

Conversion 2 and Reactor Sizing

Be more concerned with your character than with your reputation, because character is what you really are while reputation is merely what others think you are.

John Wooden, coach, UCLA Bruins

Overview. In the first chapter, the general mole balance equation was derived and then applied to the four most common types of industrial reactors. A balance equation was developed for each reactor type and these equations are summarized in Table S-1. In Chapter 2, we will evaluate these equations to size CSTRs and PFRs. To size these reactors we first define conversion, which is a measure of the reaction's progress toward completion, and then rewrite all the balance equations in terms of conversion. These equations are often referred to as the design equations. Next, we show how one may size a reactor (i.e., determine the reactor volume necessary to achieve a specified conversion) once the relationship between the reaction rate, $-r_A$, and conversion, X , is known. In addition to being able to size CSTRs and PFRs once given $-r_A = f(X)$, another goal of this chapter is to compare CSTRs and PFRs and the overall conversions for reactors arranged in series. It is also important to arrive at the best arrangement of reactors in series.

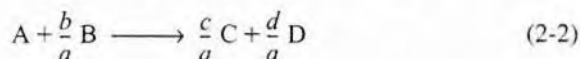
After completing this chapter you will be able to size CSTRs and PFRs given the rate of reaction as a function of conversion and to calculate the overall conversion and reactor volumes for reactors arranged in series.

2.1 Definition of Conversion

In defining conversion, we choose one of the reactants as the basis of calculation and then relate the other species involved in the reaction to this basis. In virtually all instances it is best to choose the limiting reactant as the basis of calculation. We develop the stoichiometric relationships and design equations by considering the general reaction



The uppercase letters represent chemical species and the lowercase letters represent stoichiometric coefficients. Taking species A as our *basis of calculation*, we divide the reaction expression through by the stoichiometric coefficient of species A, in order to arrange the reaction expression in the form



to put every quantity on a "per mole of A" basis, our limiting reactant.

Now we ask such questions as "How can we quantify how far a reaction [e.g., Equation (2-2)] proceeds to the right?" or "How many moles of C are formed for every mole A consumed?" A convenient way to answer these questions is to define a parameter called *conversion*. The conversion X_A is the number of moles of A that have reacted per mole of A fed to the system:

Definition of X

$$X_A = \frac{\text{Moles of A reacted}}{\text{Moles of A fed}}$$

Because we are defining conversion with respect to our basis of calculation [A in Equation (2-2)], we eliminate the subscript A for the sake of brevity and let $X \equiv X_A$. For irreversible reactions, the maximum conversion is 1.0, i.e., complete conversion. For reversible reactions, the maximum conversion is the equilibrium conversion X_e (i.e., $X_{\max} = X_e$).

2.2 Batch Reactor Design Equations

In most batch reactors, the longer a reactant stays in the reactor, the more the reactant is converted to product until either equilibrium is reached or the reactant is exhausted. Consequently, in batch systems the conversion X is a function of the time the reactants spend in the reactor. If N_{A0} is the number of moles of A initially in the reactor, then the total number of moles of A that have reacted after a time t is $[N_{A0}X]$

$$\begin{aligned} \left[\begin{array}{l} \text{Moles of A reacted (consumed)} \end{array} \right] &= \left[\begin{array}{l} \text{Moles of A fed} \end{array} \right] \cdot \left[\frac{\text{Moles of A reacted}}{\text{Moles of A fed}} \right] \\ \left[\begin{array}{l} \text{Moles of A} \\ \text{reacted} \\ \text{(consumed)} \end{array} \right] &= [N_{A0}] \cdot [X] \end{aligned} \quad (2-3)$$

Now, the number of moles of A that remain in the reactor after a time t , N_A , can be expressed in terms of N_{A0} and X :

$$\left[\begin{array}{c} \text{Moles of A} \\ \text{in reactor} \\ \text{at time } t \end{array} \right] = \left[\begin{array}{c} \text{Moles of A} \\ \text{initially fed} \\ \text{to reactor at} \\ t = 0 \end{array} \right] - \left[\begin{array}{c} \text{Moles of A that} \\ \text{have been con-} \\ \text{sumed by chemical} \\ \text{reaction} \end{array} \right]$$

$$[N_A] = [N_{A0}] - [N_{A0}X]$$

The number of moles of A in the reactor after a conversion X has been achieved is

$$N_A = N_{A0} - N_{A0}X = N_{A0}(1 - X) \quad (2-4)$$

When no spatial variations in reaction rate exist, the mole balance on species A for a batch system is given by the following equation [cf. Equation (1-5)]:

$$\frac{dN_A}{dt} = r_A V \quad (2-5)$$

This equation is valid whether or not the reactor volume is constant. In the general reaction, Equation (2-2), reactant A is disappearing; therefore, we multiply both sides of Equation (2-5) by -1 to obtain the mole balance for the batch reactor in the form

$$-\frac{dN_A}{dt} = (-r_A)V$$

The rate of disappearance of A, $-r_A$, in this reaction might be given by a rate law similar to Equation (1-2), such as $-r_A = kC_A C_B$.

For batch reactors, we are interested in determining how long to leave the reactants in the reactor to achieve a certain conversion X . To determine this length of time, we write the mole balance, Equation (2-5), in terms of conversion by differentiating Equation (2-4) with respect to time, remembering that N_{A0} is the number of moles of A initially present and is therefore a constant with respect to time.

$$\frac{dN_A}{dt} = 0 - N_{A0} \frac{dX}{dt}$$

Combining the above with Equation (2-5) yields

$$-N_{A0} \frac{dX}{dt} = r_A V$$

For a batch reactor, the design equation in differential form is

$$\left[N_{A0} \frac{dX}{dt} = -r_A V \right] \quad (2-6)$$

We call Equation (2-6) the differential form of the **design equation** for batch reactor because we have written the mole balance in terms of conversion. The differential forms of the batch reactor mole balances, Equations (2-5) and (2-6), are often used in the interpretation of reaction rate data (Chapter 5) and for reactors with heat effects (Chapter 9), respectively. Batch reactors are frequently used in industry for both gas-phase and liquid-phase reactions. The laboratory bomb calorimeter reactor is widely used for obtaining reaction rate data (see Section 9.3). Liquid-phase reactions are frequently carried out in batch reactors when small-scale production is desired or operating difficulties rule out the use of continuous flow systems.

