# Chapter 4

# Introduction to Reactor Design

## 4.1 GENERAL DISCUSSION

So far we have considered the mathematical expression called the *rate equation* which describes the progress of a homogeneous reaction. The rate equation for a reacting component $i$ is an intensive measure, and it tells how rapidly component $i$ forms or disappears in a given environment as a function of the conditions there, or

$$r_i = \frac{1}{V}\left(\frac{dN_i}{dt}\right)_{\text{by reaction}} = f(\text{conditions within the region of volume } V)$$

This is a differential expression.

In reactor design we want to know what size and type of reactor and method of operation are best for a given job. Because this may require that the conditions in the reactor vary with position as well as time, this question can only be answered by a proper integration of the rate equation for the operation. This may pose difficulties because the temperature and composition of the reacting fluid may vary from point to point within the reactor, depending on the endothermic or exothermic character of the reaction, the rate of heat addition or removal from the system, and the flow pattern of fluid through the vessel. In effect, then, many factors must be accounted for in predicting the performance of a reactor. How best to treat these factors is the main problem of reactor design.

Equipment in which homogeneous reactions are effected can be one of three general types; the *batch*, the *steady-state flow*, and the *unsteady-state flow* or *semibatch* reactor. The last classification includes all reactors that do not fall into the first two categories. These types are shown in Fig. 4.1.

Let us briefly indicate the particular features and the main areas of application of these reactor types. Naturally these remarks will be amplified further along in the text. The batch reactor is simple, needs little supporting equipment, and is therefore ideal for small-scale experimental studies on reaction kinetics. Industrially it is used when relatively small amounts of material are to be treated. The steady-state flow reactor is ideal for industrial purposes when large quantities of material are to be processed and when the rate of reaction is fairly high to extremely high. Supporting equipment needs are great; however, extremely good
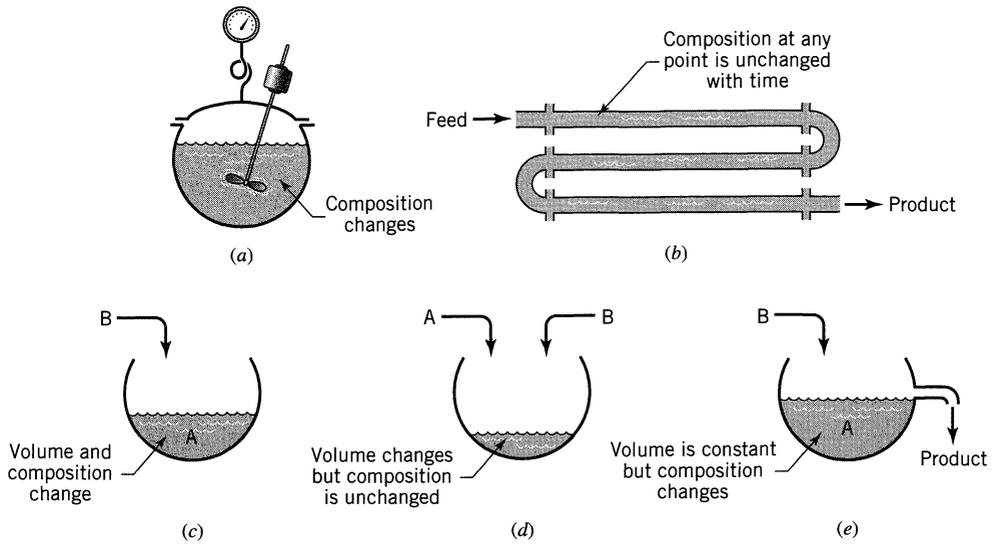
**Figure 4.1** Broad classification of reactor types. (*a*) The batch reactor. (*b*) The steady-state flow reactor. (*c*), (*d*), and (*e*) Various forms of the semibatch reactor.

product quality control can be obtained. As may be expected, this is the reactor that is widely used in the oil industry. The semibatch reactor is a flexible system but is more difficult to analyze than the other reactor types. It offers good control of reaction speed because the reaction proceeds as reactants are added. Such reactors are used in a variety of applications from the calorimetric titrations in the laboratory to the large open hearth furnaces for steel production.

The starting point for all design is the *material balance* expressed for any reactant (or product). Thus, as illustrated in Fig. 4.2, we have

$$
\begin{pmatrix}
\text{rate of} \\
\text{reactant} \\
\text{flow into} \\
\text{element} \\
\text{of volume}
\end{pmatrix}
=
\begin{pmatrix}
\text{rate of} \\
\text{reactant} \\
\text{flow out} \\
\text{of element} \\
\text{of volume}
\end{pmatrix}
+
\begin{pmatrix}
\text{rate of reactant} \\
\text{loss due to} \\
\text{chemical reaction} \\
\text{within the element} \\
\text{of volume}
\end{pmatrix}
+
\begin{pmatrix}
\text{rate of} \\
\text{accumulation} \\
\text{of reactant} \\
\text{in element} \\
\text{of volume}
\end{pmatrix}
\quad \textbf{(1)}
$$
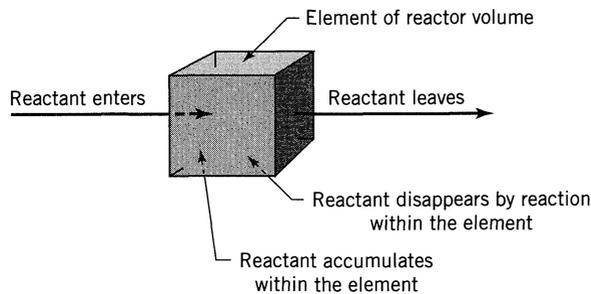


**Figure 4.2** Material balance for an element of volume of the reactor.
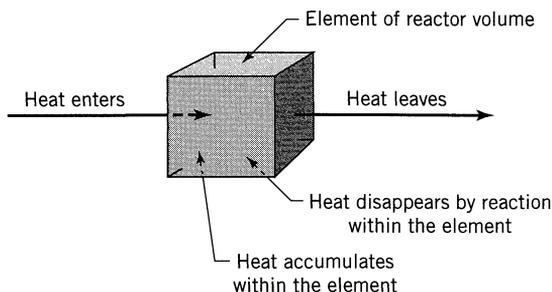
**Figure 4.3** Energy balance for an element of volume of the reactor.

Where the composition within the reactor is uniform (independent of position), the accounting may be made over the whole reactor. Where the composition is not uniform, it must be made over a differential element of volume and then integrated across the whole reactor for the appropriate flow and concentration conditions. For the various reactor types this equation simplifies one way or another, and the resultant expression when integrated gives the basic *performance equation* for that type of unit. Thus, in the batch reactor the first two terms are zero; in the steady-state flow reactor the fourth term disappears; for the semibatch reactor all four terms may have to be considered.

In nonisothermal operations *energy balances* must be used in conjunction with material balances. Thus, as illustrated in Fig. 4.3, we have

$$
\begin{pmatrix} \text{rate of heat} \\ \text{flow into} \\ \text{element of} \\ \text{volume} \end{pmatrix} = \begin{pmatrix} \text{rate of heat} \\ \text{flow out of} \\ \text{element of} \\ \text{volume} \end{pmatrix} + \begin{pmatrix} \text{rate of} \\ \text{disappearance} \\ \text{of heat by} \\ \text{reaction within} \\ \text{element of} \\ \text{volume} \end{pmatrix} + \begin{pmatrix} \text{rate of} \\ \text{accumulation} \\ \text{of heat within} \\ \text{element of} \\ \text{volume} \end{pmatrix} \quad (2)
$$

Again, depending on circumstances, this accounting may be made either about a differential element of reactor or about the reactor as a whole.

The material balance of Eq. 1 and the energy balance of Eq. 2 are tied together by their third terms because the heat effect is produced by the reaction itself.

Since Eqs. 1 and 2 are the starting points for all design, we consider their integration for a variety of situations of increasing complexity in the chapters to follow.

When we can predict the response of the reacting system to changes in operating conditions (how rates and equilibrium conversion change with temperature and pressure), when we are able to compare yields for alternative designs (adiabatic versus isothermal operations, single versus multiple reactor units, flow versus batch system), and when we can estimate the economics of these various alternatives, then and only then will we feel sure that we can arrive at the design well fitted for the purpose at hand. Unfortunately, real situations are rarely simple.
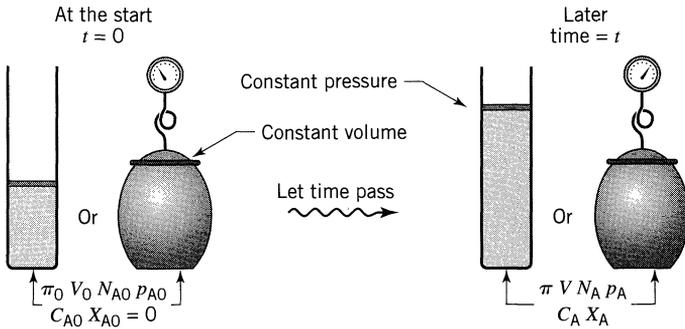
**Figure 4.4** Symbols used for batch reactors.

Should we explore all reasonable design alternatives? How sophisticated should our analysis be? What simplifying assumptions should we make? What shortcuts should we take? Which factors should we ignore and which should we consider? And how should the reliability and completeness of the data at hand influence our decisions? Good engineering judgment, which only comes with experience, will suggest the appropriate course of action.

## Symbols and Relationship between $C_A$ and $X_A$

For the reaction $aA + bB \rightarrow rR$, with inerts $iI$, Figs. 4.4 and 4.5 show the symbols commonly used to tell what is happening in the batch and flow reactors. These figures show that there are two related measures of the extent of reaction, the concentration $C_A$ and the conversion $X_A$. However, the relationship between $C_A$ and $X_A$ is often not obvious but depends on a number of factors. This leads to three special cases, as follows.

