

University of Anbar

College of Engineering

**Chemical and Petrochemical Engineering
Department**

Chemical Reaciior Design

Third Year

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Lecture No.6

Introduction to Reactor Design:

In reactor design, we want to know what size and type of reactor and method of operation are best for a given job. 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.

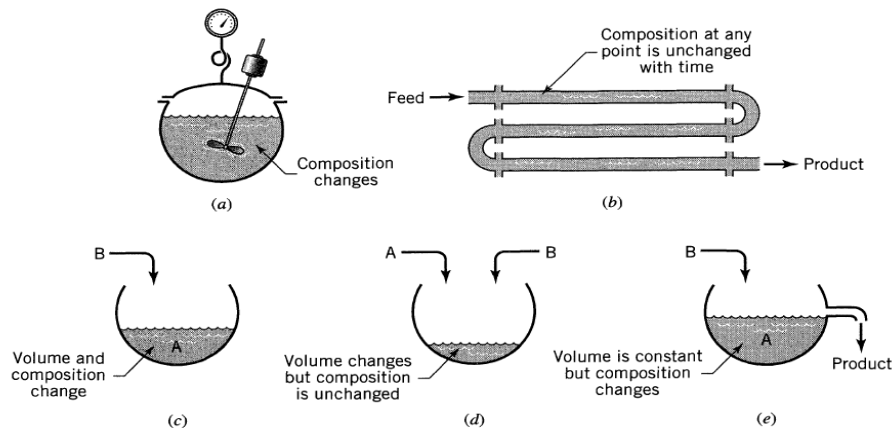


Figure 4.1 Broad classification of reactor types. (a) The batch reactor. (b) The steady-state flow reactor. (c), (d), and (e) Various forms of the semibatch reactor.

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

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

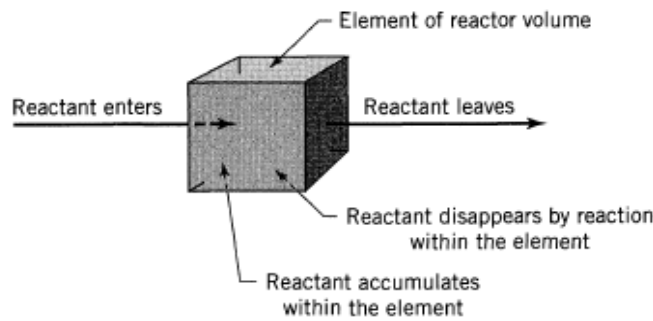


Figure 4.2 Material balance for an element of volume of the reactor.

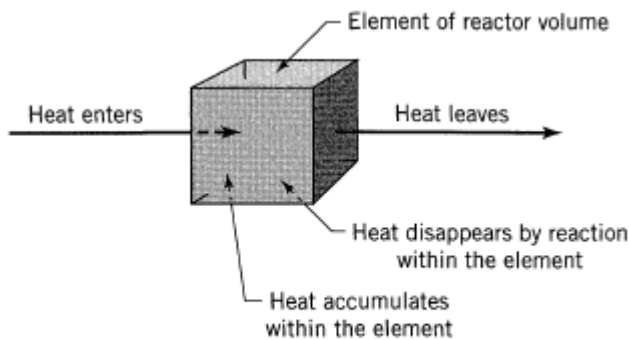


Figure 4.3 Energy balance for an element of volume of the reactor.

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

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

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:

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

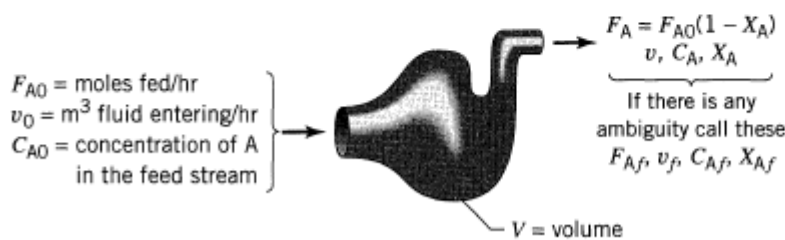


Figure 4.5 Symbols used for flow reactors.

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 $V = V_0(1 + \epsilon_A X_A)$.

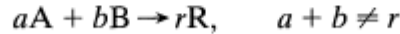
$$\left. \begin{aligned} X_A &= \frac{C_{A0} - C_A}{C_{A0} + \epsilon_A C_A} \quad \text{and} \quad dX_A = -\frac{C_{A0}(1 + \epsilon_A)}{(C_{A0} + \epsilon_A C_A)^2} dC_A \\ \frac{C_A}{C_{A0}} &= \frac{1 - X_A}{1 + \epsilon_A X_A} \quad \text{and} \quad \frac{dC_A}{C_{A0}} = -\frac{1 + \epsilon_A}{(1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

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

To follow changes in the other components we have

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

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 $\left(\frac{T_0\pi}{T\pi_0} \right)$ by $\left(\frac{z_0 T_0\pi}{z T\pi} \right)$, where z is the compressibility factor. To change to another key reactant, say B, note that

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

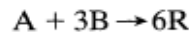
For liquids or isothermal gases with no change pressure and density

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

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).