For a constant-volume batch reactor, $V = V_0$, Equation (2-5) can be arranged into the form

$$\frac{1}{V_0} \frac{dN_A}{dt} = \frac{d(N_A/V_0)}{dt} = \frac{dC_A}{dt} \quad (2-7)$$

Constant-volume
batch reactor

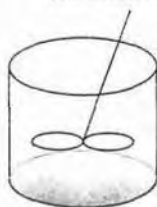
$$\frac{dC_A}{dt} = r_A$$

As previously mentioned, the differential form of the mole balance, e.g., Equation (2-7), is used for analyzing rate data in a batch reactor as we will see in Chapters 5 and 9.

To determine the time to achieve a specified conversion X , we first separate the variables in Equation (2-6) as follows

$$dt = N_{A0} \frac{dX}{-r_A V} \quad (2-8)$$

Batch time t
to achieve a
conversion X



Batch
Design
Equation

This equation is now integrated with the limits that the reaction begins at time equal zero where there is no conversion initially (i.e., $t = 0$, $X = 0$). Carrying out the integration, we obtain the time t necessary to achieve a conversion X in a batch reactor

$$t = N_{A0} \int_0^X \frac{dX}{-r_A V} \quad (2-9)$$

The longer the reactants are left in the reactor, the greater will be the conversion. Equation (2-6) is the differential form of the design equation, and Equation (2-9) is the integral form of the design equation for a batch reactor.

2.3 Design Equations for Flow Reactors

For a batch reactor, we saw that conversion increases with time spent in the reactor. For continuous-flow systems, this time usually increases with increasing

reactor volume, e.g., the bigger/longer the reactor, the more time it will take the reactants to flow completely through the reactor and thus, the more time to react. Consequently, the conversion X is a function of reactor volume V . If F_{A0} is the molar flow rate of species A fed to a system operated at steady state, the molar rate at which species A is reacting *within* the entire system will be $F_{A0}X$.

$$[F_{A0}] \cdot [X] = \frac{\text{Moles of A fed}}{\text{time}} \cdot \frac{\text{Moles of A reacted}}{\text{Mole of A fed}}$$

$$[F_{A0} \cdot X] = \frac{\text{Moles of A reacted}}{\text{time}}$$

The molar feed rate of A to the system *minus* the rate of reaction of A within the system *equals* the molar flow rate of A leaving the system F_A . The preceding sentence can be written in the form of the following mathematical statement:

$$\left[\begin{array}{c} \text{Molar flow rate} \\ \text{at which A is} \\ \text{fed to the system} \end{array} \right] - \left[\begin{array}{c} \text{Molar rate at} \\ \text{which A is} \\ \text{consumed within} \\ \text{the system} \end{array} \right] = \left[\begin{array}{c} \text{Molar flow rate} \\ \text{at which A leaves} \\ \text{the system} \end{array} \right]$$

$$[F_{A0}] - [F_{A0}X] = [F_A]$$

Rearranging gives

$$\boxed{F_A = F_{A0}(1 - X)} \quad (2-10)$$

The entering molar flow rate of species A, F_{A0} (mol/s), is just the product of the entering concentration, C_{A0} (mol/dm³), and the entering volumetric flow rate, v_0 (dm³/s):

Liquid phase

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

For liquid systems, C_{A0} is commonly given in terms of molarity, for example,

$$C_{A0} = 2 \text{ mol/dm}^3$$

For gas systems, C_{A0} can be calculated from the entering temperature and pressure using the ideal gas law or some other gas law. For an ideal gas (see Appendix B):

Gas phase

$$C_{A0} = \frac{P_{A0}}{RT_0} = \frac{y_{A0}P_0}{RT_0}$$

The entering molar flow rate is

$$F_{A0} = v_0 C_{A0} = v_0 \frac{y_{A0} P_0}{RT_0}$$

where C_{A0} = entering concentration, mol/dm³

y_{A0} = entering mole fraction of A

P_0 = entering total pressure, e.g., kPa

$P_{A0} = y_{A0} P_0$ = entering partial pressure of A, e.g., kPa

T_0 = entering temperature, K

R = ideal gas constant (e.g., $R = 8.314 \frac{\text{kPa} \cdot \text{dm}^3}{\text{mol} \cdot \text{K}}$; see Appendix B)

The size of the reactor will depend on the flow rate, reaction kinetics, reactor conditions, and desired conversion. Let's first calculate the entering molar flow rate.

Example 2-1 Using the Ideal Gas Law to Calculate C_{A0} and F_{A0}

A gas of pure A at 830 kPa (8.2 atm) enters a reactor with a volumetric flow rate, v_0 , of 2 dm³/s at 500 K. Calculate the entering concentration of A, C_{A0} , and the entering molar flow rate, F_{A0} .

