

The fact that we can model a PFR with a large number of CSTRs is an important result.

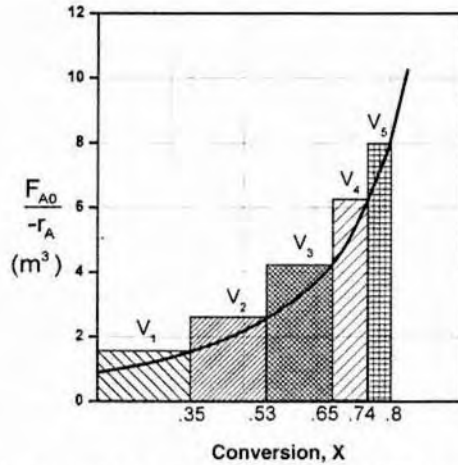


Figure 2-6 Levenspiel plot showing comparison of CSTRs in series with one PFR.

From Figure 2-6, we note a very important observation! The total volume to achieve 80% conversion for five CSTRs of equal volume in series is roughly the same as the volume of a PFR. As we make the volume of each CSTR smaller and increase the number of CSTRs, the total volume of the CSTRs in series and the volume of the PFR will become identical. *That is, we can model a PFR with a large number of CSTRs in series.* This concept of using many CSTRs in series to model a PFR will be used later in a number of situations, such as modeling catalyst decay in packed-bed reactors or transient heat effects in PFRs.

### 2.5.2 PFRs in Series

We saw that two CSTRs in series gave a smaller total volume than a single CSTR to achieve the same conversion. This case does not hold true for the two plug-flow reactors connected in series shown in Figure 2-7.

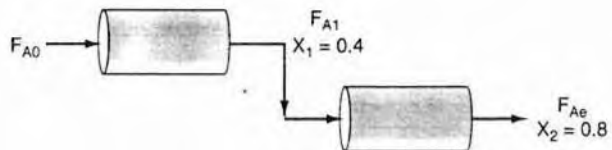


Figure 2-7 Two PFRs in series.

PRF in series We can see from Figure 2-8 and from the following equation

$$\int_0^{X_2} F_{A0} \frac{dX}{-r_A} \equiv \int_0^{X_1} F_{A0} \frac{dX}{-r_A} + \int_{X_1}^{X_2} F_{A0} \frac{dX}{-r_A}$$

that it is immaterial whether you place two plug-flow reactors in series or have one continuous plug-flow reactor; the total reactor volume required to achieve the same conversion is identical!

The overall conversion of two PRFs in series is the same as one PRF with the same total volume.

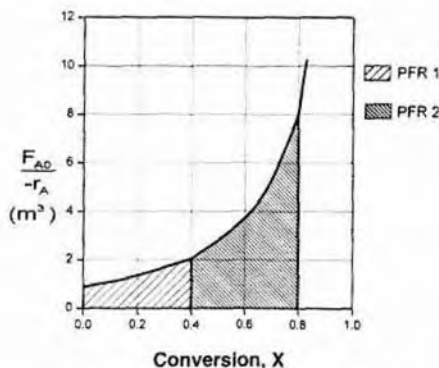


Figure 2-8 Levenspiel plot for two PFRs in series.

### Example 2-6 Sizing Plug-Flow Reactors in Series

Using either the data in Table 2-3 or Figure 2-2, calculate the reactor volumes  $V_1$  and  $V_2$  for the plug-flow sequence shown in Figure 2-7 when the intermediate conversion is 40% and the final conversion is 80%. The entering molar flow rate is the same as in the previous examples, 0.4 mol/s.

*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

In addition to graphical integration, we could have used numerical methods to size the plug-flow reactors. In this example, we shall use Simpson's rule (see Appendix A.4) to evaluate the integrals.

Simpson's  
three-point rule

$$\int_{X_0}^{X_2} f(X) dX = \frac{\Delta X}{3} [f(X_0) + 4f(X_1) + f(X_2)] \quad (\text{A-2})$$

For the first reactor,  $X_0 = 0$ ,  $X_1 = 0.2$ ,  $X_2 = 0.4$ , and  $\Delta X = 0.2$ .

$$V = F_{A0} \int_0^{0.4} \frac{dX}{-r_A} = \frac{\Delta X}{3} \left[ \frac{F_{A0}}{-r_A(0)} + 4 \frac{F_{A0}}{-r_A(0.2)} + \frac{F_{A0}}{-r_A(0.4)} \right] \quad (\text{E2-6.})$$

Selecting the appropriate values from Table 2-3, we get

$$V_1 = \left( \frac{0.2}{3} \right) [0.89 + 4(1.33) + 2.05] \text{m}^3 = 0.551 \text{m}^3$$

$$\boxed{V_1 = 551 \text{ dm}^3}$$

For the second reactor,

$$\begin{aligned} V_2 &= F_{A0} \int_{0.4}^{0.8} \frac{dX}{-r_A} \\ &= \frac{\Delta X}{3} \left[ \frac{F_{A0}}{-r_A(0.4)} + 4 \frac{F_{A0}}{-r_A(0.6)} + \frac{F_{A0}}{-r_A(0.8)} \right] \quad (\text{E2-6.}) \\ &= \left( \frac{0.2}{3} \right) [2.05 + 4(3.54) + 8.0] \text{m}^3 = \frac{0.2}{3} (24.21 \text{ m}^3) = 1.614 \text{m}^3 \end{aligned}$$

$$\boxed{V_2 = 1614 \text{ dm}^3}$$

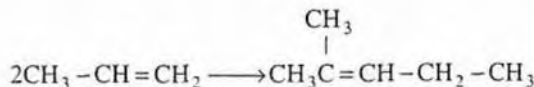
The total volume is then

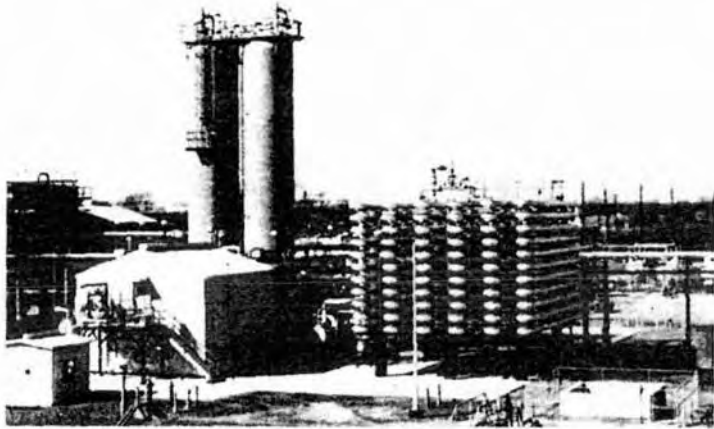
$$V = V_1 + V_2 = 551 \text{ dm}^3 + 1614 \text{ dm}^3 = 2165 \text{ dm}^3$$

