

# ELEMENTS OF CHEMICAL REACTION ENGINEERING

SIXTH EDITION

H. SCOTT FOGLER



INTERNATIONAL SERIES IN THE  
PHYSICAL AND CHEMICAL ENGINEERING SCIENCES



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of Chemical  
Reaction  
Engineering*

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H. SCOTT FOGLER

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*Dedicated to*

*Janet Meadors Fogler*

*For her companionship, encouragement,  
sense of humor, love, and support throughout the years*

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# Contents

INTRODUCTION					xix
ABOUT THE AUTHOR					xxxiii
CHAPTER 1	MOLE BALANCES				1
1.1	The Rate of Reaction, $-r_A$	4			
1.2	The General Mole Balance Equation (GMBE)		8		
1.3	Batch Reactors (BRs)	10			
1.4	Continuous-Flow Reactors	12			
1.4.1	Continuous-Stirred Tank Reactor (CSTR)		12		
1.4.2	Tubular Reactor	14			
1.4.3	Packed-Bed Reactor (PBR)	18			
1.4.4	Well-Mixed "Fluidized" Catalytic Bed Reactor		20		
1.5	Industrial Reactors	24			
1.6	And Now... A Word from Our Sponsor—Safety 1 (AWFOS–S1 Safety)	25			
1.6.1	What Is Chemical Process Safety?		25		
1.6.2	Why Study Process Safety?		25		
CHAPTER 2	CONVERSION AND REACTOR SIZING				35
2.1	Definition of Conversion	36			
2.2	Batch Reactor Design Equations	36			
2.3	Design Equations for Flow Reactors	39			
2.3.1	CSTR (Also Known as a Backmix Reactor or a Vat)		40		
2.3.2	Tubular Flow Reactor (PFR)	40			
2.3.3	Packed-Bed Reactor (PBR)	41			
2.4	Sizing Continuous-Flow Reactors	42			

2.5	<b>Reactors in Series</b>	<b>51</b>
2.5.1	CSTRs in Series	52
2.5.2	PFRs in Series	56
2.5.3	Combinations of CSTRs and PFRs in Series	57
2.5.4	Comparing the CSTR and PFR Volumes and Reactor Sequencing	61
2.6	<b>Some Further Definitions</b>	<b>62</b>
2.6.1	Space Time	62
2.6.2	Space Velocity	64
2.7	<b>And Now... A Word from Our Sponsor—Safety 2 (AWFOS–S2 The NFPA Diamond)</b>	<b>66</b>

## CHAPTER 3 RATE LAWS 75

3.1	<b>Basic Definitions</b>	<b>76</b>
3.1.1	Relative Rates of Reaction	77
3.2	<b>The Rate Law</b>	<b>78</b>
3.2.1	Power Law Models and Elementary Rate Laws	79
3.2.2	Nonelementary Rate Laws	82
3.2.3	Reversible Reactions	86
3.3	<b>The Reaction-Rate Constant</b>	<b>89</b>
3.3.1	The Rate Constant $k$ and Its Temperature Dependence	89
3.3.2	Interpretation of the Activation Energy	90
3.3.3	The Arrhenius Plot	96
3.4	<b>Molecular Simulations</b>	<b>100</b>
3.4.1	Historical Perspective	100
3.4.2	Stochastic Modeling of Reactions	101
3.5	<b>Present Status of Our Approach to Reactor Sizing and Design</b>	<b>103</b>
3.6	<b>And Now... A Word from Our Sponsor—Safety 3 (AWFOS–S3 The GHS Diamond)</b>	<b>104</b>

## CHAPTER 4 STOICHIOMETRY 117

4.1	<b>Batch Reactors (BRs)</b>	<b>119</b>
4.1.1	Batch Concentrations for the Generic Reaction, Equation (2-2)	121
4.2	<b>Flow Systems</b>	<b>125</b>
4.2.1	Equations for Concentrations in Flow Systems	126
4.2.2	Liquid-Phase Concentrations	126
4.2.3	Gas-Phase Concentrations	127
4.3	<b>Reversible Reactions and Equilibrium Conversion</b>	<b>138</b>
4.4	<b>And Now... A Word from Our Sponsor—Safety 4 (AWFOS–S4 The Swiss Cheese Model)</b>	<b>143</b>

## CHAPTER 5 ISOTHERMAL REACTOR DESIGN: CONVERSION 155

5.1	<b>Design Structure for Isothermal Reactors</b>	<b>156</b>
5.2	<b>Batch Reactors (BRs)</b>	<b>160</b>
5.2.1	Batch Reaction Times	161

5.3	<b>Continuous-Stirred Tank Reactors (CSTRs)</b>	<b>168</b>
5.3.1	A Single CSTR	168
5.3.2	CSTRs in Series	171
5.4	<b>Tubular Reactors</b>	<b>178</b>
5.4.1	Liquid-Phase Reactions in a PFR $\therefore v = v_0$	179
5.4.2	Gas-Phase Reactions in a PFR [ $v = v_0(1 + \epsilon X)/(T/T_0)(P_0/P)$ ]	180
5.4.3	Effect of $\epsilon$ on Conversion	180
5.5	<b>Pressure Drop in Reactors</b>	<b>185</b>
5.5.1	Pressure Drop and the Rate Law	185
5.5.2	Flow Through a Packed Bed	187
5.5.3	Pressure Drop in Pipes	191
5.5.4	Analytical Solution for Reaction with Pressure Drop	194
5.5.5	Robert the Worrier Wonders: What If...	198
5.6	<b>Synthesizing the Design of a Chemical Plant</b>	<b>208</b>
5.7	<b>And Now... A Word from Our Sponsor—Safety 5</b> (AWFOS–S5 A Safety Analysis of the Incident Algorithm)	<b>210</b>

## CHAPTER 6 ISOTHERMAL REACTOR DESIGN: MOLES AND MOLAR FLOW RATES 229

6.1	The Moles and Molar Flow Rate Balance Algorithms	230
6.2	Mole Balances on CSTRs, PFRs, PBRs, and Batch Reactors	230
6.2.1	Liquid Phase	230
6.2.2	Gas Phase	232
6.3	Application of the PFR Molar Flow Rate Algorithm to a Microreactor	234
6.4	Membrane Reactors	239
6.5	Unsteady-State Operation of Stirred Reactors	248
6.6	Semibatch Reactors	249
6.6.1	Motivation for Using a Semibatch Reactor	249
6.6.2	Semibatch Reactor Mole Balances	249
6.6.3	Equilibrium Conversion	255
6.7	<b>And Now... A Word from Our Sponsor—Safety 6</b> (AWFOS–S6 The BowTie Diagram)	<b>256</b>

## CHAPTER 7 COLLECTION AND ANALYSIS OF RATE DATA 269

7.1	The Algorithm for Data Analysis	270
7.2	Determining the Reaction Order for Each of Two Reactants Using the Method of Excess	272
7.3	Integral Method	273
7.4	Differential Method of Analysis	277
7.4.1	Graphical Differentiation Method	278
7.4.2	Numerical Method	278
7.4.3	Finding the Rate-Law Parameters	279
7.5	Nonlinear Regression	284
7.5.1	Concentration–Time Data	287
7.5.2	Model Discrimination	290

7.6	Reaction-Rate Data from Differential Reactors	290
7.7	Experimental Planning	297
7.8	And Now... A Word from Our Sponsor—Safety 7 (AWFOS–S7 Laboratory Safety)	297

## CHAPTER 8 MULTIPLE REACTIONS 309

8.1	Definitions	310
8.1.1	Types of Reactions	310
8.1.2	Selectivity	311
8.1.3	Yield	312
8.1.4	Conversion	313
8.2	Algorithm for Multiple Reactions	313
8.2.1	Modifications to the Chapter 6 CRE Algorithm for Multiple Reactions	314
8.3	Parallel Reactions	316
8.3.1	Selectivity	316
8.3.2	Maximizing the Desired Product for One Reactant	316
8.3.3	Reactor Selection and Operating Conditions	322
8.4	Reactions in Series	325
8.5	Complex Reactions	335
8.5.1	Complex Gas-Phase Reactions in a PBR	335
8.5.2	Complex Liquid-Phase Reactions in a CSTR	339
8.5.3	Complex Liquid-Phase Reactions in a Semibatch Reactor	341
8.6	Membrane Reactors to Improve Selectivity in Multiple Reactions	343
8.7	Sorting It All Out	348
8.8	The Fun Part	348
8.9	And Now... A Word from Our Sponsor—Safety 8 (AWFOS–S8 The Fire Triangle)	349
8.9.1	The Fire Triangle	350
8.9.2	Defining Some Important Terms	350
8.9.3	Ways to Prevent Fires	350
8.9.4	Ways to Protect from Fires	351

## CHAPTER 9 REACTION MECHANISMS, PATHWAYS, BIOREACTIONS, AND BIOREACTORS 367

9.1	Active Intermediates and Nonelementary Rate Laws	368
9.1.1	Pseudo-Steady-State Hypothesis (PSSH)	369
9.1.2	If Two Molecules Must Collide, How Can the Rate Law Be First Order?	372
9.1.3	Searching for a Mechanism	373
9.1.4	Chain Reactions	377
9.2	Enzymatic Reaction Fundamentals	377
9.2.1	Enzyme–Substrate Complex	378
9.2.2	Mechanisms	380
9.2.3	Michaelis–Menten Equation	383
9.2.4	Batch Reactor Calculations for Enzyme Reactions	389

<b>9.3</b>	<b>Inhibition of Enzyme Reactions</b>	<b>391</b>
9.3.1	Competitive Inhibition	392
9.3.2	Uncompetitive Inhibition	394
9.3.3	Noncompetitive Inhibition (Mixed Inhibition)	396
9.3.4	Substrate Inhibition	398
<b>9.4</b>	<b>Bioreactors and Biosynthesis</b>	<b>399</b>
9.4.1	Cell Growth	403
9.4.2	Rate Laws	404
9.4.3	Stoichiometry	407
9.4.4	Mass Balances	413
9.4.5	Chemostats	418
9.4.6	CSTR Bioreactor Operation	418
9.4.7	Washout	419
<b>9.5</b>	<b>And Now... A Word from Our Sponsor—Safety 9 (AWFOS–S9 Process Safety Triangle)</b>	<b>422</b>
9.5.1	Levels of the Process Safety Triangle	422
9.5.2	Application to Process Safety	423
9.5.3	Examples of Process Safety Triangle	424

## CHAPTER 10 CATALYSIS AND CATALYTIC REACTORS

441

<b>10.1</b>	<b>Catalysts</b>	<b>441</b>
10.1.1	Definitions	442
10.1.2	Catalyst Properties	443
10.1.3	Catalytic Gas–Solid Interactions	445
10.1.4	Classification of Catalysts	446
<b>10.2</b>	<b>Steps in a Catalytic Reaction</b>	<b>447</b>
10.2.1	Mass Transfer Step 1: Diffusion from the Bulk to the External Surface of the Catalyst—An Overview	450
10.2.2	Mass Transfer Step 2: Internal Diffusion—An Overview	451
10.2.3	Adsorption Isotherms	452
10.2.4	Surface Reaction	458
10.2.5	Desorption	460
10.2.6	The Rate-Limiting Step	461
<b>10.3</b>	<b>Synthesizing a Rate Law, Mechanism, and Rate-Limiting Step</b>	<b>463</b>
10.3.1	Is the Adsorption of Cumene Rate-Limiting?	466
10.3.2	Is the Surface Reaction Rate-Limiting?	470
10.3.3	Is the Desorption of Benzene the Rate-Limiting Step (RLS)?	471
10.3.4	Summary of the Cumene Decomposition	473
10.3.5	Reforming Catalysts	474
10.3.6	Rate Laws Derived from the Pseudo-Steady-State Hypothesis (PSSH)	478
10.3.7	Temperature Dependence of the Rate Law	479
<b>10.4</b>	<b>Heterogeneous Data Analysis for Reactor Design</b>	<b>479</b>
10.4.1	Deducing a Rate Law from the Experimental Data	481
10.4.2	Finding a Mechanism Consistent with Experimental Observations	482
10.4.3	Evaluation of the Rate-Law Parameters	484
10.4.4	Reactor Design	486

10.5	Reaction Engineering in Microelectronic Fabrication	490
10.5.1	Overview	490
10.5.2	Chemical Vapor Deposition (CVD)	490
10.6	Model Discrimination	493
10.7	Catalyst Deactivation	496
10.7.1	Types of Catalyst Deactivation	498
10.7.2	Decay in Packed-Bed Reactors	505
10.8	Reactors That Can Be Used to Help Offset Catalyst Decay	507
10.8.1	Temperature–Time Trajectories	508
10.8.2	Moving-Bed Reactors	510
10.8.3	Straight-Through Transport Reactors (STTR)	515
10.9	And Now... A Word from Our Sponsor—Safety 10 (AWFOS–S10 Exxon Mobil Torrance Refinery Explosion Involving a Straight-Through Transport Reactor [STTR])	519

CHAPTER 11 NONISOTHERMAL REACTOR DESIGN: THE STEADY-  
STATE ENERGY BALANCE AND ADIABATIC  
PFR APPLICATIONS 541

11.1	Rationale	542
11.2	The Energy Balance	543
11.2.1	First Law of Thermodynamics	543
11.2.2	Evaluating the Work Term	544
11.2.3	Overview of Energy Balances	546
11.3	The User-Friendly Energy Balance Equations	551
11.3.1	Dissecting the Steady-State Molar Flow Rates to Obtain the Heat of Reaction	551
11.3.2	Dissecting the Enthalpies	553
11.3.3	Relating $\Delta H_{R_x}(T)$ , $\Delta H_{R_x}^{\circ}(T_R)$ , and $\Delta C_P$	554
11.4	Adiabatic Operation $\therefore Q = 0$	557
11.4.1	Adiabatic Energy Balance	557
11.4.2	Adiabatic Tubular Reactor	558
11.5	Adiabatic Equilibrium Conversion	566
11.5.1	Equilibrium Conversion	566
11.6	Reactor Staging with Interstage Cooling or Heating	571
11.6.1	Exothermic Reactions	571
11.6.2	Endothermic Reactions	571
11.7	Optimum Feed Temperature	575
11.8	And Now... A Word from Our Sponsor—Safety 11 (AWFOS–S11 Acronyms)	579

CHAPTER 12 STEADY-STATE NONISOTHERMAL REACTOR  
DESIGN: FLOW REACTORS WITH HEAT EXCHANGE 591

12.1	Steady-State Tubular Reactor with Heat Exchange	592
12.1.1	Deriving the Energy Balance for a PFR	592
12.1.2	Applying the Algorithm to Flow Reactors with Heat Exchange	594
12.2	Balance on the Heat-Transfer Fluid	595
12.2.1	Co-Current Flow	595
12.2.2	Countercurrent Flow	597

12.3	Examples of the Algorithm for PFR/PBR Design with Heat Effects	598	
12.3.1	Applying the Algorithm to an Exothermic Reaction	603	
12.3.2	Applying the Algorithm to an Endothermic Reaction	610	
12.4	CSTR with Heat Effects	619	
12.4.1	Heat Added to the Reactor, $\dot{Q}$	620	
12.5	Multiple Steady States (MSS)	630	
12.5.1	Heat-Removed Term, $R(T)$	632	
12.5.2	Heat-Generated Term, $G(T)$	633	
12.5.3	Ignition–Extinction Curve	634	
12.6	Nonisothermal Multiple Chemical Reactions	637	
12.6.1	Energy Balance for Multiple Reactions in Plug-Flow Reactors	637	
12.6.2	Energy Balance for Multiple Reactions in a CSTR	642	
12.6.3	Series Reactions in a CSTR	642	
12.6.4	Complex Reactions in a PFR	645	
12.7	Radial and Axial Temperature Variations in a Tubular Reactor	652	
12.8	And Now... A Word from Our Sponsor—Safety 12 (AWFOS–S12 Safety Statistics)	652	
12.8.1	The Process Safety Across the Chemical Engineering Curriculum Web site	652	
12.8.2	Safety Statistics	653	
12.8.3	Additional Resources CCPS and SChE	654	

## CHAPTER 13 UNSTEADY-STATE NONISOTHERMAL REACTOR DESIGN 681

13.1	The Unsteady-State Energy Balance	682	
13.2	Energy Balance on Batch Reactors (BRs)	684	
13.2.1	Adiabatic Operation of a Batch Reactor	686	
13.2.2	Case History of a Batch Reactor with Interrupted Isothermal Operation Causing a <b>Runaway Reaction</b>	693	
13.3	Batch and Semibatch Reactors with a Heat Exchanger	700	
13.3.1	Startup of a CSTR	702	
13.3.2	Semibatch Operation	707	
13.4	Nonisothermal Multiple Reactions	711	
13.5	And Now... A Word from Our Sponsor—Safety 13 (AWFOS–S13 Safety Analysis of the T2 Laboratories Incident)	723	

## CHAPTER 14 MASS TRANSFER LIMITATIONS IN REACTING SYSTEMS 739

14.1	Diffusion Fundamentals	740	
14.1.1	Definitions	741	
14.1.2	Molar Flux: $W_A$	742	
14.1.3	Fick's First Law	743	
14.2	Binary Diffusion	744	
14.2.1	Evaluating the Molar Flux	744	
14.2.2	Diffusion and Convective Transport	744	
14.2.3	Boundary Conditions	746	
14.2.4	Temperature and Pressure Dependence of $D_{AB}$	746	

14.3	Modeling Diffusion with Chemical Reaction	748
14.3.1	Diffusion through a Stagnant Film to a Particle	748
14.4	The Mass Transfer Coefficient	750
14.5	Mass Transfer to a Single Particle	752
14.5.1	First-Order Rate Laws	752
14.5.2	Limiting Regimes	754
14.6	The Shrinking Core Model	758
14.6.1	Dust Explosions, Particle Dissolution, and Catalyst Regeneration	758
14.7	Mass Transfer–Limited Reactions in Packed Beds	763
14.8	Robert the Worrier	766
14.9	What If . . . ? (Parameter Sensitivity)	770
14.10	And Now . . . A Word from Our Sponsor—Safety 14 (AWFOS–S14 Sugar Dust Explosion)	778