Solution

We again recall that for an ideal gas:

$$C_{A0} = \frac{P_{A0}}{RT_0} = \frac{y_{A0} P_0}{RT_0} \quad (\text{E2-1.1})$$

where $P_0 = 830$ kPa (8.2 atm)

$y_{A0} = 1.0$ (Pure A)

$T_0 =$ initial temperature = 500K

$R = 8.314$ dm³ · kPa/mol · K (Appendix B)

Substituting the given parameter values into Equation (E2-1.1) yields

$$C_{A0} = \frac{(1)(830 \text{ kPa})}{(8.314 \text{ dm}^3 \cdot \text{kPa/mol} \cdot \text{K})(500\text{K})} = 0.20 \frac{\text{mol}}{\text{dm}^3}$$

We could also solve for the partial pressure in terms of the concentration:

$$P_{A0} = C_{A0} RT_0 \quad (\text{E2-1.2})$$

However, since pure A enters, the total pressure and partial pressure entering are the same. The entering molar flow rate, F_{A0} , is just the product of the entering concentration, C_{A0} , and the entering volumetric flow rate, v_0 :

$$F_{A0} = C_{A0}v_0 = (0.2 \text{ mol/dm}^3)(2 \text{ dm}^3/\text{s}) = (0.4 \text{ mol/s})$$

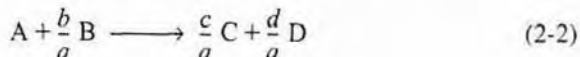
$$F_{A0} = 0.4 \text{ mol/s}$$

This feed rate ($F_{A0} = 0.4 \text{ mol/s}$) is in the range of that which is necessary to form several million pounds of product per year. We will use this value of F_{A0} together with either Table 2-2 or Figure 2-1 to size and evaluate a number of reactor schemes in Examples 2-2 through 2-5.

Now that we have a relationship [Equation (2-10)] between the molar flow rate and conversion, it is possible to express the design equations (i.e., mole balances) in terms of conversion for the *flow* reactors examined in Chapter 1.

2.3.1 CSTR (also known as a Backmix Reactor or Vat)

Recall that the CSTR is modeled as being well mixed such that there are no spatial variations in the reactor. The CSTR mole balance, Equation (1-7), when applied to species A in the reaction



can be arranged to

$$V = \frac{F_{A0} - F_A}{-r_A} \quad (2-11)$$

We now substitute for F_A in terms of F_{A0} and X

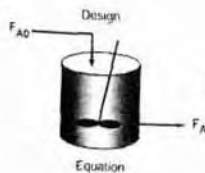
$$F_A = F_{A0} - F_{A0}X \quad (2-12)$$

and then substitute Equation (2-12) into (2-11)

$$V = \frac{F_{A0} - (F_{A0} - F_{A0}X)}{-r_A}$$

Simplifying, we see the CSTR volume necessary to achieve a specified conversion X is

$$V = \frac{F_{A0}X}{(-r_A)_{\text{exit}}} \quad (2-13)$$



Perfect mixing

Evaluate $-r_A$ at CSTR exit.

Because the reactor is *perfectly mixed*, the exit composition from the reactor is identical to the composition inside the reactor, and the rate of reaction is evaluated at the exit conditions.

2.3.2 Tubular Flow Reactor (PFR)

We model the tubular reactor as having the fluid flowing in plug flow, i.e., no radial gradients in concentration, temperature, or reaction rate.¹ As the reactants enter and flow axially down the reactor, they are consumed and the conversion increases along the length of the reactor. To develop the PFR design equation we first multiply both sides of the tubular reactor design equation (1-12) by -1 . We then express the mole balance equation for species A in the reaction as

$$\frac{-dF_A}{dV} = -r_A \quad (2-14)$$

For a flow system, F_A has previously been given in terms of the entering molar flow rate F_{A0} and the conversion X

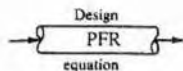
$$F_A = F_{A0} - F_{A0}X \quad (2-12)$$

differentiating

$$dF_A = -F_{A0}dX$$

and substituting into (2-14), gives the differential form of the design equation for a plug-flow reactor (PFR):

$$F_{A0} \frac{dX}{dV} = -r_A \quad (2-15)$$



We now separate the variables and integrate with the limits $V = 0$ when $X = 0$ to obtain the plug-flow reactor volume necessary to achieve a specified conversion X :

$$V = F_{A0} \int_0^X \frac{dX}{-r_A} \quad (2-16)$$

To carry out the integrations in the batch and plug-flow reactor design equations (2-9) and (2-16), as well as to evaluate the CSTR design equation (2-13), we need to know how the reaction rate $-r_A$ varies with the concentration (hence conversion) of the reacting species. This relationship between reaction rate and concentration is developed in Chapter 3.

¹ This constraint will be removed when we extend our analysis to nonideal (industrial) reactors in Chapters 13 and 14.

2.3.3 Packed-Bed Reactor

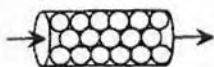
Packed-bed reactors are tubular reactors filled with catalyst particles. The derivation of the differential and integral forms of the design equations for packed-bed reactors are analogous to those for a PFR [cf. Equations (2-15) and (2-16)]. That is, substituting Equation (2-12) for F_A in Equation (1-15) gives

PBR design
equation

$$F_{A0} \frac{dX}{dW} = -r'_A \quad (2-17)$$

The differential form of the design equation [i.e., Equation (2-17)] **must** be used when analyzing reactors that have a pressure drop along the length of the reactor. We discuss pressure drop in packed-bed reactors in Chapter 4.

In the *absence* of pressure drop, i.e., $\Delta P = 0$, we can integrate (2-17) with limits $X = 0$ at $W = 0$ to obtain



$$W = F_{A0} \int_0^X \frac{dX}{-r'_A} \quad (2-18)$$

Equation (2-18) can be used to determine the catalyst weight W necessary to achieve a conversion X when the total pressure remains constant.

2.4 Applications of the Design Equations for Continuous-Flow Reactors

In this section, we are going to show how we can size CSTRs and PFRs (i.e., determine their reactor volumes) from knowledge of the rate of reaction, $-r_A$, as a function of conversion, X . The rate of disappearance of A, $-r_A$, is almost always a function of the concentrations of the various species present. When only one reaction is occurring, each of the concentrations can be expressed as a function of the conversion X (see Chapter 3); consequently, $-r_A$ can be expressed as a function of X .