**Note:** This is the same volume we calculated for a single PFR to achieve 80% conversion in Example 2-4.

### 2.5.3 Combinations of CSTRs and PFRs in Series

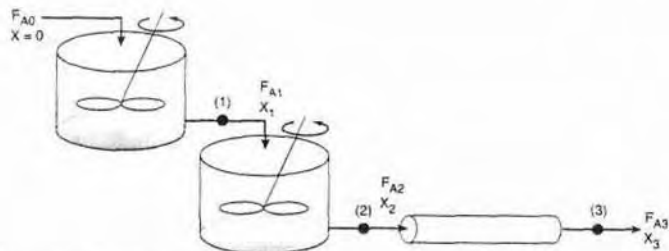
The final sequences we shall consider are combinations of CSTRs and PFRs in series. An industrial example of reactors in series is shown in the photo in Figure 2-9. This sequence is used to dimerize propylene into isohexanes, e.g.,





**Figure 2-9** Dimersol G (an organometallic catalyst) unit (two CSTRs and one tubular reactor in series) to dimerize propylene into isohexanes. Institut Français du Pétrole process. [Photo courtesy of Editions Technip (Institut Français du Pétrole).]

A schematic of the industrial reactor system in the Figure 2-9 is shown in Figure 2-10.



**Figure 2-10** Schematic of a real system.

For the sake of illustration, let's assume the reaction carried out in the reactors in Figure 2-10 follows the same  $\left(\frac{F_{A0}}{-r_A}\right)$  vs.  $X$  curve given by Table 2-3.

The volumes of the first two CSTRs in series (see Example 2-5) are:

$$\text{Reactor 1} \quad V_1 = \frac{F_{A0}X_1}{-r_{A1}} \quad (2-13)$$

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

Starting with the differential form of PFR design equation

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

In this series arrangement  $-r_{A2}$  is evaluated at  $X_2$  for the second CSTR.

Rearranging and integrating between limits, when  $V = 0$ , then  $X = X_2$ , and when  $V = V_3$ , then  $X = X_3$ .

$$\text{Reactor 3} \quad V_3 = \int_{X_2}^{X_3} \frac{F_{A0}}{-r_A} dX \quad (2-25)$$

The corresponding reactor volumes for each of the three reactors can be found from the shaded areas in Figure 2-11.

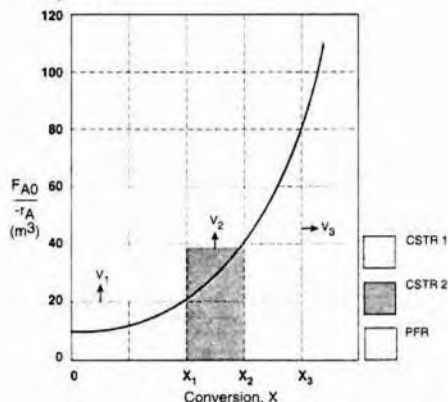
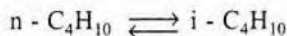


Figure 2-11 Levenspiel plot to determine the reactor volumes  $V_1$ ,  $V_2$ , and  $V_3$ .

The  $F_{A0}/-r_A$  curves we have been using in the previous examples are typical of those found in isothermal reaction systems. We will now consider a real reaction system that is carried out adiabatically. Isothermal reaction systems are discussed in Chapter 4 and adiabatic systems in Chapter 8.

### Example 2-7 An Adiabatic Liquid-Phase Isomerization

The isomerization of butane



was carried out adiabatically in the liquid phase and the data in Table E2-7.1 were obtained. (Example 8.4 shows how the data in Table E2-7.1 were generated.)

TABLE E2-7.1 RAW DATA

$X$	0.0	0.2	0.4	0.6	0.65
$-r_A$ (kmol/m <sup>3</sup> · h)	39	53	59	38	25

Don't worry how we got this data or why the  $(1/-r_A)$  looks the way it does, we will see how to construct this table in Chapter 8. It is real data for a real reaction carried out adiabatically, and the reactor scheme shown in Figure E2-7.1 is used.

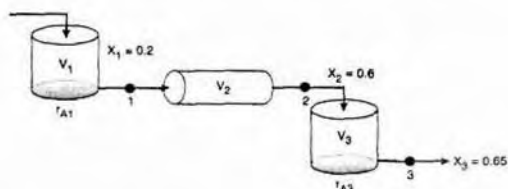


Figure E2-7.1 Reactors in series.

Calculate the volume of each of the reactors for an entering molar flow rate of *n*-butane of 50 kmol/hr.