## CHAPTER 15 DIFFUSION AND REACTION

791

15.1	Diffusion and Reactions in Homogeneous Systems	792
15.2	Diffusion and Reactions in Spherical Catalyst Pellets	793
15.2.1	Effective Diffusivity	793
15.2.2	Derivation of the Differential Equation Describing Diffusion and Reaction in a Single Spherical Catalyst Pellet	795
15.2.3	Writing the Diffusion with the Catalytic Reaction Equation in Dimensionless Form	798
15.2.4	Solution to the Differential Equation for a First-Order Reaction	801
15.3	The Internal Effectiveness Factor	802
15.3.1	Isothermal First-Order Catalytic Reactions	802
15.3.2	Effectiveness Factors with Volume Change with Reaction	806
15.3.3	Internal-Diffusion-Limited Reactions Other Than First Order	806
15.3.4	Weisz–Prater Criterion for Internal Diffusion Limitations	807
15.4	Falsified Kinetics	809
15.5	Overall Effectiveness Factor	811
15.6	Estimation of Diffusion- and Reaction-Limited Regimes	816
15.6.1	Mears Criterion for External Diffusion Limitations	816
15.7	Mass Transfer and Reaction in a Packed Bed	817
15.8	Determination of Limiting Situations from Reaction-Rate Data	823
15.9	Multiphase Reactors in the Professional Reference Shelf	824
15.9.1	Slurry Reactors	825
15.9.2	Trickle Bed Reactors	826
15.10	Fluidized Bed Reactors	826
15.11	Chemical Vapor Deposition (CVD)	826
15.12	And Now . . . A Word from Our Sponsor—Safety 15 (AWFOS–S15 Critical Thinking Questions Applied to Safety)	826

**CHAPTER 16 RESIDENCE TIME DISTRIBUTIONS OF CHEMICAL REACTORS 843**

<b>16.1</b>	<b>General Considerations</b>	<b>844</b>
16.1.1	<i>Residence Time Distribution (RTD) Function</i>	<b>845</b>
<b>16.2</b>	<b>Measurement of the RTD</b>	<b>846</b>
16.2.1	<i>Pulse Input Experiment</i>	<b>847</b>
16.2.2	<i>Step Tracer Experiment</i>	<b>852</b>
<b>16.3</b>	<b>Characteristics of the RTD</b>	<b>853</b>
16.3.1	<i>Integral Relationships</i>	<b>853</b>
16.3.2	<i>Mean Residence Time</i>	<b>854</b>
16.3.3	<i>Other Moments of the RTD</i>	<b>855</b>
16.3.4	<i>Normalized RTD Function, <math>E(\theta)</math></i>	<b>859</b>
16.3.5	<i>Internal-Age Distribution, <math>I(\alpha)</math></i>	<b>859</b>
<b>16.4</b>	<b>RTD in Ideal Reactors</b>	<b>860</b>
16.4.1	<i>RTDs in Batch and Plug-Flow Reactors</i>	<b>860</b>
16.4.2	<i>Single-CSTR RTD</i>	<b>861</b>
16.4.3	<i>Laminar-Flow Reactor (LFR)</i>	<b>863</b>
<b>16.5</b>	<b>PFR/CSTR Series RTD</b>	<b>866</b>
<b>16.6</b>	<b>Diagnostics and Troubleshooting</b>	<b>869</b>
16.6.1	<i>General Comments</i>	<b>869</b>
16.6.2	<i>Simple Diagnostics and Troubleshooting Using the RTD for Ideal Reactors</i>	<b>870</b>
<b>16.7</b>	<b>And Now... A Word from Our Sponsor—Safety 16 (AWFOS–S16 Critical Thinking Actions)</b>	<b>876</b>

**CHAPTER 17 PREDICTING CONVERSION DIRECTLY FROM THE RESIDENCE TIME DISTRIBUTION 887**

<b>17.1</b>	<b>Modeling Nonideal Reactors Using the RTD</b>	<b>888</b>
17.1.1	<i>Modeling and Mixing Overview</i>	<b>888</b>
17.1.2	<i>Mixing</i>	<b>888</b>
<b>17.2</b>	<b>Zero Adjustable Parameter Models</b>	<b>890</b>
17.2.1	<i>Segregation Model</i>	<b>890</b>
17.2.2	<i>Maximum Mixedness Model</i>	<b>900</b>
<b>17.3</b>	<b>Using Software Packages Such as Polymath to Find Maximum Mixedness Conversion</b>	<b>907</b>
17.3.1	<i>Comparing Segregation and Maximum Mixedness Predictions</i>	<b>909</b>
<b>17.4</b>	<b>Tanks-in-Series One Parameter Model, <math>n</math></b>	<b>910</b>
17.4.1	<i>Find the Number of T-I-S to Model the Real Reactor</i>	<b>911</b>
17.4.2	<i>Calculating Conversion for the T-I-S Model</i>	<b>912</b>
17.4.3	<i>Tanks-in-Series versus Segregation for a First-Order Reaction</i>	<b>912</b>
<b>17.5</b>	<b>RTD and Multiple Reactions</b>	<b>912</b>
17.5.1	<i>Segregation Model</i>	<b>912</b>
17.5.2	<i>Maximum Mixedness</i>	<b>913</b>
<b>17.6</b>	<b>And Now... A Word from Our Sponsor—Safety 17 (AWFOS–S17 Brief Case History on an Air Preheater)</b>	<b>917</b>

## CHAPTER 18 MODELS FOR NONIDEAL REACTORS 929

- 18.1 **Some Guidelines for Developing Models** **930**
  - 18.1.1 *One-Parameter Models* **932**
  - 18.1.2 *Two-Parameter Models* **932**
- 18.2 **Flow and Axial Dispersion of Inert Tracers in Isothermal Reactors** **933**
  - 18.2.1 *Balances on Inert Tracers* **933**
  - 18.2.2 *Boundary Conditions for Flow and Reaction* **935**
- 18.3 **Flow, Reaction, and Axial Dispersion** **937**
  - 18.3.1 *Balance Equations* **937**
  - 18.3.2 *Solution for a Closed-Closed System* **938**
- 18.4 **Flow, Reaction, and Axial Dispersion in Isothermal Laminar-Flow Reactors and Finding *Meno*** **941**
  - 18.4.1 *Determine the Dispersion Coefficient ( $D_a$ ) and the Péclet Number ( $Pe_v$ )* **941**
  - 18.4.2 *Correlations for  $D_a$*  **944**
  - 18.4.3 *Dispersion in Packed Beds* **944**
  - 18.4.4 *Experimental Determination of  $D_a$*  **944**
- 18.5 **Tanks-in-Series Model versus Dispersion Model** **951**
- 18.6 **Numerical Solutions to Flows with Dispersion and Reaction** **952**
- 18.7 **Nonisothermal Flow with Radial and Axial Variations in a Tubular Reactor** **956**
  - 18.7.1 *Molar Flux* **956**
  - 18.7.2 *Energy Flux* **958**
  - 18.7.3 *Energy Balance* **958**
- 18.8 **Two-Parameter Models—Modeling Real Reactors with Combinations of Ideal Reactors** **964**
  - 18.8.1 *Real CSTR Modeled Using Bypassing and Dead Space* **965**
  - 18.8.2 *Real CSTR Modeled as Two CSTRs with Interchange* **968**
  - 18.8.3 *Other Models of Nonideal Reactors Using CSTRs and PFRs* **972**
  - 18.8.4 *Applications to Pharmacokinetic Modeling* **973**
- 18.9 **And Now... A Word from Our Sponsor—Safety 18 (AWFOS–S18 An Algorithm for Management of Change (MoC))** **974**

## APPENDIX A NUMERICAL TECHNIQUES 991

- A.1 **Useful Integrals in Chemical Reactor Design** **991**
- A.2 **Equal-Area Graphical Differentiation** **992**
- A.3 **Solutions to Differential Equations** **994**
  - A.3.A *First-Order Ordinary Differential Equations* **994**
  - A.3.B *Coupled Differential Equations* **994**
  - A.3.C *Second-Order Ordinary Differential Equations* **995**
- A.4 **Numerical Evaluation of Integrals** **995**
- A.5 **Semi-Log Graphs** **997**
- A.6 **Software Packages** **997**

## APPENDIX B IDEAL GAS CONSTANT AND CONVERSION FACTORS 999

APPENDIX C	THERMODYNAMIC RELATIONSHIPS INVOLVING THE EQUILIBRIUM CONSTANT	1003
APPENDIX D	SOFTWARE PACKAGES	1009
D.1	Polymath	1009
D.1.A	About Polymath ( <a href="http://www.umich.edu/~elements/6e/software/polymath.html">http://www.umich.edu/~elements/6e/software/polymath.html</a> )	1009
D.1.B	Polymath Tutorials ( <a href="http://www.umich.edu/~elements/6e/software/polymath-tutorial.html">http://www.umich.edu/~elements/6e/software/polymath-tutorial.html</a> )	1010
D.1.C	Living Example Problems	1010
D.2	Wolfram	1010
D.3	Python	1011
D.4	MATLAB	1011
D.5	Excel	1011
D.6	COMSOL ( <a href="http://www.umich.edu/~elements/6e/12chap/comsol.html">http://www.umich.edu/~elements/6e/12chap/comsol.html</a> )	1012
D.7	Aspen	1013
D.8	Visual Encyclopedia of Equipment—Reactors Section	1013
D.9	Reactor Lab	1013
APPENDIX E	RATE-LAW DATA	1015
APPENDIX F	NOMENCLATURE	1017
APPENDIX G	OPEN-ENDED PROBLEMS	1021
G.1	Chem-E-Car	1021
G.2	Effective Lubricant Design	1021
G.3	Peach Bottom Nuclear Reactor	1021
G.4	Underground Wet Oxidation	1022
G.5	Hydrodesulfurization Reactor Design	1022
G.6	Continuous Bioprocessing	1022
G.7	Methanol Synthesis	1022
G.8	Cajun Seafood Gumbo	1022
G.9	Alcohol Metabolism	1023
G.10	Methanol Poisoning	1024
G.11	Safety	1024
APPENDIX H	USE OF COMPUTATIONAL CHEMISTRY SOFTWARE PACKAGES	1025
H.1	Computational Chemical Reaction Engineering	1025
APPENDIX I	HOW TO USE THE CRE WEB RESOURCES	1027
I.1	CRE Web Resources Components	1027
INDEX		1029

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# Introduction

The man who has ceased to learn ought not to be allowed  
to wander around loose in these dangerous days.

—M. M. Coady

## A. Who Is the Intended Audience?

This book was written with today's students in mind. It provides instantaneous access to information; does not waste time on extraneous details; cuts right to the point; uses more bullets to make information easier to access; and includes new, novel problems on chemical reaction engineering (e.g., solar energy).<sup>1</sup> The interaction between the text and Web site (<http://www.umich.edu/~elements/6e/>) breaks new ground and provides one of the most comprehensive active learning resources available. With the advent of sliders in both Wolfram and Python, students can explore the reactions and the reactor in which they occur, by carrying out simulation experiments and then writing a set of conclusions to describe what they found.

This book and interactive Web site are intended for use as both an undergraduate-level and a graduate-level text in chemical reaction engineering. The undergraduate course/courses usually focus on Chapters 1–13; the graduate course material includes topics such as diffusion limitations, effectiveness factors (discussed in Chapters 14 and 15), nonideal reactors, and residence time distribution (discussed in Chapters 16–18) along with the additional material and Professional Reference Shelf (PRS) on the Web site.

This edition emphasizes chemical reactor safety by ending each chapter with a safety lesson called *And Now... A Word From Our Sponsor-Safety (AWFOS-S)*. These lessons can also be found on the Web site at <http://umich.edu/~safeche/>.

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<sup>1</sup> This Introduction is a condensed version of the full Preface/Introduction found on the Web site (<http://www.umich.edu/~elements/6e/toc/Preface-Complete.pdf>).

## B. What Are the Goals of This Book?

### B.1 To Have Fun Learning Chemical Reaction Engineering (CRE)

Chemical reaction engineering (CRE) is a great subject that is fun to learn and is the heart of chemical engineering. I have tried to provide a little Michigan humor as we go. Take a look at the humorous YouTube videos (e.g., “Black Widow” or “Chemical Engineering Gone Wrong”) that illustrate certain principles in the text. These videos were made by chemical engineering students at the universities of Alabama and Michigan. In addition, I have found that students enjoy the Interactive Computer Games (ICGs) that, along with the videos, are linked from the CRE homepage (<http://www.umich.edu/~elements/6e/index.html>).

### B.2 To Develop a Fundamental Understanding of Reaction Engineering

The second goal of this book is to help the reader clearly understand the fundamentals of CRE. This goal is achieved by presenting a structure that allows the reader to solve reaction engineering problems through reasoning rather than through memorization and recall of numerous equations and the restrictions and conditions under which each equation applies (<http://www.umich.edu/~elements/6e/toc/Preface-Complete.pdf>).

### B.3 To Enhance Thinking Skills

A third goal of this text is to enhance critical thinking skills and creative thinking skills. How does the book help enhance your critical and creative thinking skills? We discuss ways to achieve this enhancement in Table P-2, Critical Thinking Questions; Table P-3, Critical Thinking Actions; and Table P-4, Practicing Creative Thinking, in the complete preface on the CRE Web site (<http://www.umich.edu/~elements/6e/toc/Preface-Complete.pdf>) and also from the Problem Solving Web site (<http://umich.edu/~scps/>).

## C. What Is the Structure of CRE?

### C.1 What Are the Concepts That Form the Foundation of CRE?

The strategy behind the presentation of material is to build continually on a few basic ideas in CRE to solve a wide variety of problems. The building blocks of CRE and the primary algorithm allow us to solve isothermal CRE problems through logic rather than memorization. We start with the Mole Balance Building Block (Chapter 1) and then place the other blocks one at a time on top of the others until we reach the Evaluate Block (Chapter 5), by which time we can solve a multitude of isothermal CRE problems. As we study each block, we need to make sure we understand everything in that block and be sure not to cut corners by leaving anything out so we don't wind up with a stack of cylindrical blocks. An animation of what happens to such a stack is shown at the end of Lecture 1 notes (<http://www.umich.edu/%7EElements/6e/lectures/umich.html>).

For nonisothermal reactions, we replace the “Combine” building block in Figure I-1 with the “Energy Balance” building block because nonisothermal reactions almost always require a computer-generated solution. Consequently,

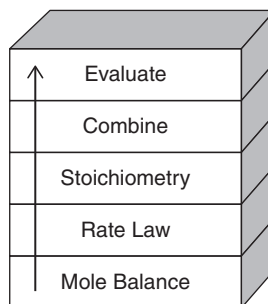


Figure I-1 Building blocks.

we don't need the "Combine" block because the computer combines everything for us. From these pillars and building blocks, we construct our CRE algorithm:

**Mole Balance + Rate Laws + Stoichiometry + Energy Balance + Combine → Solution**

## C.2 What Is the Sequence of Topics in Which This Book Can Be Used?

Margin Notes

The selection and order of topics and chapters are shown in Figure P-3 in the Complete Preface/Introduction on the Web site (<http://www.umich.edu/~elements/6e/toc/Preface-Complete.pdf>). There are notes in the margins, which are meant to serve two purposes. First, they act as guides or commentary as one reads through the material. Second, they identify key equations and relationships that are used to solve CRE problems.

## D. What Are the Components of the CRE Web Site?

The interactive companion Web site material has been significantly updated and is a novel, and integral part of this book. The main purposes of the Web site are to serve as an interactive part of the text with enrichment resources. The home page for the CRE Web site (<http://www.umich.edu/~elements/6e/index.html>) is shown in Figure I-2. For discussion of how to use the Web site and text interactively, see Appendix I.

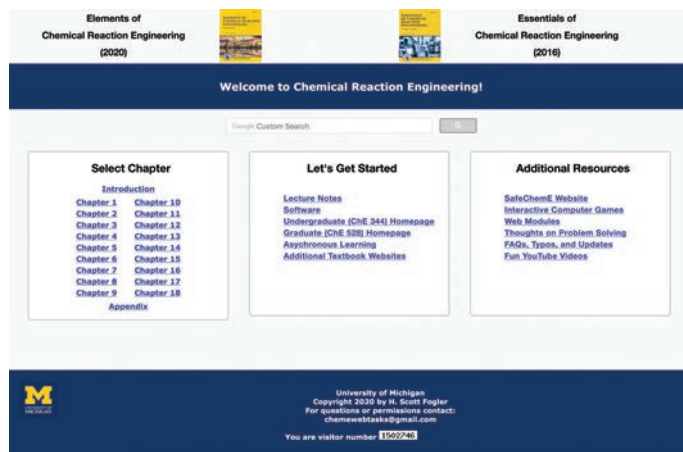


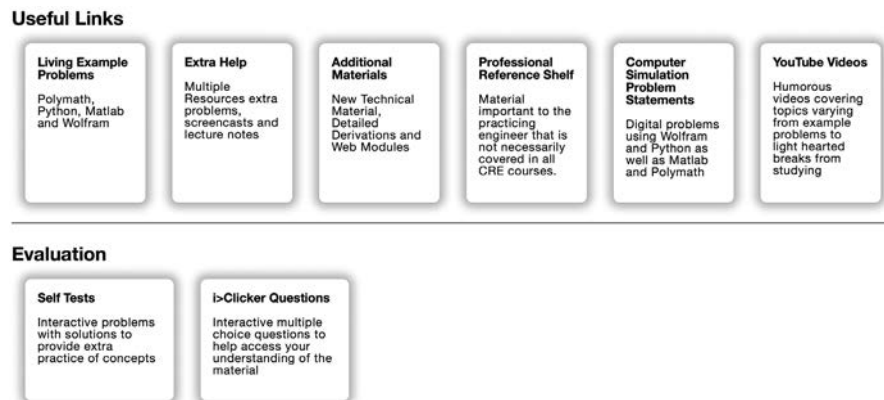
Figure I-2 Screen shot of the book's companion Web site (<http://www.umich.edu/~elements/6e/index.html>).