**Special Case 1. Constant Density Batch and Flow Systems.** This includes most liquid reactions and also those gas reactions run at constant temperature and density. Here $C_A$ and $X_A$ are related as follows:

$$\left.\begin{array}{ll} X_A = 1 - \dfrac{C_A}{C_{A0}} & \text{and} \quad dX_A = -\dfrac{dC_A}{C_{A0}} \\[2mm] \dfrac{C_A}{C_{A0}} = 1 - X_A & \text{and} \quad dC_A = -C_{A0}dX_A \end{array}\right\} \quad \text{for} \quad \varepsilon_A = \dfrac{V_{X_A=1} - V_{X_A=0}}{V_{X_A=0}} = 0 \quad (3)$$
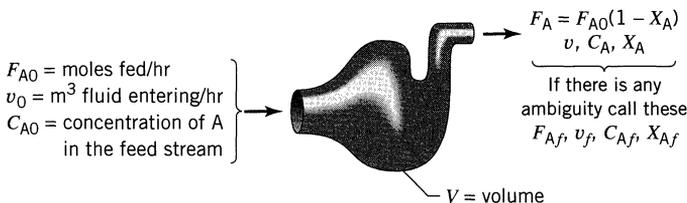


**Figure 4.5** Symbols used for flow reactors.

To relate the changes in B and R to A we have

$$\frac{C_{A0} - C_A}{a} = \frac{C_{B0} - C_B}{b} = \frac{C_R - C_{R0}}{r} \quad \text{or} \quad \frac{C_{A0}X_A}{a} = \frac{C_{B0}X_B}{b} \tag{4}$$

**Special Case 2. Batch and Flow Systems of Gases of Changing Density but with $T$ and $\pi$ Constant.** Here the density changes because of the change in number of moles during reaction. In addition, we require that the volume of a fluid element changes linearly with conversion, or $V = V_0(1 + \varepsilon_A X_A)$.

$$\left.\begin{array}{ll} X_A = \dfrac{C_{A0} - C_A}{C_{A0} + \varepsilon_A C_A} & \text{and} \quad dX_A = -\dfrac{C_{A0}(1 + \varepsilon_A)}{(C_{A0} + \varepsilon_A C_A)^2}\, dC_A \\[4mm] \dfrac{C_A}{C_{A0}} = \dfrac{1 - X_A}{1 + \varepsilon_A X_A} & \text{and} \quad \dfrac{dC_A}{C_{A0}} = -\dfrac{1 + \varepsilon_A}{(1 + \varepsilon_A X_A)^2}\, dX_A \end{array}\right\} \text{for}$$

$$\varepsilon_A = \frac{V_{X_A=1} - V_{X_A=0}}{V_{X_A=0}} \neq 0 \tag{5}$$

To follow changes in the other components we have

$$\begin{array}{ll} \text{between} \\ \text{reactants} \end{array} \left\{\begin{array}{l} \varepsilon_A X_A = \varepsilon_B X_B \\[3mm] \dfrac{a\varepsilon_A}{C_{A0}} = \dfrac{b\varepsilon_B}{C_{B0}} \end{array}\right. \quad \begin{array}{l} \text{for products} \\ \text{and inerts} \end{array} \left\{\begin{array}{l} \dfrac{C_R}{C_{A0}} = \dfrac{(r/a)X_A + C_{R0}/C_{A0}}{1 + \varepsilon_A X_A} \\[3mm] \dfrac{C_I}{C_{I0}} = \dfrac{1}{1 + \varepsilon_A X_A} \end{array}\right. \tag{6}$$

**Special Case 3. Batch and Flow Systems for Gases in General (varying $\rho$, $T$, $\pi$)** which react according to

$$a\text{A} + b\text{B} \rightarrow r\text{R}, \qquad a + b \neq r$$

Pick one reactant as the basis for determining the conversion. We call this the *key reactant*. Let A be the key. Then for *ideal gas* behavior,

$$X_A = \frac{1 - \dfrac{C_A}{C_{A0}}\left(\dfrac{T\pi_0}{T_0\pi}\right)}{1 + \varepsilon_A \dfrac{C_A}{C_{A0}}\left(\dfrac{T\pi_0}{T_0\pi}\right)} \quad \text{or} \quad \frac{C_A}{C_{A0}} = \frac{1 - X_A}{1 + \varepsilon_A X_A}\left(\frac{T_0\pi}{T\pi_0}\right)$$

$$X_A = \frac{\dfrac{C_{B0}}{C_{A0}} - \dfrac{C_B}{C_{A0}}\left(\dfrac{T\pi_0}{T_0\pi}\right)}{\dfrac{b}{a} + \varepsilon_A \dfrac{C_B}{C_{A0}}\left(\dfrac{T\pi_0}{T_0\pi}\right)} \quad \text{or} \quad \frac{C_B}{C_{A0}} = \frac{\dfrac{C_{B0}}{C_{A0}} - \dfrac{b}{a}X_A}{1 + \varepsilon_A X_A}\left(\frac{T_0\pi}{T\pi_0}\right)$$

$$\frac{C_R}{C_{A0}} = \frac{\dfrac{C_{R0}}{C_{A0}} + \dfrac{r}{a}X_A}{1 + \varepsilon_A X_A}\left(\frac{T_0\pi}{T\pi_0}\right)$$

For high-pressure nonideal gas behavior replace $\left(\dfrac{T_0\pi}{\tau_0\pi_0}\right)$ by $\left(\dfrac{z_0 T_0\pi}{zT\pi}\right)$, where $z$ is the compressibility factor. To change to another key reactant, say B, note that

$$\frac{a\varepsilon_A}{C_{A0}} = \frac{b\varepsilon_B}{C_{B0}} \quad \text{and} \quad \frac{C_{A0}X_A}{a} = \frac{C_{B0}X_B}{b}$$

For liquids or isothermal gases with no change pressure and density

$$\varepsilon_A \to 0 \quad \text{and} \quad \left(\frac{T_0\pi}{T\pi_0}\right) \to 1$$

and the preceding expressions simplify greatly.

## EXAMPLE 4.1   A BALANCE FROM STOICHIOMETRY

Consider a feed $C_{A0} = 100$, $C_{B0} = 200$, $C_{i0} = 100$ to a steady-flow reactor. The isothermal gas-phase reaction is

$$A + 3B \to 6R$$

If $C_A = 40$ at the reactor exit, what is $C_B$, $X_A$, and $X_B$ there?

### SOLUTION

First sketch what is known (see Fig. E4.1).



$-A + 3B \to 6R$

$C_{A0} = 100$
$C_{B0} = 200$
$C_{i0} = 100$

$C_A = 40$
$C_B = ?$
$X_A = ?$
$X_B = ?$
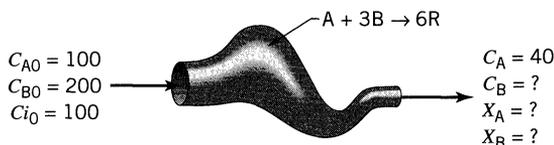
**Figure E4.1**

Next recognize that this problem concerns Special Case 2. So evaluate $\varepsilon_A$ and $\varepsilon_B$. For this take 400 volumes of gas

$$\left. \begin{array}{ll} \text{at } X_A = 0 & V = 100A + 200B + 100i = 400 \\ \text{at } X_A = 1 & V = 0A - 100B + 600R + 100i = 600 \end{array} \right\} \quad \varepsilon_A = \frac{600 - 400}{400} = \frac{1}{2}$$

Then from the equations in the text

$$\varepsilon_B = \frac{\varepsilon_A C_{B0}}{b C_{A0}} = \frac{(1/2)(200)}{3(100)} = \frac{1}{3}$$

$$X_A = \frac{C_{A0} - C_A}{C_{A0} + \varepsilon_A C_A} = \frac{100 - 40}{100 + (1/2)40} = \frac{60}{120} = \underline{\underline{0.5}}$$

$$X_B = \frac{b C_{A0} X_A}{C_{B0}} = \frac{3(100)(0.5)}{200} = \underline{\underline{0.75}}$$

$$C_B = C_{B0}\left(\frac{1 - X_B}{1 + \varepsilon_B X_B}\right) = \frac{200(1 - 0.75)}{1 + (1/3)(0.75)} = \underline{\underline{40}}$$ ∎

## PROBLEMS

The following four problems consider an isothermal single-phase flow reactor operating at steady-state and constant pressure.

**4.1.** Given a gaseous feed, $C_{A0} = 100$, $C_{B0} = 200$, $A + B \rightarrow R + S$, $X_A = 0.8$. Find $X_B$, $C_A$, $C_B$.

**4.2.** Given a dilute aqueous feed, $C_{A0} = C_{B0} = 100$, $A + 2B \rightarrow R + S$, $C_A = 20$. Find $X_A$, $X_B$, $C_B$.

**4.3.** Given a gaseous feed, $C_{A0} = 200$, $C_{B0} = 100$, $A + B \rightarrow R$, $C_A = 50$. Find $X_A$, $X_B$, $C_B$.

**4.4.** Given a gaseous feed, $C_{A0} = C_{B0} = 100$, $A + 2B \rightarrow R$, $C_B = 20$. Find $X_A$, $X_B$, $C_A$.

In the following two problems a continuous stream of fluid enters a vessel at temperature $T_0$ and pressure $\pi_0$, reacts there, and leaves at $T$ and $\pi$.

**4.5.** Given a gaseous feed, $T_0 = 400$ K, $\pi_0 = 4$ atm, $C_{A0} = 100$, $C_{B0} = 200$, $A + B \rightarrow 2R$, $T = 300$ K, $\pi = 3$ atm, $C_A = 20$. Find $X_A$, $X_B$, $C_B$.

**4.6.** Given a gaseous feed, $T_0 = 1000$ K, $\pi_0 = 5$ atm, $C_{A0} = 100$, $C_{B0} = 200$, $A + B \rightarrow 5R$, $T = 400$ K, $\pi = 4$ atm, $C_A = 20$. Find $X_A$, $X_B$, $C_B$.

**4.7.** *A Commercial Popcorn Popping Popcorn Popper.* We are constructing a 1-liter popcorn popper to be operated in steady flow. First tests in this unit show that 1 liter/min of raw corn feed stream produces 28 liter/min of mixed exit stream. Independent tests show that when raw corn pops its volume goes from 1 to 31. With this information determine what fraction of raw corn is popped in the unit.

# Chapter 5

# Ideal Reactors for a Single Reaction

In this chapter we develop the performance equations for a single fluid reacting in the three ideal reactors shown in Fig. 5.1. We call these *homogeneous reactions*. Applications and extensions of these equations to various isothermal and noniso-thermal operations are considered in the following four chapters.

In the *batch reactor*, or BR, of Fig. 5.1a the reactants are initially charged into a container, are well mixed, and are left to react for a certain period. The resultant mixture is then discharged. This is an unsteady-state operation where composition changes with time; however, at any instant the composition throughout the reactor is uniform.

