As with the PFR, the PBR is assumed to have no radial gradients in concentration, temperature, or reaction rate. The generalized mole balance on species A over catalyst weight ΔW results in the equation

$$\begin{array}{ccccccc} \textbf{\textit{In}} & - & \textbf{\textit{Out}} & + & \textbf{\textit{Generation}} & = & \textbf{\textit{Accumulation}} \\ F_{A|W} & - & F_{A|(W+\Delta W)} & + & r'_A\,\Delta W & = & 0 \end{array} \tag{1-14}$$

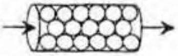
The dimensions of the generation term in Equation (1-14) are

$$(r'_A)\,\Delta W \equiv \frac{moles\ A}{(time)(mass\ of\ catalyst)} \cdot (mass\ of\ catalyst) \equiv \frac{moles\ A}{time}$$

which are, as expected, the same dimensions of the molar flow rate F_A. After dividing by ΔW and taking the limit as $\Delta W \to 0$, we arrive at the differential form of the mole balance for a packed-bed reactor:

Use differential form of design equation for catalyst decay and pressure drop.

$$\boxed{\frac{dF_A}{dW} = r'_A} \tag{1-15}$$



When pressure drop through the reactor (see Section 4.5) and catalyst decay (see Section 10.7) are neglected, the integral form of the packed-catalyst-bed design equation can be used to calculate the catalyst weight.

Use integral form only for no ΔP and no catalyst decay.

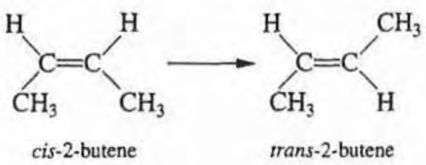
$$W = \int_{F_{A0}}^{F_A} \frac{dF_A}{r'_A} = \int_{F_A}^{F_{A0}} \frac{dF_A}{-r'_A} \tag{1-16}$$

W is the catalyst weight necessary to reduce the entering molar flow rate of species A, F_{A0}, to a flow rate F_A.

For some insight into things to come, consider the following example of how one can use the tubular reactor design Equation (1-11).

Example 1–1 How Large Is It?

Consider the liquid phase *cis – trans* isomerization of 2–butene



which we will write symbolically as

$$A \longrightarrow B$$

The first order ($-r_A = kC_A$) reaction is carried out in a tubular reactor in which the volumetric flow rate, v, is constant, i.e., $v = v_0$.

1. Sketch the concentration profile.
2. Derive an equation relating the reactor volume to the entering and exitin concentrations of A, the rate constant k, and the volumetric flow rate v.
3. Determine the reactor volume necessary to reduce the exiting concentration t 10% of the entering concentration when the volumetric flow rate is 1 dm^3/min (i.e., liters/min) and the specific reaction rate, k, is 0.23 min^{-1}.

Solution

1. Species A is consumed as we move down the reactor, and as a result, both the molar flow rate of A and the concentration of A will decrease as we move. Because the volumetric flow rate is constant, $v = v_0$, one can use Equatio (1-8) to obtain the concentration of A, $C_A = F_A/v_0$, and then by compariso with Figure 1-12 plot the concentration of A as a function of reactor volum as shown in Figure E1-1.1.

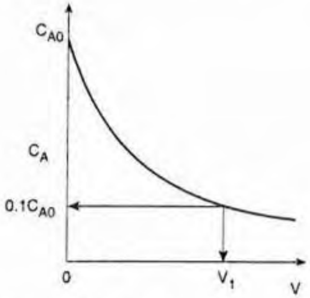


Figure E1-1.1 Concentration profile.

2. Derive an equation relating V, v_0, k, C_{A0}, and C_A.

For a tubular reactor, the mole balance on species A (j = A) was shown to be given by Equation (1-11). Then for species A (j = A) results

$$\frac{dF_A}{dV} = r_A \tag{1-11}$$

For a first-order reaction, the rate law (discussed in Chapter 3) is

$$-r_A = kC_A \tag{E1-1.1}$$

Reactor sizing

Because the volumetric flow rate, v, is constant ($v = v_0$), as it is for most liquid-phase reactions,

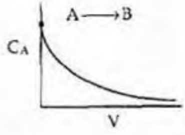
$$\frac{dF_A}{dV} = \frac{d(C_A v)}{dV} = \frac{d(C_A v_0)}{dV} = v_0 \frac{dC_A}{dV} = r_A \tag{E1-1.2}$$

Multiplying both sides of Equation (E1-1.2) by minus one and then substituting Equation (E1-1.1) yields

$$-\frac{v_0 dC_A}{dV} = -r_A = kC_A \tag{E1-1.3}$$

Rearranging gives

$$-\frac{v_0}{k}\left(\frac{dC_A}{C_A}\right)=dV$$



$C_A = C_{A0}\exp - (kV/v)$

Using the conditions at the entrance of the reactor that when $V = 0$, then $C_A = C_{A0}$,

$$-\frac{v_0}{k}\int_{C_{A0}}^{C_A}\frac{dC_A}{C_A}=\int_0^V dV \qquad \text{(E1-1.4)}$$

Carrying out the integration of Equation (E1-1.4) gives

$$\boxed{V=\frac{v_0}{k}\,ln\,\frac{C_{A0}}{C_A}} \qquad \text{(E1-1.5)}$$

3. We want to find the volume, V_1, at which $C_A = \frac{1}{10}C_{A0}$ for $k = 0.23\ \text{min}^{-1}$ and $v_0 = 10\ \text{dm}^3/\text{min}$.