**The objectives of the Web site are fourfold:**

- (1) To facilitate the interactive learning of CRE by using the companion Web site and Wolfram and Python sliders to explore Living Example Problems to gain a deep understanding of the reaction and the reactors in which they take place.
- (2) To provide additional technical material in the extended material and in the Professional Reference Shelf.
- (3) To provide tutorial information and self-assessment exercises such as the i>clicker questions.
- (4) To make the learning of CRE fun through the use of interactive games, LEP simulations, and computer experiments, which allow one to use Inquiry-Based Learning (IBL) to explore the concepts of CRE.

### D.1 How to Use the Web Site

I would like to expand a bit on a couple of things that we use extensively, namely the useful links. These items can be accessed by clicking on the Chapter number on the Home Page. After clicking on Chapter 1 shown in Figure I-3, one will arrive at



**Figure I-3** Access to useful links  
 (<http://www.umich.edu/~elements/6e/01chap/obj.html#/>).

The important point I want to make here is the list of all resources shown in Figures I-3 and I-4. In addition to listing the objectives for this chapter, you will find all the major hot buttons, such as

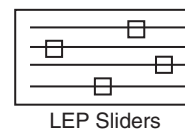


Figure I-4 Useful links.

The *Living Example Problems* (LEPs), including COMSOL, have all numerical Example Problems programmed and ready for use with the click of a button. The *Extra Help* includes interactive notes, screen casts, and techniques that facilitate learning and studying. The *Additional Material* and *Professional Reference Shelf* provide expanded derivations and material that is relevant to CRE, but did not make the final cut owing to limitations of the thickness of the book; that is, students can't concentrate about CRE if their backpacks are so heavy they are suffering from carrying them. The *Self Tests* and *i>Clicker Questions* help readers gauge their level of understanding.

## D.2 Living Example Problems (LEPs)

What are LEPs? LEPs are **Living Example Problems** that are really simulations that can be used to carry out experiments on the reactor and the reactions occurring inside the reactor. Here, rather than being stuck with the parameter values the author gives, the LEPs allow you to change the value of a parameter and see its effect on the reactor's operation. LEPs have been unique to this book since their invention and inclusion in the Third Edition of this title, published in 1999. However, Wolfram and Python have allowed us to take LEPs to a new level, resulting in a minor paradigm shift. The LEPs use simulation software, which can be downloaded directly onto one's own computer in order to "play with" the key variables and assumptions. Using the LEPs to explore the problem and asking "What if...?" questions provide students with the opportunity to practice critical and creative thinking skills. To guide students in using these simulations, questions for each chapter are given on the Web site (e.g., <http://www.umich.edu/~elements/6e/12chap/obj.html>).<sup>2</sup> In this edition, there are more than 80 interactive simulations (LEPs) provided on the Web site. It is the author's strong belief that using the LEP sliders will develop an intuitive feel for Chemical Reaction Engineering (CRE).



The simulations labeled **Stop and Smell the Roses** are comprehensive-interactive simulations that will provide significant insight and an intuitive feel for the reactor and the reaction when you take the time to explore the parameters using the Wolfram or Python sliders. #wellworthyourtime



<sup>2</sup> See Introduction section D and Appendix I for ideas on how to use the LEPs.

Figure I-5 shows a screen shot of the LEPs for Chapter 5. One simply clicks on the hot button of the desired programming language (Wolfram, Python) and the program loads, then uses the sliders to explore the reactors operating variables and the property parameters.

## Chapter 5: Isothermal Reactor Design: Conversion

### Living Example Problems

**Note:** When downloading Python code files over Chrome browser, you may see a security warning. We assure you that these files are secure and you may keep them on your computer.

Living Example Problem	Polymath™ Code	Python Code	MATLAB Code	Wolfram CDF Code *	AspenTech™
Example 5-3 Plug-flow reactor	<a href="#">LEP-5-3.pol</a>	<a href="#">LEP-5-3.py</a>	<a href="#">LEP-5-3.zip</a>	<a href="#">LEP-5-3.cdf</a>	
Example 5-4 Pressure Drop in a Packed Bed		<a href="#">LEP-5-4.py</a>		<a href="#">LEP-5-4.cdf</a>	
Example 5-5 Effect of pressure drop on conversion	<a href="#">LEP-5-5.pol</a>	<a href="#">LEP-5-5.py</a>	<a href="#">LEP-5-5.zip</a>	<a href="#">LEP-5-5.cdf</a>	
Example 5-6 Robert Worries what if...	<a href="#">LEP-5-6.pol</a>	<a href="#">LEP-5-6.py</a>		<a href="#">LEP-5-6.cdf</a>	
Example 5-7 Calculating X in a reactor with Pressure drop	<a href="#">LEP-5-7.pol</a>	<a href="#">LEP-5-7.py</a>	<a href="#">LEP-5-7.zip</a>	<a href="#">LEP-5-7.cdf</a>	Tutorial, ASPEN Backup File
Example 5-8 Reversible gas-phase reaction in a packed bed with pressure drop	<a href="#">LEP-5-8.pol</a>	<a href="#">LEP-5-8.py</a>	<a href="#">LEP-5-8.zip</a>	<a href="#">LEP-5-8.cdf</a>	

1. **LEP** : Click [here](#) to view LEP Tutorials
2. **Polymath** : Click [here](#) to view Polymath Tutorials
3. **Python** : Click [here](#) to view Python Tutorials
4. **MATLAB** : Click [here](#) to view MATLAB Tutorials
5. **Wolfram** : Click [here](#) to download Wolfram CDF Player. You can run the CDF code, download Wolfram CDF Player for free. Click [here](#) to view Wolfram Tutorials

Figure I-5 Living Example Problems (LEPs).

It has been shown that students using **inquiry-based learning (IBL)** have a much greater understanding of information than students educated by traditional methods (*Univers. J. Educ. Res.*, 2(1), 37–41 (2014)).<sup>3,4</sup> The learning was most definitely enhanced when it came to questions that required interpretation such as, “Why did the temperature profile go through a minimum?” Each chapter has a section on Computer Simulations and Experiments that will guide students in practicing **IBL**. Students have commented that the Wolfram slider LEPs are a very efficient way to study the operation of a chemical reactor. For example, one can carry out a simulation experiment on the reactor (e.g., LEP 13-2) to investigate what conditions would lead to unsafe operation.

<sup>3</sup> Ibid, Adbi, A.

<sup>4</sup> Documentation of the advantages of IBL can be found at *Studies in Higher Education*, 38(9), 1239–1258 (2013), <https://www.tandfonline.com/doi/abs/10.1080/03075079.2011.616584>.

You will note the tutorials listed just below the screen shot of the Living Example Problems page. There are 11 Polymath tutorials, and one LEP tutorial for each Polymath, Wolfram, Python, and MATLAB in later chapters. There are also six COMSOL tutorials. To access the LEP software you want to use, that is, Polymath, Wolfram, Python, or MATLAB, just click on the appropriate hot button, and then load and run the LEPs in the software you have chosen. Homework problems using the LEPs have been added to each chapter that requires the use of Wolfram, Python, and Polymath. The use of the LEP sliders will allow students to vary the reaction and reactor parameters to get a thorough understanding of the Computer Simulation Problems.

### D.3 Extra Help

The components of Extra Help are shown in Figure I-6.

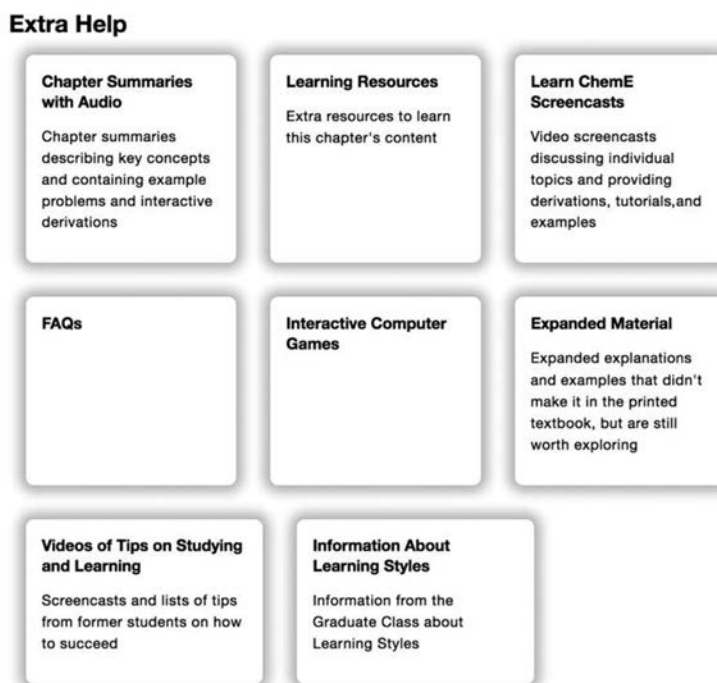


Figure I-6 Screen shot of Extra Help.

The *Learning Resources* give an overview of the material in each chapter through the Interactive *Summary Notes*. These notes include on-demand derivations of key equations, audio explanations, additional resources such as *Interactive Computer Games* (ICGs), computer simulations and experiments, Web modules of novel applications of CRE, solved problems, study aids, *Frequently Asked Questions* (FAQs), Microsoft PowerPoint lecture slides, and links to *LearnChemE videos*. The Web modules consist of a number of examples that apply key CRE concepts to both standard and nonstandard reaction engineering problems (e.g., glow sticks, the use of wetlands to degrade toxic chemicals, and pharmacokinetics of death from a cobra bite). The Web modules can be loaded directly

from the CRE Web site ([http://www.umich.edu/~elements/6e/web\\_mod/index.html](http://www.umich.edu/~elements/6e/web_mod/index.html)). These resources are described in Appendix I.

#### D.4 Additional Material

The additional material shown in Figure I-7 includes derivations, examples, and novel applications of CRE principles that build on the CRE algorithm in the text.

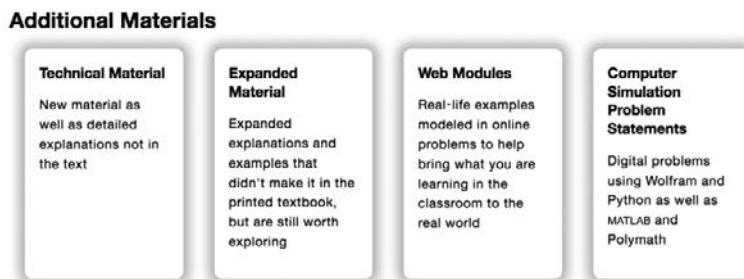


Figure I-7 Screen shot of Additional Materials.

#### D.5 Professional Reference Shelf

This material is important to the practicing engineer, such as details of the industrial reactor design for the oxidation of  $\text{SO}_2$  and design of spherical reactors and other material that is typically not included in the majority of chemical reaction engineering courses.

#### D.6 Computer Simulations, Experiments, and Problems

As discussed in section D.2, these problems help guide students to understand how the parameters and operating conditions affect the reaction and the reactors. These problems are in the printed version of the second edition of *Essentials of Chemical Reaction Engineering*, and the sixth edition of *Elements of Chemical Reaction Engineering*, but not in the printed version of the fifth edition of *Elements of Chemical Reaction Engineering*.

#### D.7 YouTube Videos

Here, you will find links to humorous YouTube videos made by students in Professor Alan Lane's 2008 chemical reaction engineering class at the University of Alabama, as well as videos from the University of Michigan's 2011 CRE class, which includes the ever-popular chemical engineering classic, "Reaction Engineering Gone Wrong." If you have a humorous YouTube video on CRE, I would be happy to consider linking to it.

## D.8 COMSOL

The COMSOL Multiphysics software is a partial differential equation solver that is used with Chapters 13 and 18 to view both axial and radial temperature and concentration profiles. For users of this text, COMSOL has provided a special Web site that includes a step-by-step tutorial, along with examples. See Figure 18-15 on page 964 and also (<https://www.comsol.com/books/elements-of-chemical-reaction-engineering-5th/models>). Further details are given in the Living Example Problems on the Web site.

## E. Why Do We Assign Homework Problems?

The working of homework problems facilitates a *true understanding* of CRE. After reading a chapter, the student may feel they have an understanding of the material. However, when attempting a new or slightly different application of CRE in a homework problem, students sometimes need to go back and reread different parts of the chapter to get the level of understanding needed to eventually solve the homework problem. **Polymath** is a most user-friendly software and is recommended to solve these end-of-chapter problems.

I would like to point out research has shown (*J. Exp. Psychol. Learn. Mem. Cogn.*, 40, 106–114 (2014)) that if you ask a question of the material before reading the material you will have greater retention. Consequently, the first question of every chapter will have such a question on that chapter's material. For Chapter 1, the question is, "Is the generation term,  $G$ , the only term in the mole balance that varies for each type of reactor?" The questions that follow are qualitative in Q1-2<sub>A</sub> and Q2-3<sub>A</sub>, and so on.

It is recommended that students first work through *Computer Simulation Problems* that use MATLAB, Python, and Wolfram before going on to other problems. These example problems are a key resource. The subscript letter (A, B, C, or D) after each problem number denotes the difficulty of the problem (i.e., A = easy; D = difficult). The A- and B-level problems should be worked before tackling the more challenging homework problems in a given chapter.

## F. Are There Other Web Site Resources?

**CRE Web Site** (<http://www.umich.edu/~elements/6e/index.html>). A complete description of all the educational resources and ways to use them can be found in Appendix I.

**Safety Web Site.** During the past two years, a safety Web site has been developed for all core chemical engineering courses (<http://umich.edu/~safeche/>). A section at the end of each chapter called *And Now... A Word From Our Sponsor-Safety (AWFOS-S)* has taken the tutorials and distributed them in chapters throughout the text. A safety module for both the T2 Laboratory incident ([http://umich.edu/~safeche/assets/pdf/courses/Problems/CRE/344ReactionEngrModule\(1\)PS-T2.pdf](http://umich.edu/~safeche/assets/pdf/courses/Problems/CRE/344ReactionEngrModule(1)PS-T2.pdf)) and the Monsanto incident ([http://umich.edu/~safeche/assets/pdf/courses/Problems/CRE/344ReactionEngrModule\(2\)PS-Monsanto.pdf](http://umich.edu/~safeche/assets/pdf/courses/Problems/CRE/344ReactionEngrModule(2)PS-Monsanto.pdf)) can be found on the safety Web site. A safety algorithm is included in both of these modules.

### **What Entertainment Is on the Web Site?**

**A. YouTube Videos.** The humorous videos are discussed in Section D, what are the components of the CRE Web site, above.

**B. Interactive Computer Games (ICGs).** Students have found the Interactive Computer Games to be both fun and extremely useful for reviewing the important chapter concepts and then applying them to real problems in a unique and entertaining fashion. The following ICGs are available on the Web site:

- Quiz Show I (Ch. 1)
- Reactor Staging (Ch. 2)
- Quiz Show II (Ch. 4)
- Murder Mystery (Ch. 5)
- Tic Tac (Ch. 5)
- Ecology (Ch. 7)
- The Great Race (Ch. 8)
- Enzyme Man (Ch. 9)
- Catalysis (Ch. 10)
- Heat Effects I (Ch. 12)
- Heat Effects II (Ch. 12)

As you play these interactive games, you will be asked a number of questions related to the corresponding material in the textbook. The ICG keeps track of all the correct answers and at the end of the game displays a coded performance number that reflects how well you mastered the material in the text. Instructors have a manual to decode the performance number.

### **G. How Can One's Critical Thinking and Creative Thinking Skills Be Enhanced?**

(<http://umich.edu/~scps/html/probsolv/strategy/crit-n-creat.htm>)

A third goal of this book is to enhance critical and creative thinking skills. How does one enhance their critical thinking skills? Answer: By learning how to ask critical thinking questions and taking critical thinking actions of the type given on the Web site in Tables P-2 and P-3. Further discussion is found in the Complete Preface-Introduction on the Web site (<http://www.umich.edu/~elements/6e/toc/Preface-Complete.pdf>).

The goal to enhance creative thinking skills is achieved by using a number of problems that are open-ended to various degrees. With these, students can practice their *creative skills* by exploring the example problems, as outlined at the beginning of the homework problems of each chapter, and by making up and solving an original problem using the suggestions in Table P-4 on the Web site (<http://www.umich.edu/~elements/6e/toc/Preface-Complete.pdf>).

One of the major goals at the undergraduate level is to bring students to the point where they can solve complex reaction problems, such as multiple reactions with heat effects, and then ask “What if . . . ?” questions and look for optimum operating conditions and unsafe operating conditions. The solution to one problem exemplifies this goal: the Manufacture of Styrene (Chapter 12, Problem P12-26<sub>C</sub>). This problem is particularly interesting because two reactions are endothermic and one is exothermic.

- (1) Ethylbenzene → Styrene + Hydrogen: Endothermic
- (2) Ethylbenzene → Benzene + Ethylene: Endothermic
- (3) Ethylbenzene + Hydrogen → Toluene + Methane: Exothermic

The student could get further practice in critical and creative thinking skills by adding any of the following exercises (x), (y), and (z) to any of the end-of-chapter homework problems.

- (x) How could you make this problem easier? More difficult?
- (y) Critique your answer by writing a critical thinking question.
- (z) Describe two ways you could work this problem incorrectly.

## H. What's New in This Edition?

This textbook and Web site interaction is a mini paradigm shift in active learning. There is a symbiotic relationship between the Web site and the textbook that allows the student to get an intuitive feel of the reactions and reactors. Here the students use the software packages of Wolfram, Python, MATLAB, and Polymath to explore the reactions and the reactors. In addition, this edition maintains all the strengths of the previous editions of *Elements of Chemical Reaction Engineering* by using algorithms that allow students to learn chemical reaction engineering through logic rather than memorization. Figure I-8 shows the Extra Help associated with the Chapter 1 material.