The first of the two ideal steady-state flow reactors is variously known as the plug flow, slug flow, piston flow, ideal tubular, and unmixed flow reactor, and it is shown in Fig. 5.1b. We refer to it as the *plug flow reactor*, or PFR, and to this pattern of flow as *plug flow*. It is characterized by the fact that the flow of fluid through the reactor is orderly with no element of fluid overtaking or mixing with any other element ahead or behind. Actually, there may be lateral mixing of fluid in a plug flow reactor; however, there must be no mixing or diffusion along
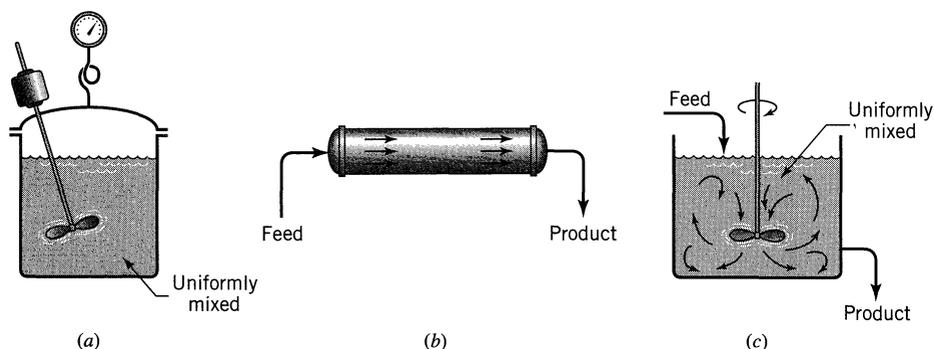


**Figure 5.1** The three types of ideal reactors: (a) batch reactor, or BR; (b) plug flow reactor, or PFR; and (c) mixed flow reactor, or MFR.

the flow path. The necessary and sufficient condition for plug flow is for the residence time in the reactor to be the same for all elements of fluid.*

The other ideal steady-state flow reactor is called the mixed reactor, the backmix reactor, the ideal stirred tank reactor, the C* (meaning C-star), CSTR, or the CFSTR (constant flow stirred tank reactor), and, as its names suggest, it is a reactor in which the contents are well stirred and uniform throughout. Thus, the exit stream from this reactor has the same composition as the fluid within the reactor. We refer to this type of flow as *mixed flow*, and the corresponding reactor the *mixed flow reactor*, or MFR.

These three ideals are relatively easy to treat. In addition, one or other usually represents the best way of contacting the reactants—no matter what the operation. For these reasons, we often try to design real reactors so that their flows approach these ideals, and much of the development in this book centers about them.

In the treatment to follow it should be understood that the term $V$, called the reactor volume, really refers to the volume of fluid in the reactor. When this differs from the internal volume of reactor, then $V_r$ designates the internal volume of reactor while $V$ designates the volume of reacting fluid. For example, in solid catalyzed reactors with voidage $\varepsilon$ we have

$$V = \varepsilon V_r$$

For homogeneous systems, however, we usually use the term $V$ alone.

## 5.1 IDEAL BATCH REACTOR

Make a material balance for any component A. For such an accounting we usually select the limiting component. In a batch reactor, since the composition is uniform throughout at any instant of time, we may make the accounting about the whole reactor. Noting that no fluid enters or leaves the reaction mixture during reaction, Eq. 4.1, which was written for component A, becomes

$$\underset{=\,0}{\text{input}} = \underset{=\,0}{\text{output}} + \text{disappearance} + \text{accumulation}$$

or

$$+ \begin{pmatrix} \text{rate of loss of reactant A} \\ \text{within reactor due to} \\ \text{chemical reaction} \end{pmatrix} = - \begin{pmatrix} \text{rate of accumulation} \\ \text{of reactant A} \\ \text{within the reactor} \end{pmatrix} \quad \textbf{(1)}$$

Evaluating the terms of Eq. 1, we find

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

$$\begin{array}{l} \text{accumulation of A,} \\ \text{moles/time} \end{array} = \frac{dN_A}{dt} = \frac{d[N_{A0}(1 - X_A)]}{dt} = -N_{A0}\frac{dX_A}{dt}$$

---

* The necessary condition follows directly from the definition of plug flow. However, the sufficient condition—that the same residence times implies plug flow—can be established only from the second law of thermodynamics.

By replacing these two terms in Eq. 1, we obtain

$$(-r_A)V = N_{A0}\frac{dX_A}{dt} \tag{2}$$

Rearranging and integrating then gives

$$t = N_{A0}\int_0^{X_A}\frac{dX_A}{(-r_A)V} \tag{3}$$

This is the general equation showing the time required to achieve a conversion $X_A$ for either isothermal or nonisothermal operation. The volume of reacting fluid and the reaction rate remain under the integral sign, for in general they both change as reaction proceeds.

This equation may be simplified for a number of situations. If the density of the fluid remains constant, we obtain

$$t = C_{A0}\int_0^{X_A}\frac{dX_A}{-r_A} = -\int_{C_{A0}}^{C_A}\frac{dC_A}{-r_A} \qquad \text{for } \varepsilon_A = 0 \tag{4}$$

For all reactions in which the volume of reacting mixture changes proportionately with conversion, such as in single gas-phase reactions with significant density changes, Eq. 3 becomes

$$t = N_{A0}\int_0^{X_A}\frac{dX_A}{(-r_A)V_0(1 + \varepsilon_A X_A)} = C_{A0}\int_0^{X_A}\frac{dX_A}{(-r_A)(1 + \varepsilon_A X_A)} \tag{5}$$

In one form or another, Eqs. 2 to 5 have all been encountered in Chapter 3. They are applicable to both isothermal and nonisothermal operations. For the latter the variation of rate with temperature, and the variation of temperature with conversion, must be known before solution is possible. Figure 5.2 is a graphical representation of two of these equations.
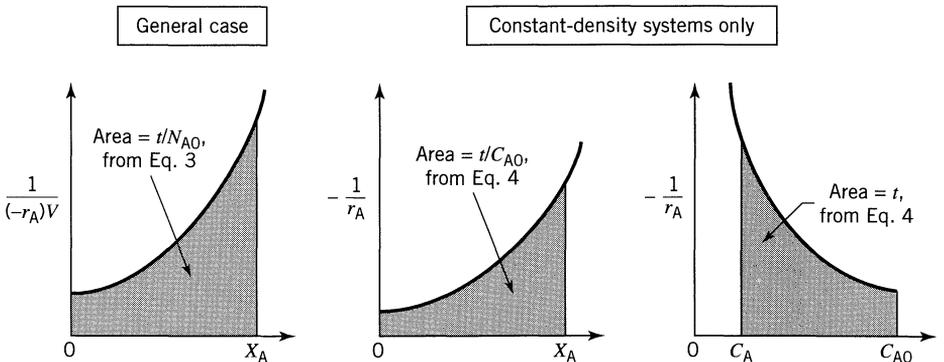


**Figure 5.2** Graphical representation of the performance equations for batch reactors, isothermal or nonisothermal.

## Space-Time and Space-Velocity

Just as the reaction time $t$ is the natural performance measure for a batch reactor, so are the space-time and space-velocity the proper performance measures of flow reactors. These terms are defined as follows:

Space-time:

$$\tau = \frac{1}{s} = \left( \begin{array}{c} \text{time required to process one} \\ \text{reactor volume of feed measured} \\ \text{at specified conditions} \end{array} \right) = [\text{time}] \tag{6}$$

Space-velocity:

$$s = \frac{1}{\tau} = \left( \begin{array}{c} \text{number of reactor volumes of} \\ \text{feed at specified conditions which} \\ \text{can be treated in unit time} \end{array} \right) = [\text{time}^{-1}] \tag{7}$$

Thus, a space-velocity of 5 hr$^{-1}$ means that five reactor volumes of feed at specified conditions are being fed into the reactor per hour. A space-time of 2 min means that every 2 min one reactor volume of feed at specified conditions is being treated by the reactor.

Now we may arbitrarily select the temperature, pressure, and state (gas, liquid, or solid) at which we choose to measure the volume of material being fed to the reactor. Certainly, then, the value for space-velocity or space-time depends on the conditions selected. If they are of the stream entering the reactor, the relation between $s$ and $\tau$ and the other pertinent variables is

$$\tau = \frac{1}{s} = \frac{C_{A0}V}{F_{A0}} = \frac{\left( \dfrac{\text{moles A entering}}{\text{volume of feed}} \right)(\text{volume of reactor})}{\left( \dfrac{\text{moles A entering}}{\text{time}} \right)} \tag{8}$$

$$= \frac{V}{v_0} = \frac{(\text{reactor volume})}{(\text{volumetric feed rate})}$$

It may be more convenient to measure the volumetric feed rate at some standard state, especially when the reactor is to operate at a number of temperatures. If, for example, the material is gaseous when fed to the reactor at high temperature but is liquid at the standard state, care must be taken to specify precisely what state has been chosen. The relation between the space-velocity and space-time for actual feed conditions (unprimed symbols) and at standard conditions (designated by primes) is given by

$$\tau' = \frac{1}{s'} = \frac{C'_{A0}V}{F_{A0}} = \tau \frac{C'_{A0}}{C_{A0}} = \frac{1}{s} \frac{C'_{A0}}{C_{A0}} \tag{9}$$

In most of what follows, we deal with the space-velocity and space-time based on feed at actual entering conditions; however, the change to any other basis is easily made.

## 5.2 STEADY-STATE MIXED FLOW REACTOR

The performance equation for the mixed flow reactor is obtained from Eq. 4.1, which makes an accounting of a given component within an element of volume of the system. But since the composition is uniform throughout, the accounting may be made about the reactor as a whole. By selecting reactant A for consideration, Eq. 4.1 becomes

$$\text{input} = \text{output} + \text{disappearance by reaction} + \overset{=\,0}{\text{accumulation}} \qquad \textbf{(10)}$$

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

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

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

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

Introducing these three terms into Eq. 10, we obtain

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

which on rearrangement becomes

or

$$\boxed{\begin{array}{c} \dfrac{V}{F_{A0}} = \dfrac{\tau}{C_{A0}} = \dfrac{\Delta X_A}{-r_A} = \dfrac{X_A}{-r_A} \\[2mm] \tau = \dfrac{1}{s} = \dfrac{V}{v_0} = \dfrac{VC_{A0}}{F_{A0}} = \dfrac{C_{A0}X_A}{-r_A} \end{array}}$$

any $\varepsilon_A$     **(11)**



$C_{A0}$
$X_{A0} = 0$
$v_0$
$F_{A0}$

$V, X_A$
$C_A, (-r_A)$

$C_{Af} = C_A$
$X_{Af} = X_A$
$v_f$
$(-r_A)_f = (-r_A)$
$F_A$

Uniform throughout
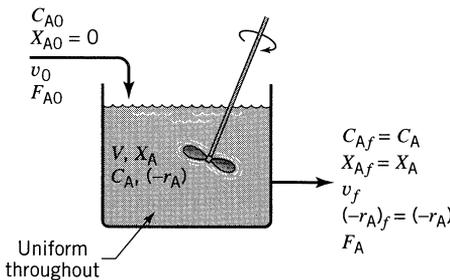
**Figure 5.3** Notation for a mixed reactor.

where $X_A$ and $r_A$ are measured at exit stream conditions, which are the same as the conditions within the reactor.