Substituting C_{A0}, C_A, v_0, and k in Equation (E1-1.5), we have

$$V=\frac{10\ \text{dm}^3/\text{min}}{0.23\ \text{min}^{-1}}\ln\frac{C_{A0}}{0.1C_{A0}}=\frac{10\ \text{dm}^3}{0.23}\ln 10 = 100\ \text{dm}^3\ \text{(i.e., 100 L; 0.1 m}^3\text{)}$$

We see that a reactor volume of 0.1 m^3 is necessary to convert 90% of species A entering into product B for the parameters given.

In the remainder of this chapter we look at slightly more detailed drawings of some typical industrial reactors and point out a few of the advantages and disadvantages of each.[2]

1.5 Industrial Reactors

When is a batch reactor used?

Be sure to view actual photographs of industrial reactors on the CD-ROM and on the Web site. There are also links to view reactors on different web sites. The CD-ROM also includes a portion of the *Visual Encyclopedia of Equipment*—Chemical Reactors developed by Dr. Susan Montgomery and her students at University of Michigan.

Links

[1] Liquid-Phase Reactions. Semibatch reactors and CSTRs are used primarily for liquid-phase reactions. A semibatch reactor (Figure 1-15) has essentially the same disadvantages as the batch reactor. However, it has the advantages of temperature control by regulation of the feed rate and the capability of minimizing unwanted side reactions through the maintenance of a low concentration of one of the reactants. The semibatch reactor is also used for two-phase reactions in which a gas usually is bubbled continuously through the liquid.

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[2] *Chem. Eng.*, *63*(10), 211 (1956). See also *AIChE Modular Instruction Series E*, 5 (1984).

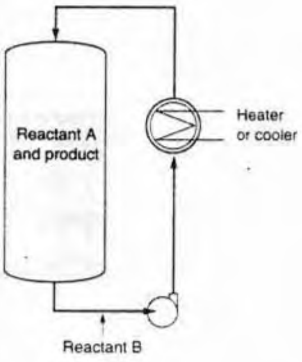


Figure 1-15(a) Semibatch reactor. [Excerpted by special permission from *Chem. Eng.*, *63*(10), 211 (Oct. 1956). Copyright 1956 by McGraw-Hill, Inc., New York, NY 10020.]

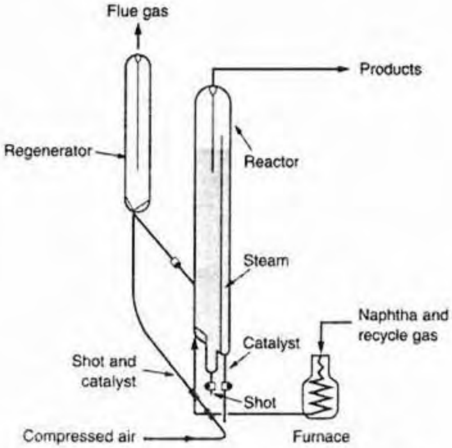


Figure 1-15(b) Fluidized-bed catalytic reactor. [Excerpted by special permission from *Chem. Eng.*, *63*(10), 211 (Oct. 1956). Copyright 1956 by McGraw-Hill, Inc., New York, NY 10020.]

What are the advantages and disadvantages of a CSTR?

A CSTR is used when intense agitation is required. Figure 1-7(a) showed a cutaway view of a Pfaudler CSTR/batch reactor. Table 1-1 gives the typical sizes (along with that of the comparable size of a familiar object) and costs for batch and CSTR reactors. All reactors are glass lined and the prices include heating/cooling jacket, motor, mixer, and baffles. The reactors can be operated at temperatures between 20 and 450°F and at pressures up to 100 psi.

TABLE 1-1. REPRESENTATIVE PFAUDLER CSTR/BATCH REACTOR SIZES AND 2004 PRICES

Volume	*Price*	*Volume*	*Price*
5 Gallons (wastebasket)	$29,000	1000 Gallons (2 Jacuzzis)	$85,000
50 Gallons (garbage can)	$38,000	4000 Gallons (8 Jacuzzis)	$150,000
500 Gallons (Jacuzzi)	$70,000	8000 Gallons (gasoline tanker)	$280,000

The CSTR can either be used by itself or, in the manner shown in Figure 1-16, as part of a series or battery of CSTRs. It is relatively easy to maintain good temperature control with a CSTR because it is well mixed. There is, however, the disadvantage that the conversion of reactant per volume of reactor is the smallest of the flow reactors. Consequently, very large reactors are necessary to obtain high conversions. An industrial flow sheet for the manufacture of nitrobenzene from benzene using a cascade of CSTRs is shown and described in the Professional Reference Shelf for Chapter 1 on the CD-ROM.

Reference Shelf

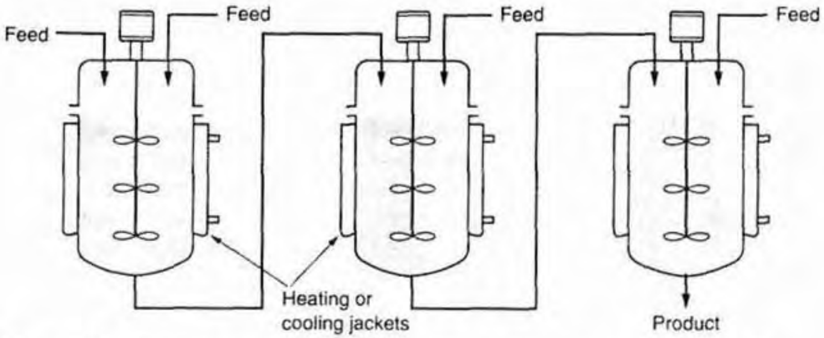


Figure 1-16 Battery of stirred tanks. [Excerpted by special permission from *Chem. Eng.*, *63*(10), 211 (Oct. 1956). Copyright 1956 by McGraw-Hill, Inc., New York, NY 10020.]

