University of Anbar

College of Engineering

Chemical and Petrochemical Engineering Department

Chemical Reacior Design

Third Year

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Lecture No. 7

B STEADY-STATE MIXED FLOW REACTOR:

$$\text{input} = \text{output} + \text{disappearance by reaction} + \underbrace{\text{accumulation}}_{=0} \quad \textbf{(10)}$$

As shown in Fig. 5.3, if $F_{A0} = v_0 C_{A0}$ is the molar feed rate of component A to the reactor, then considering the reactor as a whole we have

$$\text{input of A, moles/time} = F_{A0}(1 - X_{A0}) = F_{A0}$$

$$\text{output of A, moles/time} = F_A = F_{A0}(1 - X_A)$$

$$\begin{array}{c}\text{disappearance of A}\\ \text{by reaction,}\\ \text{moles/time}\end{array} = (-r_A)V = \left(\frac{\text{moles A reacting}}{(\text{time})(\text{volume of fluid})}\right)\left(\begin{array}{c}\text{volume of}\\ \text{reactor}\end{array}\right)$$

Introducing these three terms into Eq. 10, we obtain

$$F_{A0}X_A = (-r_A)V$$

which on rearrangement becomes

or

$$\frac{V}{F_{A0}} = \frac{\tau}{C_{A0}} = \frac{\Delta X_A}{-r_A} = \frac{X_A}{-r_A}$$
$$\tau = \frac{1}{s} = \frac{V}{v_0} = \frac{VC_{A0}}{F_{A0}} = \frac{C_{A0}X_A}{-r_A} \qquad \text{any } \varepsilon_A \qquad \textbf{(11)}$$

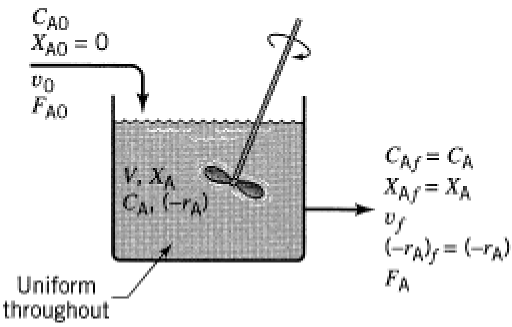

Figure 5.3 Notation for a mixed reactor.

For the special case of constant-density systems $X_A = 1 - C_A/C_{A0}$, in which case the performance equation for mixed reactors can also be written in terms of concentrations or

or

$$\frac{V}{F_{A0}} = \frac{X_A}{-r_A} = \frac{C_{A0} - C_A}{C_{A0}(-r_A)}$$
$$\tau = \frac{V}{v} = \frac{C_{A0}X_A}{-r_A} = \frac{C_{A0} - C_A}{-r_A} \qquad \varepsilon_A = 0 \qquad \textbf{(13)}$$

Figure 5.4 is a graphical representation of these mixed flow performance equations. For any specific kinetic form the equations can be written out directly.

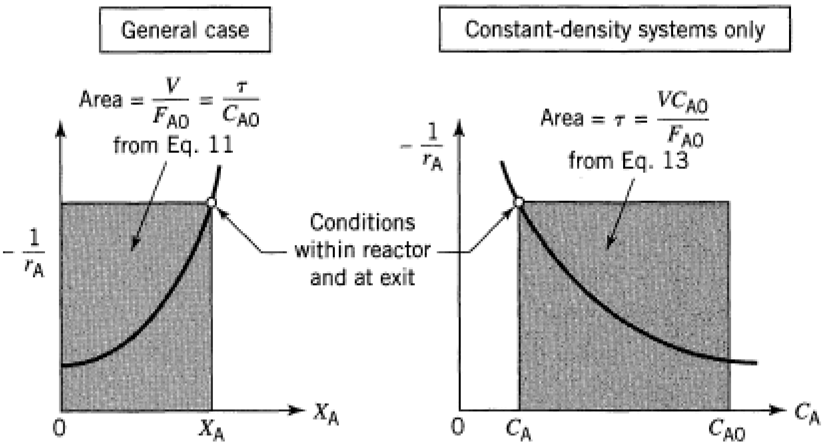

Figure 5.4 Graphical representation of the design equations for mixed flow reactor.