### Chapter 1: Mole Balances

#### Extra Help

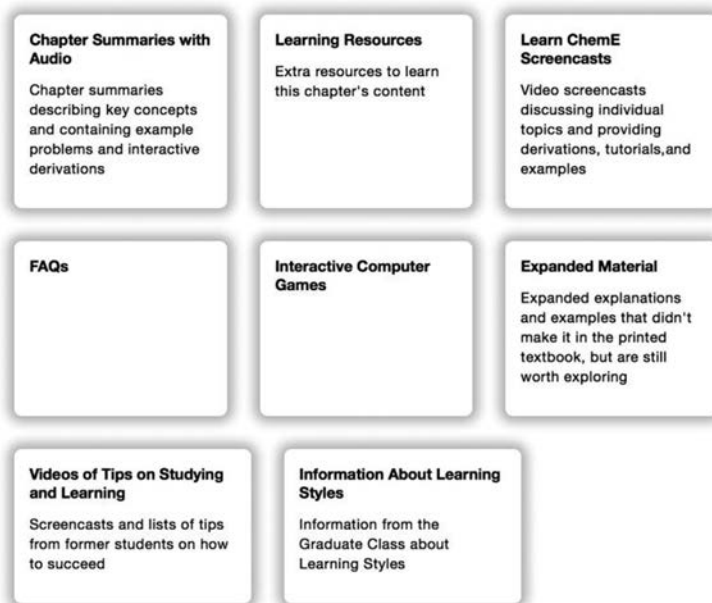




Figure I-8 Screen shot of Extra Help.

The Web site has been greatly expanded to address the Felder/Solomon Inventory of Different Learning Styles<sup>5</sup> through interactive Summary Notes, i>clicker questions and Interactive Computer Games (ICGs). For example, as discussed in Appendix I the Global Learner can get an overview of the chapter

<sup>5</sup> <https://www.engr.ncsu.edu/stem-resources/legacy-site/>

material from the Summary Notes; the Sequential Learner can use all the i>clicker questions and  hot buttons; and the active learner can interact with the ICGs and use the  hot buttons in the Summary Notes.

The Web site for this new edition provides thorough interactive example problems using Polymath, Wolfram, Python, and MATLAB. These software packages are used to perform experiments on the reactor and the reactions and to then write a set of conclusions describing what the experiments revealed. In addition, there is a Safety Section at the end of each chapter that is linked to the safety Web site (<http://umich.edu/~safeche/>).

As with the past edition, an Aspen tech tutorial is provided for four example problems on the CRE Web site (<http://www.umich.edu/~elements/6e/software/aspen.html>).

### **And most importantly we have to always remember that:**

*Hopefully all intensive laws tend often to have exceptions. Very important concepts take orderly, responsible statements. Virtually all laws intrinsically are natural thoughts. General observations become laws under experimentation.*

## **I. How Do I Say Thank You?**

There are so many colleagues and students who contributed to this book that it would require another chapter to thank them all in an appropriate manner. I again acknowledge all my friends, students, and colleagues for their contributions to the sixth edition of *Elements of Chemical Reaction Engineering*. I would like to give special recognition as follows.

First of all, I am indebted to Ame and Catherine Vennema family, whose gift of an endowed chair greatly facilitated the completion of this project. My colleague Dr. Nihat Gürmen coauthored the original Web site during the writing of the fourth edition of *Elements of Chemical Reaction Engineering*. He has been a wonderful colleague to work with. I also would like to thank University of Michigan undergraduate ChE students who served early on as webmasters for the CRE Web site namely Arthur Shih, Maria Quigley, Brendan Kirchner, and Ben Griessmann. More recently CSE students, Jun Kyungjun Kim, Elsa Wang, Wen He, Kiran Thwardas, Tony Hanchi Zhang, Arav Agarwal, and Lisa Ju Young Kim worked on both the CRE Web site and the Safety Web site.

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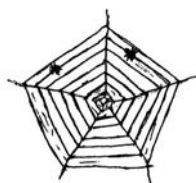
helped with preparation of the additional material for the book, especially the Safety Web site, as well as related material. Kaushik Nagaraj developed and provided the MATLAB coding for the simulations in Section 3.4 while Jakub Wlodarczyk (Warsaw University of Technology, Poland) checked all of the i>clicker questions and solutions. Students from Indian Institute of Technology, Bombay, who contributed to AWFOS-S at the end of each chapter include Kaushik Nagaraj, Triesha Singh, Reshma Kalyan Sundaram, Kshitiz Parihar, Manan Agarwal, Kushal Mittal, and Sahil Kulkarni. Vaibav Jain from IIT Delhi worked on the Solutions Manual. From the University of Michigan, Kara Steshetz, Alec Driesenga, Maeve Gillis, and Lydia Peters also worked on the Safety material.

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Finally, to my wife Janet, love and thanks. Not only did she type the first edition of this book—can you believe on a Royal Select typewriter!—she also was a sounding board for so many things in this edition. She was always willing to help with the wording and sentence structure. For example, I often asked her, “Is this the correct phrase or word to use here?” or “Should I mention Jofostan here?” Jan also helped me learn that creativity involves knowing what to leave out. Without her enormous help and support the project would never have been possible.

HSF  
Ann Arbor, Michigan  
May 2020



Updates, FAQs, Web Modules, LEPs, exciting new applications, and typographical errors can all be accessed from the Home page on the companion Web site:

[www.umich.edu/~elements/6e/index.html](http://www.umich.edu/~elements/6e/index.html)

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# About the Author



**H. Scott Fogler** is the Ame and Catherine Vennema professor of chemical engineering and the Arthur F. Thurnau professor at the University of Michigan in Ann Arbor. He was recognized as a 2020 Michigan Distinguished Professor of the year, and was the 2009 National President of the American Institute of Chemical Engineers (AIChE), a 50,000-member organization. He received his B.S. from the University of Illinois and his M.S. and Ph.D. from the University of Colorado.

He is also the author of the *Essentials of Chemical Reaction Engineering, Second Edition*, and coauthor, with Steven LeBlanc and Benjamin Rizzo, of *Strategies for Creative Problem Solving, Third Edition*.

Professor Fogler's research interests include flow and reaction in porous media, wax and asphaltene deposition, asphaltene flocculation kinetics, gelation kinetics, colloidal phenomena, and catalyzed dissolution. He has been research advisor to 49 Ph.D. students and has more than 250 refereed publications in these areas. Fogler has chaired ASEE's Chemical Engineering Division, served as director of the AIChE, and earned the Warren K. Lewis Award from AIChE for contributions to chemical engineering education. He also received the Chemical Manufacturers Association's National Catalyst Award, and the 2010 Malcom E. Pruitt Award from the Council for Chemical Research (CCR), and the 2019 Van Antwerpen Award from AIChE. He is the recipient of 12 named lectureships and is associate editor of *Energy & Fuels*. On April 15, 2016, Scott received a *doctor honoris causa* degree from the Universitat Rovira i Virgili, Tarragona, Spain.

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# *Mole Balances* 1

The first step to knowledge  
is to know that we are ignorant.

—Socrates (470–399 B.C.)

## **The Wide, Wild World of Chemical Reaction Engineering**

How is a chemical  
engineer different  
from other  
engineers?

Chemical kinetics is the study of chemical reaction rates and reaction mechanisms. The study of chemical reaction engineering (CRE) combines the study of chemical kinetics with the reactors in which the reactions occur. Chemical kinetics and reactor design are at the heart of producing almost all industrial chemicals, such as the manufacture of phthalic anhydride shown in Figure 1-1. It is primarily a knowledge of chemical kinetics and reactor design that distinguishes the chemical engineer from other engineers. The selection of a reaction system that operates in the safest and most efficient manner can be the key to the economic success or failure of a chemical plant. For example, if a reaction system produces a large amount of undesirable product, subsequent purification and separation of the desired product could make the entire process economically unfeasible.

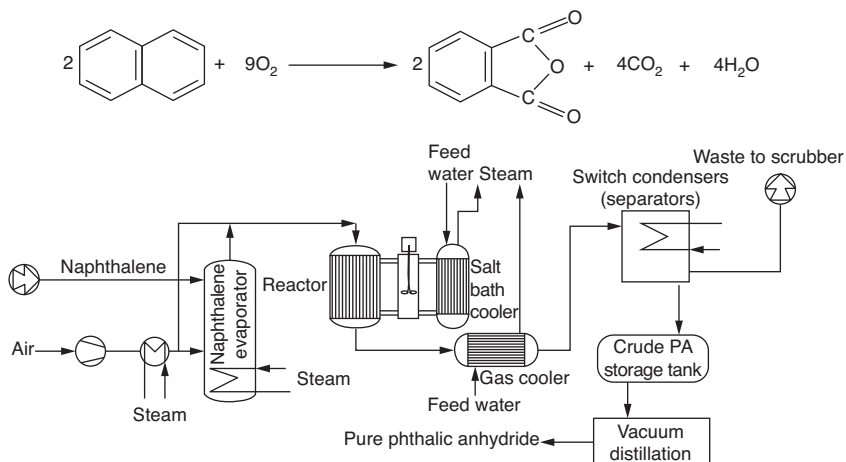
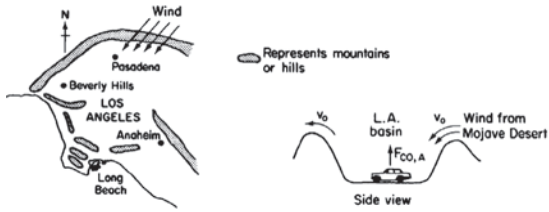
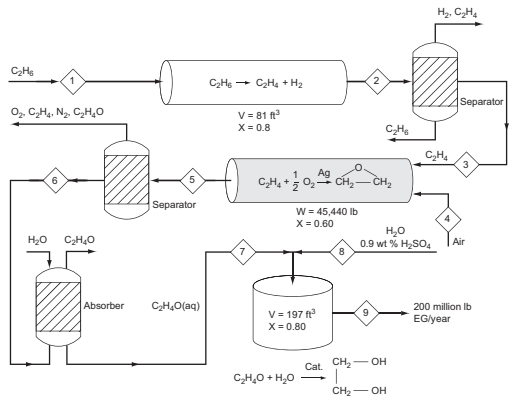


Figure 1-1 Manufacture of phthalic anhydride.

The chemical reaction engineering (CRE) principles learned here can also be applied in many areas, such as waste water treatment, microelectronics, nanoparticles fabrication, and pharmacokinetics of living systems, in addition to the more traditional areas of the manufacture of chemicals and pharmaceuticals. Some of the examples that illustrate the wide application of CRE principles in this book are shown in Figure 1-2. These examples, which can be found either in the text or as Web modules ([www.umich.edu/~elements/6e/index.html](http://www.umich.edu/~elements/6e/index.html)), include modeling smog in the Los Angeles (L.A.) basin (Chapter 1 Web module), the digestive system of a hippopotamus (Chapter 2 Web module), molecular CRE (Chapter 3 Web module), use of wetlands to degrade toxic chemicals (Chapter 6 on the CRE Web site); pharmacokinetics of cobra bites (Chapter 8 Web module); free-radical scavengers used in the design of motor oils (Chapter 9); enzyme kinetics (Chapter 9) and drug delivery pharmacokinetics (Chapter 9 on the CRE Web site). Also shown in Figure 1-2 are the manufacture of ethylene glycol (antifreeze), where three of the most common types of industrial reactors are used (Chapters 5 and 6). Other examples shown are heat effects, runaway reactions, and plant safety (Chapters 11–13); and increasing the octane number of gasoline and the manufacture of computer chips (Chapter 10).



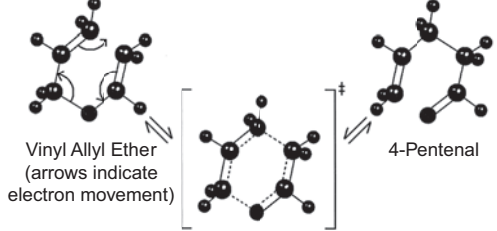
Smog (Ch. 1 on CRE Web site)



Chemical Plant for Ethylene Glycol (Ch. 5)

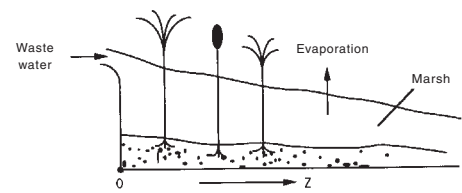


Hippo Digestion (Ch. 2 on CRE Web site)



Transition State (dashed lines show transition state electron delocalization)

Molecular CRE (Ch. 3 on CRE Web site)



Wetlands Remediation of Pollutants (Ch. 6 on CRE Web site)



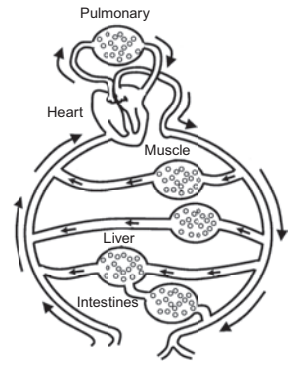
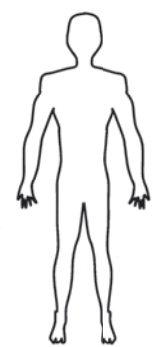
Pharmacokinetics of Cobra Bites  
Multiple Reactions in a Batch (Body) Reactor

Cobra Bites (Ch. 8 on the CRE Web site)

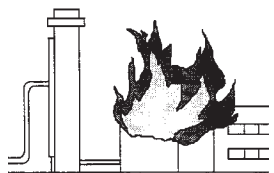


Effective Lubricant Design Scavenging Free Radicals

Lubricant Design (Ch. 9)



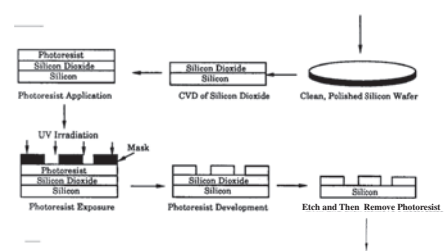
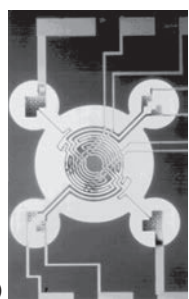
Pharmacokinetics (Ch. 9 on CRE Web site)



Nitroaniline Plant Explosion  
Exothermic Reactions That Run Away

Plant Safety (Ch.11 to Ch.13)

(<http://www.umich.edu/~safeche/index.html>)



Microelectronic Fabrication Steps (Ch. 10)

Figure 1-2 The wide world of CRE applications.

**Overview.** This chapter develops the first building block of chemical reaction engineering, *mole balances*, which will be used continually throughout the text. After completing this chapter, you will be able to:

- Describe and define the rate of reaction
- Derive the general mole balance equation
- Apply the general mole balance equation to the four most common types of industrial reactors

Before entering into discussions of the conditions that affect chemical reaction rates mechanisms and reactor design, it is necessary to account for the various chemical species entering, leaving, reacting, and accumulating in a system. This accounting process is achieved through overall mole balances on individual species in the reacting system. In this chapter, we develop a general mole balance that can be applied to any species (usually a chemical compound) entering, leaving, reacting, and accumulating within the reaction system volume. After defining the rate of reaction,  $-r_A$ , we show how the general mole balance equation (GMBE) may be used to develop a preliminary form of the design equations of the most common industrial reactors (<http://encyclopedia.che.engin.umich.edu/Pages/Reactors/menu.html>).

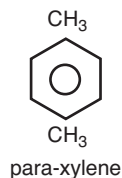
- Batch Reactor (BR)
- Continuous-Stirred Tank Reactor (CSTR)
- Plug-Flow Reactor (PFR)
- Packed-Bed Reactor (PBR)

In developing these equations, the assumptions pertaining to the modeling of each type of reactor are delineated. Finally, a brief summary and series of short review questions and problems are given at the end of the chapter.

## 1.1 The Rate of Reaction, $-r_A$

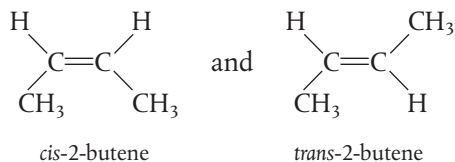
The rate of reaction tells us how fast the number of moles of one chemical species are being consumed to form another chemical species. The term *chemical species* refers to any chemical component or element with a given *identity*. The *identity* of a chemical species is determined by the *kind*, *number*, and *configuration* of that species' atoms. For example, the species para-xylene is made up of a

Identify  
– Kind  
– Number  
– Configuration



fixed number of specific atoms in a definite molecular arrangement or configuration. The structure shown illustrates the kind, number, and configuration of atoms on a molecular level. Even though two chemical compounds have exactly the same kind and number of atoms of each element, they could still be different species because of different configurations. For example, 2-butene

has four carbon atoms and eight hydrogen atoms; however, the atoms in this compound can form two different arrangements.



As a consequence of the different configurations, these two isomers display different chemical and physical properties. Therefore, we consider them as two different species, even though each has the same number of atoms of each element.

When has a chemical reaction taken place?

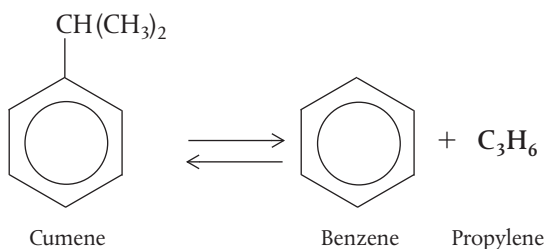
We say that a *chemical reaction* has taken place when a detectable number of molecules of one or more species have lost their identity and assumed a new form by a change in the kind or number of atoms in the compound and/or by a change in structure or configuration of these atoms. In this classical approach to chemical change, it is assumed that the total mass is neither created nor destroyed when a chemical reaction occurs. The mass referred to is the total collective mass of all the different species in the system. However, when considering the individual species involved in a particular reaction, we do speak of the rate of disappearance of mass of a particular species. *The rate of disappearance of a species, say species A, is the number of A molecules that lose their chemical identity per unit time per unit volume through the breaking and subsequent re-forming of chemical bonds during the course of the reaction.* In order for a particular species to “appear” in the system, some prescribed fraction of another species must lose its chemical identity.

Definition of Rate of Reaction

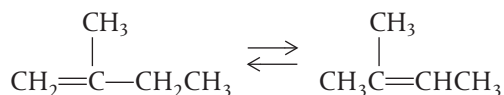
There are three basic ways a species may lose its chemical identity: decomposition, combination, and isomerization. In *decomposition*, the molecule loses its identity by being broken down into smaller molecules, atoms, or atom fragments. For example, if benzene and propylene are formed from a cumene molecule,

A species can lose its identity by

- Decomposition
- Combination
- Isomerization



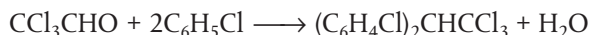
the cumene molecule has lost its identity (i.e., disappeared) by breaking its bonds to form these molecules. A second way that a molecule may lose its chemical identity is through *combination* with another molecule or atom. In the above reaction, the propylene molecule would lose its chemical identity if the reaction were carried out in the reverse direction, so that it combined with benzene to form cumene. The third way a species may lose its chemical identity is through *isomerization*, such as the reaction



Here, although the molecule neither adds other molecules to itself nor breaks into smaller molecules, it still loses its identity through a change in configuration.

