Assignment 3 - solutions

1. The gas phase reaction

   $A + B \rightarrow C + D$

   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 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 dm^3/min. The pressure-drop parameter, α, is α = 0.0099 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 mol/dm^3
   X = 0.5
   W = 100 kg
   v_0 = 100 dm^3/min
   α = 0.0099 kg^{-1}
   E = 10,000 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:

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

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

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

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

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

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

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

2. The gas-phase reaction

   A → B + C

   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 dm^3 PFR at 300 K and a volumetric flow rate of 5 dm^3/s, the conversion is 80%. When a mixture of 50% A and 50% inert (I) is fed to a 10 dm^3 CSTR at 320 K and a volumetric flow rate of 5 dm^3/s, the conversion is also 80%. What is the activation energy in cal/mol?

PFR @ 300 K

$V = 10\ dm^3$.

$v_0 = 5\ dm^3/s$

$X = 0.8$

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

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

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

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

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

CSTR @ 320 K

Design equation: $V = \frac{F_{A0}X}{-r_A} = \frac{v_0 X}{k}\frac{1+0.5X}{1-X}$ $\quad (\delta = 1, y = 0.5;\ \varepsilon = 0.5)$

$$k = \frac{v_0 X}{V}\frac{1+0.5X}{1-X}$$

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

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

E = 8081 cal/mol.

3. The gaseous reaction

   A → B

   has a unimolecular reaction rate constant of 0.0015 min^{-1} at 80 ^oF. 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 ^oF. 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 F = 300K
   260 F = 400 K

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

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

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

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

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

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

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

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

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

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

Number of pipes = 15.

4. At present the elementary liquid-phase reaction

   A + B → C +D

   takes place in a plug flow reactor using equimolar quantities of A and B. Conversion is 96%, $C_{A0} = C_{B0} = 1$ mol/lt. 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:

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

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

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 3%. Is it worth?