Links

If you are not able to afford to purchase a new reactor, it may be possible to find a used reactor that may fit your needs. Previously owned reactors are much less expensive and can be purchased from equipment clearinghouses such as Aaron Equipment Company (*www.aaronequipment.com*) or Loeb Equipment Supply (*www.loebequipment.com/*).

What are the advantages and disadvantages of a PFR?

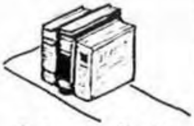
[2] Gas-Phase Reactions. The tubular reactor (i.e., plug-flow reactor [PFR]) is relatively easy to maintain (no moving parts), and it usually produces the highest conversion per reactor volume of any of the flow reactors. The disadvantage of the tubular reactor is that it is difficult to control temperature within the reactor, and hot spots can occur when the reaction is exothermic. The tubular reactor is commonly found either in the form of one long tube or as one of a number of shorter reactors arranged in a tube bank as shown in Figures 1-8(a) and (b). Most homogeneous liquid-phase flow reactors are CSTRs, whereas most homogeneous gas-phase flow reactors are tubular.

CSTR: liquids
PFR: gases

The costs of PFRs and PBRs (without catalyst) are similar to the costs of heat exchangers and can be found in *Plant Design and Economics for Chemical Engineers*, 5th ed., by M. S. Peters and K. D. Timmerhaus (New York: McGraw-Hill, 2002). From Figure 15-12 of the Peters and Timmerhaus book, one can get an estimate of the purchase cost per foot of $1 for a 1-in. pipe and $2 per foot for a 2-in. pipe for single tubes and approximately $20 to $50 per square foot of surface area for fixed-tube sheet exchangers.

A packed-bed (also called a fixed-bed) reactor is essentially a tubular reactor that is packed with solid catalyst particles (Figure 1-13). This heterogeneous reaction system is most often used to catalyze gas reactions. This reactor has the same difficulties with temperature control as other tubular reactors; in addition, the catalyst is usually troublesome to replace. On occasion, channeling of the gas flow occurs, resulting in ineffective use of parts of the reactor bed. The advantage of the packed-bed reactor is that for most reactions it gives the highest conversion per weight of catalyst of any catalytic reactor.

Another type of catalytic reactor in common use is the fluidized-bed (Figure 1-15[b]) reactor, which is analogous to the CSTR in that its contents, though heterogeneous, are well mixed, resulting in an even temperature distribution throughout the bed. The fluidized-bed reactor can only be approximately modeled as a CSTR (Example 10.3); for higher precision it requires a model of its own (Section PRS12.3). The temperature is relatively uniform throughout, thus avoiding hot spots. This type of reactor can handle large amounts of feed and solids and has good temperature control; consequently, it is used in a large number of applications. The advantages of the ease of catalyst replacement or regeneration are sometimes offset by the high cost of the reactor and catalyst regeneration equipment. A thorough discussion of a gas-phase industrial reactor and process can be found on the Professional Reference Shelf of the CD-ROM for Chapter 1. The process is the manufacture of paraffins from synthesis gas (CO and H_2) in a straight-through transport reactor (see Chapter 10).



Reference Shelf

In this chapter, and on the CD-ROM, we've introduced each of the major types of industrial reactors: batch, semibatch, stirred tank, tubular, fixed bed (packed bed), and fluidized bed. Many variations and modifications of these commercial reactors are in current use; for further elaboration, refer to the detailed discussion of industrial reactors given by Walas.[3]

The CD-ROM describes industrial reactors, along with typical feed and operating conditions. In addition, two solved example problems for Chapter 1 can be found on the CD.

Solved Problems

Closure. The goal of this text is to weave the fundamentals of chemical reaction engineering into a structure or algorithm that is easy to use and apply to a variety of problems. We have just finished the first building block of this algorithm: mole balances. This algorithm and its corresponding building blocks will be developed and discussed in the following chapters:

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

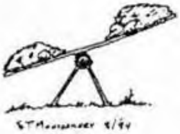
With this algorithm, one can approach and solve chemical reaction engineering problems through logic rather than memorization.

---

[3] S. M. Walas, *Reaction Kinetics for Chemical Engineers* (New York: McGraw-Hill, 1959), Chapter 11.

SUMMARY

Each chapter summary gives the key points of the chapter that need to be remembered and carried into succeeding chapters.



1. A mole balance on species j, which enters, leaves, reacts, and accumulates in a system volume V, is

$$F_{j0}-F_j+\int^V r_j\,dV=\frac{dN_j}{dt} \tag{S1-1}$$

If, and only if, the contents of the reactor are well mixed, then a mole balance (Equation S1-1) on species A gives

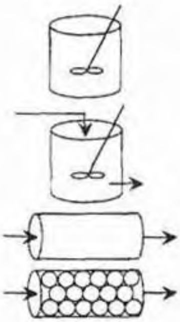
$$F_{A0}-F_A+r_AV=\frac{dN_A}{dt} \tag{S1-2}$$

2. The kinetic rate law for r_j is:
   - Solely a function of properties of reacting materials and reaction conditions (e.g., concentration [activities], temperature, pressure, catalyst or solvent [if any])
   - The rate of formation of species j per unit volume (e.g., mol/s·dm^3)
   - An intensive quantity (i.e., it does not depend on the total amount)
   - An algebraic equation, not a differential equation (e.g., $-r_A=kC_A$, $-r_A=kC_A^2$)

   For homogeneous catalytic systems, typical units of $-r_j$ may be gram moles per second per liter; for heterogeneous systems, typical units of r_j' may be gram moles per second per gram of catalyst. By convention, $-r_A$ is the rate of disappearance of species A and r_A is the rate of formation of species A.

