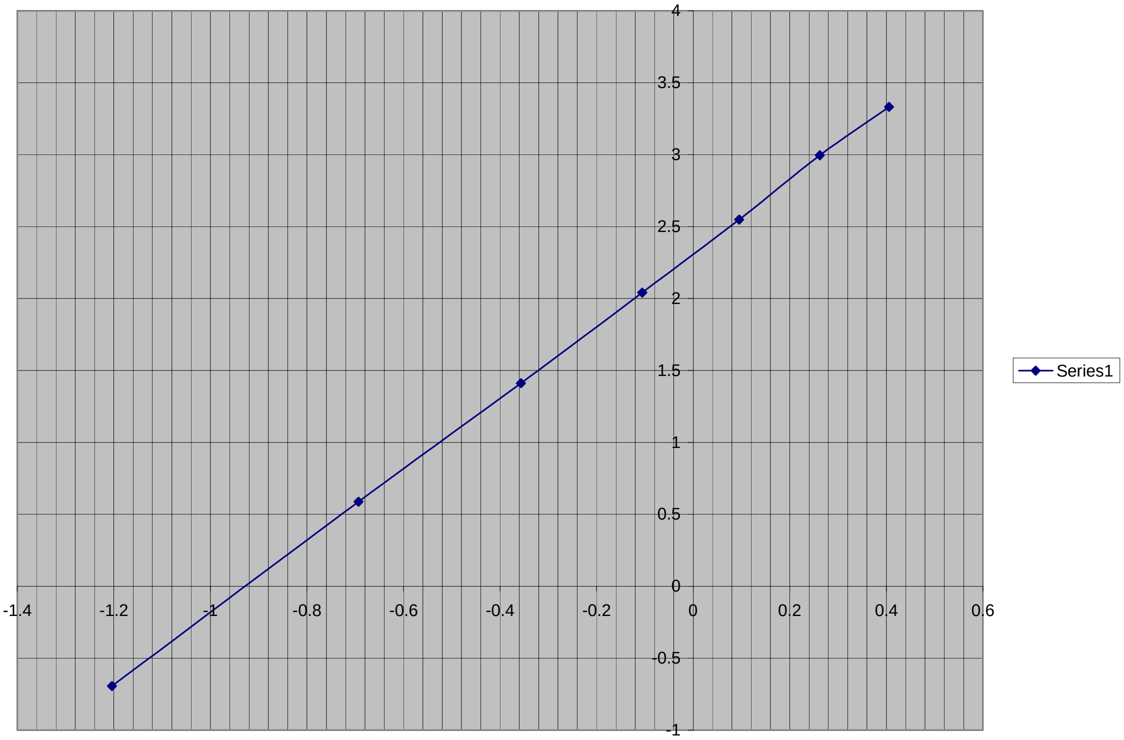
$$\tau_{PFR} = 4.6866$$

$$V_{PFR} = 4.6866 \cdot 20 = 93.73\,\text{lit}$$

2. Rate versus concentration data for a reaction is given below. Find the order of the reaction and the reaction rate.

Con. (mol/liter)	1.5	1.3	1.1	0.9	0.7	0.5	0.3
Rate (mol/lit-sec)	28	20	12.8	7.7	4.1	1.8	0.5

16 points



n=2.52
k=10.1

3. An elementary irreversible liquid-phase reaction $A + B \rightarrow C$ is carried out in a CSTR. A and B are fed at molar rates of 1.25 mol/s and 1 mol/s respectively, at a temperature of 300 K. The reactor is jacketed and the jacket temperature can be assumed to be 310 K. An agitator contributes a work of 20.9 kW to the reactor. The volumetric flow rate is 5 lit/s. Additionally:

$$H_A^0(298\,K) = -20\,\text{kcal/mol} \quad H_B^0(298\,K) = -25\,\text{kcal/mol} \quad H_C^0(298\,K) = -60\,\text{kcal/mol}$$

$$C_{pA} = C_{pB} = 40\ \frac{\text{cal}}{\text{mol}\cdot\text{K}},\ C_{pC} = 55\frac{\text{cal}}{\text{mol}\cdot\text{K}}$$

$$k = 0.01\frac{\text{lit}}{\text{mol}\cdot\text{s}}\ \text{at 300 K},\ \ U\cdot A = 75\frac{\text{cal}}{\text{s}\cdot\text{K}},\ E = 8\ \text{kcal/mol}$$

Determine the volume of the reactor for 60% conversion of A.