To summarize this point, we say that a given number of molecules (i.e., moles) of a particular chemical species have reacted or disappeared when the molecules have lost their chemical identity.

The rate at which a given chemical reaction proceeds can be expressed in different ways by referring it to different chemical species in the reaction. To illustrate, consider the reaction of chloral with chlorobenzene in the presence of fuming sulfuric acid to produce the banned insecticide DDT (dichlorodiphenyl trichloroethane).



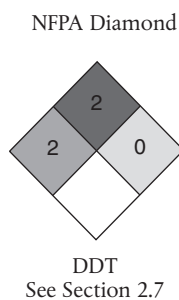
Letting the symbol A represent chloral, B be chlorobenzene, C be DDT, and D be  $\text{H}_2\text{O}$ , we obtain



What is  $-r_A$ ?

The rate of reaction,  $-r_A$ , is the number of moles of A (e.g., chloral) reacting (disappearing) per unit time per unit volume ( $\text{mol}/\text{dm}^3\cdot\text{s}$ ).

The numerical value of the rate of disappearance of reactant A,  $-r_A$ , is a positive number.



### Example 1-1 Rates of Disappearance and Formation

Chloral is being consumed at a rate of 10 moles per second per  $\text{m}^3$  when reacting with chlorobenzene to form DDT and water in the reaction described above. In symbol form, the reaction is written as



Write the rates of disappearance and formation (i.e., generation;  $\text{mol}/\text{m}^3\cdot\text{s}$ ) for each species in this reaction when the rate of reaction of chloral [A] ( $-r_A$ ) is  $10 \text{ mol}/\text{m}^3\cdot\text{s}$ .

#### Solution

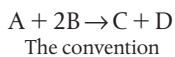
- (a) *Chloral*[A]: Rate of disappearance of A =  $-r_A = 10 \text{ mol}/\text{m}^3\cdot\text{s}$   
Rate of formation of A =  $r_A = -10 \text{ mol}/\text{m}^3\cdot\text{s}$
- (b) *Chlorobenzene*[B]: For every mole of chloral that disappears, two moles of chlorobenzene [B] also disappear.  
Rate of disappearance of B =  $-r_B = -2r_A = 20 \text{ mol}/\text{m}^3\cdot\text{s}$   
Rate of formation of B =  $r_B = -20 \text{ mol}/\text{m}^3\cdot\text{s}$
- (c) *DDT*[C]: For every mole of chloral that disappears, one mole of DDT [C] appears.  $r_C = -r_A$   
Rate of disappearance of C =  $-r_C = -10 \text{ mol}/\text{m}^3\cdot\text{s}$   
Rate of formation of C =  $r_C = -r_A = -(-10 \text{ mol}/\text{m}^3\cdot\text{s}) = 10 \text{ mol}/\text{m}^3\cdot\text{s}$
- (d) *Water*[D]: Same relationship to chloral as the relationship to DDT  
Rate of formation of D =  $r_D = 10 \text{ mol}/\text{m}^3\cdot\text{s}$   
Rate of disappearance of D =  $-r_D = -10 \text{ mol}/\text{m}^3\cdot\text{s}$

$$\begin{aligned} -r_A &= 10 \text{ mol A}/\text{m}^3\cdot\text{s}^\dagger \\ r_A &= -10 \text{ mol A}/\text{m}^3\cdot\text{s} \\ \text{Equation (3-1) page 77} \end{aligned}$$

Then

$$\begin{aligned} \frac{r_A}{-1} &= \frac{r_B}{-2} = \frac{r_C}{1} = \frac{r_D}{1} \\ r_B &= 2(r_A) = -20 \text{ mol B}/\text{m}^3\cdot\text{s} \\ -r_B &= 20 \text{ mol B}/\text{m}^3\cdot\text{s} \\ r_C &= -r_A = 10 \text{ mol C}/\text{m}^3\cdot\text{s} \\ r_D &= -r_A = 10 \text{ mol D}/\text{m}^3\cdot\text{s} \end{aligned}$$

<sup>†</sup> Tutorial Video: <https://www.youtube.com/watch?v=6mAqX31RRJU>



$-r_A = 10 \text{ mol A/m}^3\cdot\text{s}$
$r_A = -10 \text{ mol A/m}^3\cdot\text{s}$
$-r_B = 20 \text{ mol B/m}^3\cdot\text{s}$
$r_B = -20 \text{ mol B/m}^3\cdot\text{s}$
$r_C = 10 \text{ mol C/m}^3\cdot\text{s}$

**Analysis:** The purpose of this example is to better understand the convention for the rate of reaction. The symbol  $r_j$  is the rate of formation (generation) of species  $j$ . If species  $j$  is a reactant, the numerical value of  $r_j$  will be a negative number. If species  $j$  is a product, then  $r_j$  will be a positive number. The rate of reaction,  $-r_A$ , is the rate of disappearance of reactant A and must be a positive number. A mnemonic relationship to help remember how to obtain relative rates of reaction of A to B, and so on, is given by Equation (3-1) on page 77.

In Equation (3-1) in Chapter 3, we will delineate the prescribed relationship between the rate of formation of one species,  $r_j$  (e.g., DDT [C]), and the rate of disappearance of another species,  $-r_i$  (e.g., chlorobenzene [B]), in a chemical reaction.

Heterogeneous reactions involve more than one phase. In heterogeneous reaction systems, the rate of reaction is usually expressed in measures other than volume, such as reaction surface area or catalyst weight. For a gas–solid catalytic reaction, the gas molecules must interact with the solid catalyst surface for the reaction to take place, as described in Chapter 10.

What is  $-r'_A$ ?

The dimensions of this heterogeneous reaction rate,  $-r'_A$  (prime), are the number of moles of A reacting per unit time per unit mass of catalyst (e.g., mol/s·g catalyst).

Definition of  $r_j$

Most of the introductory discussions on chemical reaction engineering in this book focus on homogeneous systems, in which case we simply say that  $r_j$  is the rate of formation of species  $j$  per unit volume. It is the number of moles of species  $j$  generated per unit volume per unit time.

We can say four things about the reaction rate  $r_j$ :  $r_j$  is

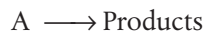
The rate law does not depend on the type of reactor used!!

- **The rate of formation of species  $j$  (mole/time/volume)**
- **An algebraic equation**
- **Independent of the type of reactor (e.g., batch or continuous flow) in which the reaction is carried out**
- **Solely a function of the properties of the reacting materials and reaction conditions (e.g., species concentration, temperature, pressure, or type of catalyst, if any) at a point in the system**

What is  $-r_A$  a function of?

However, because the properties and reaction conditions of the reacting materials may vary with position in a chemical reactor,  $r_j$  can in turn be a function of position and can vary from point to point in the system. This concept is utilized in flow reactors.

The *reaction-rate law* relates the rate of reaction to species concentration and temperature as will be shown in Chapter 3. The chemical reaction-rate-law is essentially an algebraic equation involving concentration, not a differential equation.<sup>1</sup> For example, the algebraic form of the rate law,  $-r_A$  for the reaction



may be a linear function of concentration,

$$-r_A = kC_A \quad (1-1)$$

<sup>1</sup> For further elaboration on this point, see *Chem. Eng. Sci.*, 25, 337 (1970); B. L. Crynes and H. S. Fogler, eds., *AIChE Modular Instruction Series E: Kinetics*, 1, 1 New York: AIChE, 1981; and R. L. Kabel, "Rates," *Chem. Eng. Commun.*, 9, 15 (1981).

or it may be some other algebraic function of concentration, such as Equation 3-6 shown in Chapter 3,

$$-r_A = kC_A^2 \quad (1-2)$$

or

$$-r_A = \frac{k_1 C_A}{1 + k_2 C_A}$$

The rate law is an algebraic equation.

The convention

For a given reaction, the particular concentration dependence that the rate law follows (i.e.,  $-r_A = kC_A$  or  $-r_A = kC_A^2$  or ...) must be determined from *experimental observation*. Equation (1-2) states that the rate of disappearance of A is equal to a rate constant  $k$  (which is a function of temperature) times the square of the concentration of A. As noted earlier, by convention,  $r_A$  is the rate of formation of A; consequently,  $-r_A$  is the rate of disappearance of A. Throughout this book, the phrase *rate of generation* means exactly the same as the phrase *rate of formation*, and these phrases are used interchangeably.

## 1.2 The General Mole Balance Equation (GMBE)

To perform a mole balance on any system, the system boundaries must first be specified. The volume enclosed by these boundaries is referred to as the *system volume*. We shall perform a mole balance on species  $j$  in a system volume, where species  $j$  represents the particular chemical species of interest, such as water or NaOH (Figure 1-3).

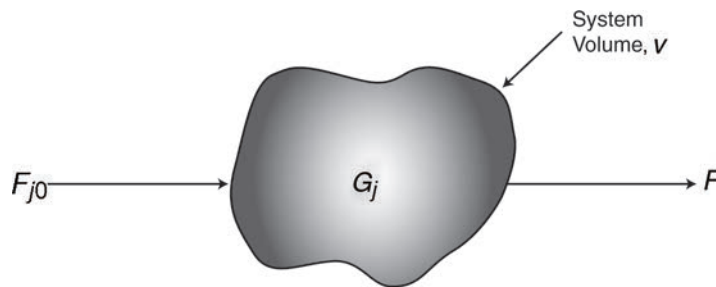


Figure 1-3 Mole balance on species  $j$  in a system volume,  $V$ .

A mole balance on species  $j$  at any instant in time,  $t$ , yields the following equation:

	$\left[ \begin{array}{c} \text{Rate of flow} \\ \text{of } j \text{ into} \\ \text{the system} \\ \text{(moles/time)} \end{array} \right]$	-	$\left[ \begin{array}{c} \text{Rate of flow} \\ \text{of } j \text{ out of} \\ \text{the system} \\ \text{(moles/time)} \end{array} \right]$	+	$\left[ \begin{array}{c} \text{Rate of generation} \\ \text{of } j \text{ by chemical} \\ \text{reaction within} \\ \text{the system} \\ \text{(moles/time)} \end{array} \right]$	=	$\left[ \begin{array}{c} \text{Rate of} \\ \text{accumulation} \\ \text{of } j \text{ within} \\ \text{the system} \\ \text{(moles/time)} \end{array} \right]$
Mole balance	<b>In</b>		<b>Out</b>		<b>Generation</b>		<b>Accumulation</b>
	$F_{j0}$	-	$F_j$	+	$G_j$	=	$\frac{dN_j}{dt}$ (1-3)

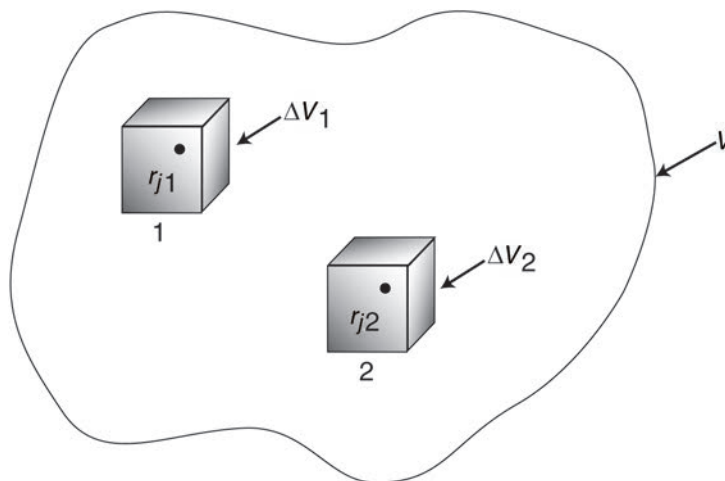
*Accumulation:* In this equation,  $N_j$  represents the number of moles of species  $j$  in the system at time  $t$  and  $\left(\frac{dN_j}{dt}\right)$  is the rate of accumulation of species  $j$  within the system volume.

*Generation:* If all the system variables (e.g., temperature, catalytic activity, and concentration of the chemical species) are spatially uniform throughout the system volume, the rate of generation of species  $j$ ,  $G_j$  (moles/time) is just the product of the reaction volume,  $V$ , and the rate of formation of species  $j$ ,  $r_j$ .

$$G_j = r_j \cdot V$$

$$\frac{\text{moles}}{\text{time}} = \frac{\text{moles}}{\text{time} \cdot \text{volume}} \cdot \text{volume}$$

Now suppose that the rate of formation of species  $j$  for the reaction varies with position in the system volume. That is, it has a value  $r_{j1}$  at location 1, which is surrounded by a small volume,  $\Delta V_1$ , within which the rate is uniform; similarly, the reaction rate has a value  $r_{j2}$  at location 2 and an associated volume,  $\Delta V_2$ , and so on (Figure 1-4).



**Figure 1-4** Dividing up the system volume,  $V$ .

The rate of generation,  $\Delta G_{j1}$ , in terms of  $r_{j1}$  and subvolume  $\Delta V_1$ , is

$$\Delta G_{j1} = r_{j1} \Delta V_1$$

Similar expressions can be written for  $\Delta G_{j2}$  and the other system subvolumes,  $\Delta V_i$ . The total rate of generation within the system volume is the sum of all the rates of generation in each of the subvolumes. If the total system volume is divided into  $M$  subvolumes, the total rate of generation is

$$G_j = \sum_{i=1}^M \Delta G_{ji} = \sum_{i=1}^M r_{ji} \Delta V_i$$

By taking the appropriate limits (i.e., let  $M \rightarrow \infty$  and  $\Delta V \rightarrow 0$ ) and making use of the definition of an integral, we can rewrite the foregoing equation in the form

$$G_j = \int^V r_j dV$$

From this equation, we see that  $r_j$  will be an indirect function of position, since the properties of the reacting materials and reaction conditions (e.g., concentration, temperature) can have different values at different locations in the reactor volume.

We now replace  $G_j$  in Equation (1-3), that is,

$$F_{j0} - F_j + G_j = \frac{dN_j}{dt} \quad (1-3)$$

by its integral form to yield a form of the general mole balance equation for any chemical species  $j$  that is entering, leaving, reacting, and/or accumulating within any system volume  $V$ .

This is a basic equation for chemical reaction engineering.

$$F_{j0} - F_j + \int^V r_j dV = \frac{dN_j}{dt} \quad (1-4)$$

From this general mole balance equation, we can develop the *design* equations for the various types of industrial reactors: batch, semibatch, and continuous-flow. Upon evaluation of these equations, we can determine the time (batch), reactor volume or catalyst weight (continuous-flow) necessary to convert a specified amount of the reactants into products.

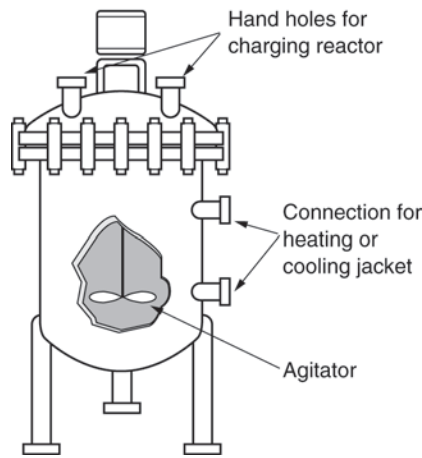
### 1.3 Batch Reactors (BRs)

When is a batch reactor used?

A batch reactor is used for small-scale operation, for testing new processes that have not been fully developed, for the manufacture of expensive products, and for processes that are difficult to convert to continuous operations. The reactor can be charged (i.e., filled) through the holes at the top (see Figure 1-5(a)). The batch reactor has the advantage of high conversions that can be obtained by leaving the reactant in the reactor for long periods of time, but it also has the disadvantages of high labor costs per batch, the variability of products from batch to batch, and the difficulty of large-scale production (see Industrial Reactor Photos in *Professional Reference Shelf [PRS]* (<http://www.umich.edu/~elements/6e/01chap/prof-reactors.html>) on the CRE Web sites, [www.umich.edu/~elements/6e/index.html](http://www.umich.edu/~elements/6e/index.html)). Also see <http://encyclopedia.che.engin.umich.edu/Pages/Reactors/menu.html>.



Reference Shelf



**Figure 1-5(a)** Simple homogeneous batch reactor (BR). [Excerpted by special permission from *Chem. Eng.*, 63(10), 211 (Oct. 1956). Copyright 1956 by McGraw-Hill, Inc., New York, NY 10020.]



**Figure 1-5(b)** Batch reactor mixing patterns. Further descriptions and photos of the batch reactors can be found in both the *Visual Encyclopedia of Equipment* and in the *Professional Reference Shelf* on the CRE Web site.

Also see <http://encyclopedia.che.engin.umich.edu/Pages/Reactors/Batch/Batch.html>.

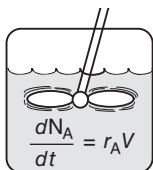
A batch reactor has neither inflow nor outflow of reactants or products while the reaction is being carried out:  $F_{j0} = F_j = 0$ . The resulting general mole balance on species  $j$  is

$$\frac{dN_j}{dt} = \int^V r_j dV$$

If the reaction mixture is perfectly mixed (Figure 1-5(b)) so that there is no variation in the rate of reaction throughout the reactor volume, we can take  $r_j$  out of the integral, integrate, and write the differential form of the mole balance, that is,

Perfect mixing

$$\boxed{\frac{dN_j}{dt} = r_j V} \tag{1-5}$$



Batch Reactor

Let's consider the isomerization of species A in a batch reactor



As the reaction proceeds, the number of moles of A decreases and the number of moles of B increases, as shown in Figure 1-6.