More generally, if the feed on which conversion is based, subscript 0, enters the reactor partially converted, subscript $i$, and leaves at conditions given by subscript $f$, we have

$$\frac{V}{F_{A0}} = \frac{\Delta X_A}{(-r_A)_f} = \frac{X_{Af} - X_{Ai}}{(-r_A)_f}$$

or $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad$ (12)

$$\tau = \frac{VC_{A0}}{F_{A0}} = \frac{C_{A0}(X_{Af} - X_{Ai})}{(-r_A)_f}$$

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
$$\boxed{\begin{array}{c} \dfrac{V}{F_{A0}} = \dfrac{X_A}{-r_A} = \dfrac{C_{A0} - C_A}{C_{A0}(-r_A)} \\[2mm] \tau = \dfrac{V}{v} = \dfrac{C_{A0}X_A}{-r_A} = \dfrac{C_{A0} - C_A}{-r_A} \end{array}} \qquad \varepsilon_A = 0 \qquad (13)$$

These expressions relate in a simple way the four terms $X_A$, $-r_A$, $V$, $F_{A0}$; thus, knowing any three allows the fourth to be found directly. In design, then, the size of reactor needed for a given duty or the extent of conversion in a reactor of given size is found directly. In kinetic studies each steady-state run gives, without integration, the reaction rate for the conditions within the reactor. The ease of interpretation of data from a mixed flow reactor makes its use very attractive in kinetic studies, in particular with messy reactions (e.g., multiple reactions and solid catalyzed reactions).

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.
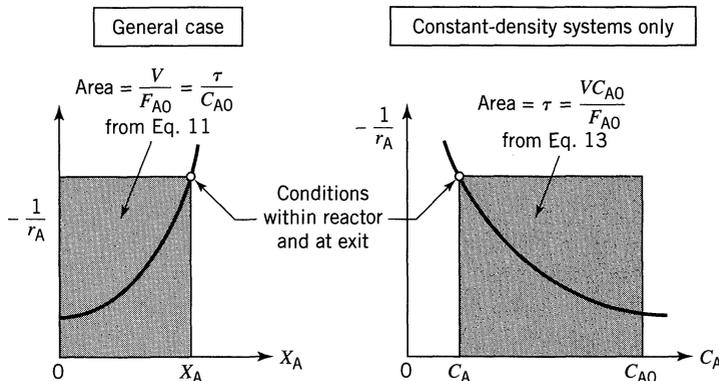


**Figure 5.4** Graphical representation of the design equations for mixed flow reactor.

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

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

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

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

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

$$\boxed{k\tau = \frac{C_{A0} - C_A}{C_A^2} \quad \text{or} \quad C_A = \frac{-1 + \sqrt{1 + 4k\tau C_{A0}}}{2k\tau}} \qquad \textbf{(15)}$$

Similar expressions can be written for any other form of rate equation. These expressions can be written either in terms of concentrations or conversions. Using conversions is simpler for systems of changing density, while either form can be used for sytems of constant density.

---

**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.
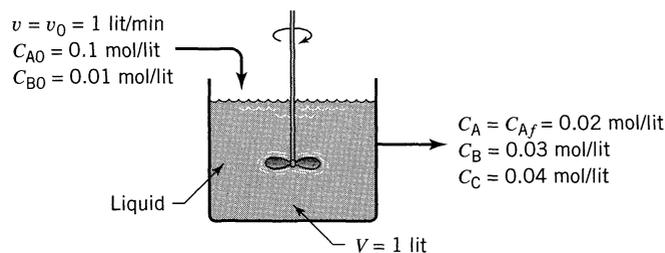


**Figure E5.1**

## 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 ($2A \rightarrow R$). 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, $2A \rightarrow R$, 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 | $v_0$ | $C_A$ | $X_A$ | $(-r_A) = \dfrac{v_0 C_{A0} X_A}{V}$ | $\log C_A$ | $\log(-r_A)$ |
| 1 | 10.0 | 85.7 | 0.25 | $\dfrac{(10)(100)(0.25)}{0.1} = 2500$ | 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

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

These values are tabulated in column 5 of Table E5.2.

Having paired values of $r_A$ and $C_A$ (see Table E5.2) we are ready to test various kinetic expressions. Instead of separately testing for first-order (plot $r_A$ vs. $C_A$), second-order (plot $r_A$ vs. $C_A^2$), etc., let us test directly for $n$th-order kinetics. For this take logarithms of $-r_A = kC_A^n$, giving

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

For $n$th-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
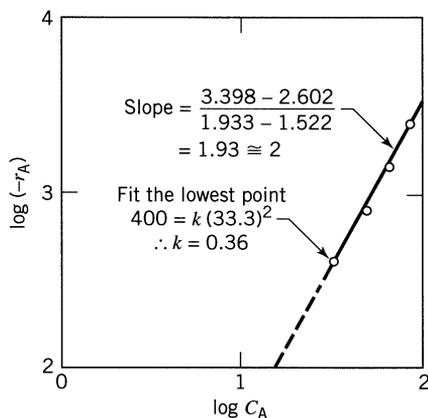


**Figure E5.2**

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

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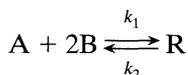
with rate equation

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

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.
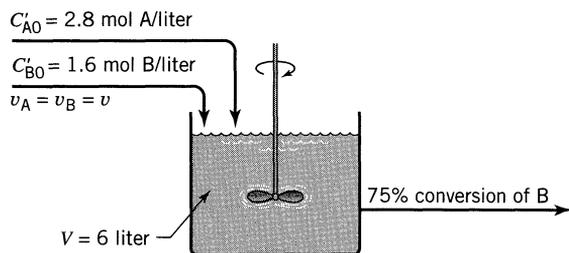


Figure E5.3

*SOLUTION*

The concentration of components in the mixed feed stream is

$$C_{A0} = 1.4 \text{ mol/liter}$$

$$C_{B0} = 0.8 \text{ mol/liter}$$

$$C_{R0} = 0$$

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

$$C_A = 1.4 - 0.6/2 = 1.1 \text{ mol/liter}$$

$$C_B = 0.8 - 0.6 = 0.2 \text{ mol/liter} \quad \text{or} \quad 75\% \text{ conversion}$$

$$C_R = 0.3 \text{ mol/liter}$$

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

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

■

## 5.3 STEADY-STATE PLUG FLOW REACTOR

In a plug flow reactor the composition of the fluid varies from point to point along a flow path; consequently, the material balance for a reaction component must be made for a differential element of volume $dV$. Thus for reactant A, Eq. 4.1 becomes

$$\text{input} = \text{output} + \text{disappearance by reaction} + \overset{= 0}{\text{accumulation}} \qquad (10)$$

Referring to Fig. 5.5, we see for volume $dV$ that

$$\text{input of A, moles/time} = F_A$$

$$\text{output of A, moles/time} = F_A + dF_A$$

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

Introducing these three terms in Eq. 10, we obtain

$$F_A = (F_A + dF_A) + (-r_A)dV$$

Noting that

$$dF_A = d[F_{A0}(1 - X_A)] = -F_{A0}dX_A$$

We obtain on replacement

$$F_{A0}dX_A = (-r_A)dV \qquad (16)$$
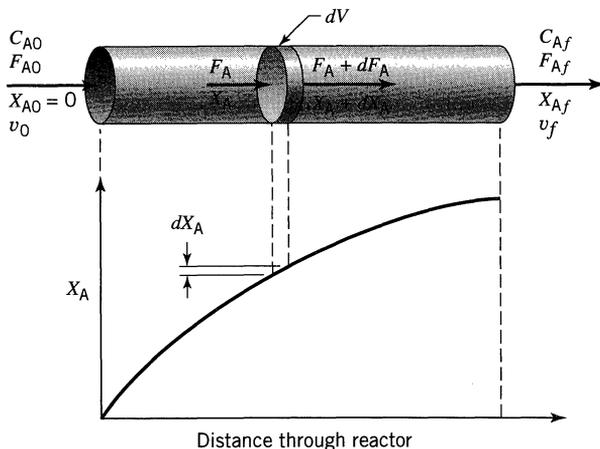


**Figure 5.5** Notation for a plug flow reactor.

This, then, is the equation which accounts for A in the differential section of reactor of volume $dV$. For the reactor as a whole the expression must be integrated. Now $F_{A0}$, the feed rate, is constant, but $r_A$ is certainly dependent on the concentration or conversion of materials. Grouping the terms accordingly, we obtain

$$\int_0^V \frac{dV}{F_{A0}} = \int_0^{X_{Af}} \frac{dX_A}{-r_A}$$

Thus

or

$$\boxed{\begin{array}{l} \dfrac{V}{F_{A0}} = \dfrac{\tau}{C_{A0}} = \displaystyle\int_0^{X_{Af}} \dfrac{dX_A}{-r_A} \\[3mm] \tau = \dfrac{V}{v_0} = \dfrac{VC_{A0}}{F_{A0}} = C_{A0}\displaystyle\int_0^{X_{Af}} \dfrac{dX_A}{-r_A} \end{array}} \qquad \text{any } \varepsilon_A \qquad (17)$$

Equation 17 allows the determination of reactor size for a given feed rate and required conversion. Compare Eqs. 11 and 17. The difference is that in plug flow $r_A$ varies, whereas in mixed flow $r_A$ is constant.