*Solution*

Taking the reciprocal of  $-r_A$  and multiplying by  $F_{A0}$  we obtain Table E2-7.2.

$$\text{E.g., at } X = 0: \frac{F_{A0}}{-r_A} = \frac{50 \text{ kmol/h}}{39 \text{ kmol/h} \cdot \text{m}^3} = 1.28 \text{ m}^3$$

TABLE E2-7.2 PROCESSED DATA

$X$	0.0	0.2	0.4	0.6	0.65
$-r_A$ (kmol/m <sup>3</sup> · h)	39	53	59	38	25
$[F_{A0}/-r_A]$ (m <sup>3</sup> )	1.28	0.94	0.85	1.32	2.0

(a) For the first CSTR,  $\frac{F_{A0}}{-r_A} = 0.94$   
when  $X = 0.2$ , then

$$V_1 = \frac{F_{A0}}{-r_A} X_1 = (0.94 \text{ m}^3)(0.2) = 0.188 \text{ m}^3 \quad (\text{E2-7.1})$$

$$\boxed{V_1 = 0.188 \text{ m}^3 = 188 \text{ dm}^3} \quad (\text{E2-7.2})$$

(b) For the PFR,

$$V_2 = \int_{0.2}^{0.6} \left( \frac{F_{A0}}{-r_A} \right) dX$$

Using Simpson's three-point formula with  $\Delta X = (0.6 - 0.2)/2 = 0.2$ , and  $X_1 = 0$ ,  $X_2 = 0.4$ , and  $X_3 = 0.6$ .

$$V_2 = \int_{0.2}^{0.6} \frac{F_{A0}}{-r_A} (dX) = \frac{\Delta X}{3} \left[ \frac{F_{A0}}{-r_A} \Big|_{X=0.2} + 4 \frac{F_{A0}}{-r_A} \Big|_{X=0.4} + \frac{F_{A0}}{-r_A} \Big|_{X=0.6} \right]$$

$$= \frac{0.2}{3} [0.94 + 4(0.85) + 1.32] \text{m}^3 \quad (\text{E2-7.7})$$

$$\boxed{V_2 = 0.38 \text{ m}^3 = 380 \text{ dm}^3} \quad (\text{E2-7.8})$$

(c) For the last reactor and the second CSTR, mole balance on A for the CSTR

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

$$F_{A2} - F_{A3} + r_{A3}V_3 = 0 \quad (\text{E2-7.9})$$

Rearranging

$$V_3 = \frac{F_{A3} - F_{A2}}{-r_{A3}} \quad (\text{E2-7.10})$$

$$F_{A2} = F_{A0} - F_{A0}X_2$$

$$F_{A3} = F_{A0} - F_{A0}X_3$$

$$V_3 = \frac{(F_{A0} - F_{A0}X_2) - (F_{A0} - F_{A0}X_3)}{-r_{A3}}$$

Simplifying

$$\boxed{V_3 = \left( \frac{F_{A0}}{-r_{A3}} \right) (X_3 - X_2)} \quad (\text{E2-7.11})$$

We find from Table E2-7.2 that at  $X_3 = 0.65$ , then  $\frac{F_{A0}}{-r_{A3}} = 2.0 \text{ m}^3$

$$V_3 = 2 \text{ m}^3 (0.65 - 0.6) = 0.1 \text{ m}^3$$

$$\boxed{V_3 = 0.1 \text{ m}^3 = 100 \text{ dm}^3} \quad (\text{E2-7.12})$$

A Levenspiel plot of  $(F_{A0}/-r_A)$  vs.  $X$  is shown in Figure E2-7.2.

## 2.5.4 Comparing the CSTR and PFR Reactor Volumes and Reactor Sequencing

If we look at Figure E7-2.2, the area under the curve (PFR volume) between  $X = 0$  and  $X = 0.2$ , we see that the PFR area is greater than the rectangular area corresponding to the CSTR volume, i.e.,  $V_{\text{PFR}} > V_{\text{CSTR}}$ . However, if we compare the areas under the curve between  $X = 0.6$  and  $X = 0.65$ , we see that the

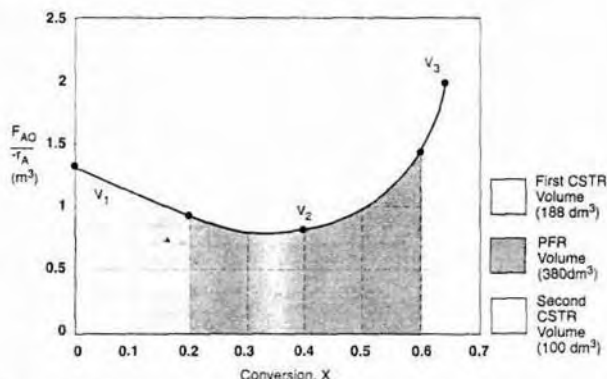
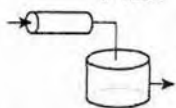
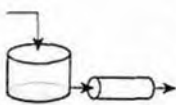


Figure E2-7.2 Levenspiel plot for adiabatic reactors in series.

Which arrangement is best?



or



area under the curve (PFR volume) is smaller than the rectangular area corresponding to the CSTR volume, i.e.,  $V_{\text{CSTR}} > V_{\text{PFR}}$ . This result often occurs when the reaction is carried out adiabatically, which is discussed when we look at heat effects in Chapter 8.

In the *sequencing of reactors* one is often asked, “Which reactor should go first to give the highest overall conversion? Should it be a PFR followed by a CSTR, or two CSTRs, then a PFR, or ...?” The answer is “**It depends.**” It depends not only on the shape of the Levenspiel plots ( $F_{A0}/-r_A$ ) versus  $X$ , but also on the relative reactor sizes. As an exercise, examine Figure E2-7.2 to learn if there is a better way to arrange the two CSTRs and one PFR. Suppose you were given a Levenspiel plot of ( $F_{A0}/-r_A$ ) vs.  $X$  for three reactors in series along with their reactor volumes  $V_{\text{CSTR1}} = 3 \text{ m}^3$ ,  $V_{\text{CSTR2}} = 2 \text{ m}^3$ , and  $V_{\text{PFR}} = 1.2 \text{ m}^3$  and asked to find the highest possible conversion  $X$ . What would you do? The methods we used to calculate reactor volumes all apply, except the procedure is reversed and a trial-and-error solution is needed to find the exit overall conversion from each reactor. See Problem P2-5<sub>B</sub>.