3. Mole balances on species A in four common reactors are as follows:

TABLE S-1 SUMMARY OF REACTOR MOLE BALANCES



Reactor	*Comment*	*Mole Balance Differential Form*	*Algebraic Form*	*Integral Form*
Batch	No spatial variations	$\frac{dN_A}{dt}=r_AV$		$t_1=\int_{N_{A1}}^{N_{A0}}\frac{dN_A}{-r_AV}$
CSTR	No spatial variations, steady state	—	$V=\frac{F_{A0}-F_A}{-r_A}$	—
PFR	Steady state	$\frac{dF_A}{dV}=r_A$		$V_1=\int_{F_{A1}}^{F_{A0}}\frac{dF_A}{-r_A}$
PBR	Steady state	$\frac{dF_A}{dW}=r_A'$		$W_1=\int_{F_{A1}}^{F_{A0}}\frac{dF_A}{-r_A'}$

CD-ROM MATERIAL

Summary Notes

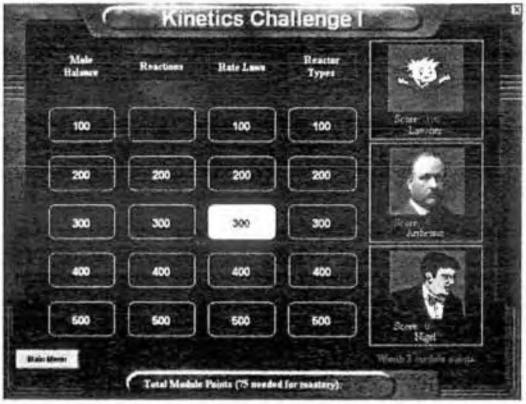
- **Learning Resources**
  1. *Summary Notes*
  2. *Web Material*
     - A. Problem-Solving Algorithm
     - B. Getting Unstuck on a Problem
       This site on the web and CD-ROM gives tips on how to overcome mental barriers in problem solving.
     - C. Smog in L.A. basin

B. Getting Unstuck

C. Smog in L.A.

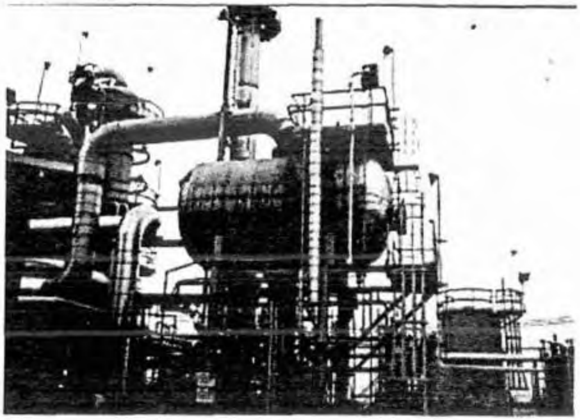
Fotografiert von ©2002 Hank Good.

3. *Interactive Computer Modules*
   - A. Quiz Show I



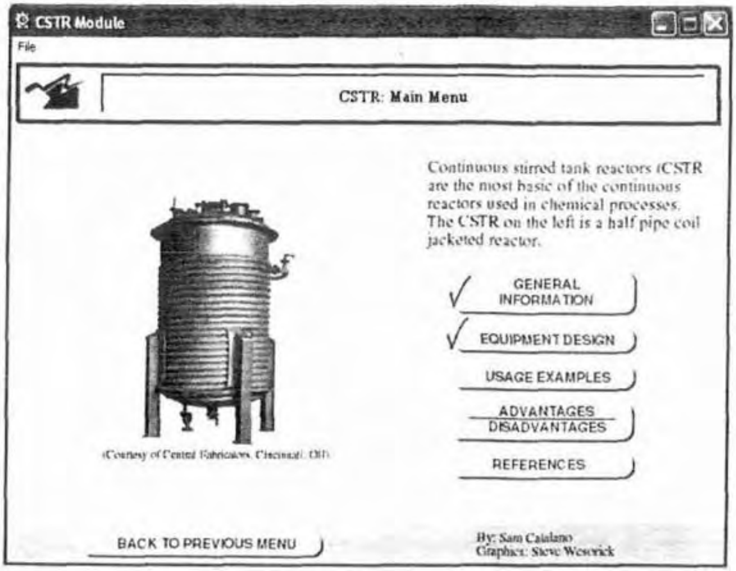
Living Example Problem
Smog in L.A.

4. *Solved Problems*
   A. CDP1-A_B Batch Reactor Calculations: A Hint of Things to Come
   B. P1-14_B Modeling Smog in the L.A. Basin
- **FAQ [Frequently Asked Questions]**—In Updates/FAQ icon section
- **Professional Reference Shelf**
  1. **Photos of Real Reactors**



Reference Shelf

2. **Reactor Section of the *Visual Encyclopedia of Equipment***
   This section of the CD-ROM shows industrial equipment and discusses its operation. The reactor portion of this encyclopedia is included on the CD-ROM accompanying this book.



Continuous stirred tank reactors (CSTR are the most basic of the continuous reactors used in chemical processes. The CSTR on the left is a half pipe coil jacketed reactor.