As a more general expression for plug flow reactors, if the feed on which conversion is based, subscript 0, enters the reactor partially converted, subscript $i$, and leaves at a conversion designated by subscript $f$, we have

$$\frac{V}{F_{A0}} = \int_{X_{Ai}}^{X_{Af}} \frac{dX_A}{-r_A}$$

or

$$\tau = C_{A0} \int_{X_{Ai}}^{X_{Af}} \frac{dX_A}{-r_A} \qquad (18)$$

For the special case of *constant-density systems*

$$X_A = 1 - \frac{C_A}{C_{A0}} \quad \text{and} \quad dX_A = -\frac{dC_A}{C_{A0}}$$

in which case the performance equation can be expressed in terms of concentrations, or

or

$$\boxed{\begin{array}{l} \dfrac{V}{F_{A0}} = \dfrac{\tau}{C_{A0}} = \displaystyle\int_0^{X_{Af}} \dfrac{dX_A}{-r_A} = -\dfrac{1}{C_{A0}}\displaystyle\int_{C_{A0}}^{C_{Af}} \dfrac{dC_A}{-r_A} \\[3mm] \tau = \dfrac{V}{v_0} = C_{A0}\displaystyle\int_0^{X_{Af}} \dfrac{dX_A}{-r_A} = -\displaystyle\int_{C_{A0}}^{C_{Af}} \dfrac{dC_A}{-r_A} \end{array}} \quad \varepsilon_A = 0 \qquad (19)$$
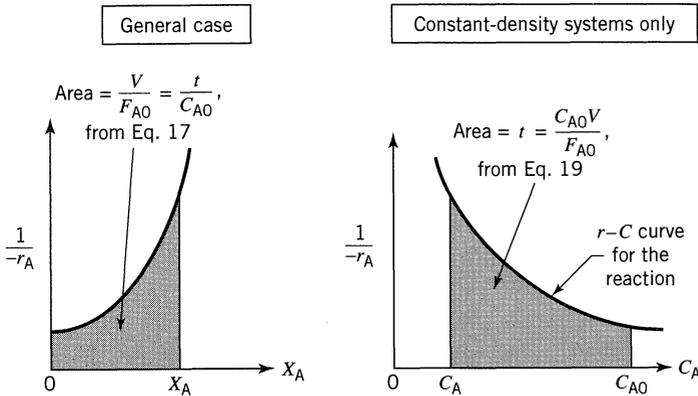
**Figure 5.6** Graphical representation of the performance equations for plug flow reactors.

These performance equations, Eqs. 17 to 19, can be written either in terms of concentrations or conversions. For systems of changing density it is more convenient to use conversions; however, there is no particular preference for constant density systems. Whatever its form, the performance equations interrelate the *rate of reaction*, the *extent of reaction*, the *reactor volume*, and the *feed rate*, and if any one of these quantities is unknown it can be found from the other three.

Figure 5.6 displays these performance equations and shows that the space-time needed for any particular duty can always be found by numerical or graphical integration. However, for certain simple kinetic forms analytic integration is possible—and convenient. To do this, insert the kinetic expression for $r_A$ in Eq. 17 and integrate. Some of the simpler integrated forms for plug flow are as follows:

*Zero-order homogeneous reaction*, any constant $\varepsilon_A$

$$k\tau = \frac{kC_{A0}V}{F_{A0}} = C_{A0}X_A \tag{20}$$

*First-order irreversible reaction*, A $\rightarrow$ products, any constant $\varepsilon_A$,

$$\boxed{k\tau = -(1 + \varepsilon_A)\ln(1 - X_A) - \varepsilon_A X_A} \tag{21}$$

*First-order reversible reaction*, A $\rightleftarrows$ rR, $C_{R0}/C_{A0} = M$, kinetics approximated or fitted by $-r_A = k_1 C_A - k_2 C_R$ with an observed equilibrium conversion $X_{Ae}$, any constant $\varepsilon_A$,

$$k_1\tau = \frac{M + rX_{Ae}}{M + r}\left[-(1 + \varepsilon_A X_{Ae})\ln\left(1 - \frac{X_A}{X_{Ae}}\right) - \varepsilon_A X_A\right] \tag{22}$$

*Second-order irreversible reaction*, A + B $\rightarrow$ products with equimolar feed or 2A $\rightarrow$ products, any constant $\varepsilon_A$,

$$C_{A0}k\tau = 2\varepsilon_A(1 + \varepsilon_A)\ln(1 - X_A) + \varepsilon_A^2 X_A + (\varepsilon_A + 1)^2 \frac{X_A}{1 - X_A} \tag{23}$$

Where the density is constant, put $\varepsilon_A = 0$ to obtain the simplified performance equation.

By comparing the batch expressions of Chapter 3 with these plug flow expressions we find:

(1) For *systems of constant density* (constant-volume batch and constant-density plug flow) the performance equations are identical, $\tau$ for plug flow is equivalent to $t$ for the batch reactor, and the equations can be used interchangeably.

(2) For *systems of changing density* there is no direct correspondence between the batch and the plug flow equations and the correct equation must be used for each particular situation. In this case the performance equations cannot be used interchangeably.

The following illustrative examples show how to use these expressions.

**EXAMPLE 5.4** **PLUG FLOW REACTOR PERFORMANCE**

A homogeneous gas reaction $A \rightarrow 3R$ has a reported rate at 215°C

$$-r_A = 10^{-2}C_A^{1/2}, \quad [\text{mol/liter} \cdot \text{sec}]$$

Find the space-time needed for 80% conversion of a 50% A–50% inert feed to a plug flow reactor operating at 215°C and 5 atm ($C_{A0} = 0.0625$ mol/liter).
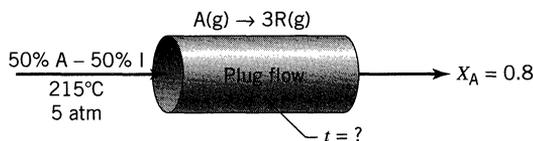


**Figure E5.4a**

**SOLUTION**

For this stoichiometry and with 50% inerts, two volumes of feed gas would give four volumes of completely converted product gas; thus

$$\varepsilon_A = \frac{4-2}{2} = 1$$

in which case the plug flow performance equation, Eq. 17, becomes

$$\tau = C_{A0}\int_0^{X_{Af}}\frac{dX_A}{-r_A} = C_{A0}\int_0^{X_{Af}}\frac{dX_A}{kC_{A0}^{1/2}\left(\dfrac{1-X_A}{1+\varepsilon_AX_A}\right)^{1/2}} = \frac{C_{A0}^{1/2}}{k}\int_0^{0.8}\left(\frac{1+X_A}{1-X_A}\right)^{1/2}dX_A \quad \text{(i)}$$

The integral can be evaluated in any one of three ways: graphically, numerically, or analytically. Let us illustrate these methods.

**Table E5.4**

| $X_A$ | $\dfrac{1 + X_A}{1 - X_A}$ | $\left(\dfrac{1 + X_A}{1 - X_A}\right)^{1/2}$ |
|---|---|---|
| 0 | 1 | 1 |
| 0.2 | $\dfrac{1.2}{0.8} = 1.5$ | 1.227 |
| 0.4 | 2.3 | 1.528 |
| 0.6 | 4 | 2 |
| 0.8 | 9 | 3 |

*Graphical Integration.*   First evaluate the function to be integrated at selected values (see Table E5.4) and plot this function (see Fig. E5.4*b*).
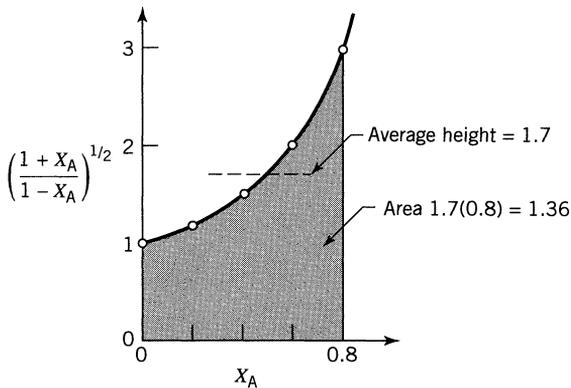


**Figure E5.4*b***

Counting squares or estimating by eye we find

$$\text{Area} = \int_0^{0.8} \left(\frac{1 + X_A}{1 - X_A}\right)^{1/2} dX_A = (1.70)(0.8) = \underline{\underline{1.36}}$$

*Numerical Integration.*   Using Simpson's rule, applicable to an even number of uniformly spaced intervals on the $X_A$ axis, we find for the data of Table E5.4,

$$\int_0^{0.8} \left(\frac{1 + X_A}{1 - X_A}\right)^{1/2} dX_A = (\text{average height})(\text{total width})$$

$$= \left[\frac{1(1) + 4(1.227) + 2(1.528) + 4(2) + 1(3)}{12}\right](0.8)$$

$$= \underline{\underline{1.331}}$$

**Analytical Integration.** From a table of integrals

$$\int_0^{0.8} \left(\frac{1 + X_A}{1 - X_A}\right)^{1/2} dX_A = \int_0^{0.8} \frac{1 + X_A}{\sqrt{1 - X_A^2}} dX_A$$

$$= \left(\text{arc sin } X_A - \sqrt{1 - X_A^2}\right) \Big|_0^{0.8} = \underline{\underline{1.328}}$$

The method of integration recommended depends on the situation. In this problem probably the numerical method is the quickest and simplest and gives a good enough answer for most purposes.