A particularly simple functional dependence, yet one that occurs often, is the first-order dependence

$$-r_A = kC_A = kC_{A0}(1-X)$$

Here, k is the specific reaction rate and is a function only of temperature, and C_{A0} is the entering concentration. We note in Equations (2-13) and (2-16) the reactor volume in a function of the reciprocal of $-r_A$. For this first-order dependence, a plot of the reciprocal rate of reaction ($1/-r_A$) as a function of conversion yields a curve similar to the one shown in Figure 2-1, where

$$\frac{1}{-r_A} = \frac{1}{kC_{A0}} \left(\frac{1}{1-X} \right)$$

To illustrate the design of a series of reactors, we consider the isothermal gas-phase isomerization



We are going to the laboratory to determine the rate of chemical reaction as a function of the conversion of reactant A. The laboratory measurements given in Table 2-1 show the chemical reaction rate as a function of conversion. The temperature was 500 K (440°F), the total pressure was 830 kPa (8.2 atm), and the initial charge to the reactor was pure A.

If we know $-r_A$ as a function of X , we can size any isothermal reaction system.

TABLE 2-1 RAW DATA

X	$-r_A$ (mol/m ³ ·s)
0	0.45
0.1	0.37
0.2	0.30
0.4	0.195
0.6	0.113
0.7	0.079
0.8	0.05

Recalling the CSTR and PFR design equations, (2-13) and (2-16), we see that the reactor volume varies with the reciprocal of $-r_A$, $(1/-r_A)$, e.g., $V = \left(\frac{1}{-r_A}\right)(F_{A0}X)$. Consequently, to size reactors, we convert the rate data in Table 2-1 to reciprocal rates, $(1/-r_A)$, in Table 2-2.

TABLE 2-2 PROCESSED DATA -1

X	0.0	0.1	0.2	0.4	0.6	0.7	0.8
$-r_A \left(\frac{\text{mol}}{\text{m}^3 \cdot \text{s}}\right)$	0.45	0.37	0.30	0.195	0.113	0.079	0.05
$(1/-r_A) \left(\frac{\text{m}^3 \cdot \text{s}}{\text{mol}}\right)$	2.22	2.70	3.33	5.13	8.85	12.7	20

These data are used to arrive at a plot of $(1/-r_A)$ as a function of X , shown in Figure 2-1.

We can use this figure to size flow reactors for different entering molar flow rates. Before sizing flow reactors let's first consider some insights. If a

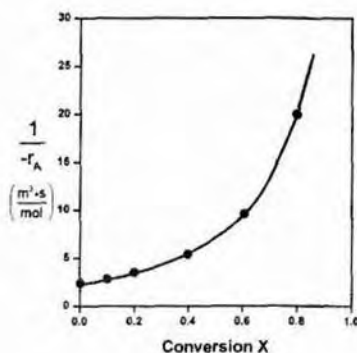


Figure 2-1 Processed data -1.

reaction is carried out isothermally, the rate is usually greatest at the start of the reaction when the concentration of reactant is greatest (i.e., when there is negligible conversion [$X \cong 0$]). Hence $(1/-r_A)$ will be small. Near the end of the reaction, when the reactant has been mostly used up and thus the concentration of A is small (i.e., the conversion is large), the reaction rate will be small. Consequently, $(1/-r_A)$ is large.

For all irreversible reactions of greater than zero order (see Chapter 3 for zero-order reactions), as we approach complete conversion where all the limiting reactant is used up, i.e., $X = 1$, the reciprocal rate approaches infinity as does the reactor volume, i.e.

$$A \rightarrow B + C \quad \text{As } X \rightarrow 1, -r_A \rightarrow 0, \text{ thus, } \frac{1}{-r_A} \rightarrow \infty \text{ therefore } V \rightarrow \infty$$

“To infinity
and beyond”
—Buzz Lightyear

Consequently, we see that an infinite reactor volume is necessary to reach complete conversion, $X = 1.0$

For reversible reactions (e.g., $A \rightleftharpoons B$), the maximum conversion is the equilibrium conversion X_e . At equilibrium, the reaction rate is zero ($r_A \cong 0$). Therefore,

$$A \rightleftharpoons B + C \quad \text{As } X \rightarrow X_e, -r_A \rightarrow 0, \text{ thus, } \frac{1}{-r_A} \rightarrow \infty \text{ and therefore } V \rightarrow \infty$$

and we see that an infinite reactor volume would also be necessary to obtain the exact equilibrium conversion, $X = X_e$.

To size a number of reactors for the reaction we have been considering, we will use $F_{A0} = 0.4$ mol/s (calculated in Example 2-1) to add another row to the processed data shown in Table 2-2 to obtain Table 2-3.

TABLE 2-3 PROCESSED DATA -2

X	0.0	0.1	0.2	0.4	0.6	0.7	0.8
$-r_A \left(\frac{\text{mol}}{\text{m}^3 \cdot \text{s}} \right)$	0.45	0.37	0.30	0.195	0.113	0.079	0.05
$(1/-r_A) \left(\frac{\text{m}^3 \cdot \text{s}}{\text{mol}} \right)$	2.22	2.70	3.33	5.13	8.85	12.7	20
$[F_{A0}/-r_A](\text{m}^3)$	0.89	1.08	1.33	2.05	3.54	5.06	8.0

We shall use the data in this table for the next five Example Problems.

Plotting $\left(\frac{F_{A0}}{-r_A} \right)$ as a function of X using the data in Table 2-3 we obtain the plot shown in Figure 2.2.