As an example, for constant density systems $C_A/C_{A0} = 1 - X_A$, thus the performance expression *for first-order reaction* becomes

$$k\tau = \frac{X_A}{1 - X_A} = \frac{C_{A0} - C_A}{C_A} \qquad \text{for } \varepsilon_A = 0 \tag{14a}$$

On the other hand, for linear expansion

$$V = V_0(1 + \varepsilon_A X_A) \quad \text{and} \quad \frac{C_A}{C_{A0}} = \frac{1 - X_A}{1 + \varepsilon_A X_A}$$

thus *for first-order reaction* the performance expression of Eq. 11 becomes

$$k\tau = \frac{X_A(1 + \varepsilon_A X_A)}{1 - X_A} \qquad \text{for any } \varepsilon_A \tag{14b}$$

For *second-order reaction*, A → products, $-r_A = kC_A^2$, $\varepsilon_A = 0$, the performance equation of Eq. 11 becomes

$$k\tau = \frac{C_{A0} - C_A}{C_A^2} \quad \text{or} \quad C_A = \frac{-1 + \sqrt{1 + 4k\tau C_{A0}}}{2k\tau} \tag{15}$$

EXAMPLE 5.1 REACTION RATE IN A MIXED FLOW REACTOR

One liter per minute of liquid containing A and B (C_{A0} = 0.10 mol/liter, C_{B0} = 0.01 mol/liter) flow into a mixed reactor of volume V = 1 liter. The materials react in a complex manner for which the stoichiometry is unknown. The outlet stream from the reactor contains A, B, and C (C_{Af} = 0.02 mol/liter, C_{Bf} = 0.03 mol/liter, C_{Cf} = 0.04 mol/liter), as shown in Fig. E5.1. Find the rate of reaction of A, B, and C for the conditions within the reactor.

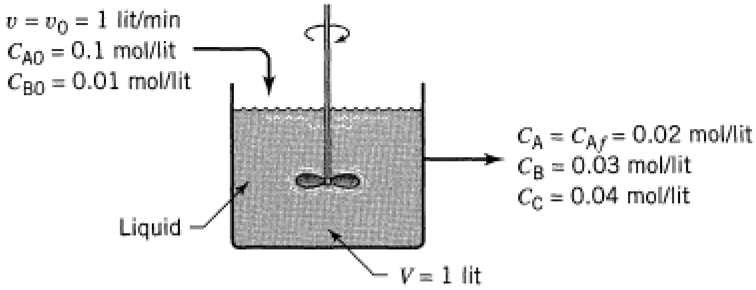

Figure E5.1

SOLUTION

For a liquid in a mixed flow reactor $\varepsilon_A = 0$ and Eq. 13 applies to each of the reacting components, giving for the rate of disappearance:

$$-r_A = \frac{C_{A0} - C_A}{\tau} = \frac{C_{A0} - C_A}{V/v} = \frac{0.10 - 0.02}{1/1} = \underline{\underline{0.08 \text{ mol/liter} \cdot \text{min}}}$$

$$-r_B = \frac{C_{B0} - C_B}{\tau} = \frac{0.01 - 0.03}{1} = \underline{\underline{-0.02 \text{ mol/liter} \cdot \text{min}}}$$

$$-r_C = \frac{C_{C0} - C_C}{\tau} = \frac{0 - 0.04}{1} = \underline{\underline{-0.04 \text{ mol/liter} \cdot \text{min}}}$$

Thus A is disappearing while B and C are being formed. ■

EXAMPLE 5.2 ***KINETICS FROM A MIXED FLOW REACTOR***

Pure gaseous reactant A (C_{A0} = 100 millimol/liter) is fed at a steady rate into a mixed flow reactor (V = 0.1 liter) where it dimerizes (2A → R). For different gas feed rates the following data are obtained:

Run number	1	2	3	4
v_0, liter/hr	10.0	3.0	1.2	0.5
C_{Af}, millimol/liter	85.7	66.7	50	33.4

Find a rate equation for this reaction.

SOLUTION

For this stoichiometry, 2A → R, the expansion factor is

$$\varepsilon_A = \frac{1-2}{2} = -\frac{1}{2}$$

and the corresponding relation between concentration and conversion is

$$\frac{C_A}{C_{A0}} = \frac{1-X_A}{1+\varepsilon_A X_A} = \frac{1-X_A}{1-\frac{1}{2}X_A}$$

or

$$X_A = \frac{1-C_A/C_{A0}}{1+\varepsilon_A C_A/C_{A0}} = \frac{1-C_A/C_{A0}}{1-C_A/2C_{A0}}$$

The conversion for each run is then calculated and tabulated in column 4 of Table E5.2.

Table E5.2

	Given		Calculated			
Run	v_0	C_A	X_A	$(-r_A) = \frac{v_0 C_{A0} X_A}{V}$	log C_A	log $(-r_A)$
1	10.0	85.7	0.25	$\frac{(10)(100)(0.25)}{0.1} = 2500$	1.933	3.398
2	3.0	66.7	0.50	1500	1.824	3.176
3	1.2	50	0.667	800	1.699	2.903
4	0.5	33.3	0.80	400	1.522	2.602

From the performance equation, Eq. 11, the rate of reaction for each run is given by

$$(-r_A) = \frac{v_0 C_{A0} X_A}{V}, \qquad \left[\frac{\text{millimol}}{\text{liter} \cdot \text{hr}}\right]$$

$$\log(-r_A) = \log k + n \log C_A$$

For nth-order kinetics this data should give a straight line on a log $(-r_A)$ vs. log C_A plot. From columns 6 and 7 of Table E5.2 and as shown in Fig. E5.2, the