16 points

Use equation 8-50 from the text ±

$$\frac{\dot{Q} - \dot{W}}{F_{A0}} - X\Delta H_{Rx} = \sum \theta_{\text{i}} \tilde{C}_{pi}(T - T_{i0})$$

$$\Delta H_{Rx} = -60 + 20 + 25 = -15\,\text{kcal/mol}$$

$$\frac{(U\cdot A\cdot(T_a - T) - \dot{W})}{F_{A0}} - X\left(\Delta H_{Rx}(T_R) + \Delta\hat{C}_p(T - T_R)\right) = \sum \theta_{\text{i}} \tilde{C}_{pi}(T - T_{i0})$$

$$T = \frac{F_{A0}X\left(-\Delta H_{Rx}(T_R) + \Delta\hat{C}_p \cdot T_R\right) + F_{A0}(\theta_A\tilde{C}_{pA} + \theta_B\tilde{C}_{pB})T_0 + UAT_a - \dot{W}}{F_{A0}(\theta_A\tilde{C}_{pA} + \theta_B\tilde{C}_{pB}) + UA + F_{A0}X\Delta\hat{C}_p}$$

$$\Delta\hat{C}_p = 55 - 40 - 40 = -25\frac{cal}{mol - K}$$

$$T = \frac{1.25\cdot 0.6\left(15{,}000 - 25\cdot 298\right) + 1.25\cdot(1\cdot 40 + 0.8\cdot 40)\cdot 300 + 75\cdot 310 + 5000}{1.25\cdot(1\cdot 40 + 0.8\cdot 40) + 75 + 1.25\cdot 0.6\cdot(-25)}$$

$$T = 416.5\ \text{K}$$

$$\ln\frac{k_2}{k_1} = \frac{-E}{R}\left(\frac{1}{T_1} - \frac{1}{T_2}\right) = \frac{-8000}{1.987}\left(\frac{1}{416.5} - \frac{1}{300}\right)$$

$$k_2 = 0.4268$$

$$V = \frac{F_{A0}X}{-r_A} = \frac{C_{A0}vX}{kC_{A0}^2(1 - X)(\theta_B - X)} = \frac{vX}{kC_{A0}(1 - X)(\theta_B - X)}$$

$$C_{A0} = 1.25/5 = 0.25\frac{\text{mol}}{\text{lit}},\ v = 5\,\frac{\text{lit}}{\text{s}}$$

$$V = \frac{5\cdot 0.6}{0.4268\cdot 0.25\cdot(1 - 0.6)(0.8 - 0.6)} = 351.43\ \text{liters}$$

4. Mechanism of a catalytic reaction $A \rightarrow B$ is shown below.

$$A + S \underset{k_{-A}}{\overset{k_A}{\rightleftarrows}} A \cdot S$$

$$A \cdot S \underset{k_{-S}}{\overset{k_S}{\rightleftarrows}} B \cdot S$$

$$B \cdot S \underset{k_{-D}}{\overset{k_D}{\rightleftarrows}} B + S$$

Write down the rates of adsorption, surface reaction and desorption and derive an effective rate when, surface reaction is rate controlling.

16 points

$$r_{AD} = k_A (p_A C_v - \frac{C_{A \cdot S}}{K_A})$$

$$\frac{r_{AD}}{k_A} = 0$$

$$r_S = k_s (C_{A \cdot S} - \frac{C_{B \cdot S}}{K_S})$$

$$r_D = k_D (C_{B \cdot S} - p_B C_v / K_{DB})$$

$$\frac{r_D}{k_D} = 0$$

$$C_{A \cdot S} = K_A p_A C_v$$

$$C_{B \cdot S} = \frac{p_B C_v}{K_{DB}} = K_B p_B C_v$$

Substitute into r_S

$$r_S = k_s (K_A p_A C_v - \frac{K_B p_B C_v}{K_S}) = k_s (K_A p_A C_v - \frac{K_A K_B p_B C_v}{K_S K_A})$$

$$= k_s (K_A p_A C_v - \frac{K_A p_B C_v}{K_P}) = k_S K_A C_v (p_A - \frac{p_B}{K_P})$$

$$C_t = C_v + C_{A \cdot S} + C_{B \cdot S} = C_v + K_A p_A C_v + K_B p_B C_v$$

$$C_v = \frac{C_t}{(1 + K_A p_A + K_B p_B)}$$

$$r_S = k_S K_A (p_A - \frac{p_B}{K_P}) \cdot \frac{C_t}{(1 + K_A p_A + K_B p_B)}$$

$$\boxed{r_S = \frac{k_S K_A C_t (p_A - \frac{p_B}{K_P})}{(1 + K_A p_A + K_B p_B)}}$$