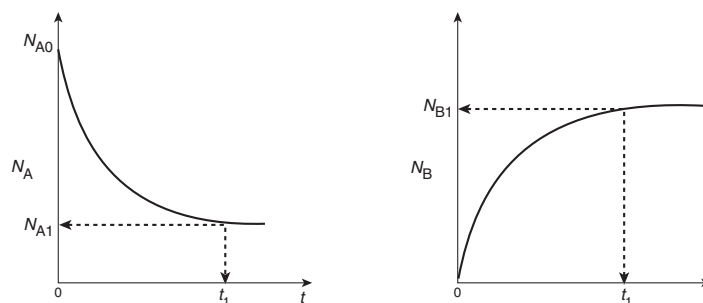


Figure 1-6 Mole-time trajectories.

We might ask what time,  $t_1$ , is necessary to reduce the initial number of moles from  $N_{A0}$  to a final desired number  $N_{A1}$ . Applying Equation (1-5) to the isomerization

$$\frac{dN_A}{dt} = r_A V$$

rearranging,

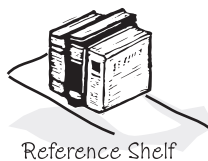
$$dt = \frac{dN_A}{r_A V}$$

and integrating with limits that at  $t = 0$ , then  $N_A = N_{A0}$ , and at  $t = t_1$ , then  $N_A = N_{A1}$ , we obtain

$$t_1 = \int_{N_{A1}}^{N_{A0}} \frac{dN_A}{-r_A V} \quad (1-6)$$

This equation is the integral form of the mole balance on a batch reactor. It gives the time,  $t_1$ , necessary to reduce the number of moles from  $N_{A0}$  to  $N_{A1}$  and also to form  $N_{B1}$  moles of B.

## 1.4 Continuous-Flow Reactors



Reference Shelf

Continuous-flow reactors are almost always operated at steady state. We will consider three types: the *continuous-stirred tank reactor* (CSTR), the *plug-flow reactor* (PFR), and the *packed-bed reactor* (PBR). Detailed physical descriptions of these reactors can be found in both the *Professional Reference Shelf* (PRS) (<http://www.umich.edu/~elements/6e/01chap/prof.html>) of Chapter 1 and in the *Visual Encyclopedia of Equipment* (<http://encyclopedia.che.engin.umich.edu/Pages/Reactors/CSTR/CSTR.html>), and on the CRE Web site.

### 1.4.1 Continuous-Stirred Tank Reactor (CSTR)

A type of reactor commonly used in industrial processing is the stirred tank operated continuously (Figure 1-7). It is referred to as the *continuous-stirred tank reactor* (CSTR) or *vat*, or *backmix reactor*, and is primarily used for

What is a CSTR used for?

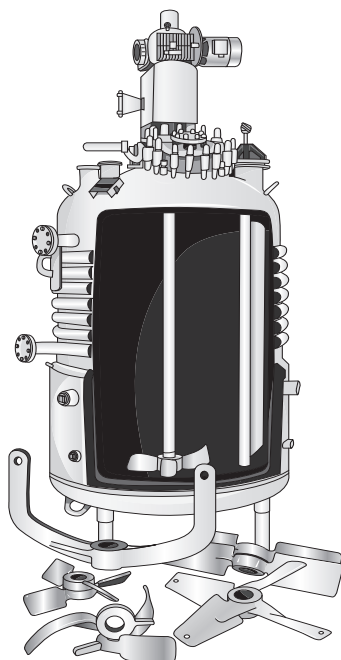


Figure 1-7(a) CSTR/batch reactor.

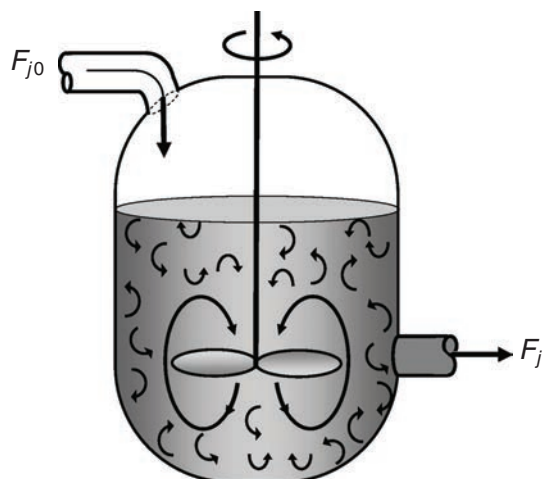


Figure 1-7(b) CSTR mixing patterns.

Also see <http://encyclopedia.che.engin.umich.edu/Pages/Reactors/CSTR/CSTR.html>.

*liquid-phase reactions*. It is normally operated **at steady state** and is assumed to be **perfectly mixed**; consequently, there is no time dependence or position dependence of the temperature, concentration, or reaction rate inside the CSTR. That is, every variable is the same at every point inside the reactor. Because the temperature and concentration are identical everywhere within the reaction vessel, they are the same at the *exit point* as they are elsewhere in the tank. Thus, the temperature and concentration in the exit stream are modeled as being the same as those inside the reactor. In systems where mixing is highly *nonideal*, the well-mixed model is inadequate, and we must resort to other modeling techniques, such as residence time distributions, to obtain meaningful results. This topic of nonideal mixing is discussed in Chapters 16 and 17, while nonideal flow reactors are discussed in Chapter 18.

When the general mole balance equation

$$\text{GMBE} \quad F_{j0} - F_j + \int^V r_j dV = \frac{dN_j}{dt} \quad (1-4)$$

is applied to a CSTR operated at steady state (i.e., conditions do not change with time),

$$\frac{dN_j}{dt} = 0$$

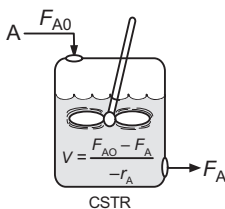
in which there are no spatial variations in the rate of reaction (i.e., perfect mixing),

The ideal CSTR is assumed to be perfectly mixed.

$$\int^V r_j dV = Vr_j$$

it takes the familiar form, which is sometimes called *the design equation* for a CSTR

$$V = \frac{F_{j0} - F_j}{-r_j} \quad (1-7)$$



The CSTR design equation gives the reactor volume  $V$  necessary to reduce the entering molar flow rate of species  $j$  from  $F_{j0}$  to the exit molar flow rate  $F_j$ , when species  $j$  is disappearing at a rate of  $-r_j$ . We note that the CSTR is modeled such that the conditions in the exit stream (e.g., concentration and temperature) **are identical** to those in the tank. The molar flow rate  $F_j$  is just the product of the concentration of species  $j$  and the volumetric flow rate  $v$

$$F_j = C_j \cdot v$$

$$\frac{\text{moles}}{\text{time}} = \frac{\text{moles}}{\text{volume}} \cdot \frac{\text{volume}}{\text{time}} \quad (1-8)$$

Applying Equation (1-8) at the entrance of the reactor one obtains

$$F_{j0} = C_{j0} \cdot v_0$$

Consequently, we can substitute for  $F_{j0}$  and  $F_j$  into Equation (1-7) to write a balance on species  $A$  in terms of concentration, as

$$V = \frac{v_0 C_{A0} - v C_A}{-r_A} \quad (1-9)$$

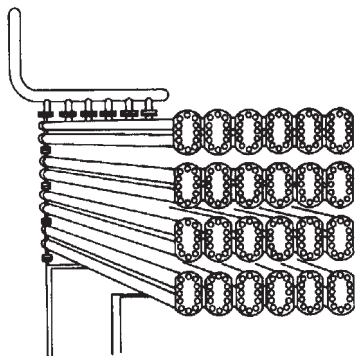
The ideal CSTR mole balance equation is an algebraic equation, not a differential equation.

### 1.4.2 Tubular Reactor

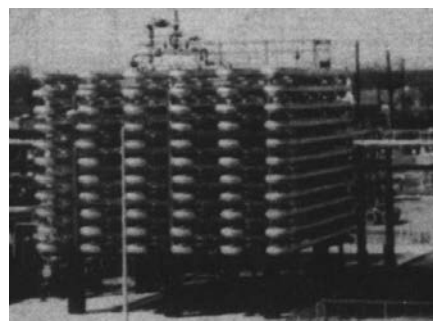
When is a tubular reactor most often used?

In addition to the CSTR and batch reactors, another type of reactor commonly used in industry is the *tubular reactor*. It consists of a cylindrical pipe and is normally operated at steady state, as is the CSTR. Tubular reactors are used most often for *gas-phase reactions*. A schematic and a photograph of industrial tubular reactors are shown in Figure 1-8.

In the tubular reactor, the reactants are continually consumed as they flow down the length of the reactor. In modeling the tubular reactor, we assume that the concentration varies continuously in the axial direction through the reactor. Consequently, the *reaction rate*, which is a function of concentration for all but zero-order reactions (cf. Equation 3-2), will *also* vary axially. For the purposes of the material presented here, we consider systems in which the flow field may be modeled by that of a plug-flow profile (e.g., uniform radial



**Figure 1-8(a)** Tubular reactor schematic. Longitudinal tubular reactor. [Excerpted by special permission from *Chem. Eng.*, 63(10), 211 (Oct. 1956). Copyright 1956 by McGraw-Hill, Inc., New York, NY 10020.]

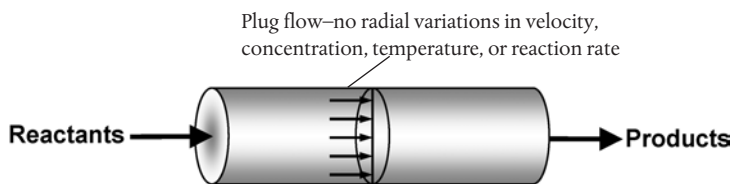


**Figure 1-8(b)** Tubular reactor photo. Tubular reactor for production of Dimersol G. (Photo courtesy of Editions Techniq Institut Français du Pétrole.)

Also see <http://encyclopedia.che.engin.umich.edu/Pages/Reactors/PFR/PFR.html>.

velocity in turbulent flow), as shown in Figure 1-9. That is, there is no radial variation in reaction rate, and the reactor is referred to as a *plug-flow reactor* (PFR). (The laminar-flow reactor (LFR) is discussed in Chapters 16–18, along with a discussion of nonideal reactors.)

Also see PRS and  
*Visual Encyclopedia of  
Equipment.*



**Figure 1-9** Plug-flow tubular reactor.

The general mole balance equation is given by Equation (1-4):

$$F_{j0} - F_j + \int^V r_j dV = \frac{dN_j}{dt} \quad (1-4)$$

The equation we will use to design PFRs at steady state can be developed in two ways: (1) directly from Equation (1-4) by differentiating with respect to volume  $V$ , and then rearranging the result or (2) from a mole balance on species  $j$  in a differential segment of the reactor volume  $\Delta V$ . Let's choose the second way to arrive at the differential form of the PFR mole balance. The differential volume,  $\Delta V$ , shown in Figure 1-10, will be chosen sufficiently small such that there are no spatial variations in reaction rate within this volume. Thus the generation term,  $\Delta G_j$ , is

$$\Delta G_j = \int^{\Delta V} r_j dV = r_j \Delta V$$

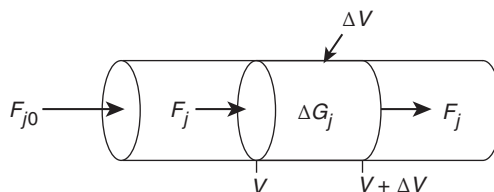


Figure 1-10 Mole balance on species  $j$  in volume  $\Delta V$ .

$\left[ \begin{array}{c} \text{Molar flow} \\ \text{rate of species } j \\ \text{In at } V \\ \text{moles/time} \end{array} \right]$	-	$\left[ \begin{array}{c} \text{Molar flow} \\ \text{rate of species } j \\ \text{Out at } (V + \Delta V) \\ \text{moles/time} \end{array} \right]$	+	$\left[ \begin{array}{c} \text{Molar rate of} \\ \text{Generation} \\ \text{of species } j \\ \text{within } \Delta V \\ \text{moles/time} \end{array} \right]$	=	$\left[ \begin{array}{c} \text{Molar rate of} \\ \text{Accumulation} \\ \text{of species } j \\ \text{within } \Delta V \\ \text{moles/time} \end{array} \right]$
<b>In</b>	-	<b>Out</b>	+	<b>Generation</b>	=	<b>Accumulation</b>
$F_j _V$	-	$F_j _{V+\Delta V}$	+	$r_j \Delta V$	=	0 (1-10)

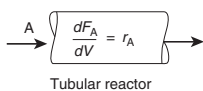
Dividing Equation (1-10) by  $\Delta V$  and rearranging

$$\left[ \frac{F_j|_{V+\Delta V} - F_j|_V}{\Delta V} \right] = r_j$$

we note the term in brackets resembles the definition of a derivative

$$\lim_{\Delta x \rightarrow 0} \left[ \frac{f(x + \Delta x) - f(x)}{\Delta x} \right] = \frac{df}{dx}$$

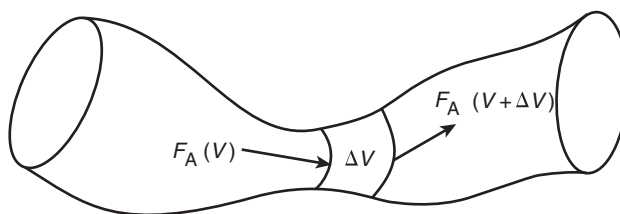
Taking the limit as  $\Delta V$  approaches zero, we obtain the differential form of steady-state mole balance on a PFR



$$\boxed{\frac{dF_j}{dV} = r_j} \quad (1-11)$$

We could have made the cylindrical reactor on which we carried out our mole balance an irregularly shaped reactor, such as the one shown in Figure 1-11 for reactant species A. However, we see that by applying Equation (1-10), the result would yield the same equation (i.e., Equation (1-11)). For species A, the mole balance is

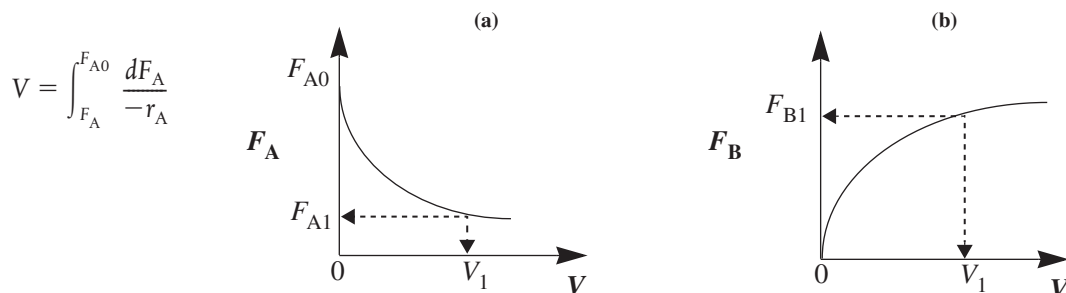
$$\boxed{\frac{dF_A}{dV} = r_A} \quad (1-12)$$

Picasso's  
reactor**Figure 1-11** Pablo Picasso's reactor.

Consequently, we see that Equation (1-11) applies equally well to our model of tubular reactors of variable and constant cross-sectional area, although it is doubtful that one would find a reactor of the shape shown in Figure 1-11 unless it were designed by Pablo Picasso or perhaps one of his followers.

The conclusion drawn from the application of the design equation to Picasso's reactor is an important one: the degree of completion of a reaction achieved in an ideal plug-flow reactor (PFR) does not depend on its shape, only on its total volume.

Let's again consider the isomerization  $A \rightarrow B$ , this time in a PFR. As the reactants proceed down the reactor, A is consumed by chemical reaction and B is produced. Consequently, the molar flow rate  $F_A$  decreases as shown in Figure 1-12(a) while  $F_B$  increases as the reactor volume  $V$  increases, as shown in Figure 1-12(b).

**Figure 1-12** Profiles of molar flow rates in a PFR.

We now ask, "What is the reactor volume  $V_1$  necessary to reduce the entering molar flow rate of A from  $F_{A0}$  to an exit flow rate  $F_{A1}$ ?" Rearranging Equation (1-12) in the form

$$dV = \frac{dF_A}{r_A}$$

and integrating with limits at  $V = 0$ , then  $F_A = F_{A0}$ , and at  $V = V_1$ , then  $F_A = F_{A1}$

$$V_1 = \int_{F_{A0}}^{F_{A1}} \frac{dF_A}{r_A} = \int_{F_{A1}}^{F_{A0}} \frac{dF_A}{-r_A} \quad (1-13)$$

$V_1$  is the volume necessary to reduce the entering molar flow rate  $F_{A0}$  to some specified value  $F_{A1}$  and also the volume necessary to produce a molar flow rate of B of  $F_{B1}$ .

### 1.4.3 Packed-Bed Reactor (PBR)

The principal difference between reactor design calculations involving homogeneous reactions and those involving fluid–solid heterogeneous reactions is that for the latter, the reaction takes place on the surface of the catalyst (see Figure 10-5). The greater the mass of a given catalyst, the greater the reactive surface area. Consequently, the reaction rate is based on mass of solid catalyst,  $W$ , rather than on reactor volume,  $V$ . For a fluid–solid heterogeneous system, the rate of reaction of a species A,  $-r'_A$ , is defined as

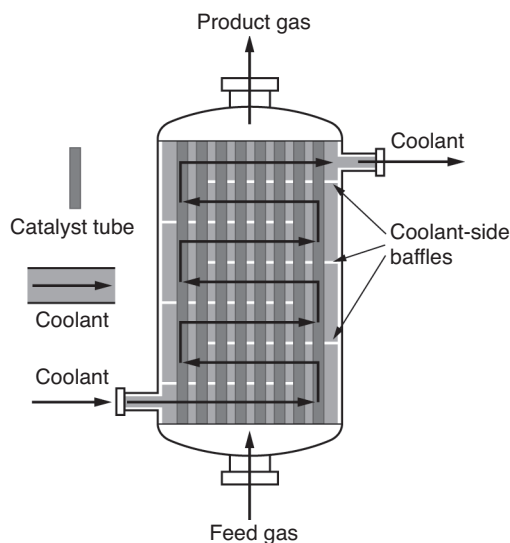
$$-r'_A = \text{mol A reacted}/(\text{time} \times \text{mass of catalyst})$$

The mass of solid catalyst is used because the amount of catalyst is what is important to the rate of product formation. We note that by multiplying the heterogeneous reaction rate,  $-r'_A$ , by the bulk catalyst density,  $\rho_b$   $\left(\frac{\text{mass}}{\text{volume}}\right)$ , we can obtain the reaction rate per unit volume,  $-r_A$ .

$$-r_A = \rho_b (-r'_A)$$

$$\left(\frac{\text{mol}}{\text{dm}^3 \cdot \text{s}}\right) = \left(\frac{\text{g}}{\text{dm}^3}\right)\left(\frac{\text{mol}}{\text{g} \cdot \text{s}}\right)$$

The reactor volume that contains the catalyst is of secondary significance. Figure 1-13 shows a schematic of an industrial catalytic reactor with vertical tubes packed with solid catalyst.