Levenspiel plot

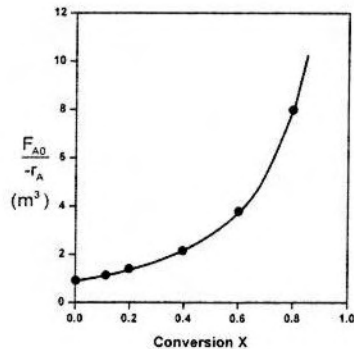


Figure 2-2 Levenspiel plot of processed data -2.

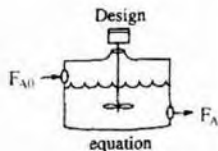
Example 2-2 Sizing a CSTR

The reaction described by the data in Table 2-2



is to be carried out in a CSTR. Species A enters the reactor at a molar flow rate of 0.4 mol/s.

- Using the data in either Table 2-2, Table 2-3, or Figure 2-1, calculate the volume necessary to achieve 80% conversion in a CSTR.
- Shade the area in Figure 2-2 that would give the CSTR volume necessary to achieve 80% conversion.



Solutions

(a) Equation (2-13) gives the volume of a CSTR as a function of F_{A0} , X , and $-r_A$:

$$V = \frac{F_{A0}X}{(-r_A)_{\text{exit}}} \quad (2-13)$$

In a CSTR, the composition, temperature, and conversion of the effluent stream are identical to that of the fluid within the reactor, because perfect mixing is assumed. Therefore, we need to find the value of $-r_A$ (or reciprocal thereof) at $X = 0.8$. From either Table 2-2 or Figure 2-1, we see that when $X = 0.8$, then

$$\left(\frac{1}{-r_A}\right)_{X=0.8} = 20 \frac{\text{m}^3 \cdot \text{s}}{\text{mol}}$$

Substitution into Equation (2-13) for an entering molar flow rate, F_{A0} , of 0.4 mol A/s and $X = 0.8$ gives

$$V = 0.4 \frac{\text{mol}}{\text{s}} \left(\frac{20 \text{ m}^3 \cdot \text{s}}{\text{mol}} \right) (0.8) = 6.4 \text{ m}^3 \quad (\text{E2-2.1})$$

$$V = 6.4 \text{ m}^3 = 6400 \text{ dm}^3 = 6400 \text{ l}$$

(b) Shade the area in Figure 2-2 that yields the CSTR volume. Rearranging Equation (2-13) gives

$$V = \left[\frac{F_{A0}}{-r_A} \right] X \quad (2-13)$$

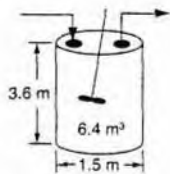
In Figure E2-2.1, the volume is equal to the area of a rectangle with a height ($F_{A0}/-r_A = 8 \text{ m}^3$) and a base ($X = 0.8$). This rectangle is shaded in the figure.

$$V = \left[\frac{F_{A0}}{-r_A} \right]_{X=0.8} (0.8) \quad (\text{E2-2.2})$$

$V = \text{Levenspiel rectangle area} = \text{height} \times \text{width}$

$$V = [8 \text{ m}^3][0.8] = 6.4 \text{ m}^3$$

The CSTR volume necessary to achieve 80% conversion is 6.4 m³ when operated at 500 K, 830 kPa (8.2 atm), and with an entering molar flow rate of A of 0.4 mol/s. This volume corresponds to a reactor about 1.5 m in diameter and 3.6 m high. It's a large CSTR, but this is a gas-phase reaction, and CSTRs are normally not used for gas-phase reactions. CSTRs are used primarily for liquid-phase reactions.



Plots of $1/-r_A$ vs. X are sometimes referred to as Levenspiel plots (after Octave Levenspiel)

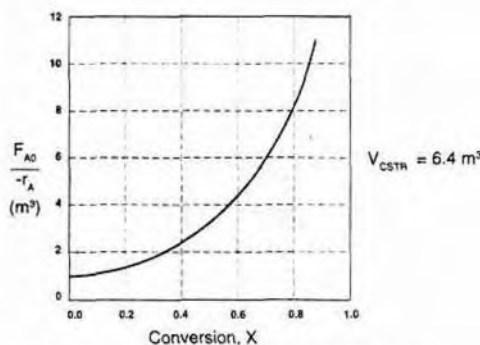


Figure E2-2.1 Levenspiel CSTR plot.

Example 2-3 Sizing a PFR

The reaction described by the data in Tables 2-1 and 2-2 is to be carried out in a PFR. The entering molar flow rate of A is 0.4 mol/s.

- First, use one of the integration formulas given in Appendix A.4 to determine the PFR reactor volume necessary to achieve 80% conversion.
- Next, shade the area in Figure 2-2 that would give the PFR the volume necessary to achieve 80% conversion.
- Finally, make a qualitative sketch of the conversion, X , and the rate of reaction, $-r_A$, down the length (volume) of the reactor.

Solution

We start by repeating rows (1) and (4) of Table 2-3.

TABLE 2-3 PROCESSED DATA -2

X	0.0	0.1	0.2	0.4	0.6	0.7	0.8
$[F_{A0}/-r_A](m^3)$	0.89	1.08	1.33	2.05	3.54	5.06	8.0

- For the PFR, the differential form of the mole balance is

$$F_{A0} \frac{dX}{dV} = -r_A \quad (2-15)$$

Rearranging and integrating gives

$$V = F_{A0} \int_0^{0.8} \frac{dX}{-r_A} = \int_0^{0.8} \frac{F_{A0}}{-r_A} dX \quad (2-16)$$

We shall use the *five point quadrature* formula (A-23) given in Appendix A.4 to numerically evaluate Equation (2-16). For the five-point formula with a final conversion of 0.8, gives for four equal segments between $X = 0$ and $X = 0.8$ with a segment length of $\Delta X = \frac{0.8}{4} = 0.2$. The function inside the integral is evaluated at $X = 0$, $X = 0.2$, $X = 0.4$, $X = 0.6$, and $X = 0.8$.