So with the integral evaluated, Eq. (i) becomes

$$\underline{\underline{\tau}} = \frac{(0.0625 \text{ mol/liter})^{1/2}}{(10^{-2} \text{ mol}^{1/2}/\text{liter}^{1/2} \cdot \text{sec})} (1.33) = \underline{\underline{33.2 \text{ sec}}}$$

∎

## EXAMPLE 5.5    *PLUG FLOW REACTOR VOLUME*

The homogeneous gas decomposition of phosphine

$$4PH_3(g) \rightarrow P_4(g) + 6H_2$$
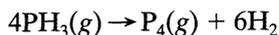
proceeds at 649°C with the first-order rate

$$-r_{PH_3} = (10/\text{hr}) \, C_{PH_3}$$

What size of plug flow reactor operating at 649°C and 460 kPa can produce 80% conversion of a feed consisting of 40 mol of pure phosphine per hour?
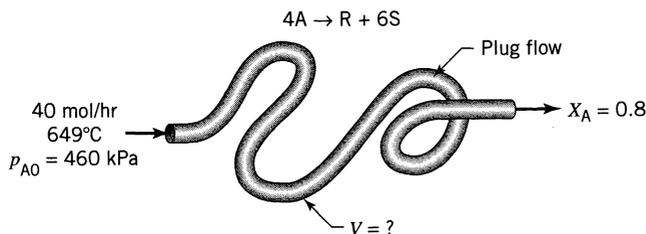


**Figure E5.5**

## SOLUTION

Let $A = PH_3$, $R = P_4$, $S = H_2$. Then the reaction becomes

$$4A \rightarrow R + 6S$$

with

$$-r_A = (10/\text{hr})\, C_A$$

The volume of plug flow reactor is given by Eq. 21

$$V = \frac{F_{A0}}{kC_{A0}}\left[(1 + \varepsilon_A)\ln\frac{1}{1 - X_A} - \varepsilon_A X_A\right]$$

Evaluating the individual terms in this expression gives

$$F_{A0} = 40\,\text{mol/hr}$$

$$k = 10/\text{hr}$$

$$C_{A0} = \frac{p_{A0}}{RT} = \frac{460\,000\,\text{Pa}}{(8.314\,\text{Pa}\cdot\text{m}^3/\text{mol}\cdot\text{K})(922\,\text{K})} = 60\,\text{mol/m}^3$$

$$\varepsilon_A = \frac{7 - 4}{4} = 0.75$$

$$X_A = 0.8$$

hence the volume of reactor

$$\underline{V} = \frac{40\,\text{mol/hr}}{(10/\text{hr})(60\,\text{mol/m}^3)}\left[(1 + 0.75)\ln\frac{1}{0.2} - 0.75(0.8)\right] = 0.148\,\text{m}^3$$

$$= \underline{\underline{148\,\text{liters}}}$$

■

## EXAMPLE 5.6 *TEST OF A KINETIC EQUATION IN A PLUG FLOW REACTOR*

We suspect that the gas reaction between A, B, and R is an elementary reversible reaction

$$A + B \underset{k_2}{\overset{k_1}{\rightleftarrows}} R$$
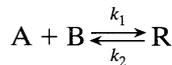
and we plan to test this with experiments in an isothermal plug flow reactor.

(a) Develop the isothermal performance equation for these kinetics for a feed of A, B, R, and inerts.

(b) Show how to test this equation for an equimolar feed of A and B.

## SOLUTION

**(a)** Feed of A, B, R, and inerts. For this elementary reaction the rate is

$$-r_A = k_1 C_A C_B - k_2 C_R = k_1 \frac{N_A}{V} \frac{N_B}{V} - k_2 \frac{N_R}{V}$$

At constant pressure, basing expansion and conversion on substance A,

$$-r_A = k_1 \frac{N_{A0} - N_{A0}X_A}{V_0(1 + \varepsilon_A X_A)} \frac{N_{B0} - N_{A0}X_A}{V_0(1 + \varepsilon_A X_A)} - k_2 \frac{N_{R0} + N_{A0}X_A}{V_0(1 + \varepsilon_A X_A)}$$

Letting $M = C_{B0}/C_{A0}$, $M' = C_{R0}/C_{A0}$, we obtain

$$-r_A = k_1 C_{A0}^2 \frac{(1 - X_A)(M - X_A)}{(1 + \varepsilon_A X_A)^2} - k_2 C_{A0} \frac{M' + X_A}{1 + \varepsilon_A X_A}$$

Hence, the design equation for plug flow, Eq. 17, becomes

$$\tau = C_{A0} \int_0^{X_{Af}} \frac{dX_A}{-r_A} = \int_0^{X_{Af}} \frac{(1 + \varepsilon_A X_A)^2 dX_A}{k_1 C_{A0}(1 - X_A)(M - X_A) - k_2(M' + X_A)(1 + \varepsilon_A X_A)}$$

In this expression $\varepsilon_A$ accounts for the stoichiometry and for inerts present in the feed.

**(b)** Equimolar feed of A and B. For $C_{A0} = C_{B0}$, $C_{R0} = 0$, and no inerts, we have $M = 1$, $M' = 0$, $\varepsilon_A = -0.5$; hence the expression for part a reduces to

$$\tau = \int_0^{X_{Af}} \frac{(1 - 0.5X_A)^2 \, dX_A}{k_1 C_{A0}(1 - X_A)^2 - k_2 X_A(1 - 0.5X_A)} \overset{\underset{\text{call}}{}}{\underset{\text{this}}{=}} \int_0^{X_{Af}} f(X_A) dX_A \qquad \textbf{(i)}$$

Having $V$, $v_0$, and $X_A$ data from a series of experiments, separately evaluate the left side and the right side of Eq. (i). For the right side, at various $X_A$



Eq. (i) predicts a
straight line
correlation

$t = V/v_0$
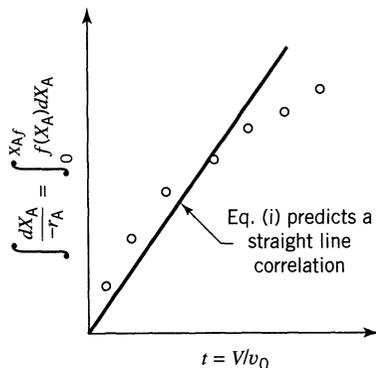
**Figure E5.6**

evaluate $f(X_A)$, then integrate graphically to give $\int f(X_A)dX_A$ and then make the plot of Fig. E5.6. If the data fall on a reasonably straight line, then the suggested kinetic scheme can be said to be satisfactory in that it fits the data. ∎

## Holding Time and Space Time for Flow Reactors

We should be clearly aware of the distinction between these two measures of time, $\bar{t}$ and $\tau$. They are defined as follows:

$$\tau = \begin{pmatrix} \text{time needed to} \\ \text{treat one reactor} \\ \text{volume of feed} \end{pmatrix} = \frac{V}{v_0} = \frac{C_{A0}V}{F_{A0}}, \quad [\text{hr}] \qquad \textbf{(6) or (8)}$$

$$\bar{t} = \begin{pmatrix} \text{mean residence time} \\ \text{of flowing material} \\ \text{in the reactor} \end{pmatrix} = C_{A0} \int_0^{X_A} \frac{dX_A}{(-r_A)(1 + \varepsilon_A X_A)}, \quad [\text{hr}] \qquad \textbf{(24)}$$

For constant density systems (all liquids and constant density gases)

$$\tau = \bar{t} = \frac{V}{v}$$

For changing density systems $\bar{t} \neq \tau$ and $\bar{t} \neq V/v_0$ in which case it becomes difficult to find how these terms are related.

As a simple illustration of the difference between $\bar{t}$ and $\tau$, consider two cases of the steady-flow popcorn popper of Problem 4.7 which takes in 1 liter/min of raw corn and produces 28 liters/min of product popcorn.

Consider three cases, called X, Y, and Z, which are shown in Fig. 5.7. In the first case (case X) all the popping occurs at the back end of the reactor. In the
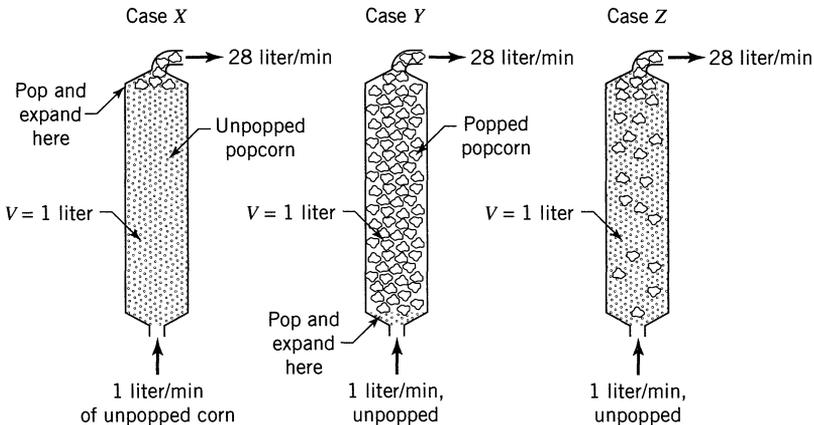


**Figure 5.7** For the same $\tau$ value the $\bar{t}$ values differ in these three cases.

second case (case Y) all the popping occurs at the front end of the reactor. In the third case (case Z) the popping occurs somewhere between entrance and exit. In all three cases

$$\tau_X = \tau_Y = \tau_Z = \frac{V}{v_0} = \frac{1 \text{ liter}}{1 \text{ liter/min}} = 1 \text{ min}$$

irrespective of where the popping occurs. However, we see that the residence time in the three cases is very different, or

$$\bar{t}_X = \frac{1 \text{ liter}}{1 \text{ liter/min}} = 1 \text{ min}$$

$$\bar{t}_Y = \frac{1 \text{ liter}}{28 \text{ liter/min}} \cong 2 \text{ sec}$$

$\bar{t}_Z$ is somewhere between 2 and 60 s, depending on the kinetics

Note that the value of $\bar{t}$ depends on what happens in the reactor, while the value of $\tau$ is independent of what happens in the reactor.

This example shows that $\bar{t}$ and $\tau$ are not, in general, identical. Now which is the natural performance measure for reactors? For batch systems Chapter 3 shows that it is the time of reaction; however, holding time does not appear anywhere in the performance equations for flow systems developed in this chapter, Eqs. 13 to 19, while it is seen that space-time or $V/F_{A0}$ does naturally appear. Hence, $\tau$ or $V/F_{A0}$ is the proper performance measure for flow systems.

The above simple example shows that in the special case of constant fluid density the space-time is equivalent to the holding time; hence, these terms can be used interchangeably. This special case includes practically all liquid phase reactions. However, for fluids of changing density, e.g., nonisothermal gas reactions or gas reactions with changing number of moles, a distinction should be made between $\tau$ and $\bar{t}$ and the correct measure should be used in each situation.

## Summary of Performance Equations

Tables 5.1 and 5.2 present the integrated performance equations for single ideal reactors.

### REFERENCES

Corcoran, W. H., and Lacey, W. N., *Introduction to Chemical Engineering Problems*, McGraw Hill, New York, 1970, p. 103.

Pease, R. N., *J. Am. Chem. Soc.*, **51,** 3470 (1929).

