## Chemical Reaction Engineering Chapter 3

P3-10<sub>A</sub> (a) Write the rate law for the following reactions assuming each reaction follows an elementary rate law.

$$C_2H_6 \longrightarrow C_2H_4 + H$$

(2) 
$$C_2H_4 + \frac{1}{2}O_2 \rightarrow CH_2 - CH_2$$

(3) 
$$(CH_3)_3COOC(CH_3)_3 \rightleftharpoons C_2H_6 + 2CH_3COCH_3$$

$$nC_4H_{10} \iff iC_4H_{10}$$

(5) 
$$CH_3COOC_2H_5 + C_4H_9OH \rightleftharpoons CH_3COOC_4H_9 + C_2H_5OH$$

(b) Write the rate law for the reaction

$$2A + B \rightarrow C$$

if the reaction (1) is second order in B and overall third order, (2) is zero order in A and first order in B, (3) is zero order in both A and B, and (4) is first order in A and overall zero order.

- (c) Find and write the rate laws for the following reactions
  - (1)  $H_2 + Br_2 \rightarrow 2HBr$
  - $(2) H<sub>2</sub> + I<sub>2</sub> \rightarrow 2HI$

P3-11<sub>A</sub> Set up a stoichiometric table for each of the following reactions and express the concentration of each species in the reaction as a function of conversion

evaluating all constants (e.g.,  $\varepsilon$ ,  $\Theta$ ). Then, assume the reaction follows an elementary rate law, and write the reaction rate solely as a function of conversion, i.e.,  $-r_A = f(X)$ .

(a) For the liquid-phase reaction

$$CH_2$$
—OH  
 $CH_2$ — $CH_2$  +  $H_2O$   $H_2SO_4$   $CH_2$ —OH

the initial concentrations of ethylene oxide and water are 1 lb-mol/ft³ and 3.47 lb-mol/ft³ (62.41 lb/ft³  $\div$  18), respectively. If k=0.1 dm³/mol  $\cdot$  s at 300 K with E=12,500 cal/mol, calculate the space-time volume for 90% conversion at 300 K and at 350 K.

(b) For the isothermal, isobaric gas-phase pyrolysis

$$^{\cdot}C_2H_6 \longrightarrow C_2H_4 + H_2$$

pure ethane enters the flow reactor at 6 atm and 1100 K. How would your equation for the concentration and reaction rate change if the reaction were to be carried out in a constant-volume batch reactor?

(c) For the isothermal, isobaric, catalytic gas-phase oxidation

$$C_2H_4 + \frac{1}{2}O_2 \longrightarrow CH_2 - CH_3$$

the feed enters a PBR at 6 atm and 260°C and is a stoichiometric mixture of only oxygen and ethylene.

(d) For the isothermal, isobaric, catalytic gas-phase reaction is carried out in a PBR

the feed enters a PBR at 6 atm and 170°C and is a stoichiometric mixture. What catalyst weight is required to reach 80% conversion in a fluidized CSTR at 170°C and 270°C? The rate constant is defined wrt benzene and  $v_0 = 50 \ \rm dm^3/min$ .

$$k_{\rm B} = \frac{53 \text{ mol}}{\text{kgcat} \cdot \text{min atm}^3}$$
 at 300 K with  $E = 80 \text{ kJ/mol}$ 

P3-13<sub>B</sub>. The formation of nitroanalyine (an important intermediate in dyes—called fast orange) is formed from the reaction of orthonitrochlorobenzene (ONCB) and aqueous ammonia. (See Table 3-1 and Example 9-2.)

$$\begin{array}{c|c} \operatorname{NO_2} & \operatorname{NO_2} \\ & + 2\operatorname{NH_3} \end{array} + \operatorname{NH_2} \\ + \operatorname{NH_4CL} \end{array}$$

The liquid-phase reaction is first order in both ONCB and ammonia with k = 0.0017 m<sup>3</sup>/kmol min at 188°C with E = 11,273 cal/mol. The initial entering concentrations of ONCB and ammonia are 1.8 kmol/m<sup>3</sup> and 6.6 kmol/m<sup>3</sup>, respectively (more on this reaction in Chapter 9).

- (a) Write the rate law for the rate of disappearance of ONCB in terms of concentration.
- (b) Set up a stoichiometric table for this reaction for a flow system.
- (c) Explain how part (a) would be different for a batch system.
- (d) Write  $-r_{\Delta}$  solely as a function of conversion.  $-r_{\Delta} =$
- (e) What is the initial rate of reaction (X = 0) at 188°C?  $-r_A = \frac{1}{25}$  at 25°C?  $-r_A = \frac{1}{25}$
- (f) What is the rate of reaction when X = 0.90 at  $188^{\circ}C$ ?  $-r_{A} =$  \_\_\_\_\_\_ at  $25^{\circ}C$ ?  $-r_{A} =$  \_\_\_\_\_ at  $288^{\circ}C$ ?  $-r_{A} =$  \_\_\_\_\_ at  $288^{\circ}C$ ?  $-r_{A} =$  \_\_\_\_\_
- (g) What would be the corresponding CSTR reactor volume at 25°C to achieve 90% conversion at 25°C and at 288°C for a molar feed rate of 2 mol/min

at 25°C? 
$$V =$$
\_\_\_\_\_  
at 288°C?  $V =$ \_\_\_\_\_

P3-15<sub>B</sub> The gas-phase reaction

$$\frac{1}{2}N_2 + \frac{3}{5}H_2 \longrightarrow NH_3$$

is to be carried out isothermally. The molar feed is 50%  $\rm H_2$  and 50%  $\rm N_2$ , at a pressure of 16.4 atm and 227°C.

- (a) Construct a complete stoichiometric table.
- (b) What are C<sub>AO</sub>, δ, and ε? Calculate the concentrations of ammonia and hydrogen when the conversion of H<sub>2</sub> is 60%. (Ans. C<sub>H<sub>2</sub></sub> = 0.1 mol/dm<sup>3</sup>)
- (c) Suppose by chance the reaction is elementary with k<sub>N2</sub> = 40 dm³/mol/s. Write the rate of reaction solely as a function of conversion for (1) a flow system and (2) a constant volume batch system.
- P3-16<sub>B</sub> Calculate the equilibrium conversion and concentrations for each of the following reactions.
  - (a) The liquid-phase reaction

$$A + B \longrightarrow C$$

with  $C_{A0} = C_{B0} = 2 \text{ mol/dm}^3$  and  $K_C = 10 \text{ dm}^3/\text{mol}$ 

(b) The gas-phase reaction

$$A \longrightarrow 3C$$

carried out in a flow reactor with no pressure drop. Pure A enters at a temperature of 400 K and 10 atm. At this temperature,  $K_C = 0.25 (\text{dm}^3/\text{mol})^2$ .

- (c) The gas-phase reaction in part (b) carried out in a constant-volume batch reactor.
- (d) The gas-phase reaction in part (b) carried out in a constant-pressure batch reaction.