$$V = \frac{\Delta X}{3} \left[\frac{F_{A0}}{-r_A(X=0)} + \frac{4F_{A0}}{-r_A(X=0.2)} + \frac{2F_{A0}}{-r_A(X=0.4)} + \frac{4F_{A0}}{-r_A(X=0.6)} + \frac{F_{A0}}{-r_A(X=0.8)} \right]$$

Using values of $F_{A0}/(-r_A)$ in Table 2-3 yields

$$V = \left(\frac{0.2}{3}\right) [0.89 + 4(1.33) + 2(2.05) + 4(3.54) + 8.0] \text{dm}^3 = \left(\frac{0.2}{3}\right) (32.47 \text{ m}^3)$$

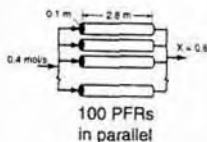
$$V = 2.165 \text{ m}^3 = 2165 \text{ dm}^3$$

The PFR reactor volume necessary to achieve 80% conversion is 2165 dm³. This volume could result from a bank of 100 PFRs that are each 0.1 m in diameter with a length of 2.8 m (e.g., see Figures 1-8(a) and (b)).

(b) The integral in Equation (2-16) can also be evaluated from the area under the curve of a plot of $(F_{A0}/-r_A)$ versus X .

$$V = \int_0^{0.8} \frac{F_{A0}}{-r_A} dX = \text{Area under the curve between } X = 0 \text{ and } X = 0.8$$

(see appropriate shaded area in Figure E2-3.1)



PFR

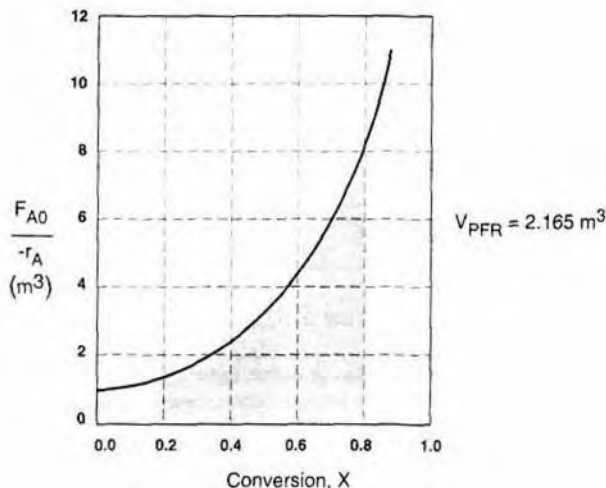


Figure E2-3.1 Levenspiel PFR plot.

The area under the curve will give the tubular reactor volume necessary to achieve the specified conversion of A. For 80% conversion, the shaded area is roughly equal to 2165 dm³ (2.165 m³).

(c) Sketch the profiles of $-r_A$ and X down the length of the reactor.

Solution

We know that as we proceed down the reactor and more and more of the reactant is consumed, the concentration of reactant decreases, as does the rate of disappearance of A. However, the conversion increases as more and more reactant is converted to product. For $X = 0.2$, we calculate the corresponding reactor volume using Simpson's rule (given in Appendix A.4 as Equation [A-21]) with $\Delta X = 0.1$ and the data in rows 1 and 4 in Table 2-3.

$$V = F_{A0} \int_0^{0.2} \frac{dX}{-r_A} = \frac{\Delta X}{3} \left[\frac{F_{A0}}{-r_A(X=0)} + \frac{4F_{A0}}{-r_A(X=0.1)} + \frac{F_{A0}}{-r_A(X=0.2)} \right]$$

$$= \left[\frac{0.1}{3} [0.89 + 4(1.08) + 1.33] \right] \text{m}^3 = \frac{0.1}{3} (6.54 \text{ m}^3) = 0.218 \text{ m}^3 = 218 \text{ dm}^3$$

$$= 218 \text{ dm}^3$$

For $X = 0.4$, we can again use Simpson's rule with $\Delta X = 0.2$ to find the reactor volume necessary for a conversion of 40%.

$$V = \frac{\Delta X}{3} \left[\frac{F_{A0}}{-r_A(X=0)} + \frac{4F_{A0}}{-r_A(X=0.2)} + \frac{F_{A0}}{-r_A(X=0.4)} \right]$$

$$= \left[\frac{0.2}{3} [0.89 + 4(1.33) + 2.05] \right] \text{m}^3 = 0.551 \text{ m}^3$$

$$= 551 \text{ dm}^3$$

We can continue in this manner to arrive at Table E2-3.1.

TABLE E2-3.1. CONVERSION AND REACTION RATE PROFILES

X	0	0.2	0.4	0.6	0.8
$-r_A \left(\frac{\text{mol}}{\text{m}^3 \cdot \text{s}} \right)$	0.45	0.30	0.195	0.113	0.05
$V \text{ (dm}^3\text{)}$	0	218	551	1093	2165

The data in Table E2-3.1 are plotted in Figures E2-3.2 (a) and (b).

One observes that the reaction rate, $-r_A$, decreases as we move down the reactor while the conversion increases. These plots are typical for reactors operated isothermally.

For isothermal reactions, the conversion increases and the rate decreases as we move down the PFR.

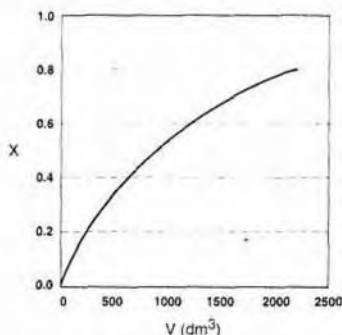


Figure E2-3.2(a) Conversion profile.