The previous examples show that *if* we know the molar flow rate to the reactor and the reaction rate as a function of conversion, *then* we can calculate the reactor volume necessary to achieve a specified conversion. The reaction rate does not depend on conversion alone, however. It is also affected by the initial concentrations of the reactants, the temperature, and the pressure. Consequently, the experimental data obtained in the laboratory and presented in Table 2-1 as  $-r_A$  as a function of  $X$  are useful only in the design of full-scale reactors that are to be operated at the *identical conditions* as the laboratory experiments (temperature, pressure, initial reactant concentrations). However,

Given  $V$  and

$\left[ \frac{1}{-r_A} \text{ vs. } X \right]$  find  $X$



such circumstances are **seldom** encountered and we must revert to the methods we describe in Chapter 3 to obtain  $-r_A$  as a function of  $X$ .

Only need  $-r_A = f(X)$  to size flow reactors

**It is important to understand that if the rate of reaction is available or can be obtained solely as a function of conversion,  $-r_A = f(X)$ , or if it can be generated by some intermediate calculations, one can design a variety of reactors or a combination of reactors.**

Chapter 3 shows how to find  $-r_A = f(X)$ .

Ordinarily, laboratory data are used to formulate a rate law, and then the reaction rate–conversion functional dependence is determined using the rate law. The preceding sections show that with the reaction rate–conversion relationship, different reactor schemes can readily be sized. In Chapter 3, we show how we obtain this relationship between reaction rate and conversion from rate law and reaction stoichiometry.

## 2.6 Some Further Definitions

Before proceeding to Chapter 3, some terms and equations commonly used in reaction engineering need to be defined. We also consider the special case of the plug-flow design equation when the volumetric flow rate is constant.

### 2.6.1 Space Time

The space time,  $\tau$ , is obtained by dividing reactor volume by the volumetric flow rate entering the reactor:

$\tau$  is an important quantity!

$$\tau \equiv \frac{V}{v_0} \quad (2-26)$$

The space time is the time necessary to process one reactor volume of fluid based on entrance conditions. For example, consider the tubular reactor shown in Figure 2-12, which is 20 m long and  $0.2 \text{ m}^3$  in volume. The dashed line in Figure 2-12 represents  $0.2 \text{ m}^3$  of fluid directly upstream of the reactor. The time it takes for this fluid to enter the reactor completely is the space time. It is also called the *holding time* or *mean residence time*.



Space time or mean residence time,  
 $\tau = V/v_0$

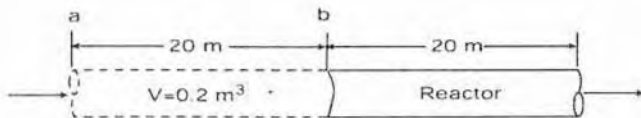


Figure 2-12 Tubular reactor showing identical volume upstream.

For example, if the volumetric flow rate were  $0.01 \text{ m}^3/\text{s}$ , it would take the upstream volume shown by the dashed lines a time  $\tau$

$$\tau = \frac{0.2 \text{ m}^3}{0.01 \text{ m}^3/\text{s}} = 20 \text{ s}$$

to enter the reactor. In other words, it would take 20 s for the fluid at point a to move to point b, which corresponds to a space time of 20 s.

In the absence of dispersion, which is discussed in Chapter 14, the space time is equal to the mean residence time in the reactor,  $t_m$ . This time is the average time the molecules spend in the reactor. A range of typical processing times in terms of the space time (residence time) for industrial reactors is shown in Table 2-4.

TABLE 2-4 TYPICAL SPACE TIME FOR INDUSTRIAL REACTORS<sup>2</sup>

Reactor Type	Mean Residence Time Range	Production Capacity
Batch	15 min to 20 h	Few kg/day to 100,000 tons/year
CSTR	10 min to 4 h	10 to 3,000,000 tons/year
Tubular	0.5 s to 1 h	50 to 5,000,000 tons/year

Table 2-5 shows space times for six industrial reactions and reactors.

TABLE 2-5 SAMPLE INDUSTRIAL SPACE TIMES<sup>3</sup>

	Reaction	Reactor	Temperature	Pressure	Space Time
				atm	
Typical industrial reaction space times	(1) $\text{C}_2\text{H}_6 \rightarrow \text{C}_2\text{H}_4 + \text{H}_2$	PFR <sup>†</sup>	860°C	2	1 s
	(2) $\text{CH}_3\text{CH}_2\text{OH} + \text{HCH}_3\text{COOH} \rightarrow \text{CH}_3\text{CH}_2\text{COOCH}_3 + \text{H}_2\text{O}$	CSTR	100°C	1	2 h
	(3) Catalytic cracking	PBR	490°C	20	1 s < $\tau$ < 400 s
	(4) $\text{C}_6\text{H}_5\text{CH}_2\text{CH}_3 \rightarrow \text{C}_6\text{H}_5\text{CH}=\text{CH}_2 + \text{H}_2$	PBR	600°C	1	0.2 s
	(5) $\text{CO} + \text{H}_2\text{O} \rightarrow \text{CO}_2 + \text{H}_2$	PBR	300°C	26	4.5 s
	(6) $\text{C}_6\text{H}_6 + \text{HNO}_3 \rightarrow \text{C}_6\text{H}_5\text{NO}_2 + \text{H}_2\text{O}$	CSTR	50°C	1	20 min

<sup>†</sup>The reactor is tubular but the flow may or may not be ideal plug flow.

<sup>2</sup> Trambouze, Landeghem, and Wauquier, *Chemical Reactors*, p. 154, (Paris: Editions Technip, 1988; Houston: Gulf Publishing Company, 1988).

<sup>3</sup> Walas, S. M. Chemical Reactor Data, *Chemical Engineering*, 79 (October 14, 1985).

