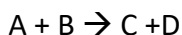


Assignment 3 - solutions

1. The gas phase reaction



Takes place isothermally at 300 K in a packed-bed reactor in which the feed is equal in A and B with $C_{A0} = 0.1 \text{ mol/dm}^3$. The reaction is second order in A and zero order in B. Currently, 50% conversion is achieved in a reactor with 100 kg catalysts for a volumetric flow rate $100 \text{ dm}^3/\text{min}$. The pressure-drop parameter, α , is $\alpha = 0.0099 \text{ kg}^{-1}$. If the activation energy is 10,000 cal/mol, what is the specific reaction rate constant at 400 K?

Data: $C_{A0} = 0.1 \text{ mol/dm}^3$

$X = 0.5$

$W = 100 \text{ kg}$

$v_0 = 100 \text{ dm}^3/\text{min}$

$\alpha = 0.0099 \text{ kg}^{-1}$

$E = 10,000 \text{ cal/mol}$

Rate law: $-r_A = kC_A^2$

Since $\varepsilon = 0$, $p = P/P_0 = (1 - \alpha W)^{1/2}$

$C_A = C_{A0} (1 - X) p$

$$-r_A = kC_{A0}^2 (1-X)^2 (1 - \alpha W)$$

PBR design equation:

$$\frac{dF_A}{dW} = -r'_A$$

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

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

$$\int_0^{0.5} \frac{dX}{(1 - X)^2} = \frac{X}{1 - X} = 1$$

$$k = \frac{v_0}{C_{A0}(W - 0.5 \alpha W^2)} = \frac{100}{0.1(1 - 0.0099 \times 100) \times 100} = 19.8 \frac{\text{dm}^6}{\text{mol.kg.min}}$$

$$k(400K) = k(300K) e^{\frac{10000}{1.987} \left(\frac{1}{300} - \frac{1}{400} \right)}$$

$$k(400K) = 1312 \frac{\text{dm}^6}{\text{mol.kg.min}}$$

2. The gas-phase reaction



Follows an elementary rate law and is to be carried out first in a PFR and then in a separate experiment in a CSTR. When pure A is fed to a 10 dm³ PFR at 300 K and a volumetric flow rate of 5 dm³/s, the conversion is 80%. When a mixture of 50% A and 50% inert (I) is fed to a 10 dm³ CSTR at 320 K and a volumetric flow rate of 5 dm³/s, the conversion is also 80%. What is the activation energy in cal/mol?

PFR @ 300 K

$$V = 10 \text{ dm}^3.$$

$$v_0 = 5 \text{ dm}^3/\text{s}$$

$$X = 0.8$$

$$C_A = C_{A0} \frac{1-X}{1+X}$$

$$-r_A = kC_A = kC_{A0} \frac{1-X}{1+X}$$

$$\text{Design equation: } \tau = C_{A0} \int_0^X \frac{dX}{-r_A} = \frac{1}{k} \int_0^X \frac{(1+X)}{(1-X)} dX = \frac{1}{k} \left[2 \ln \left(\frac{1}{1-X} \right) - X \right]$$

$$k = \frac{1}{\tau} \left[2 \ln \left(\frac{1}{1-X} \right) - X \right]$$

$$k(300\text{K}) = 1.2 \text{ s}^{-1}.$$

CSTR @ 320 K

$$\text{Design equation: } V = \frac{F_{A0}X}{-r_A} = \frac{v_0X}{k} \frac{1+0.5X}{1-X} \quad (\delta = 1, y = 0.5; \varepsilon = 0.5)$$

$$k = \frac{v_0X}{V} \frac{1+0.5X}{1-X}$$

$$k(320\text{K}) = 2.8 \text{ s}^{-1}.$$

$$\text{Activation energy: } E = R \frac{\ln \left(\frac{k(320)}{k(300)} \right)}{300^{-1} - 320^{-1}}$$

$$E = 8081 \text{ cal/mol}.$$

3. The gaseous reaction



has a unimolecular reaction rate constant of 0.0015 min^{-1} at 80°F . This reaction is to be carried out in parallel tubes 10 ft long and 1 in. inside diameter, under a pressure of 132 psig at 260°F . A production rate of 1000 lb/h of B is required. Assuming an activation energy of 25000 cal/mol, how many tubes are needed if the conversion of A is to be 90%? Assume perfect gas laws. A and B each have molecular weights of 58.

$$80^\circ\text{F} = 300\text{K}$$

$$260^\circ\text{F} = 400\text{K}$$

$$k(300\text{K}) = 0.0015 \text{ min}^{-1}$$

$$k(400\text{K}) = k(300\text{K}) e^{\frac{25000}{1.987} \left(\frac{1}{300} - \frac{1}{400} \right)}$$

$$k(400\text{K}) = 53.6 \text{ min}^{-1}$$

$$F_B = \frac{1000 \times 0.4536 \times 1000}{60 \times 58} = 130.3 \text{ mol/min}$$

$$F_{A0} = \frac{F_B}{X} = 145 \text{ mol/min}$$

$$V = F_{A0} \int_0^X \frac{dX}{-r_A}$$

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

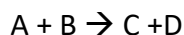
$$C_{A0} = \frac{P}{RT} = 273.6 \text{ mol/m}^3$$

$$\int_0^{0.9} \frac{dX}{(1 - X)} = 2.3$$

$$V = \frac{145 \times 2.3}{53.6 \times 273.6} = 22.7 \text{ dm}^3$$

Number of pipes = 15.

4. At present the elementary liquid-phase reaction



takes place in a plug flow reactor using equimolar quantities of A and B. Conversion is 96%, $C_{A0} = C_{B0} = 1 \text{ mol/lit}$. If a CSTR ten times as large as the plug flow reactor were hooked up in series (downstream) with the existing unit, what fraction could production be increased for that setup?

PFR:

$$-r_A = kC_A C_B = kC_{A0}^2 (1 - X)^2$$

$$\frac{kV}{F_{A0}} = \frac{X}{1 - X} = 24$$

CSTR:

$$V_{CSTR} = \frac{F_{A0}(X_2 - X_1)}{-r_A}$$

$$10V = \frac{F_{A0}(X_2 - 0.96)}{kC_{A0}^2(1 - X_2)^2}$$

$$\frac{(X_2 - 0.96)}{(1 - X_2)^2} = \frac{10kV}{F_{A0}} C_{A0}^2 = 240$$

Solving for X_2 : $X_2 = 0.99$

Connecting a CSTR of 10 times as large as the PFR increases conversion to 99%. Is it worth?