(Courtesy of Central Fabricators, Cincinnati, OH)

By: Sam Catalano
Graphics: Steve Weserick

Examples of industrial reactions and reactors

3. **The production of nitrobenzene example problem.** Here the process flowsheet is given, along with operating conditions.

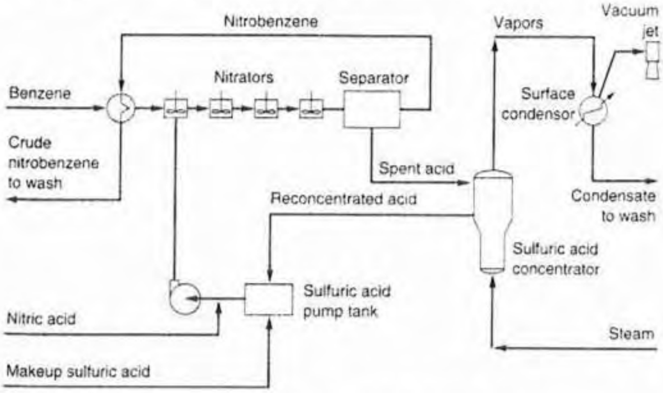


Figure PRS.A-1 Flowsheet for the manufacture of nitrobenzene.

4. **Fischer-Tropsch Reaction and Reactor Example.** A Fischer-Tropsch reaction carried out in a typical straight-through transport reactor (Riser).

Reference Shelf

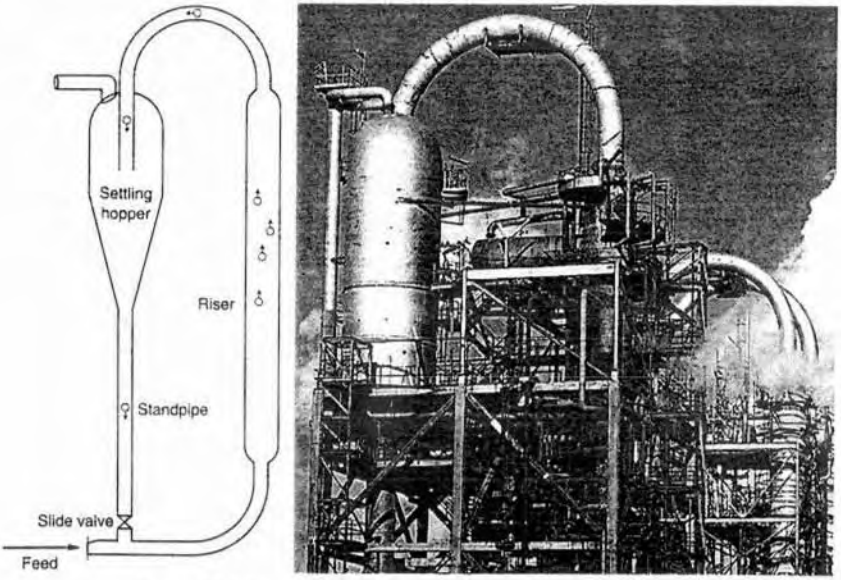


Figure PRS.B-1 The reactor is 3.5 m in diameter and 38 m tall.
[Schematic and photo courtesy of Sasol/Sastech PT Limited.]

Here photographs and schematics of the equipment along with the feed rates, reactor sizes, and principal reactions

$$\mathrm{nCO} + 2\mathrm{nH_2} \longrightarrow \mathrm{C_nH_{2n}} + \mathrm{nH_2O}$$

are also discussed in the PRS.

Homework Problems

QUESTIONS AND PROBLEMS

> I wish I had an answer for that, because I'm getting tired of answering that question.
>
> Yogi Berra, New York Yankees
> *Sports Illustrated*, June 11, 1984

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

A = ● B = ■ C = ◆ D = ◆◆

In each of the questions and problems below, rather than just drawing a box around your answer, write a sentence or two describing how you solved the problem, the assumptions you made, the reasonableness of your answer, what you learned, and any other facts that you want to include. You may wish to refer to W. Strunk and E. B. White, *The Elements of Style*, 4th Ed. (New York: Macmillan, 2000) and Joseph M. Williams, *Style: Ten Lessons in Clarity & Grace*, 6th Ed. (Glenview, Ill.: Scott, Foresman, 1999) to enhance the quality of your sentences.

🔍 = Hint on the web.

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

P1-1$_A$ **(a)** Read through the Preface. Write a paragraph describing both the content goals and the intellectual goals of the course and text. Also describe what's on the CD and how the CD can be used with the text and course.

(b) List the areas in Figure 1-1 you are most looking forward to studying.

(c) Take a quick look at the web modules and list the ones that you feel are the most novel applications of **CRE**.

(d) Visit the problem-solving web site, *www.engin.umich.edu/~cre/probsolv/closed/cep.htm*, to find ways to "Get Unstuck" on a problem and to review the "Problem-Solving Algorithm." List four ways that might help you in your solutions to the home problems.

P1-2$_A$ **(a)** After reading each page or two ask yourself a question. Make a list of the four best questions for this chapter.

(b) Make a list of the five most important things you learned from this chapter.

P1-3$_A$ Visit the web site on Critical and Creative Thinking, *www.engin.umich.edu/~cre/probsolv/strategy/crit-n-creat.htm.*

(a) Write a paragraph describing what "critical thinking" is and how you can develop your critical thinking skills.

(b) Write a paragraph describing what "creative thinking" is and then list four things you will do during the next month that will increase your creative thinking skills.

