

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.

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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.

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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

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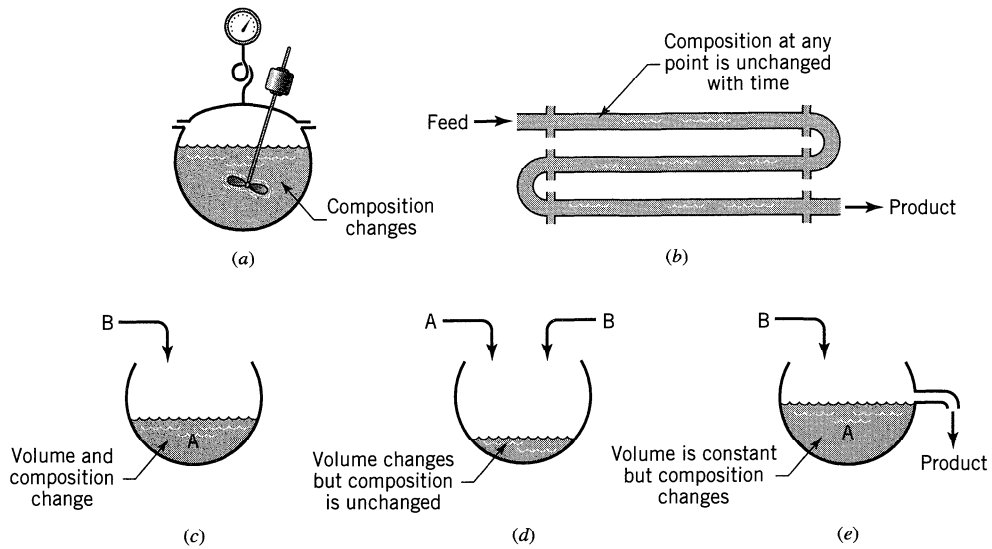


Figure 4.1 Broad classification of reactor types. (a) The batch reactor. (b) The steady-state flow reactor. (c), (d), and (e) Various forms of the semibatch reactor.

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

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

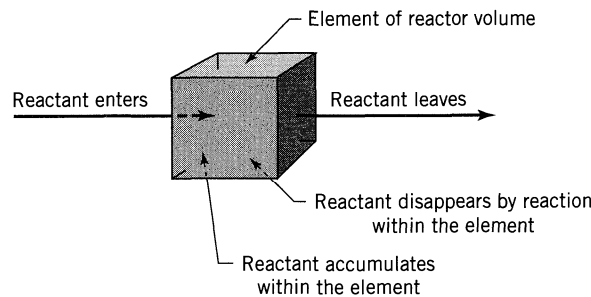


Figure 4.2 Material balance for an element of volume of the reactor.

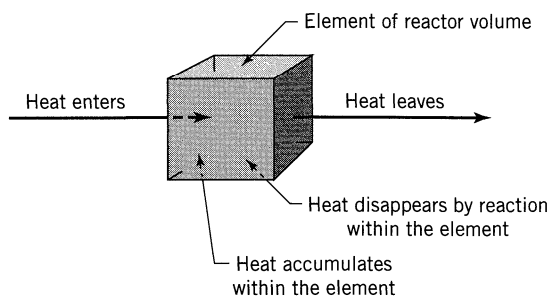


Figure 4.3 Energy balance for an element of volume of the reactor.

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

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

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.

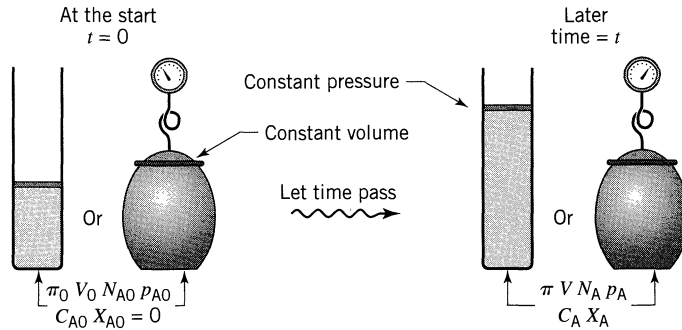


Figure 4.4 Symbols used for batch reactors.

