CHFEN 3553 Chemical Reaction Engineering

April 28, 2003; 1:00 PM – 3:00 PM

Answer all questions

1. It is well known that the integrated expressions for batch and plug flow reactors are identical when there is no volume change. What happens to these expressions when there is volume change? A first order gas-phase reaction with volume change is of interest. Derive integrated rate expressions for a batch reactor (time to reach a certain level of conversion) and a plug flow reactor (Volume or τ to reach a certain level of conversion). All of the integrals that you may need are at the back of your text. Are these expressions the same? Explain your answer.

17 points

Batch:

$$N_A = N_{A0}(1-X); \quad V = V_0(1+\varepsilon X)$$

$$-r_A V = N_{A0}\frac{dX_A}{dt}; -r_A = kC_A = k\frac{N_A}{V} = k\frac{N_{A0}(1-X)}{V_0(1+\varepsilon X)}$$

Substitute the rate expression:

$$k\frac{N_{A0}(1-X)}{V_0(1+\varepsilon X)}V_0(1+\varepsilon X) = N_{A0}\frac{dX_A}{dt}$$

Integrate

$$-\ln(1-X) = kt$$

Plug Flow Reactor

$$F_A = F_{A0}(1-X)$$

$$v = v_0(1+\varepsilon X)$$

$$F_{A0}dX = (-r_A)dV$$

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

$$\int_0^X \frac{(1-X)}{(1+\varepsilon X)}dX = k\frac{C_{A0}}{F_{A0}}V$$

$$(1+\varepsilon)\ln\frac{1}{(1-X)} - \varepsilon X = k\tau$$

In the batch reactor, the effect of volume change is not seen for the first order reaction. The difference is due to tha fact that volumetric flow rate change gets incorporated in the PFR equation.

2. The reversible (elementary) reaction $2A \Leftrightarrow C + D$ is conducted in a CSTR at a feed rate of 100 liters/min with an inlet concentration C_{A0}=1.5 mols/lit. The specific rate in the forward direction is 10 lit/mol-min and the equilibrium constant is 16. 80% of the **equilibrium conversion** is required. Find the size of a CSTR to achieve this conversion.

17 points

At equilibrium,

$$-r_A = k\left(C_A^2 - \frac{C_C C_D}{K_C}\right) = 0; C_A = C_B = C_{A0}(1-X); C_C = C_D = C_{A0}X/2$$

$$C_{A0}^2(1-X)^2 = C_{A0}^2 X^2/64;$$

Solve; $X_e = 0.8888$

Conversion desired: $X = 0.8 \cdot 0.8888 = 0.711$

$$\frac{V}{F_{A0}} = \frac{\tau}{C_{A0}} = \frac{X_A}{-r_A} = \frac{X_A}{k\left(C_A^2 - \frac{C_C C_D}{K_C}\right)}$$

$\tau = 0.627; V = 62.7$ liters

3. The conversion of an irreversible first-order, liquid-phase reaction, taking place in a PFR of 500 liter capacity is 50%. In order to increase conversion, a 300 liter CSTR is installed *upstream* of (before) the PFR. What is the exit conversion in the new system?

16 points

First order PFR

$$k\tau = \ln\frac{1}{1-X} = \ln\frac{1}{1-0.5} = k\frac{500}{v_0}$$

$$\frac{k}{v_0} = \frac{0.6932}{500}$$

First CSTR

$$k\tau = \frac{X}{1-X} \Rightarrow \frac{kV}{v_0} = \frac{X}{1-X} \Rightarrow \frac{0.6932 \cdot 300}{500} = \frac{X}{1-X}$$

$X = 0.2938$

Followed by the 500 liter PFR

$$\frac{V}{F_{A0}} = \int_{X_1}^{X_2} \frac{dX}{-r} = \int_{X_1}^{X_2} \frac{dX}{kC_{A0}(1-X)}$$

$$\frac{kV}{v_0} = -\ln(1-X_2) + \ln(1-X_1) = 0.6932$$

$X_2 = 0.65$

4. The irreversible reaction $A \rightarrow B$ was carried out in a constant volume batch reactor and the following concentration-time data were obtained. Find the reaction order and the reaction rate constant. Identify the units of the rate constant. Show the finite difference formulae that you would use to obtain $\frac{dC_A}{dt}$ clearly.

t(min)	0	5	10	15	20
C_A(mol/lit)	4.0	2.3256	1.1025	0.3306	0.01
-dCa/dt	0.38001	0.28975	0.1995	0.10925	0.01899

Formulae Used:

$$\left(\frac{dC_A}{dt}\right)_{\downarrow t=0} = \frac{-3C_{A0} + 4C_{A1} - C_{A2}}{2\Delta t}$$

Interior points

$$\left(\frac{dC_A}{dt}\right) = \frac{C_{A,i+1} - C_{A,i-1}}{2\Delta t}$$

Plot on log-log paper and take slope;

Last point

$$\left(\frac{dC_A}{dt}\right) = \frac{3C_{A5} - 4C_{A4} + C_{A3}}{2\Delta t}$$

Order = 2 and rate constant = 0.19.