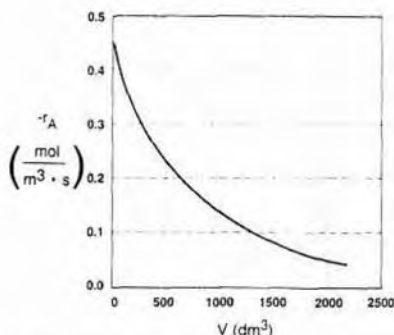


Figure E2-3.2(b) Reaction rate profile.

Example 2-4 Comparing CSTR and PFR Sizes

It is interesting to compare the volumes of a CSTR and a PFR required for the same job. To make this comparison, we shall use the data in Figure 2-2 to learn which reactor would require the smaller volume to achieve a conversion of 80%: a CSTR or a PFR. The entering molar flow rate $F_{A0} = 0.4$ mol/s, and the feed conditions are the same in both cases.

Solution

TABLE 2-3 PROCESSED DATA -2

X	0.0	0.1	0.2	0.4	0.6	0.7	0.8
$[F_{A0}/-r_A](m^3)$	0.89	1.08	1.33	2.05	3.54	5.06	8.0

The CSTR volume was 6.4 m^3 and the PFR volume was 2.165 m^3 . When we combine Figures E2-2.1 and E2-3.1 on the same graph, we see that the crosshatched area above the curve is the difference in the CSTR and PFR reactor volumes.

For isothermal reactions greater than zero order (see Chapter 3 for zero order), the CSTR volume will usually be greater than the PFR volume for the same conversion and reaction conditions (temperature, flow rate, etc.).

We see that the reason the isothermal CSTR volume is usually greater than the PFR volume is that the CSTR is always operating at the lowest reaction rate (e.g., $-r_A = 0.05$ in Figure E2-4.1(b)). The PFR on the other hand starts at a high rate at the entrance and gradually decreases to the exit rate, thereby requiring less volume because the volume is inversely proportional to the rate. However, for autocatalytic reactions, product-inhibited reactions, and nonisothermal exothermic reactions, these trends will not always be the case, as we will see in Chapters 7 and 8.

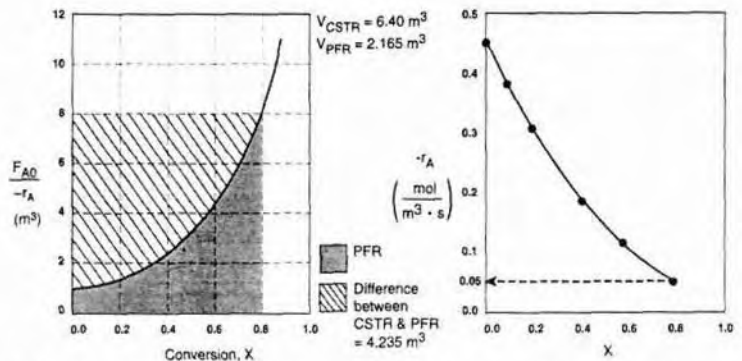


Figure E2-4.1(a) Comparison of CSTR and PFR reactor sizes.

(b) $-r_A$ as a function of X .

2.5 Reactors in Series

Many times, reactors are connected in series so that the exit stream of one reactor is the feed stream for another reactor. When this arrangement is used, it is often possible to speed calculations by defining conversion in terms of location at a point downstream rather than with respect to any single reactor. That is, the conversion X is the *total number of moles of A that have reacted up to that point per mole of A fed to the first reactor*.

Only valid for
NO side streams

For reactors in series

$$X_i = \frac{\text{Total moles of A reacted up to point } i}{\text{Moles of A fed to the first reactor}}$$



However, this definition can *only* be used when the feed stream only enters the first reactor in the series and there are *no* side streams either fed or withdrawn. The molar flow rate of A at point i is equal to moles of A fed to the first reactor minus all the moles of A reacted up to point i :

$$F_{A_i} = F_{A0} - F_{A0}X_i$$

For the reactors shown in Figure 2-3, X_1 at point $i = 1$ is the conversion achieved in the PFR, X_2 at point $i = 2$ is the total conversion achieved at this point in the PFR and the CSTR, and X_3 is the total conversion achieved by all three reactors.

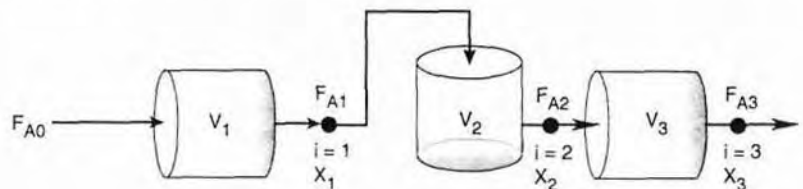


Figure 2-3 Reactors in series.

To demonstrate these ideas, let us consider three different schemes of reactors in series: two CSTRs, two PFRs, and then a combination of PFRs and CSTRs in series. To size these reactors, we shall use laboratory data that gives the reaction rate at different conversions.

2.5.1 CSTRs in Series

The first scheme to be considered is the two CSTRs in series shown in Figure 2-4.

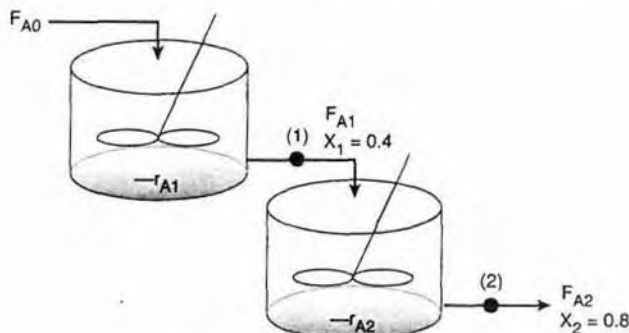


Figure 2-4 Two CSTRs in series.