**Figure 1-13** Longitudinal catalytic packed-bed reactor. Also see <http://encyclopedia.che.engin.umich.edu/Pages/Reactors/PBR/PBR.html>.

PBR  
Mole Balance

In the three idealized types of reactors just discussed (the perfectly mixed batch reactor [BR], the plug-flow tubular reactor [PFR]), and the perfectly mixed continuous-stirred tank reactor [CSTR]), the design equations (i.e., mole balances) were developed based on reactor volume. The derivation of the design equation for a packed-bed catalytic reactor (PBR) will be carried out in a manner analogous to the development of the tubular design equation. To accomplish this derivation, we simply replace the volume coordinate,  $V$ , in Equation (1-10) with the catalyst mass (i.e., weight) coordinate  $W$  (Figure 1-14).

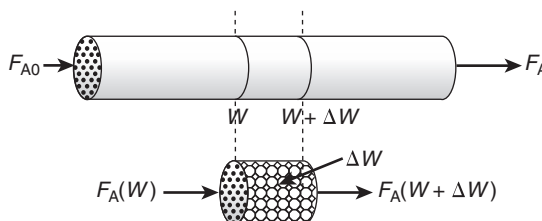


Figure 1-14 Packed-bed reactor schematic.

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  $\Delta W$  results in the equation

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

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

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

which are, as expected, the same dimensions of the molar flow rate  $F_A$ . After dividing Equation (1-14) by  $\Delta W$  and taking the limit as  $\Delta W \rightarrow 0$ , we arrive at the differential form of the mole balance for a packed-bed reactor:

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

$$\boxed{\frac{dF_A}{dW} = r'_A} \quad (1-15)$$



When pressure drop through the reactor (see Section 5.5) and catalyst decay (see Section 10.7 in Chapter 10) are neglected, the integral form of the packed-catalyst-bed design equation can be used to calculate the catalyst weight

You can use the integral form **only** when there is no  $\Delta P$  and no catalyst decay.

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

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

### 1.4.4 Well-Mixed "Fluidized" Catalytic Bed Reactor

For particulate catalytic gas-phase systems, the fluidized bed is also in common use. Depending of the flow regime, it can be modeled anywhere between a straight through transport reactor (Chapter 10) to a fluidized bed that is analogous to a CSTR (section 1.4.1), which is shown in Figure 1-15.

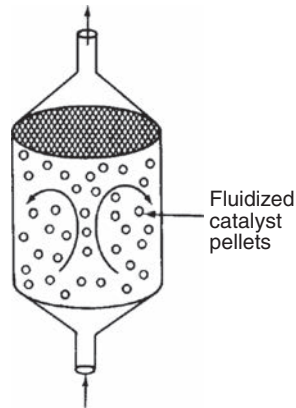


Figure 1-15 Well-mixed fluidized bed modeled as a CSTR.

A mole balance on species A in a well-mixed "fluidized" bed is

$$F_{A0} - F_A + r'_A W = 0 \quad (1-17)$$

Dividing by the catalyst weight  $W$ , we arrive at the Equation (1-18) that gives the catalyst weight necessary to reduce the molar rate entering from,  $F_{A0}$  (mol/s) to the molar rate leaving,  $F_A$ , (mol/s) when species A is disappearing at a rate,  $r'_A$  (mol/s·gcat) the design equation is

$$W = \frac{F_{A0} - F_A}{-r'_A} \quad (1-18)$$

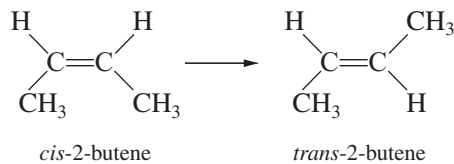
Looking Ahead



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

#### Example 1-2 How Large Is the Reactor Volume?

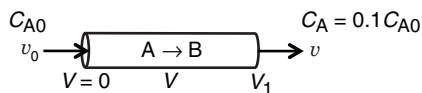
Let's consider the liquid phase *cis*-*trans* isomerization of 2-butene



which we will write symbolically as



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



1. Without solving any equations, sketch what you think the concentration profile ( $C_A$  as a function of  $V$ ) would look like.
2. Derive an equation relating the reactor volume to the entering and exiting concentrations of A, the rate constant  $k$ , and the volumetric flow rate  $v_0$ .
3. Determine the reactor volume,  $V_1$ , necessary to reduce the exiting concentration to 10% of the entering concentration, that is,  $C_A = 0.1C_{A0}$ , when the volumetric flow rate  $v_0$  is  $10 \text{ dm}^3/\text{min}$  (i.e., liters/min) and the specific reaction rate,  $k$ , is  $0.23 \text{ min}^{-1}$ .

#### Solution

1. Sketch  $C_A$  as a function of  $V$ .

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. Because the volumetric flow rate is constant,  $v = v_0$ , one can use Equation (1-8) to obtain the concentration of A,  $C_A = F_A/v_0$ , and then by comparison with the plot in Figure 1-12, obtain the concentration of A as a function of reactor volume, as shown in Figure E1-2.1.

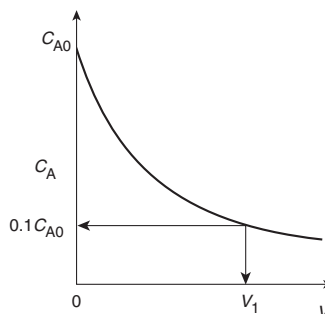


Figure E1-2.1 Concentration profile.

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 ( $j = A$ )

$$\text{Mole Balance:} \quad \frac{dF_A}{dV} = r_A \quad (1-12)$$

For a first-order reaction, the rate law (as will be discussed in Chapter 3, Equation (3-5)) is

$$\text{Rate Law:} \quad -r_A = kC_A \quad (\text{E1-2.1})$$

Reactor sizing

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

$$\frac{dF_A}{dV} = \frac{d(C_A v)}{dV} = \frac{d(C_A v_0)}{dV} = v_0 \frac{dC_A}{dV} = r_A \quad (\text{E1-2.2})$$

Multiplying both sides of Equation (E1-2.2) by minus one and then substituting Equation (E1-2.1) yields

**Combine:** 
$$-\frac{v_0 dC_A}{dV} = -r_A = kC_A \quad (\text{E1-2.3})$$

Separating the variables and rearranging gives

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

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

$$-\frac{v_0}{k} \int_{C_{A0}}^{C_A} \frac{dC_A}{C_A} = \int_0^V dV \quad (\text{E1-2.4})$$

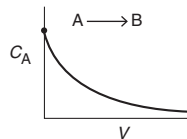
Carrying out the integration of Equation (E1-2.4) gives

**Solve:** 
$$V = \frac{v_0}{k} \ln \frac{C_{A0}}{C_A} \quad (\text{E1-2.5})$$

We can also rearrange Equation (E1-2.5) to solve for the concentration of A as a function of reactor volume to obtain

$$C_A = C_{A0} \exp(-kV/v_0)$$

Concentration profile



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

**Evaluate:**

Substituting  $C_{A0}$ ,  $C_A$ ,  $v_0$ , and  $k$  in Equation (E1-2.5), we have

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

We see that a reactor volume of  $0.1 \text{ m}^3$  is necessary to convert 90% of species A entering (i.e.,  $C_A = 0.1 C_{A0}$ ) into product B for the parameters given.

Let's now calculate the reactor volume necessary to an even smaller concentration say  $(1/100)^{\text{th}}$  of the entering concentration, that is,

$$C_A = 0.01C_{A0}$$

$$V = \frac{10 \text{ dm}^3/\text{min}}{0.23 \text{ min}^{-1}} \ln \frac{C_{A0}}{0.01 C_{A0}} = \frac{10 \text{ dm}^3}{0.23} \ln 100 = 200 \text{ dm}^3 \quad \text{Ans.}$$

Note: We see that a larger reactor (200 dm<sup>3</sup>) is needed to reduce the exit concentration to a smaller fraction of the entering concentration (e.g.,  $C_A = 0.01 C_{A0}$ ).

**Analysis:** For this irreversible liquid-phase first-order reaction (i.e.,  $-r_A = kC_A$ ) being carried out in a PFR, the concentration of the reactant decreases exponentially down the length (i.e., volume  $V$ ) of the reactor. The more that species A is consumed and converted to product B, the larger must be the reactor volume. The purpose of the example was to give a vision of the types of calculations we will be carrying out as we study chemical reaction engineering (CRE).

### Example 1-3 Numerical Solutions to Example 1-2 Problem: How Large Is the Reactor Volume?

Now we will turn Example 1-2 into a *Living Example Problem* (LEP) where we can vary parameters to learn their effect on the volume and/or exit concentrations. We could use Polymath, Wolfram, or Python to solve the combined mole balance and rate law to determine the concentration profile. In this example, we will use *Polymath*.

We begin by rewriting the mole balance, Equation (E1-2.2), in Polymath notation form

$$\text{Mole Balances} \quad \frac{d(Ca)}{d(V)} = ra/v_o \quad (\text{E1-3.1})$$

$$\frac{d(Cb)}{d(V)} = rb/v_o \quad (\text{E1-3.2})$$

$$\text{Rate Law} \quad ra = -k*Ca \quad (\text{E1-3.3})$$

$$rb = -ra \quad (\text{E1-3.4})$$

$$k = 0.23$$

$$v_o = 10$$

Polymath  
Formulation

A Polymath tutorial to solve the ordinary differential equations (ODEs) can be found on the Web site ([http://www.umich.edu/~elements/6e/tutorials/ODE\\_Equation\\_Tutorial.pdf](http://www.umich.edu/~elements/6e/tutorials/ODE_Equation_Tutorial.pdf) and [http://www.umich.edu/~elements/6e/tutorials/Polymath\\_tutorials.html](http://www.umich.edu/~elements/6e/tutorials/Polymath_tutorials.html)).

The parameter values are  $k = 0.23 \text{ min}^{-1}$ ,  $v_o = 10 \text{ dm}^3/\text{min}$  and  $C_{A0} = 10 \text{ mole/dm}^3$ . The initial and final values for the integration wrt the volume  $V$  are  $V = 0$  and  $V = 100 \text{ dm}^3$ .

The output from the Polymath solution is given in Table E1-3.1 and the axial concentration profiles for species A and B are shown in Figure E1-3.1.

TABLE E1-3.1 POLYMATH PROGRAM AND OUTPUT FOR ISOTHERMAL PFR

Differential equations	Calculated values of DEQ variables		
	Variable	Initial value	Final value
1 $d(Cb)/d(V) = rb/v_o$	1 Ca	10.	1.002588
2 $d(Ca)/d(V) = ra/v_o$	2 Cb	0	8.997412
<b>Explicit equations</b>	3 k	0.23	0.23
1 $v_o = 10$	4 ra	-2.3	-0.2305953
2 $k = 0.23$	5 rb	2.3	0.2305953
3 $ra = -k*Ca$	6 V	0	100.
4 $rb = -ra$	7 $v_o$	10.	10.

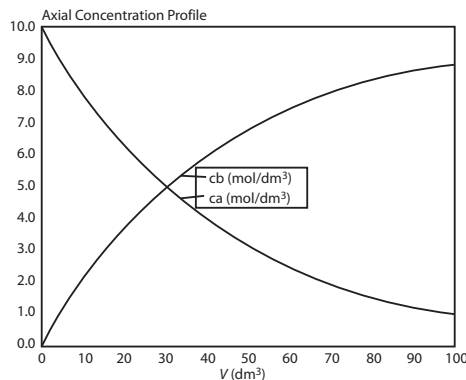
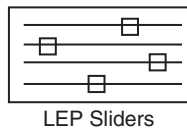


Figure E1-3.1 Axial concentration profiles for A and B.

**Analysis:** Because Polymath will be used extensively in later chapters to solve non-linear ordinary differential equations (ODEs), we introduce it here so that the reader can start to become familiar with it. Figure E1-3.1 shows how the concentrations of species A and B vary down the length of the PFR. In order to become familiar with Polymath, the reader is encouraged to solve the foxes and rabbits problem using Polymath (P1-3<sub>B</sub>(a)) and then study the dynamics of the reaction using Wolfram or Python (P1-3<sub>B</sub>(b)).

## 1.5 Industrial Reactors



<http://encyclopedia.che.engin.umich.edu/Pages/Reactors/menu.html>

Be sure to view the actual photographs of industrial reactors on the CRE Web site so you will know them when you run into them. There are also links to view reactors on different Web sites. The CRE Web site also includes a portion of the *Visual Encyclopedia of Equipment*, [encyclopedia.che.engin.umich.edu](http://encyclopedia.che.engin.umich.edu), “Chemical Reactors” developed by Dr. Susan Montgomery and her students at the University of Michigan. Also see *Professional Reference Shelf* on the CRE Web site for “Reactors for Liquid-Phase and Gas-Phase Reactions,” along with photos of industrial reactors, and Expanded Material on the CRE Web site.<sup>2</sup>

In this chapter, and on the CRE Web site, we’ve introduced each of the major types of industrial reactors: batch, stirred tank, tubular, and fixed bed (packed bed). Many variations and modifications of these commercial reactors (e.g., semibatch, fluidized bed) are in current use and these reactors will be discussed in Chapters 6 and 10, respectively. For further elaboration, refer to the detailed discussion of industrial reactors given by Walas.<sup>3</sup>

The CRE Web site describes industrial reactors, along with typical feed and operating conditions. In addition, two solved example problems for Chapter 1 can be found on the CRE Web site, <http://www.umich.edu/~elements/6e>.

<sup>2</sup> Chem. Eng., 63(10), 211 (1956). See also *AIChE Modular Instruction Series E*, 5 (1984).

<sup>3</sup> S. M. Walas, *Reaction Kinetics for Chemical Engineers*, New York: McGraw-Hill, 1959, Chap. 11.

## 1.6 *And Now... A Word from Our Sponsor–Safety 1 (AWFOS–S1 Safety)*

*A note to students:* In this sixth edition of *Elements of Chemical Reaction Engineering*, I am including a section at the end of each chapter to bring a greater awareness to process safety. A critical aspect of process safety is “anticipating” what could go wrong in a chemical process and ensuring it won’t go wrong. Equipment and processes involving exothermic chemical reactions are some of the most at risk in a chemical plant. Consequently, each chapter will end with a segment “*And Now... A Word From Our Sponsor–Safety*” (AWFOS–S). In addition, to highlight process safety across the chemical engineering curriculum, a Web site (<http://umich.edu/~safeche/>) has been developed that features a safety module specific to every core chemical engineering lecture course plus lab safety. In this chapter, we define process safety along with a very brief discussion on why it is important to study process safety.

### 1.6.1 What Is Chemical Process Safety?

Chemical process safety is a blend of engineering and management practices focused on preventing accidents, namely explosions, fires, and toxic releases that result in loss of life and property.

### 1.6.2 Why Study Process Safety?

Industrial disasters such as UCIL Bhopal, T2 Laboratories, BP Texas City, and Flixborough have collectively killed and injured thousands of people and caused billions of dollars in damage to chemical plants and nearby communities. Accidents such as these occur because chemical engineering processes are some of the most potentially dangerous due to extreme operating conditions and the use of explosive, reactive, and flammable materials. What surprises people is that most of these chemical engineering accidents, such as those listed in the Chemical Safety Board Videos on the companion Web site



**Figure 1-16** T2 Laboratories (see Chapter 13).

(<http://umich.edu/~safeche/>) were preventable. They were the result of poor engineering decisions, made by people who lacked fundamental understanding of basic chemical engineering concepts and chemical engineering safety. Thus, knowing the fundamentals of chemical engineering and process safety may save your life and the lives of innocent people, and prevent the loss of millions of dollars of material and equipment.

Engineers have an ethical and professional obligation to work only in areas for which they are competent and qualified. The best way to prevent future industrial disasters is to understand how to effectively and safely design, operate, and troubleshoot chemical processes. To prepare a prevention plan, we must take the time and effort to understand chemical processes and chemical process safety. To help achieve this understanding, the last section of every chapter has a tutorial, AWFOSS, that can help you prevent accidents.

A comparison of process safety and personal safety is very succinctly given on the Web site ([http://www.energysafetycanada.com/files/pdf/Personal\\_vs\\_Process\\_Safety\\_v3.pdf](http://www.energysafetycanada.com/files/pdf/Personal_vs_Process_Safety_v3.pdf)).

**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, Chapters 1 and 2
- Rate Law, Chapter 3
- Stoichiometry, Chapter 4
- Isothermal Reactor Design, Chapter 5
- Combine  
Evaluate
- Energy Balance, Chapters 11–13

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

*A Word of Caution: The falling CRE Tower. As we proceed through the next five chapters, we will see how these building blocks form a tower. Now, if one cuts corners when studying this material, the building blocks become cylinders and as a result the tower becomes unstable and all of the understanding of CRE falls apart. See <http://www.umich.edu/~elements/6e/01chap/assets/player/KeynoteDHTML-Player.html#3>.*

## 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

$$F_{j0} - F_j + \int^V r_j dV = \frac{dN_j}{dt} \quad (\text{S1-1})$$

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

$$F_{A0} - F_A + r_A V = \frac{dN_A}{dt} \quad (\text{S1-2})$$


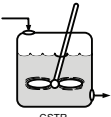
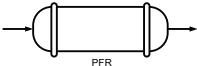
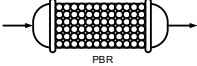
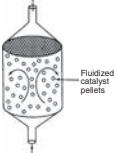
2. The kinetic rate law for  $r_j$  is

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

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 shown in Table S1-1.