## 2.6.2 Space Velocity

The space velocity (SV), which is defined as

$$SV \equiv \frac{v_0}{V} \quad SV = \frac{1}{\tau} \quad (2-26)$$

might be regarded at first sight as the reciprocal of the space time. However, there can be a difference in the two quantities' definitions. For the space time, the entering volumetric flow rate is measured at the entrance conditions, but for the space velocity, other conditions are often used. The two space velocities commonly used in industry are the liquid-hourly and gas-hourly space velocities, LHSV and GHSV, respectively. The entering volumetric flow rate,  $v_0$ , in the LHSV is frequently measured as that of a liquid feed rate at 60°F or 75°F, even though the feed to the reactor may be a vapor at some higher temperature. Strange but true. The gas volumetric flow rate,  $v_0$ , in the GHSV is normally measured at standard temperature and pressure (STP).

$$\text{LHSV} = \frac{v_0|_{\text{liquid}}}{V} \quad (2-27)$$

$$\text{GHSV} = \frac{v_0|_{\text{STP}}}{V} \quad (2-28)$$

**Example 2-8 Reactor Space Times and Space Velocities**

Calculate the space time,  $\tau$ , and space velocities for each of the reactors in Examples 2-2 and 2-3.

**Solution**

From Example 2-1, we recall the entering volumetric flow rate was given as 2 dm<sup>3</sup>/s (0.002 m<sup>3</sup>/s), and we calculated the concentration and molar flow rates for the conditions given to be  $C_{A0} = 0.2$  mol/dm<sup>3</sup> and  $F_{A0} = 0.4$  mol/s.

From Example 2-2, the CSTR volume was 6.4 m<sup>3</sup> and the corresponding space time and space velocity are

$$\tau = \frac{V}{v_0} = \frac{6.4 \text{ m}^3}{0.002 \text{ m}^3/\text{s}} = 3200 \text{ s} = 0.89 \text{ h}$$

$$SV = \frac{1}{\tau} = \frac{1}{0.89 \text{ h}} = 1.125 \text{ h}^{-1}$$

From Example 2-3, the PFR volume was 2.165 m<sup>3</sup>, and the corresponding space time and space velocity are

$$\tau = \frac{V}{v_0} = \frac{2.165 \text{ m}^3}{0.002 \text{ m}^3/\text{s}} = 1083 \text{ s} = 0.30 \text{ h}$$

$$SV = \frac{1}{\tau} = \frac{1}{0.30 \text{ h}} = 3.3 \text{ h}^{-1}$$

These space times are the times for each of the reactors to take one reactor volume of fluid and put it into the reactor.

To summarize these last examples, we have seen that in the design of reactors that are to be operated at conditions (e.g., temperature and initial concentration) identical to those at which the reaction rate data were obtained, we can size (determine the reactor volume) both CSTRs and PFRs alone or in various combinations. In principle, it may be possible to scale up a laboratory-bench or pilot-plant reaction system solely from knowledge of  $-r_A$  as a function of  $X$  or  $C_A$ . However, for most reactor systems in industry, a scale-up process cannot be achieved in this manner because knowledge of  $-r_A$  solely as a function of  $X$  is seldom, if ever, available under identical conditions. In Chapter 3, we shall see how we can obtain  $-r_A = f(X)$  from information obtained either in the laboratory or from the literature. This relationship will be developed in a two-step process. In Step 1, we will find the rate law that gives the rate as a function of concentration and in Step 2, we will find the concentrations as a function of conversion. Combining Steps 1 and 2 in Chapter 3, we obtain  $-r_A = f(X)$ . We can then use the methods developed in this chapter along with integral and numerical methods to size reactors.

#### The CRE Algorithm

- Mole Balance, Ch 1
- Rate Law, Ch 3
- Stoichiometry, Ch 3
- Combine, Ch 4
- Evaluate, Ch 4
- Energy Balance, Ch 8

### Closure

In this chapter, we have shown that if you are given the rate of reaction as a function of conversion, i.e.,  $-r_A = f(X)$ , you will be able to size CSTRs and PFRs and arrange the order of a given set of reactors to determine the best overall conversion. After completing this chapter, the reader should be able to

- a. define the parameter *conversion* and rewrite the mole balances in terms of conversion
- b. show that by expressing  $-r_A$  as a function of conversion  $X$  a number of reactors and reaction systems can be sized or a conversion calculated from a given reactor size
- c. arrange reactors in series to achieve the maximum conversion for a given Levenspiel plot

## SUMMARY

1. The conversion  $X$  is the moles of A reacted per mole of A fed.

$$\text{For batch systems:} \quad X = \frac{N_{A0} - N_A}{N_{A0}} \quad (\text{S2-1})$$

$$\text{For flow systems:} \quad X = \frac{F_{A0} - F_A}{F_{A0}} \quad (\text{S2-2})$$

For reactors in series with no side streams, the conversion at point  $i$  is

$$X_i = \frac{\text{Total moles of A reacted up to point } i}{\text{Moles A fed to the first reactor}} \quad (\text{S2-3})$$

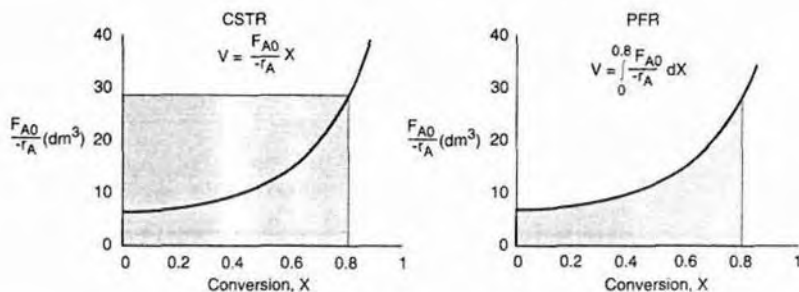
2. In terms of the conversion, the differential and integral forms of the reactor design equations become:

TABLE S2-1

	Differential Form	Algebraic Form	Integral Form
Batch	$N_{A0} \frac{dX}{dt} = -r_A V$		$t = N_{A0} \int_0^X \frac{dX}{-r_A V}$
CSTR		$V = \frac{F_{A0}(X_{\text{out}} - X_{\text{in}})}{(-r_A)_{\text{out}}}$	
PFR	$F_{A0} \frac{dX}{dV} = -r_A$		$V = F_{A0} \int_{X_{\text{in}}}^{X_{\text{out}}} \frac{dX}{-r_A}$
PBR	$F_{A0} \frac{dX}{dW} = -r'_A$		$W = F_{A0} \int_{X_{\text{in}}}^{X_{\text{out}}} \frac{dX}{-r'_A}$

3. If the rate of disappearance is given as a function of conversion, the following graphical techniques can be used to size a CSTR and a plug-flow reactor.