**Table 5.1 Performance Equations for $n$-order Kinetics and $\varepsilon_A = 0$**

| | Plug Flow or Batch | | Mixed Flow | |
|---|---|---|---|---|
| $n = 0$ <br> $-r_A = k$ | $k\tau = \dfrac{C_{A0} - C_A}{C_{A0}} = X_A$ | (20) | $\dfrac{k\tau}{C_{A0}} = \dfrac{C_{A0} - C_A}{C_{A0}} = X_A$ | |
| $n = 1$ <br> $-r_A = kC_A$ | $k\tau = \ln\dfrac{C_{A0}}{C_A} = \ln\dfrac{1}{1-X_A}$ | (3.12) | $k\tau = \dfrac{C_{A0} - C_A}{C_A} = \dfrac{X_A}{1 - X_A}$ | (14a) |
| $n = 2$ <br> $-r_A = kC_A^2$ | $k\tau C_{A0} = \dfrac{C_{A0} - C_A}{C_A} = \dfrac{X_A}{1-X_A}$ | (3.16) | $k\tau = \dfrac{(C_{A0} - C_A)}{C_A^2} = \dfrac{X_A}{C_{A0}(1 - X_A)^2}$ | (15) |
| any $n$ <br> $-r_A = kC_A^n$ | $(n-1)C_{A0}^{n-1}k\tau = \left(\dfrac{C_A}{C_{A0}}\right)^{1-n} - 1 = (1 - X_A)^{1-n} - 1$ | (3.29) | $k\tau = \dfrac{C_{A0} - C_A}{C_A^n} = \dfrac{X_A}{C_{A0}^{n-1}(1 - X_A)^n}$ | |
| $n = 1$ <br> $A \underset{2}{\overset{1}{\rightleftarrows}} R$ <br> $C_{R0} = 0$ | $k_1\tau = \left(1 - \dfrac{C_{Ae}}{C_{A0}}\right)\ln\left(\dfrac{C_{A0} - C_{Ae}}{C_A - C_{Ae}}\right) = X_{Ae}\ln\left(\dfrac{X_{Ae}}{X_{Ae} - X_A}\right)$ | (19) | $k_1\tau = \dfrac{(C_{A0} - C_A)(C_{A0} - C_{Ae})}{C_{A0}(C_A - C_{Ae})} = \dfrac{X_A X_{Ae}}{X_{Ae} - X_A}$ | |
| General rate | $\tau = \int_{C_A}^{C_{A0}} \dfrac{dC_A}{-r_A} = C_{A0}\int_0^{X_{Ae}} \dfrac{dX_A}{-r_A}$ | | $\tau = \dfrac{C_{A0} - C_A}{-r_{Af}} = \dfrac{C_{A0}X_A}{-r_{Af}}$ | (13) |

**Table 5.2** Performance Equations for $n$th-order Kinetics and $\varepsilon_A \neq 0$

| | Plug Flow | | Mixed Flow | |
|---|---|---|---|---|
| $n = 0$ <br> $-r_A = k$ | $\dfrac{k\tau}{C_{A0}} = X_A$ | (20) | $\dfrac{k\tau}{C_{A0}} = X_A$ | |
| $n = 1$ <br> $-r_A = kC_A$ | $k\tau = (1+\varepsilon_A)\ln\dfrac{1}{1-X_A} - \varepsilon_A X_A$ | (21) | $k\tau = \dfrac{X_A(1+\varepsilon_A X_A)}{1-X_A}$ | (14b) |
| $n = 2$ <br> $-r_A = kC_A^2$ | $k\tau C_{A0} = 2\varepsilon_A(1+\varepsilon_A)\ln(1-X_A) + \varepsilon_A^2 X_A + (\varepsilon_A+1)^2 \cdot \dfrac{X_A}{1-X_A}$ | (23) | $k\tau C_{A0} = \dfrac{X_A(1+\varepsilon_A X_A)^2}{(1-X_A)^2}$ | (15) |
| any $n$ <br> $-r_A = kC_A^n$ | | | $k\tau C_{A0}^{n-1} = \dfrac{X_A(1+\varepsilon_A X_A)^n}{(1-X_A)^n}$ | |
| $n = 1$ <br> $A \underset{2}{\overset{1}{\rightleftarrows}} rR$ <br> $C_{R0} = 0$ | $\dfrac{k\tau}{X_{Ae}} = (1+\varepsilon_A X_{Ae})\ln\dfrac{X_{Ae}}{X_{Ae}-X_A} - \varepsilon_A X_A$ | (22) | $\dfrac{k\tau}{X_{Ae}} = \dfrac{X_A(1+\varepsilon_A X_A)}{X_{Ae}-X_A}$ | |
| General expression | $\tau = C_{A0}\displaystyle\int_0^{X_A} \dfrac{dX_A}{-r_A}$ | (17) | $\tau = \dfrac{C_{A0}X_A}{-r_A}$ | (11) |

## PROBLEMS

**5.1.** Consider a gas-phase reaction $2A \rightarrow R + 2S$ with unknown kinetics. If a space velocity of 1/min is needed for 90% conversion of A in a plug flow reactor, find the corresponding space-time and mean residence time or holding time of fluid in the plug flow reactor.

**5.2.** In an isothermal batch reactor 70% of a liquid reactant is converted in 13 min. What space-time and space-velocity are needed to effect this conversion in a plug flow reactor and in a mixed flow reactor?

**5.3.** A stream of aqueous monomer A (1 mol/liter, 4 liter/min) enters a 2-liter mixed flow reactor, is radiated therein, and polymerizes as follows:

$$A \xrightarrow{+A} R \xrightarrow{+A} S \xrightarrow{+A} T \dots$$
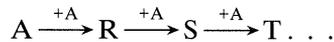
In the exit stream $C_A = 0.01$ mol/liter, and for a particular reaction product W, $C_W = 0.0002$ mol/liter. Find the rate of reaction of A and the rate of formation of W.

**5.4.** We plan to replace our present mixed flow reactor with one having double the volume. For the same aqueous feed (10 mol A/liter) and the same feed rate find the new conversion. The reaction kinetics are represented by

$$A \rightarrow R, \quad -r_A = kC_A^{1.5}$$
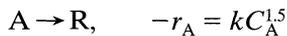
and present conversion is 70%.

**5.5.** An aqueous feed of A and B (400 liter/min, 100 mmol A/liter, 200 mmol B/liter) is to be converted to product in a plug flow reactor. The kinetics of the reaction is represented by

$$A + B \rightarrow R, \quad -r_A = 200 \, C_A C_B \frac{\text{mol}}{\text{liter} \cdot \text{min}}$$
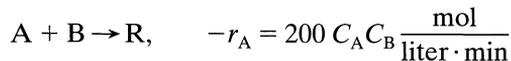
Find the volume of reactor needed for 99.9% conversion of A to product.

**5.6.** A plug flow reactor (2 m³) processes an aqueous feed (100 liter/min) containing reactant A ($C_{A0} = 100$ mmol/liter). This reaction is reversible and represented by

$$A \rightleftharpoons R, \quad -r_A = (0.04 \, \text{min}^{-1})C_A - (0.01 \, \text{min}^{-1})C_R$$
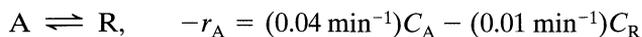
First find the equilibrium conversion and then find the actual conversion of A in the reactor.

**5.7.** The off gas from a boiling water nuclear power reactor contains a whole variety of radioactive trash, one of the most troublesome being Xe-133 (half life = 5.2 days). This off gas flows continuously through a large holdup tank in which its mean residence time is 30 days, and where we can assume that the contents are well mixed. Find the fraction of activity removed in the tank.

**5.8.** A mixed flow reactor (2 m³) processes an aqueous feed (100 liter/min) containing reactant A ($C_{A0}$ = 100 mmol/liter). The reaction is reversible and represented by

$$A \rightleftharpoons R, \quad -r_A = 0.04\, C_A - 0.01\, C_R \; \frac{\text{mol}}{\text{liter} \cdot \text{min}}$$
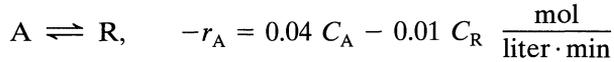
What is the equilibrium conversion and the actual conversion in the reactor?

**5.9.** A specific enzyme acts as catalyst in the fermentation of reactant A. At a given enzyme concentration in the aqueous feed stream (25 liter/min) find the volume of plug flow reactor needed for 95% conversion of reactant A ($C_{A0}$ = 2 mol/liter). The kinetics of the fermentation at this enzyme concentration is given by

$$A \xrightarrow{\text{enzyme}} R, \quad -r_A = \frac{0.1\, C_A}{1 + 0.5\, C_A} \; \frac{\text{mol}}{\text{liter} \cdot \text{min}}$$
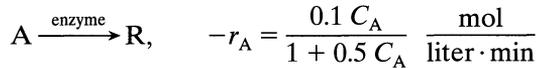
**5.10.** A gaseous feed of pure A (2 mol/liter, 100 mol/min) decomposes to give a variety of products in a plug flow reactor. The kinetics of the conversion is represented by

$$A \rightarrow 2.5 \,(\text{products}), \quad -r_A = (10\,\text{min}^{-1})C_A$$

Find the expected conversion in a 22-liter reactor.

**5.11.** Enzyme E catalyses the fermentation of substrate A (the reactant) to product R. Find the size of mixed flow reactor needed for 95% conversion of reactant in a feed stream (25 liter/min) of reactant (2 mol/liter) and enzyme. The kinetics of the fermentation at this enzyme concentration are given by

$$A \xrightarrow{\text{enzyme}} R, \quad -r_A = \frac{0.1\, C_A}{1 + 0.5\, C_A} \; \frac{\text{mol}}{\text{liter} \cdot \text{min}}$$
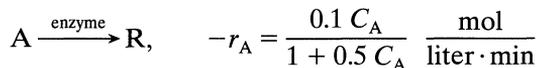
**5.12.** An aqueous feed of A and B (400 liter/min, 100 mmol A/liter, 200 mmol B/liter) is to be converted to product in a mixed flow reactor. The kinetics

of the reaction are represented by

$$A + B \rightarrow R, \qquad -r_A = 200\, C_A C_B \; \frac{\text{mol}}{\text{liter} \cdot \text{min}}$$
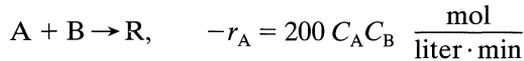
Find the volume of reactor needed for 99.9% conversion of A to product.

**5.13.** At 650°C phosphine vapor decomposes as follows:

$$4PH_3 \rightarrow P_4(g) + 6H_2, \qquad -r_{\text{phos}} = (10\ \text{hr}^{-1})C_{\text{phos}}$$

What size of plug flow reactor operating at 649°C and 11.4 atm is needed for 75% conversion of 10 mol/hr of phosphine in a 2/3 phosphine–1/3 inert feed?