(c) Write a question based on the material in this chapter that involves critical thinking and explain why it involves critical thinking.
(d) Repeat (c) for creative thinking.
(e) Brainstorm a list of ways you could work problems P-XX (to be specified by your instructor—e.g., Example E-1, or P1-15_B) incorrectly.

Web Hint

P1-4_A Surf the CD-ROM and the web (*www.engin.umich.edu/~cre*). Go on a scavenger hunt using the summary notes for Chapter 1 on the CD-ROM.
(a) What Frequently Asked Question (FAQ) is not really frequently asked?
(b) What **Derive** hot button leads to a picture of a cobra?
(c) What **Self Test** hot button leads to a picture of a rabbit?
(d) What **Example** hot button leads to a picture of a hippo?
(e) Review the objectives for Chapter 1 in the Summary Notes on the CD-ROM. Write a paragraph in which you describe how well you feel you met these objectives. Discuss any difficulties you encountered and three ways (e.g., meet with professor, classmates) you plan to address removing these difficulties.
(f) Look at the Chemical Reactor section of the *Visual Encyclopedia of Equipment* on the CD-ROM. Write a paragraph describing what you learned.
(g) View the photos and schematics on the CD-ROM under Elements of Chemical Reaction Engineering—Chapter 1. Look at the quicktime videos. Write a paragraph describing two or more of the reactors. What similarities and differences do you observe between the reactors on the web (e.g., *www.loebequipment.com*), on the CD-ROM, and in the text? How do the used reactor prices compare with those in Table 1-1?

ICM Quiz Show

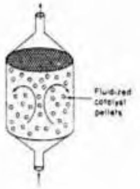
Mole Balance	Reactions	Rate Laws
100	100	100
200	200	200
300	300	300

P1-5_A Load the Interactive Computer Module (ICM) from the CD-ROM. Run the module and then record your performance number for the module which indicates your mastery of the material.
ICM Kinetics Challenge 1 Performance # ____________________

P1-6_B **Example 1-1** Calculate the volume of a CSTR for the conditions used to figure the plug-flow reactor volume in Example 1-1. Which volume is larger, the PFR or the CSTR? Explain why. Suggest two ways to work this problem incorrectly.

P1-7_A Calculate the time to reduce the number of moles of A to 1% of its initial value in a constant-volume batch reactor for the reaction and data in Example 1-1.

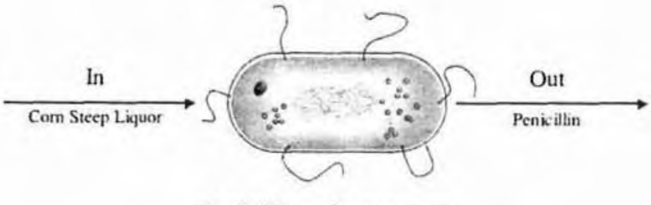
P1-8_A What assumptions were made in the derivation of the design equation for:
(a) the batch reactor?
(b) the CSTR?
(c) the plug-flow reactor (PFR)?
(d) the packed-bed reactor (PBR)?
(e) State in words the meanings of $-r_A$, $-r'_A$, and r'_A. Is the reaction rate $-r_A$ an extensive quantity? Explain.



P1-9_A Use the mole balance to derive an equation analogous to Equation (1-7) for a fluidized CSTR containing catalyst particles in terms of the catalyst weight, *W*, and other appropriate terms. *Hint:* See margin figure.

P1-10$_A$ How can you convert the general mole balance equation for a given species, Equation (1-4), to a general mass balance equation for that species?

P1-11$_B$ We are going to consider the cell as a reactor. The nutrient corn steep liquor enters the cell of the microorganism *Penicillium chrysogenum* and is decomposed to form such products as amino acids, RNA, and DNA. Write an unsteady mass balance on (a) the corn steep liquor, (b) RNA, and (c) penicillin. Assume the cell is well mixed and that RNA remains inside the cell.



Penicillium chrysogenum

P1-12$_A$ The United States produced 32.5% of the world's chemical products in 2002 according to "Global Top 50," *Chemical and Engineering News*, July 28, 2003. Table P1-12.1 lists the 10 most produced chemicals in 2002.

TABLE P1-12.1. CHEMICAL PRODUCTION

2002 Chemical	*Thousands of Metric Tons*	*1995 Rank*	*2002 Chemical*	*Thousands of Metric Tons*	*1995 Rank*
1. H_2SO_4	36,567	1	6. H_2	13,989	—
2. N_2	26,448	2	7. NH_3	13,171	6
3. C_2H_4	23,644	4	8. Cl_2	11,362	10
4. O_2	16,735	3	9. P_2O_5	10,789	—
5. C_3H_6	14,425	9	10. $C_2H_2Cl_2$	9,328	—

Reference: *Chemical and Engineering News*, July 7, 2003, *http://pubs.acs.org/cen/*

(a) What were the 10 most produced chemicals for the year that just ended? Were there any significant changes from the 1995 statistics? (See Chapter 1 of 3rd edition of *Elements of CRE*.) The same issue of *C&E News* ranks chemical companies as given in Table P1-12.2.

(b) What 10 companies were tops in sales for the year just ended? Did any significant changes occur compared to the 2002 statistics?

(c) Why do you think H_2SO_4 is the most produced chemical? What are some of its uses?

(d) What is the current annual production rate (lb/yr) of ethylene, ethylene oxide, and benzene?

(e) Why do you suspect there are so few organic chemicals in the top 10?