A. Graphical Integration Using Levenspiel Plots



The PFR integral could also be evaluated by

B. Numerical Integration

See Appendix A.4 for quadrature formulas such as the five-point quadrature formula with  $\Delta X = 0.8/4$  of five equally spaced points,  $X_1 = 0$ ,  $X_2 = 0.2$ ,  $X_3 = 0.4$ ,  $X_4 = 0.6$ , and  $X_5 = 0.8$ .

4. Space time,  $\tau$ , and space velocity, SV, are given by

$$\tau = \frac{V}{v_0} \quad (\text{S2-4})$$

$$\text{SV} = \frac{v_0}{V} \quad (\text{at STP}) \quad (\text{S2-5})$$

## CD-ROM MATERIALS

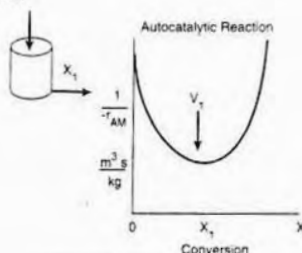
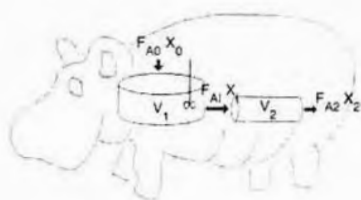
### • Learning Resources

1. Summary Notes for Chapter 2
2. Web Module

#### A. Hippopotamus Digestive System



Summary Notes



Levenspiel Plot for Autocatalytic Digestion in a CSTR

### 3. Interactive Computer Modules

#### A. Reactor Staging



Web Modules



## 4. Solved Problems

A. CDP2-A<sub>B</sub> More CSTR and PFR Calculations—No Memorization

## • FAQ [Frequently Asked Questions]

## • Professional Reference Shelf

## R2.1 Modified Levenspiel Plots

For liquids and constant volume batch reactors, the mole balance equation can be modified to

$$\tau = \int_{C_A}^{C_{A0}} \frac{dC_A}{-r_A}$$

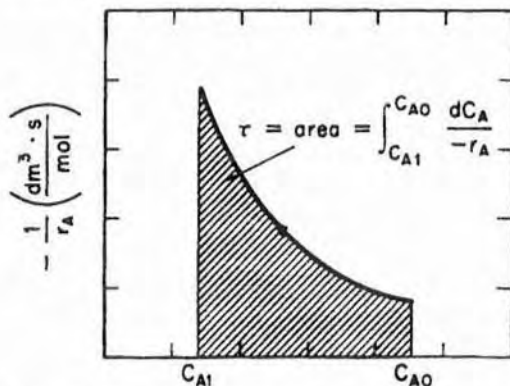
A plot of  $(1/-r_A)$  versus  $C_A$  gives Figure CD2-1.



Solved Problems



Reference Shelf

Figure CD2-1 Determining the space time,  $\tau$ .

One can use this plot to study CSTRs, PFRs, and batch reactors. This material using space time as a variable is given on the CD-ROM.

## QUESTIONS AND PROBLEMS

The subscript to each of the problem numbers indicates the level of difficulty: A, least difficult; D, most difficult.

A = ● B = ■ C = ◆ D = ◆◆



Homework Problems

Before solving the problems, state or sketch qualitatively the expected results or trends.

**P2-1<sub>A</sub>** Without referring back, make a list of the most important items you learned in this chapter. What do you believe was the overall purpose of the chapter?

**P2-2<sub>A</sub>** Go to the web site [www.engr.ncsu.edu/learningstyles/ilsweb.html](http://www.engr.ncsu.edu/learningstyles/ilsweb.html)

(a) Take the Inventory of Learning Style test, and record your learning style according to the Solomon/Felder inventory.

Global/Sequential \_\_\_\_\_

Active/Reflective \_\_\_\_\_

Visual/Verbal \_\_\_\_\_

Sensing/Intuitive \_\_\_\_\_




P2-3A

P2-4A

P2-5B



- (b) After checking the web site [www.engin.umich.edu/~cre/344/ITResources.htm](http://www.engin.umich.edu/~cre/344/ITResources.htm), suggest two ways to facilitate your learning style in each of the four categories.
- (c) Visit the problem-solving web site [www.engin.umich.edu/~cre/probsolv/closed/cep.htm](http://www.engin.umich.edu/~cre/probsolv/closed/cep.htm) to find ways to “Get Unstuck” when you get stuck on a problem and to review the “Problem-Solving Algorithm.” List four ways that might help you in your solution to the home problems.
- (d) What audio, , from the first two chapters sounds like Arnold Schwarzenegger?

(e) What Frequently Asked Question (FAQ) would you have asked?

**ICM Staging.** Load the Interactive Computer Module (ICM) from the CD-ROM. Run the module and then record the performance number, which indicates your mastery of the material. Your professor has the key to decode your performance number. Note: To run this module you *must* have Windows 2000 or a later version. ICM Reactor Staging Performance # \_\_\_\_\_.

- (a) Revisit **Examples 2-1** through **2-3**. How would your answers change if the flow rate,  $F_{A0}$ , were cut in half? If it were doubled?
- (b) **Example 2-5.** How would your answers change if the two CSTRs (one  $0.82 \text{ m}^3$  and the other  $3.2 \text{ m}^3$ ) were placed in parallel with the flow,  $F_{A0}$ , divided equally to each reactor.
- (c) **Example 2-6.** How would your answer change if the PFRs were placed in parallel with the flow,  $F_{A0}$ , divided equally to each reactor?
- (d) **Example 2-7.** (1) What would be the reactor volumes if the two intermediate conversions were changed to 20% and 50%, respectively. (2) What would be the conversions,  $X_1$ ,  $X_2$ , and  $X_3$ , if all the reactors had the same volume of  $100 \text{ dm}^3$  and were placed in the same order? (3) What is the worst possible way to arrange the two CSTRs and one PFR?
- (e) **Example 2-8.** The space time required to achieve 80% conversion in a CSTR is 5 h. The entering volumetric flow rate and concentration of reactant A are  $1 \text{ dm}^3/\text{min}$  and 2.5 molar, respectively. If possible, determine (1) the rate of reaction,  $-r_A = \underline{\hspace{2cm}}$ , (2) the reactor volume,  $V = \underline{\hspace{2cm}}$ , (3) the exit concentration of A,  $C_A = \underline{\hspace{2cm}}$ , and (4) the PFR space time for 80% conversion.