**5.14.** A stream of pure gaseous reactant A ($C_{A0}$ = 660 mmol/liter) enters a plug flow reactor at a flow rate of $F_{A0}$ = 540 mmol/min and polymerizes there as follows

$$3A \rightarrow R, \qquad -r_A = 54\ \frac{\text{mmol}}{\text{liter} \cdot \text{min}}$$
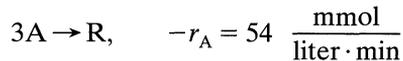
How large a reactor is needed to lower the concentration of A in the exit stream to $C_{Af}$ = 330 mmol/liter?

**5.15.** A gaseous feed of pure A (1 mol/liter) enters a mixed flow reactor (2 liters) and reacts as follows:

$$2A \rightarrow R, \qquad -r_A = 0.05\, C_A^2 \; \frac{\text{mol}}{\text{liter} \cdot \text{sec}}$$
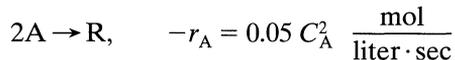
Find what feed rate (liter/min) will give an outlet concentration $C_A$ = 0.5 mol/liter.

**5.16.** Gaseous reactant A decomposes as follows:

$$A \rightarrow 3R, \qquad -r_A = (0.6\ \text{min}^{-1})C_A$$

Find the conversion of A in a 50% A–50% inert feed ($v_0$ = 180 liter/min, $C_{A0}$ = 300 mmol/liter) to a 1 m³ mixed flow reactor.

**5.17.** 1 liter/s of a 20% ozone–80% air mixture at 1.5 atm and 93°C passes through a plug flow reactor. Under these conditions ozone decomposes by homogeneous reaction

$$2O_3 \rightarrow 3O_2, \qquad -r_{\text{ozone}} = kC_{\text{ozone}}^2, \qquad k = 0.05\ \frac{\text{liter}}{\text{mol} \cdot \text{s}}$$
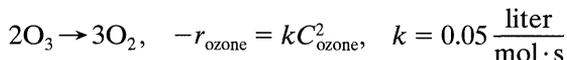
What size reactor is needed for 50% decomposition of ozone? This problem is a modification of a problem given by Corcoran and Lacey (1970).

**5.18.** An aqueous feed containing A (1 mol/liter) enters a 2-liter plug flow reactor and reacts away ($2A \rightarrow R$, $-r_A = 0.05\,C_A^2$ mol/liter · s). Find the outlet concentration of A for a feed rate of 0.5 liter/min.

**5.19.** Pure gaseous A at about 3 atm and 30°C (120 mmol/liter) is fed into a 1-liter mixed flow reactor at various flow rates. There it decomposes, and the exit concentration of A is measured for each flow rate. From the following data find a rate equation to represent the kinetics of the decomposition of A. Assume that reactant A alone affects the rate.

| $v_0$, liter/min | 0.06 | 0.48 | 1.5 | 8.1 | $A \rightarrow 3R$ |
|---|---|---|---|---|---|
| $C_A$, mmol/liter | 30 | 60 | 80 | 105 | |

**5.20.** A mixed flow reactor is being used to determine the kinetics of a reaction whose stoichiometry is $A \rightarrow R$. For this purpose various flow rates of an aqueous solution of 100 mmol A/liter are fed to a 1-liter reactor, and for each run the outlet concentration of A is measured. Find a rate equation to represent the following data. Also assume that reactant alone affects the rate.

| $v$, liter/min | 1 | 6 | 24 |
|---|---|---|---|
| $C_A$, mmol/liter | 4 | 20 | 50 |

**5.21.** We are planning to operate a batch reactor to convert A into R. This is a liquid reaction, the stoichiometry is $A \rightarrow R$, and the rate of reaction is given in Table P5.21. How long must we react each batch for the concentration to drop from $C_{A0} = 1.3$ mol/liter to $C_{Af} = 0.3$ mol/liter?

**Table P5.21**

| $C_A$, mol/liter | $-r_A$, mol/liter · min |
|---|---|
| 0.1 | 0.1 |
| 0.2 | 0.3 |
| 0.3 | 0.5 |
| 0.4 | 0.6 |
| 0.5 | 0.5 |
| 0.6 | 0.25 |
| 0.7 | 0.10 |
| 0.8 | 0.06 |
| 1.0 | 0.05 |
| 1.3 | 0.045 |
| 2.0 | 0.042 |

**5.22.** For the reaction of Problem 5.21, what size of plug flow reactor would be needed for 80% conversion of a feed stream of 1000 mol A/hr at $C_{A0} = 1.5$ mol/liter?

**5.23. (a)** For the reaction of Problem 5.21, what size of mixed flow reactor is needed for 75% conversion of a feed stream of 1000 mol A/hr at $C_{A0}$ = 1.2 mol/liter?

**(b)** Repeat part (a) with the modification that the feed rate is doubled, thus 2000 mol A/hr at $C_{A0}$ = 1.2 mol/liter are to be treated.

**(c)** Repeat part (a) with the modification that $C_{A0}$ = 2.4 mol/liter; however, 1000 mol A/hr are still to be treated down to $C_{Af}$ = 0.3 mol/liter.

**5.24.** A high molecular weight hydrocarbon gas A is fed continuously to a heated high temperature mixed flow reactor where it thermally cracks (homogeneous gas reaction) into lower molecular weight materials, collectively called R, by a stoichiometry approximated by A → 5R. By changing the feed rate different extents of cracking are obtained as follows:

| $F_{A0}$, millimol/hr | 300 | 1000 | 3000 | 5000 |
|---|---|---|---|---|
| $C_{A,out}$, millimol/liter | 16 | 30 | 50 | 60 |

The internal void volume of the reactor is $V$ = 0.1 liter, and at the temperature of the reactor the feed concentration is $C_{A0}$ = 100 millimol/liter. Find a rate equation to represent the cracking reaction.

**5.25.** The aqueous decomposition of A is studied in an experimental mixed flow reactor. The results in Table P5.25 are obtained in steady-state runs. To obtain 75% conversion of reactant in a feed, $C_{A0}$ = 0.8 mol/liter, what holding time is needed in a plug flow reactor?

**Table P5.25**

| Concentration of A, mol/liter | | Holding Time, sec |
|---|---|---|
| In Feed | In Exit Stream | |
| 2.00 | 0.65 | 300 |
| 2.00 | 0.92 | 240 |
| 2.00 | 1.00 | 250 |
| 1.00 | 0.56 | 110 |
| 1.00 | 0.37 | 360 |
| 0.48 | 0.42 | 24 |
| 0.48 | 0.28 | 200 |
| 0.48 | 0.20 | 560 |

**5.26.** Repeat the previous problem but for a mixed flow reactor.

**5.27.** HOLMES: You say he was last seen tending this vat . . . .

SIR BOSS: You mean "overflow stirred tank reactor," Mr. Holmes.

HOLMES: You must excuse my ignorance of your particular technical jargon, Sir Boss.

SIR BOSS: That's all right; however, you must find him, Mr. Holmes.

Imbibit was a queer chap; always staring into the reactor, taking deep breaths, and licking his lips, but he was our very best operator. Why, since he left, our conversion of googliox has dropped from 80% to 75%.

HOLMES (*tapping the side of the vat idly*): By the way, what goes on in the vat?

SIR BOSS: Just an elementary second-order reaction, between ethanol and googliox, if you know what I mean. Of course, we maintain a large excess of alcohol, about 100 to 1 and ....

HOLMES (*interrupting*): Intriguing, we checked every possible lead in town and found not a single clue.

SIR BOSS (*wiping away the tears*): We'll give the old chap a raise—about twopence per week—if only he'll come back.

DR. WATSON: Pardon me, but may I ask a question?

HOLMES: Why certainly, Watson.

WATSON: What is the capacity of this vat, Sir Boss?

SIR BOSS: A hundred Imperial gallons, and we always keep it filled to the brim. That is why we call it an overflow reactor. You see we are running at full capacity—profitable operation you know.

HOLMES: Well, my dear Watson, we must admit that we're stumped, for without clues deductive powers are of no avail.

WATSON: Ahh, but there is where you are wrong, Holmes. (*Then, turning to the manager*): Imbibit was a largish fellow—say about 18 stone—was he not?

SIR BOSS: Why yes, how did you know?

HOLMES (*with awe*): Amazing, my dear Watson!

WATSON (*modestly*): Why it's quite elementary, Holmes. We have all the clues necessary to deduce what happened to the happy fellow. But first of all, would someone fetch me some dill?

With Sherlock Holmes and Sir Boss impatiently waiting, Dr. Watson casually leaned against the vat, slowly and carefully filled his pipe, and—with the keen sense of the dramatic—lit it. There our story ends.

(a) What momentous revelation was Dr. Watson planning to make, and how did he arrive at this conclusion?

(b) Why did he never make it?

**5.28.** The data in Table P5.28 have been obtained on the decomposition of gaseous reactant A in a constant volume batch reactor at 100°C. The

**Table P5.28**

| $t$, sec | $p_A$, atm | $t$, sec | $p_A$, atm |
|---|---|---|---|
| 0 | 1.00 | 140 | 0.25 |
| 20 | 0.80 | 200 | 0.14 |
| 40 | 0.68 | 260 | 0.08 |
| 60 | 0.56 | 330 | 0.04 |
| 80 | 0.45 | 420 | 0.02 |
| 100 | 0.37 | | |

stoichiometry of the reaction is $2A \rightarrow R + S$. What size plug flow reactor (in liters) operating at 100°C and 1 atm can treat 100 mol A/hr in a feed consisting of 20% inerts to obtain 95% converson of A?

**5.29.** Repeat the previous problem for a mixed flow reactor.

**5.30.** The aqueous decomposition of A produces R as follows:

$$A \rightleftharpoons R$$
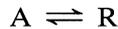
The following results are obtained in a series of steady state runs, all having no R in the feed stream.

| Space Time, $\tau$, sec | $C_{A0}$, In Feed, mol/liter | $C_{Af}$, In Exit Stream, mol/liter |
|---|---|---|
| 50 | 2.0 | 1.00 |
| 16 | 1.2 | 0.80 |
| 60 | 2.0 | 0.65 |
| 22 | 1.0 | 0.56 |
| 4.8 | 0.48 | 0.42 |
| 72 | 1.00 | 0.37 |
| 40 | 0.48 | 0.28 |
| 112 | 0.48 | 0.20 |

From this kinetic information, find the size of reactor needed to achieve 75% conversion of a feed stream of $v = 1$ liter/sec and $C_{A0} = 0.8$ mol/liter. In the reactor the fluid follows
**(a)** plug flow
**(b)** mixed flow