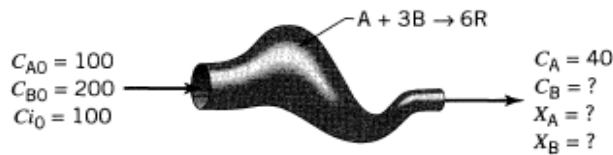


Figure E4.1

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

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

Then from the equations in the text

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

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

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

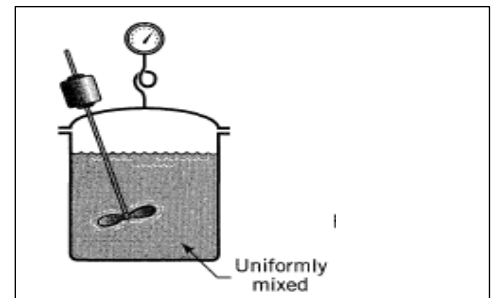
$$C_B = C_{B0} \left(\frac{1 - X_B}{1 + \epsilon_B X_B} \right) = \frac{200(1 - 0.75)}{1 + (1/3)(0.75)} = \underline{\underline{40}}$$

1. Ideal Reactors for a Single Reaction:

A. IDEAL BATCH REACTOR:

Make a material balance for any component A

$$\begin{array}{c} = 0 \quad = 0 \\ \swarrow \quad \searrow \\ \text{input} = \text{output} + \text{disappearance} + \text{accumulation} \end{array}$$



or

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

Evaluating the terms of Eq. 1, we find

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

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

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

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

Rearranging and integrating then gives

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

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

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

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

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

In one form or another, Eqs. 2 to 5 they are applicable to both isothermal and nonisothermal operations.

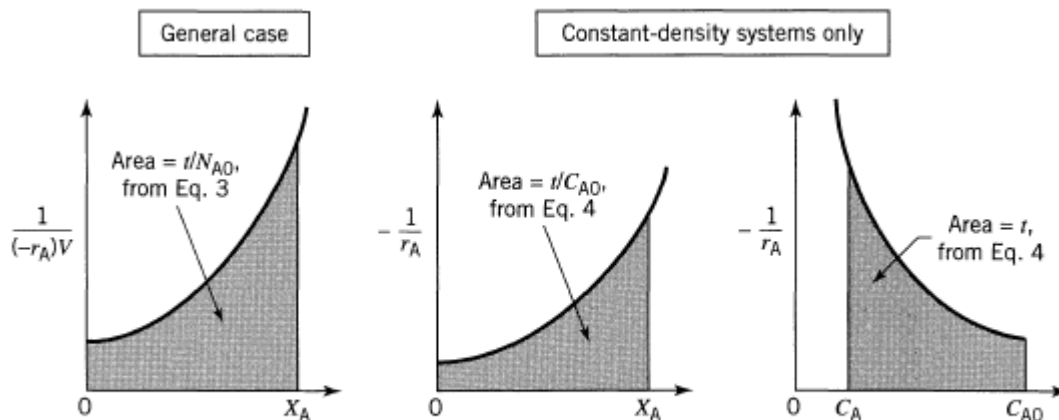


Figure 5.2 Graphical representation of the performance equations for batch reactors, isothermal or nonisothermal.

Space-Time and Space-Velocity

Space-time:

$$\tau = \frac{1}{s} = \left(\frac{\text{time required to process one}}{\text{reactor volume of feed measured}} \right) = [\text{time}] \quad (6)$$

Space-velocity:

$$s = \frac{1}{\tau} = \left(\frac{\text{number of reactor volumes of}}{\text{feed at specified conditions which}} \right) = [\text{time}^{-1}] \quad (7)$$

If they are of the stream entering the reactor, the relation between s and τ and the other pertinent variables is

$$\begin{aligned} \tau = \frac{1}{s} &= \frac{C_{A0}V}{F_{A0}} = \frac{\left(\frac{\text{moles A entering}}{\text{volume of feed}} \right) (\text{volume of reactor})}{\left(\frac{\text{moles A entering}}{\text{time}} \right)} \quad (8) \\ &= \frac{V}{v_0} = \frac{(\text{reactor volume})}{(\text{volumetric feed rate})} \end{aligned}$$