You have two CSTRs and two PFRs each with a volume of  $1.6 \text{ m}^3$ . Use Figure 2-2 to calculate the conversion for each of the reactors in the following arrangements.

- (a) Two CSTRs in series.
- (b) Two PFRs in series.
- (c) Two CSTRs in parallel with the feed,  $F_{A0}$ , divided equally between the two reactors.
- (d) Two PFRs in parallel with the feed divided equally between the two reactors.
- (e) A CSTR and a PFR in parallel with the flow equally divided. Also calculate the overall conversion,  $X_{ov}$ .

$$X_{ov} = \frac{F_{A0} - F_{ACSTR} - F_{APFR}}{F_{A0}}, \text{ with } F_{ACSTR} = \frac{F_{A0}}{2} - \frac{F_{A0}}{2} X_{CSTR}$$

$$F_{APFR} = \frac{F_{A0}}{2} (1 - X_{PFR})$$

- (f) A PFR followed by a CSTR.





- (g) A CSTR followed by a PFR.  
 (h) A PFR followed by two CSTRs. Is this arrangement a good one or is there a better one?
- P2-6<sub>A</sub>** Read the chemical reaction engineer of hippopotamus on the CD-ROM or on the web.
- (a) Write five sentences summarizing what you learned from the web module.  
 (b) Work problems (1) and (2) on the hippo module.  
 (c) The hippo has picked up a river fungus and now the effective volume of the CSTR stomach compartment is only 0.2 m<sup>3</sup>. The hippo needs 30% conversion to survive? Will the hippo survive?  
 (d) The hippo had to have surgery to remove a blockage. Unfortunately, the surgeon, Dr. No, accidentally reversed the CSTR and the PFR during the operation. **Oops!!** What will be the conversion with the new digestive arrangement? Can the hippo survive?
- P2-7<sub>B</sub>** The exothermic reaction

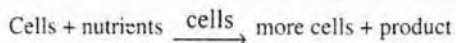


was carried out adiabatically and the following data recorded:

$X$	0	0.2	0.4	0.45	0.5	0.6	0.8	0.9
$-r_A$ (mol/dm <sup>3</sup> ·min)	1.0	1.67	5.0	5.0	5.0	5.0	1.25	0.91

The entering molar flow rate of A was 300 mol/min.

- (a) What are the PFR and CSTR volumes necessary to achieve 40% conversion? ( $V_{\text{PFR}} = 72 \text{ dm}^3$ ,  $V_{\text{CSTR}} = 24 \text{ dm}^3$ )  
 (b) Over what range of conversions would the CSTR and PFR reactor volumes be identical?  
 (c) What is the maximum conversion that can be achieved in a 10.5-dm<sup>3</sup> CSTR?  
 (d) What conversion can be achieved if a 72-dm<sup>3</sup> PFR is followed in series by a 24-dm<sup>3</sup> CSTR?  
 (e) What conversion can be achieved if a 24-dm<sup>3</sup> CSTR is followed in a series by a 72-dm<sup>3</sup> PFR?  
 (f) Plot the conversion and rate of reaction as a function of PFR reactor volume up to a volume of 100 dm<sup>3</sup>.
- P2-8<sub>B</sub>** In bioreactors, the growth is autocatalytic in that the more cells you have, the greater the growth rate



The cell growth rate,  $r_g$ , and the rate of nutrient consumption,  $r_s$ , are directly proportional to the concentration of cells for a given set of conditions. A

Levenspiel plot of  $(1/-r_s)$  a function of nutrient conversion  $X_S = (C_{S0} - C_S)/C_{S0}$  is given below in Figure P2-8.

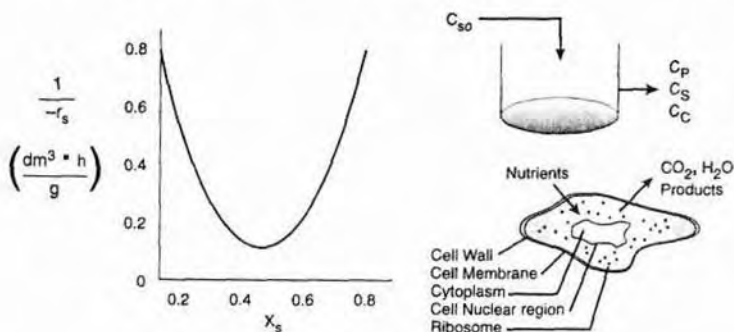


Figure P2-8 Levenspiel plot for bacteria growth.

For a nutrient feed rate of 1 kg/hr with  $C_{S0} = 0.25 \text{ g/dm}^3$ , what chemostat (CSTR) size is necessary to achieve.

- 40% conversion of the substrate.
- 80% conversion of the substrate.
- What conversion could you achieve with an 80-dm<sup>3</sup> CSTR? An 80-dm<sup>3</sup> PFR?
- How could you arrange a CSTR and PFR in series to achieve 80% conversion with the minimum total volume? Repeat for two CSTRs in series.
- Show that Monod Equation for cell growth

$$-r_s = \frac{kC_S C_C}{K_M + C_S}$$

along with the stoichiometric relationship between the cell concentration,  $C_C$ , and the substrate concentration,  $C_S$ ,

$$C_C = Y_{C/S}[C_{S0} - C_S] + C_{C0} = 0.1[C_{S0} - C_S] + 0.001$$

is consistent with Figure P2-8<sub>B</sub>.