TABLE P1-12.2. TOP COMPANIES IN SALES

Rank 2002	*Rank 2001*	*Rank 2000*	*Rank 1999*	*Rank 1995*	*Company*	*Chemical Sales [$ millions]*
1	1	2	2	1	Dow Chemical	27,609
2	2	1	1	2	Dupont	26,728
3	3	3	3	3	ExxonMobil	16,408
4	5	5	6	6	General Electric	7,651
5	4	4	4	—	Huntsman Corp.	7,200
6	8	10	9	—	PPG Industries	5,996
7	9	8	10	—	Equistar Chemicals	5,537
8	7	7	—	—	Chevron Phillips	5,473
9	—	—	—	—	Eastman Chemical	5,320
10	—	—	—	—	Praxair	5,128

References:

Rank 2002: *Chemical and Engineering News*, May 12, 2003.
Rank 2001: *Chemical and Engineering News*, May 13, 2002.
Rank 2000: *Chemical and Engineering News*, May 7, 2001.
Rank 1999: *Chemical and Engineering News*, May 1, 2000.
http://pubs.acs-org/cen/

P1-13$_A$ Referring to the text material and the additional references on commercia reactors given at the end of this chapter, fill in Table P1-13.

TABLE P1.13 COMPARISON OF REACTOR TYPES

Type of Reactor	*Characteristics*	*Kinds of Phases Present*	*Use*	*Advantages*	*Disadvantages*
Batch					
CSTR					
PFR					
PBR					

Hall of Fame

P1-14$_B$ Schematic diagrams of the Los Angeles basin are shown in Figure P1-14. The basin floor covers approximately 700 square miles ($2 \times 10^{10}\ ft^2$) and is almos completely surrounded by mountain ranges. If one assumes an inversior height in the basin of 2000 ft, the corresponding volume of air in the basin i: $4 \times 10^{13}\ ft^3$. We shall use this system volume to model the accumulation anc depletion of air pollutants. As a very rough first approximation, we shall trea the Los Angeles basin as a well-mixed container (analogous to a CSTR) ir which there are no spatial variations in pollutant concentrations.

Web Hint

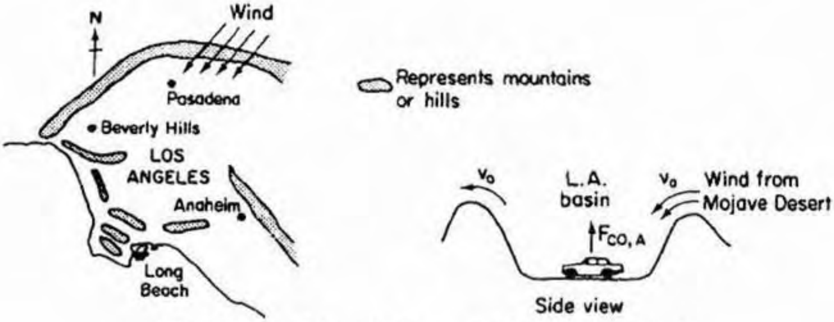


Figure P1-14 Schematic diagrams of the Los Angeles basin.

Living Example Problem

We shall perform an unsteady-state mole balance on CO as it is depleted from the basin area by a Santa Ana wind. Santa Ana winds are high-velocity winds that originate in the Mojave Desert just to the northeast of Los Angeles. Load the **Smog in Los Angeles Basin Web Module.** Use the data in the module to work part 1–14 (a) through (h) given in the module. Load the **living example polymath code** and explore the problem. For part (i), vary the parameters v_0, a, and b, and write a paragraph describing what you find.

There is heavier traffic in the L.A. basin in the mornings and in the evenings as workers go to and from work in downtown L.A. Consequently, the flow of CO into the L.A. basin might be better represented by the sine function over a 24-hour period.

P1-15$_B$ The reaction

$$A \longrightarrow B$$

is to be carried out isothermally in a continuous-flow reactor. Calculate both the CSTR and PFR reactor volumes necessary to consume 99% of A (i.e., $C_A = 0.01C_{A0}$) when the entering molar flow rate is 5 mol/h, assuming the reaction rate $-r_A$ is:

(a) $-r_A = k$ with $k = 0.05 \dfrac{\text{mol}}{\text{h}\cdot\text{dm}^3}$ (*Ans.*: $V = 99\ \text{dm}^3$)

(b) $-r_A = kC_A$ with $k = 0.0001\ \text{s}^{-1}$

(c) $-r_A = kC_A^2$ with $k = 3 \dfrac{\text{dm}^3}{\text{mol}\cdot\text{h}}$ (*Ans.*: $V_{\text{CSTR}} = 66{,}000\ \text{dm}^3$)

The entering volumetric flow rate is 10 dm³/h. (*Note*: $F_A = C_A v$. For a constant volumetric flow rate $v = v_0$, then $F_A = C_A v_0$. Also, $C_{A0} = F_{A0}/v_0 = [5\ \text{mol/h}]/[10\ \text{dm}^3/\text{h}] = 0.5\ \text{mol/dm}^3$.)

(d) Repeat **(a)**, **(b)**, and **(c)** to calculate the time necessary to consume 99.9% of species A in a 1000 dm³ constant volume batch reactor with $C_{A0} = 0.5$ mol/dm³.

P1-16$_B$ Write a one-paragraph summary of a journal article on chemical kinetics or reaction engineering. The article must have been published within the last five years. What did you learn from this article? Why is the article important?