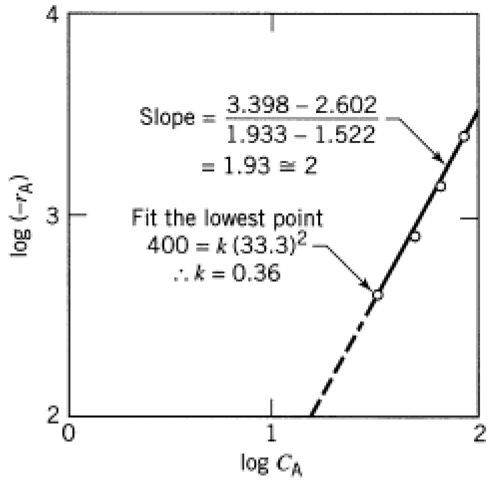

Figure E5.2

four data points are reasonably represented by a straight line of slope 2, so the rate equation for this dimerization is

$$-r_A = \left(0.36 \frac{\text{liter}}{\text{hr} \cdot \text{millimol}}\right) C_A^2, \qquad \left[\frac{\text{millimol}}{\text{liter} \cdot \text{hr}}\right]$$

Comment. If we ignore the density change in our analysis (or put $\varepsilon_A = 0$ and use $C_A/C_{A0} = 1 - X_A$) we end up with an incorrect rate equation (reaction order $n \cong 1.6$) which when used in design would give wrong performance predictions.

EXAMPLE 5.3 MIXED FLOW REACTOR PERFORMANCE

The elementary liquid-phase reaction

$$A + 2B \underset{k_2}{\overset{k_1}{\rightleftharpoons}} R$$

with rate equation

$$-r_A = -\frac{1}{2} r_B = (12.5\ \text{liter}^2/\text{mol}^2 \cdot \text{min}) C_A C_B^2 - (1.5\ \text{min}^{-1}) C_R, \qquad \left[\frac{\text{mol}}{\text{liter} \cdot \text{min}}\right]$$

is to take place in a 6-liter steady-state mixed flow reactor. Two feed streams, one containing 2.8 mol A/liter and the other containing 1.6 mol B/liter, are to be introduced at equal volumetric flow rates into the reactor, and 75% conversion of limiting component is desired (see Fig. E5.3). What should be the flow rate of each stream? Assume a constant density throughout.

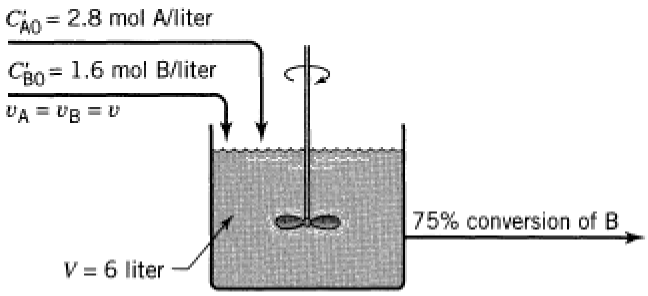

Figure E5.3

SOLUTION

The concentration of components in the mixed feed stream is

$C_{A0} = 1.4$ mol/liter , $C_{B0} = 0.8$ mol/liter , $C_{R0} = 0$

These numbers show that B is the limiting component, so for 75% conversion of B and $\varepsilon = 0$, the composition in the reactor and in the exit stream is

$C_A = 1.4 - 0.6/2 = 1.1$ mol/liter

$C_B = 0.8 - 0.6 = 0.2$ mol/liter or 75% conversion

$C_R = 0.3$ mol/liter

Writing the rate and solving the problem in terms of B we have at the conditions within the reactor

$$-r_B = 2(-r_A) = (2 \times 12.5)C_A C_B^2 - (2 \times 1.5)C_R$$

$$= \left(25 \frac{\text{liter}^2}{\text{mol}^2 \cdot \text{min}}\right)\left(1.1 \frac{\text{mol}}{\text{liter}}\right)\left(0.2 \frac{\text{mol}}{\text{liter}}\right)^2 - (3\ \text{min}^{-1})\left(0.3 \frac{\text{mol}}{\text{liter}}\right)$$

$$= (1.1 - 0.9)\frac{\text{mol}}{\text{liter} \cdot \text{min}} = 0.2 \frac{\text{mol}}{\text{liter} \cdot \text{min}}$$

For no density change, the performance equation of Eq. 13 gives

$$\tau = \frac{V}{v} = \frac{C_{B0} - C_B}{-r_B}$$

Hence the volumentric flow rate into and out of the reactor is

$$v = \frac{V(-r_B)}{C_{B0} - C_B}$$

$$\underline{\underline{v}} = \frac{(6\ \text{liter})(0.2\ \text{mol/liter}\cdot\text{min})}{(0.8 - 0.6)\ \text{mol/liter}} = \underline{\underline{6\ \text{liter/min}}}$$

or

$$\underline{\underline{3\ \text{liter/min of each of the two feed streams}}}$$