**P2-9<sub>B</sub>** The adiabatic exothermic irreversible gas-phase reaction



is to be carried out in a flow reactor for an equimolar feed of A and B. A Levenspiel plot for this reaction is shown in Figure P2-9.

- What PFR volume is necessary to achieve 50% conversion?
- What CSTR volume is necessary to achieve 50% conversion?
- What is the volume of a second CSTR added in series to the first CSTR (**Part B**) necessary to achieve an overall conversion of 80%?
- What PFR volume must be added to the first CSTR (**Part B**) to raise the conversion to 80%?
- What conversion can be achieved in a  $6 \times 10^4 \text{ m}^3$  CSTR and also in a  $6 \times 10^4 \text{ m}^3$  PFR?
- Critique the shape of Figure P2-9 and the answers (numbers) to this problem.

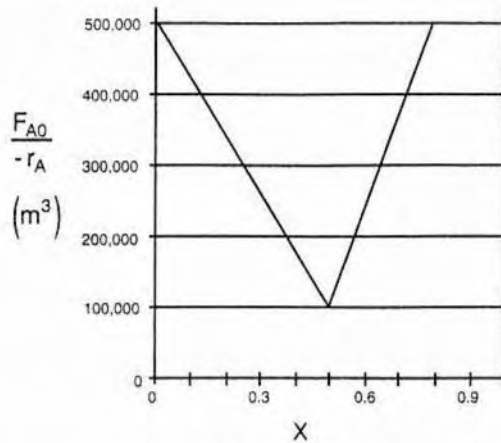


Figure P2-9 Levenspiel plot.

- P2-10<sub>A</sub>** Estimate the reactor volumes of the two CSTRs and the PFR shown in the photo in Figure 2-9.
- P2-11<sub>D</sub>** Don't calculate anything. Just go home and relax.
- P2-12<sub>B</sub>** The curve shown in Figure 2-1 is typical of a reaction carried out isothermally and the curve shown in Figure P2-12 is typical of gas-solid catalytic exothermic reaction carried out adiabatically.

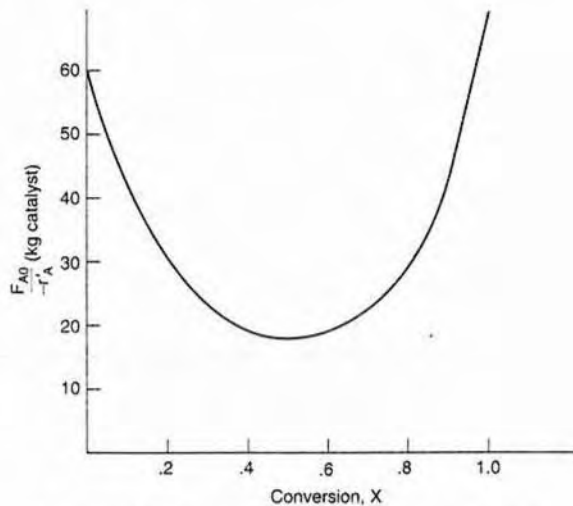
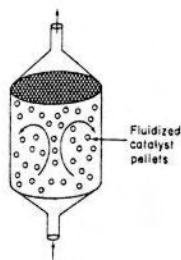


Figure P2-12 Levenspiel plot for an exothermic reaction.



- Assuming that you have a fluidized CSTR and a PBR containing equal weights of catalyst, how should they be arranged for this adiabatic reaction? In each case, use the smallest amount of catalyst weight and still achieve 80% conversion.
- What is the catalyst weight necessary to achieve 80% conversion in a fluidized CSTR?
- What fluidized CSTR weight is necessary to achieve 40% conversion?
- What PBR weight is necessary to achieve 80% conversion?
- What PBR weight is necessary to achieve 40% conversion?
- Plot the rate of reaction and conversion as a function of PBR volume.
- Write a paragraph describing how you would arrange reactors for different  $-r_A$  versus  $X$  curves.

Additional information:  $F_{A0} = 2 \text{ mol/s}$ .

• **Additional Homework Problems on the CD-ROM**

- CDP2-A<sub>B</sub>** Use Levenspiel plots to calculate PFR and CSTR reactor volumes given  $-r_A = f(X)$ . (Includes Solution) [2nd Ed. P2-12<sub>B</sub>]
- CDP2-B<sub>A</sub>** An ethical dilemma as to how to determine the reactor size in a competitor's chemical plant. [2nd Ed. P2-18<sub>B</sub>]
- CDP2-C<sub>B</sub>** Uses an unusual rate law and asks how to best arrange the reactors. This problem is a good practice problem before running the ICM "Staging." (PDF) [3rd Ed. P2-7]
- CDP2-D<sub>B</sub>** Use Levenspiel plots to calculate PFR and CSTR volumes. (PDF) [3rd Ed. P2-9]
- CDP2-E<sub>A</sub>** Use Levenspiel plots to calculate PFR and CSTR volumes.
- CDP2-F<sub>A</sub>** Use Levenspiel plots to calculate CSTR and PFR volumes for the reaction  $A + B \rightarrow C$ .

## SUPPLEMENTARY READING

- Further discussion of stoichiometry may be found in

HIMMELBLAU, D. M., and J. D. Riggs, *Basic Principles and Calculations in Chemical Engineering*, 7th ed. Upper Saddle River, N.J.: Prentice Hall, 2004, Chapters 2 and 6.

FELDER, R. M., and R. W. ROUSSEAU, *Elementary Principles of Chemical Processes*, 3rd ed. New York: Wiley, 2000, Chapter 4.

- Further discussion of the proper staging of reactors in series for various rate laws, in which a plot of  $-1/r_A$  versus  $X$  is given, is presented in

LEVENSPIEL, O., *Chemical Reaction Engineering*, 3rd ed. New York: Wiley, 1999, Chapter 6 (pp. 139–156).

HILL, C. G., *An Introduction to Chemical Engineering Kinetics and Reactor Design*. New York: Wiley, 1977, Chapter 8.