5. A first-order reaction $A \rightarrow 3B$ is taking place in a PBR. The particles are 10 mm in diameter and the intrinsic rate constant (k')is 0.8 lit/kg-cat-s. A conversion of 75% is desired. Feed at 4 mol/s, containing 40% A and 60% inerts enters the reactor at 127^0C and 5 atmospheres. The engineer designing the reactor neglects to consider that there might be internal diffusion to consider.
   a. What weight of the catalyst does the engineer pack the reactor with?
   b. If the diffusion coefficient is 0.08 cm^2/s ad bulk density of the catalyst is 2.8 kg/liter, what conversion would actually result with the catalyst packed?
   c. What weight of the catalyst did he need to use to meet the design specifications of 75% conversion? Assume that the reactor operates at constant pressure.

18 points

$\delta = 2, y_{A0} = 0.4, \varepsilon = 0.8$

PBR Equation without the effectiveness factor

$$F_{A0}\frac{dX}{dW} = -r_A^{'} = kC_A = kC_{A0}\frac{(1-X)}{(1+\varepsilon X)}$$

$$\frac{dX}{dW} = \frac{kC_{A0}}{F_{A0}}\frac{(1-X)}{(1+\varepsilon X)} = \frac{k}{v_0}\frac{(1-X)}{(1+\varepsilon X)}$$

$$\int_0^X \frac{(1+\varepsilon X)}{(1-X)}dX = \frac{k}{v_0}W = (1+\varepsilon)\ln\frac{1}{1-X} - \varepsilon X = 1.8953$$

$$Pv_0 = F_{T_0}RT$$

$$5 \cdot v_0 = 4 \cdot 0.082 \cdot 400 \Rightarrow v_0 = 26.24\frac{\text{lit}}{\text{s}}$$

$$\frac{0.8}{26.24}W = 1.8953$$

$$W = 62.17\,kg$$

PBR with internal diffusion

$$\phi = R\sqrt{\frac{k\rho}{D}} = 0.5\sqrt{\frac{0.8 \cdot 2.8}{0.08}} = 2.6457$$

$$\eta = \frac{3}{\phi^2}\left(\frac{\phi}{\tanh\phi} - 1\right) = 0.5912$$

$$= \frac{3}{2.6457^2}\left(\frac{2.6457}{0.9878} - 1\right) = 0.7193$$

Conversion with 62.17 kg

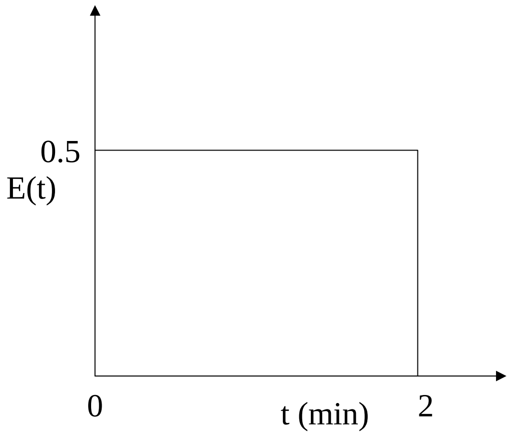
$$\frac{\eta k}{v_0}W = (1+\varepsilon)\ln\frac{1}{1-X} - \varepsilon X$$

$$\frac{0.7193 \cdot 0.8}{26.24}62.17 = (1+0.8)\ln\frac{1}{1-X} - \varepsilon X = 1.3634$$

$$X = 0.66$$

Weight to acheive 75% conversion = 62.17/0.7193=86.4 kg

6. The residence time distribution function for a reactor is given below. The reaction is ½ order, C_{A0}= 1 mol/lit and the rate constant is $2\,\frac{\text{mol}^{1/2}}{\text{lit}^{1/2}-\text{min}}$. Determine the conversion in the reactor using the segregated-flow model.



17 points

The performance equation is

$$\frac{C}{C_0}=\int_0^{\infty}\left(\frac{C}{C_0}\right)_{\text{batch}}E(t)dt$$

For a general n-th order reaction

$$(n-1)kC_0^n t=\left(\frac{C}{C_0}\right)^{1-n}-1$$

For 1/2 order reaction,

$$\left(-\frac{1}{2}\right)2(1)t=\left(\frac{C}{C_0}\right)^{\frac{1}{2}}-1$$

$$\left(\frac{C}{C_0}\right)_{\text{batch}}=(1-t)^2$$

$$\frac{C}{C_0}=\int_0^2(1-t)^2(0.5)dt=\frac{0.5}{3}\left.(1-t)^3\right|_2^0=\frac{1}{6}(1+1)=\frac{1}{3}$$

$$\overline{X}=0.6667$$