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:

$$\left. \begin{aligned} X_A &= 1 - \frac{C_A}{C_{A0}} \quad \text{and} \quad dX_A = -\frac{dC_A}{C_{A0}} \\ \frac{C_A}{C_{A0}} &= 1 - X_A \quad \text{and} \quad dC_A = -C_{A0}dX_A \end{aligned} \right\} \text{for } \varepsilon_A = \frac{V_{X_A=1} - V_{X_A=0}}{V_{X_A=0}} = 0 \quad (3)$$

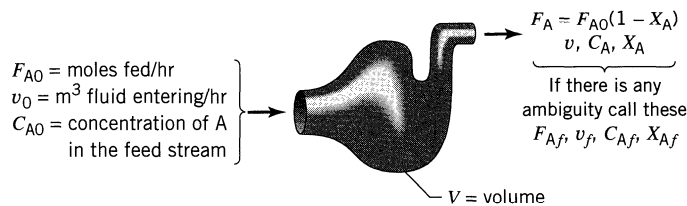


Figure 4.5 Symbols used for flow reactors.

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

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

Special Case 2. Batch and Flow Systems of Gases of Changing Density but with T and π 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 $V = V_0(1 + \varepsilon_A X_A)$.

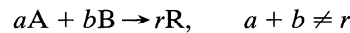
$$\left. \begin{aligned} X_A &= \frac{C_{A0} - C_A}{C_{A0} + \varepsilon_A C_A} & \text{and} & \quad dX_A = -\frac{C_{A0}(1 + \varepsilon_A)}{(C_{A0} + \varepsilon_A C_A)^2} dC_A \\ \frac{C_A}{C_{A0}} &= \frac{1 - X_A}{1 + \varepsilon_A X_A} & \text{and} & \quad \frac{dC_A}{C_{A0}} = -\frac{1 + \varepsilon_A}{(1 + \varepsilon_A X_A)^2} dX_A \end{aligned} \right\} \text{for}$$

$$\varepsilon_A = \frac{V_{X_A=1} - V_{X_A=0}}{V_{X_A=0}} \neq 0 \quad (5)$$

To follow changes in the other components we have

$$\text{between} \begin{cases} \varepsilon_A X_A = \varepsilon_B X_B \\ \frac{a\varepsilon_A}{C_{A0}} = \frac{b\varepsilon_B}{C_{B0}} \end{cases} \quad \text{for products} \begin{cases} \frac{C_R}{C_{A0}} = \frac{(r/a)X_A + C_{R0}/C_{A0}}{1 + \varepsilon_A X_A} \\ \frac{C_I}{C_{I0}} = \frac{1}{1 + \varepsilon_A X_A} \end{cases} \quad (6)$$

Special Case 3. Batch and Flow Systems for Gases in General (varying ρ , T , π) which react according to



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,

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

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

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

For high-pressure nonideal gas behavior replace $\left(\frac{T_0\pi}{\pi_0\pi_0}\right)$ by $\left(\frac{z_0T_0\pi}{zT\pi}\right)$, where z is the compressibility factor. To change to another key reactant, say B, note that

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

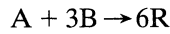
For liquids or isothermal gases with no change pressure and density

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

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



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).

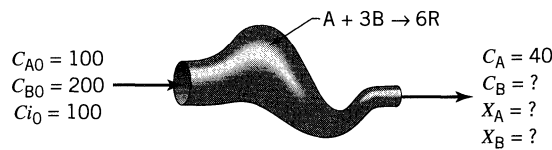


Figure E4.1

Next recognize that this problem concerns Special Case 2. So evaluate ε_A and ε_B . For this take 400 volumes of gas

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

لو فرضنا ان كل المادة A تفاعلت اذا نحتاج الى 300 من B لكن نحن لدينا 200 فقط في المتفاعلات اذا النقص 100 من B

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 π_0 , reacts there, and leaves at T and π .

- 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.