For the first reactor, the rate of disappearance of A is $-r_{A1}$ at conversion X_1 . A mole balance on reactor 1 gives

$$\text{In} - \text{Out} + \text{Generation} = 0$$

$$\text{Reactor 1: } F_{A0} - F_{A1} + r_{A1}V_1 = 0 \quad (2-19)$$

The molar flow rate of A at point 1 is

$$F_{A1} = F_{A0} - F_{A0}X_1 \quad (2-20)$$

Combining Equations (2-19) and (2-20) or rearranging

Reactor 1

$$V_1 = F_{A0} \left(\frac{1}{-r_{A1}} \right) X_1 \quad (2-21)$$

In the second reactor, the rate of disappearance of A, $-r_{A2}$, is evaluated at the conversion of the exit stream of reactor 2, X_2 . A mole balance on the second reactor

$$\text{In} - \text{Out} + \text{Generation} = 0$$

$$\text{Reactor 2: } F_{A1} - F_{A2} + r_{A2}V = 0 \quad (2-22)$$

The molar flow rate of A at point 2 is

$$F_{A2} = F_{A0} - F_{A0}X_2 \quad (2-23)$$

Combining and rearranging

$$V_2 = \frac{F_{A1} - F_{A2}}{-r_{A2}} = \frac{(F_{A0} - F_{A0}X_1) - (F_{A0} - F_{A0}X_2)}{-r_{A2}}$$

Reactor 2

$$V_2 = \frac{F_{A0}}{-r_{A2}}(X_2 - X_1) \quad (2-24)$$

For the second CSTR recall that $-r_{A2}$ is evaluated at X_2 and then use $(X_2 - X_1)$ to calculate V_2 at X_2 .

In the examples that follow, we shall use the molar flow rate of A we calculated in Example 2-1 (0.4 mol A/s) and the reaction conditions given in Table 2-3.

Example 2-5 Comparing Volumes for CSTRs in Series

For the two CSTRs in series, 40% conversion is achieved in the first reactor. What is the volume of each of the two reactors necessary to achieve 80% overall conversion of the entering species A?

TABLE 2-3 PROCESSED DATA -2

X	0.0	0.1	0.2	0.4	0.6	0.7	0.8
$[F_{A0}/-r_A](\text{m}^3)$	0.89	1.09	1.33	2.05	3.54	5.06	8.0

Solution

For reactor 1, we observe from either Table 2-3 or Figure E2-5.1 that when $X = 0.4$, then

$$\left(\frac{F_{A0}}{-r_{A1}}\right)_{X=0.4} = 2.05 \text{ m}^3$$

then

$$V_1 = \left(\frac{F_{A0}}{-r_{A1}}\right)_{X_1} X_1 = \left(\frac{F_{A0}}{-r_{A1}}\right)_{0.4} (0.4) = (2.05)(0.4) = 0.82 \text{ m}^3 = 820 \text{ dm}^3$$

For reactor 2, when $X_2 = 0.8$, then $\left(\frac{F_{A0}}{-r_{A2}}\right)_{X=0.8} = 8.0 \text{ m}^3$

$$V_2 = \left(\frac{F_{A0}}{-r_{A2}}\right)(X_2 - X_1) \quad (2-24)$$

$$V_2 = (8.0 \text{ m}^3)(0.8 - 0.4) = 3.2 \text{ m}^3 = 3200 \text{ dm}^3$$

$$V_2 = 3200 \text{ dm}^3 \text{ (liters)}$$

To achieve the same overall conversion, the total volume for two CSTRs in series is less than that required for one CSTR.

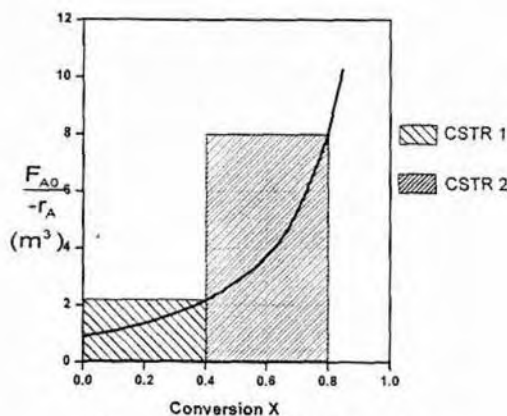


Figure E2-5.1 Two CSTRs in series.

Note again that for CSTRs in series the rate $-r_{A1}$ is evaluated at a conversion of 0.4 and rate $-r_{A2}$ is evaluated at a conversion of 0.8. The total volume for these two reactors in series is

$$V = V_1 + V_2 = 0.82 \text{ m}^3 + 3.2 \text{ m}^3 = 4.02 \text{ m}^3 = 4020 \text{ dm}^3$$

By comparison, the volume necessary to achieve 80% conversion in **one** CSTR is

$$V = \left(\frac{F_{A0}}{-r_{A1}} \right) X = (8.0)(0.8) = 6.4 \text{ m}^3 = 6400 \text{ dm}^3$$

Notice in Example 2-5 that the sum of the two CSTR reactor volumes (4.02 m^3) in series is less than the volume of one CSTR (6.4 m^3) to achieve the same conversion.

Approximating a PFR by a large number of CSTRs in series

Consider approximating a PFR with a number of small, equal-volume CSTRs of V_i in series (Figure 2-5). We want to compare the *total volume* of all the CSTRs with the volume of one plug-flow reactor for the same conversion, say 80%.

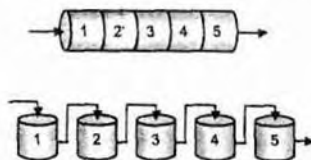


Figure 2-5 Modeling a PFR with CSTRs in series.

We need only $-r_A = f(x)$ and F_{A0} to size reactors.