17 points

5. An elementary second order adiabatic reaction $A + B \rightarrow C + D$ is taking place in a CSTR. The feed to the reactor is equimolar A and B at concentrations of 2.4 mol/liter. The entering temperature is 300 K. The volumetric flow rate is 15 lit/min. Following are some other data characterizing the reaction.

$$C_{p_A} = 20 \text{ Btu/lb.mol-}^0\text{F}$$

$$C_{p_B} = 15 \text{ Btu/lb.mol-}^0\text{F}$$

$$C_{p_C} = 15 \text{ Btu/lb.mol-}^0\text{F}$$

$$C_{p_d} = 20 \text{ Btu/lb.mol-}^0\text{F}$$

$$\Delta H_{Rx}(300K) = -7000 \text{ cal/mole of A}$$

$$k(300\ K) = 0.00045 \text{ l/mol-min}$$

$$E = 12{,}000 \text{ cal/mol}$$

What volume of the reactor is required for 75% conversion?

16 points

Energy Balance

$$\text{T=T}_0 + \frac{X \cdot -\Delta H_{Rx}}{\sum \theta_i C_{pi}}$$

Cps are given in Btu/lb-mole F, which is the same as cal/mole K.

$$\text{T=300+}\frac{0.75 \cdot 7000}{(20+15)} = 450K$$

$$k(450) = 0.00045 \exp\left[\frac{12000}{1.987}\left(\frac{1}{300} - \frac{1}{450}\right)\right] = 0.3694 lit/mol - \text{min}$$

$$V = \frac{F_{A0}X}{-r_A} = \frac{C_{A0}vX}{kC_{A0}^2(1-X)^2} = \frac{vX}{kC_{A0}(1-X)^2} = 203.05\ liters$$

6. A first-order, gas-phase reaction $A \rightarrow 2B$ is performed in a PBR at 400 K and 10 atm. Feed rate is 5 mol/s containing 20% A and the rest inerts. The PBR is packed with 8 mm-diameter spherical porous particles. The intrinsic reaction rate is given as: $r_A^{'} = 3.75\, C_A$ mol/kg(cat)-s . Bulk density of the catalyst is 2.3 kg/liter. The diffusivity is 0.1 cm^2/s. The pressure drop parameter alpha is found to be 9.8×10^{-4} kg^{-1}.
    a. What is the value of the internal effectiveness factor? What does it signify?

b. How much catalyst (kg) is required to obtain a conversion of 75% in the reactor?
c. Find the pressure at the exit of the reactor.

17 points

$$\phi = R\sqrt{\frac{k\rho}{D}} = 0.4\sqrt{\frac{3.75\cdot 2.3}{0.1}} = 3.714$$

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

$$F_{A0}\frac{dX}{dW} = -r_A^{'} = kC_A = \eta k C_{A0}\frac{(1-X)}{(1+\varepsilon X)}\frac{P}{P_0}$$

$$= \eta k C_{A0}\frac{(1-X)}{(1+\varepsilon X)}(1-\alpha W)^{1/2}$$

$$\frac{dX}{dW} = \frac{\eta k C_{A0}}{F_{A0}}\frac{(1-X)}{(1+\varepsilon X)}(1-\alpha W)^{1/2}$$

$$\int_0^X \frac{1+\varepsilon X}{1-X}dX = \frac{\eta k}{v_0}\int_0^W (1-\alpha W)^{\frac{1}{2}} dW$$

$$(1+\varepsilon)\ln\frac{1}{(1-X)} - \varepsilon X = \frac{\eta k}{v_0}\frac{2}{3\alpha}\left[1-(1-\alpha W)^{3/2}\right]$$

$$v_0 = 16.4 lit/s; X = 0.75; \varepsilon = 0.2; \alpha = 9.8\times 10^{-4}; \eta = 0.5912;$$

$$k = 3.75$$

$$W = 11.22\ kg$$

$$\frac{P}{P_0} = (1-\alpha W)^{1/2} = 0.9944$$

$$P = 9.94\ atm$$