P1-17$_B$ **(a)** There are initially 500 rabbits (x) and 200 foxes (y) on Farmer Oat's property. Use Polymath or MATLAB to plot the concentration of foxes and rabbits as a function of time for a period of up to 500 days. The predator–prey relationships are given by the following set of coupled ordinary differential equations:

$$\frac{dx}{dt} = k_1 x - k_2 x \cdot y$$

$$\frac{dy}{dt} = k_3 x \cdot y - k_4 y$$

Constant for growth of rabbits $k_1 = 0.02\ day^{-1}$
Constant for death of rabbits $k_2 = 0.00004/(\text{day} \times \text{no. of foxes})$
Constant for growth of foxes after eating rabbits $k_3 = 0.0004/(\text{day} \times \text{no. of rabbits})$
Constant for death of foxes $k_4 = 0.04\ day^{-1}$
What do your results look like for the case of $k_3 = 0.00004/(\text{day} \times \text{no. of rabbits})$ and $t_{\text{final}} = 800$ days? Also plot the number of foxes versus the number of rabbits. Explain why the curves look the way they do.
Vary the parameters k_1, k_2, k_3, and k_4. Discuss which parameters can or cannot be larger than others. Write a paragraph describing what you find.

(b) Use Polymath or MATLAB to solve the following set of nonlinear algebraic equations:

Polymath Tutorial

$$x^3 y - 4y^2 + 3x = 1$$

$$6y^2 - 9xy = 5$$

with initial guesses of $x = 2$, $y = 2$. Try to become familiar with the edit keys in Polymath MATLAB. See the CD-ROM for instructions.

Summary Notes

Screen shots on how to run Polymath are shown at the end of Summary Notes for Chapter 1 on the CD-ROM and on the web.

P1-18$_C$ **What if:**

(a) the benzene feed stream in Example R1.3-1 in the PRS were not preheated by the product stream? What would be the consequences?

(b) you needed the cost of a 6000-gallon and a 15,000-gallon Pfaudler reactor? What would they be?

(c) the exit concentration of A in Example 1-1 were specified at 0.1% of the entering concentration?

(d) only one operator showed up to run the nitrobenzene plant. What would be some of your first concerns?

P1-19$_A$ **Enrico Fermi (1901–1954) Problems** (**EEP**). Enrico Fermi was an Italian physicist who received the Nobel Prize for his work on nuclear processes. Fermi was famous for his "Back of the Envelope Order of Magnitude Calculation" to obtain an estimate of the answer through *logic* and making reasonable assumptions. He used a process to set bounds on the answer by saying it is probably larger than one number and smaller than another and arrived at an answer that was within a factor of 10.

http://mathforum.org/workshops/sum96/interdisc/sheila2.html

Enrico Fermi Problem (EFP) #1

How many piano tuners are there in the city of Chicago? Show the steps in your reasoning.

Web Hint

1. Population of Chicago __________
2. Number of people per household __________

3. Number of households _________
4. Households with pianos _________
5. Average number of tunes per year _________
6. Etc. _________

An answer is given on the web under Summary Notes for Chapter 1.

P1-20$_A$ EFP #2. How many square meters of pizza were eaten by an undergraduate student body population of 20,000 during the Fall term 2004?

P1-21$_B$ This problem will be used in each of the following chapters to help develop critical-thinking skills.

(a) Write a question about this problem that involve critical thinking.
(b) What generalizations can you make about the results of this problem?
(c) Write a question that will expand this problem.

P1-22 New material for the 2nd printing the following changes/additions have been made to the 2nd printing.

NOTE TO INSTRUCTORS: Additional problems (cf. those from the preceding editions) can be found in the solutions manual and on the CD-ROM. These problems could be photocopied and used to help reinforce the fundamental principles discussed in this chapter.

Solved Problems

CDP1-A$_A$ Calculate the time to consume 80% of species A in a constant-volume batch reactor for a first- and a second-order reaction. (**Includes Solution**)

CDP1-B$_A$ Derive the differential mole balance equation for a foam reactor. [2nd Ed. P1-10$_B$]

SUPPLEMENTARY READING

1. For further elaboration of the development of the general balance equation, see not only the web site *www.engin.umich.edu/~cre* but also

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

   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.

   SANDERS, R. J., *The Anatomy of Skiing*. Denver, CO: Golden Bell Press, 1976.

2. A detailed explanation of a number of topics in this chapter can be found in

   CRYNES, B. L., and H. S. FOGLER, eds., *AIChE Modular Instruction Series E: Kinetics*, Vols. 1 and 2. New York: AIChE, 1981.

3. An excellent description of the various types of commercial reactors used in industry is found in Chapter 11 of

   WALAS, S. M., *Reaction Kinetics for Chemical Engineers*. New York: McGraw-Hill, 1959.

4. A discussion of some of the most important industrial processes is presented by

   MEYERS, R.A., *Handbook of Chemicals Production Processes*. New York: McGraw-Hill, 1986.

   See also

   MCKETTA, J. J., ed., *Encyclopedia of Chemical Processes and Design*. New York: Marcel Dekker, 1976.

A similar book, which describes a larger number of processes, is

AUSTIN, G. T., *Shreve's Chemical Process Industries*. 5th ed. New York McGraw-Hill, 1984.

5. The following journals may be useful in obtaining information on chemical reaction engineering: *International Journal of Chemical Kinetics, Journal of Catalysis Journal of Applied Catalysis, AIChE Journal, Chemical Engineering Science Canadian Journal of Chemical Engineering, Chemical Engineering Communications, Journal of Physical Chemistry,* and *Industrial and Engineering Chemistry Research.*

6. The price of chemicals can be found in such journals as the *Chemical Marketing Reporter, Chemical Weekly*, and *Chemical Engineering News* and on the ACS web site *http://pubs.acs.org/cen*.