TABLE S1-1 SUMMARY OF REACTOR MOLE BALANCES

Reactor	Comment	Mole Balance Differential Form	Algebraic Form	Integral Form
 BR	No spatial variations	$\frac{dN_A}{dt} = r_A V$		$t_1 = \int_{N_{A1}}^{N_{A0}} \frac{dN_A}{-r_A V}$
 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	$\frac{dF_A}{dW} = r'_A$		$W_1 = \int_{F_{A1}}^{F_{A0}} \frac{dF_A}{-r'_A}$
 Fluidized CSTR	Steady state	—	$W = \frac{F_{A0} - F_A}{-r'_A}$	—

## CRE WEB SITE MATERIALS

(<http://www.umich.edu/~elements/6e/01chap/obj.html#/>)

### Useful Links

#### Living Example Problems

Polymath, Python, Matlab and Wolfram

#### Extra Help

Multiple Resources extra problems, screencasts and lecture notes

#### Additional Materials

New Technical Material, Detailed Derivations and Web Modules

#### Professional Reference Shelf

Material important to the practicing engineer that is not necessarily covered in all CRE courses.

#### YouTube Videos

Humorous videos covering topics varying from example problems to light hearted breaks from studying

### Evaluation

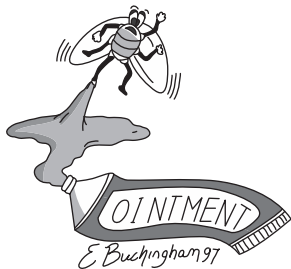
#### Self Tests

Interactive problems with solutions to provide extra practice of concepts

#### i>Clicker Questions

Interactive multiple choice questions to help access your understanding of the material

### Getting Unstuck on a Problem



([http://www.umich.edu/~elements/6e/01chap/iclicker\\_ch1\\_q1.html](http://www.umich.edu/~elements/6e/01chap/iclicker_ch1_q1.html))

### Smog in L.A. Web Module



Photograph by Radoslaw Lecyk/Shutterstock  
([http://www.umich.edu/~elements/6e/web\\_mod/la\\_basin/index.htm](http://www.umich.edu/~elements/6e/web_mod/la_basin/index.htm))

Living Example Problem:  
<http://www.umich.edu/~elements/6e/01chap/live.html>

Interactive Computer Games (<http://www.umich.edu/~elements/6e/icm/index.html>)

A. Quiz Show I (<http://www.umich.edu/~elements/6e/icm/kinchal1.html>)



This game could help prepare you for the AIChE student chapter Jeopardy Competition held each year at the Annual AIChE meeting.

## QUESTIONS, SIMULATIONS, 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, that is, A, least difficult; B, moderate difficulty; C, fairly difficult; D, (double black diamond), most difficult. A = ● B = ■ C = ◆ D = ◆◆ For example, P1-5<sub>B</sub> means “1” is the Chapter number, “5” is the problem number, “B” is the problem difficulty, in this case B means moderate difficulty.

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

### Questions

- Q1-1<sub>A</sub>** **QBR Questions Before Reading.** Research has shown (*J. Exp. Psychol. Learn. Mem. Cogn.*, 40, 106–114 (2014)) that if you ask a question of the material before reading the material you will have greater retention. Consequently, the first question of every chapter will have such a question on that chapter's material. For Chapter 1, the question is “Is the generation term, G, the only term in the mole balance that varies for each type of reactor?”
- Q1-2<sub>A</sub>** Go to Chapter 1 **Evaluation** on the Web site. Click on **i>Clicker Questions** ([http://www.umich.edu/~elements/6e/01chap/iclicker\\_ch1\\_q1.html](http://www.umich.edu/~elements/6e/01chap/iclicker_ch1_q1.html)) and view at least five i>clicker questions. Choose one that could be used as is, or a variation thereof, to be included on the next exam. You also could consider the opposite case: explaining why the question should *not* be on the next exam. In either case, explain your reasoning.
- Q1-3<sub>A</sub>** **What if...** the PFR in **Example 1-2** were replaced by a CSTR, what would be its volume?
- Q1-4<sub>A</sub>** **What if...** you were asked to rework **Example 1-2** to calculate the time to reduce the number of moles of A to 1% of its initial value for a constant volume BR, what would you say? Would you do it? If your answer is “yes,” go ahead and calculate it; if your answer is “NO, I won't do it!” then suggest two ways to work this problem incorrectly.
- Q1-5<sub>A</sub>** Read through the Introduction. Write a paragraph describing both the content goals and the intellectual goals of the course and text. Also describe what's on the Web site and how the Web site can be used with the text and course.



i>Clicker  
Questions

- Q1-6<sub>A</sub>** Go to Chapter 1 **Useful Links** (<http://www.umich.edu/~elements/6e/01chap/obj.html#/>) and click on Professional Reference Shelf to view the photos and schematics of real reactors. Write a paragraph describing two or more of the reactors. What similarities and differences do you observe between the reactors on the Web site (e.g., [www.loebequipment.com](http://www.loebequipment.com)), and in the text? How do the used reactor prices compare with those in Table 2-6?
- Q1-7<sub>A</sub>** What assumptions were made in the derivation of the design equation for: **(a)** The batch reactor (BR)? **(b)** The CSTR? **(c)** The plug-flow reactor (PFR)? **(d)** The packed-bed reactor (PBR)? **(e)** State in words the meanings of  $-r_A$  and  $r'_A$ .
- Q1-8<sub>A</sub>** Fill out the following table for each of the reactors discussed in this chapter, BR, CSTR, PBR, and Fluidized Bed:

Type of Reactor	Characteristics	Phases Present	Usage	Advantages	Disadvantages

- Q1-9<sub>A</sub>** Define Chemical Process Safety and list four reasons we need to study it and why it is particularly relevant to CRE (<http://umich.edu/~safeche/index.html>).
- Q1-10<sub>A</sub>** Go to Chapter 1 **Extra Help** on the Web site and click on **LearnChemE ScreenCasts** (<http://www.umich.edu/~elements/6e/01chap/learn-cheme-videos.html>). Choose one of the LearnChemE videos and critique it for such things as **(a)** value, **(b)** clarity, **(c)** visuals, and **(d)** how well it held your interest. (Score 1–7; 7 = outstanding, 1 = poor)
- Q1-11<sub>A</sub>** Go to Chapter 1 **Extra Help** on the Web site and click on **LearnChemE ScreenCasts** (<http://www.umich.edu/~elements/6e/01chap/learn-cheme-videos.html>) choose the **How to Study** screencast and list three ways that screencasts can help you learn the material.
- Q1-12<sub>A</sub>** Go to **Extra Help** then click on **Videos of Tips on Studying and Learning**. Go to Chapter 1 (<http://www.umich.edu/~elements/6e/01chap/obj.html#/video-tips/>).
- (a)** View one of the 5- to 6-minute video tutorials and list two of the most important points in the video. List what two things you think this screencast did well?
- (b)** After viewing the three screencasts on How to Study (<http://www.learncheme.com/student-resources/how-to-study-resources>), describe the most efficient way to study. In video 3 How to Study, the author of this book has a very different view of one of the points suggested. What do you think it is?
- (c)** View the video 13 Study Tips\*\*\*\* (4 Stars) (<https://www.youtube.com/watch?v=eVlxxHJdqI8&feature=youtu.be>). List four of the tips that you think might help your study habits.
- (d)** Rate each of the sites on video tips, (1) Not Helpful, (5) Very Helpful.

### Computer Simulations and Experiments

Before running your experiments, stop a moment and try to predict how your curves will change shape as you change a variable (cf. Q1-1<sub>A</sub>).

- P1-1<sub>A</sub>** **(a)** Revisit **Example 1-3**.

#### Wolfram and Python

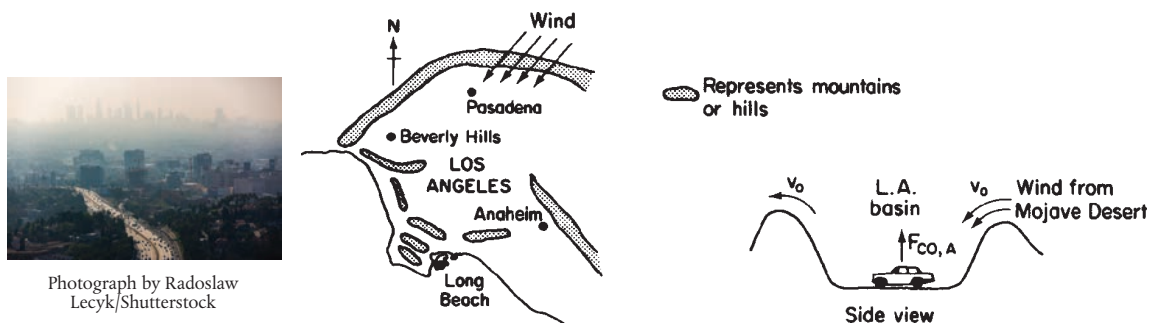
- (i) Describe how  $C_A$  and  $C_B$  change when you experiment with varying the volumetric flow rate,  $v_0$ , and the specific reaction rate,  $k$ , and then write a conclusion about your experiments.
- (ii) Click on the description of reversible reaction  $A \rightleftharpoons B$  to understand how the rate law becomes  $-r_A = k \left[ C_A - \frac{C_B}{K_e} \right]$ . Set  $K_e$  at its minimum value and vary  $k$  and  $v_0$ . Next, set  $K_e$  at its maximum value and vary  $k$  and  $v_0$ . Write a couple sentences describing how varying  $k$ ,  $v_0$ , and  $K_e$  affect the concentration profiles. We will learn more about  $K_e$  in Section 3.2.
- (iii) After reviewing *Generating Ideas and Solutions* on the Web site ([http://www.umich.edu/~elements/6e/toc/SCPS,3rdEdBook\(Ch07\).pdf](http://www.umich.edu/~elements/6e/toc/SCPS,3rdEdBook(Ch07).pdf)), choose one of the brainstorming techniques (e.g., lateral thinking) to suggest two questions that should be included in this problem.

**Polymath**

- (iv) Modify the Polymath program to consider the case where the reaction is reversible as discussed in part (ii) above with  $K_e = 3$ . How do your results (i.e.,  $C_A$ ) compare with the irreversible reaction case?

**Problems**

- P1-2<sub>B</sub>** Schematic diagrams of the Los Angeles basin are shown in Figure P1-2<sub>B</sub>. The basin floor covers approximately 700 square miles ( $2 \times 10^{10}$  ft<sup>2</sup>) and is almost completely surrounded by mountain ranges. If one assumes an inversion height in the basin of 2,000 ft, the corresponding volume of air in the basin is  $4 \times 10^{13}$  ft<sup>3</sup>. We shall use this system volume to model the accumulation and depletion of air pollutants. As a very rough first approximation, we shall treat the Los Angeles basin as a well-mixed container (analogous to a CSTR) in which there are no spatial variations in pollutant concentrations.



**Figure P1-2<sub>B</sub>** Schematic diagrams of the Los Angeles basin.

([http://www.umich.edu/~elements/6e/web\\_mod/la\\_basin/index.htm](http://www.umich.edu/~elements/6e/web_mod/la_basin/index.htm))

We shall perform an unsteady-state mole balance (Equation (1–4)) 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 parts 1–12 (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.

- P1-3<sub>B</sub>** This problem focuses on using Polymath, an ordinary differential equation (ODE) solver, and also a non-linear equation (NLE) solver. These equation solvers will be used extensively in later chapters. Information on how to obtain and load the Polymath Software is given in **Appendix D** and on the CRE Web site.

- (a) Professor Sven Köttlov has a son-in-law, Stěpán Dolež, who has a farm near Riča, Jofostan where there are initially 500 rabbits ( $x$ ) and 200 foxes ( $y$ ). 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  $k_1 = 0.02 \text{ day}^{-1}$   
 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  $k_4 = 0.04 \text{ day}^{-1}$

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. **Polymath Tutorial** (<https://www.youtube.com/watch?v=nyjmt6cTiL4>)

- (b) Using Wolfram and/or Python in the Chapter 1 LEP on the Web site, what parameters would you change to convert the foxes versus rabbits plot from an oval to a circle? Suggest reasons that could cause this shape change to occur.
- (c) We will now consider the situation in which the rabbits contracted a deadly virus also called *rabbit measles* (*measlii*). The death rate is  $r_{\text{Death}} = k_D x$  with  $k_D = 0.005 \text{ day}^{-1}$ . Now plot the fox and rabbit concentrations as a function of time and also plot the foxes versus rabbits. Describe, if possible, the minimum growth rate at which the death rate does not contribute to the net decrease in the total rabbit population.
- (d) Use Polymath or MATLAB to solve the following set of nonlinear algebraic equations

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

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

with initial guesses of  $x = 2$ ,  $y = 2$ . Try to become familiar with the edit keys in Polymath and MATLAB. See the CRE Web site for instructions. You will need to know how to use this solver in later chapters involving CSTRs.

**Screen shots on how to run Polymath are shown at the end of Summary Notes for Chapter 1 or on the CRE Web site, [www.umich.edu/~elements/6e/software/polymath-tutorial.html](http://www.umich.edu/~elements/6e/software/polymath-tutorial.html).**

### Interactive Computer Games

- P1-4<sub>A</sub>** Find the Interactive Computer Games (ICG) on the CRE Web site (<http://www.umich.edu/~elements/6e/icg/index.html>). Read the description of the Kinetic Challenge module (<http://www.umich.edu/~elements/6e/icm/kinchal1.html>) and then go to the installation instructions (<http://www.umich.edu/~elements/6e/icm/install.html>) to install the module on your computer. Play this game and then record your performance number, which indicates your mastery of the material.

Jeopardy Game  
Held at Annual  
AIChE Student  
Chapter Meeting

ICM Quiz Show ICG

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

ICG Kinetics Challenge 1 Performance # \_\_\_\_\_

### Problems

- P1-5<sub>A</sub>** **OEQ** (*Old Exam Question*) The reaction



takes place in an unsteady CSTR. The feed is only A and B in equimolar proportions. Which of the following sets of equations gives the correct set of mole balances on A, B, and C? Species A and B are disappearing and species C is being formed. Circle the correct answer where all the mole balances are correct.

(a)  $F_{B0} - F_A - \int^V r_A dV = \frac{dN_A}{dt}$

$$F_{B0} - F_B - \int^V r_A dV = \frac{dN_B}{dt}$$

$$-F_C + 2 \int^V r_A dV = \frac{dN_C}{dt}$$

(b)  $F_{A0} - F_A + \int^V r_A dV = \frac{dN_A}{dt}$

$$F_{A0} - F_B + \int^V r_A dV = \frac{dN_B}{dt}$$

$$-F_C - 2 \int^V r_A dV = \frac{dN_C}{dt}$$

$$\begin{array}{ll}
 \text{(c)} & F_{A0} - F_A + \int_0^V r_A dV = \frac{dN_A}{dt} \\
 & F_{A0} - F_B + \int_0^V r_A dV = \frac{dN_B}{dt} \\
 & F_C + \int_0^V r_C dV = \frac{dN_C}{dt} \\
 \text{(d)} & F_{B0} - F_A - \int_0^V r_A dV = \frac{dN_A}{dt} \\
 & F_{B0} - F_{A0} - \int_0^V r_A dV = \frac{dN_B}{dt} \\
 & -F_C + \int_0^V r_C dV = \frac{dN_C}{dt}
 \end{array}$$

(e) None of the above.

This problem was written in honor of Ann Arbor, Michigan's own Grammy winning artist, Bob Seger ([https://www.youtube.com/channel/UComKJVf5rNLL\\_RfC\\_rbt7qg/videos](https://www.youtube.com/channel/UComKJVf5rNLL_RfC_rbt7qg/videos)).

**P1-6<sub>B</sub>** The reaction



is to be carried out isothermally in a continuous-flow reactor. The entering volumetric flow rate  $v_0$  is  $10 \text{ dm}^3/\text{h}$ . Note:  $F_A = C_A v$ . For a constant volumetric flow rate  $v = v_0$ , then  $F_A = C_A v_0$ . Also,  $C_{A0} = F_{A0}/v_0 = ([5 \text{ mol/h}]/[10 \text{ dm}^3/\text{h}]) = 0.5 \text{ mol}/\text{dm}^3$ .

Calculate both the CSTR and PFR volumes necessary to consume 99% of A (i.e.,  $C_A = 0.01C_{A0}$ ) when the entering molar flow rate is  $5 \text{ mol/h}$ , assuming the reaction rate  $-r_A$  is

(a)  $-r_A = k$  with  $k = 0.05 \frac{\text{mol}}{\text{h} \cdot \text{dm}^3}$  (Ans:  $V_{\text{CSTR}} = 99 \text{ dm}^3$ )

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

(c)  $-r_A = kC_A^2$  with  $k = 300 \frac{\text{dm}^3}{\text{mol} \cdot \text{h}}$  (Ans:  $V_{\text{CSTR}} = 660 \text{ dm}^3$ )

(d) Repeat (a), (b), and/or (c) to calculate the time necessary to consume 99.9% of species A in a  $1000 \text{ dm}^3$  constant-volume batch reactor with  $C_{A0} = 0.5 \text{ mol}/\text{dm}^3$ .

**P1-7<sub>A</sub>** **Enrico Fermi (1901–1954) Problems (EFP)**. 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 then to make 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.

See <http://mathforum.org/workshops/sum96/interdisc/sheila2.html>.

**Enrico Fermi Problem**

(a) **EFP #1**. How many piano tuners are there in the city of Chicago? Show the steps in your reasoning.

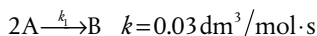
1. Population of Chicago \_\_\_\_\_
2. Number of people per household \_\_\_\_\_
3. And so on, \_\_\_\_\_

An answer is given on the CRE Web site under Summary Notes for Chapter 1.

(b) **EFP #2**. How many square meters of pizza were eaten by an undergraduate student body population of 20,000 during the Fall term 2016?

(c) **EFP #3**. How many bathtubs of water will the average person drink in a lifetime?

**P1-8<sub>A</sub>** **What is wrong with this solution?** The irreversible liquid-phase second-order reaction ( $-r = kC_A^2$ )



is carried out in a CSTR. The entering concentration of A,  $C_{A0}$ , is 2 molar, and the exit concentration of A,  $C_A$  is 0.1 molar. The volumetric flow rate,  $v_0$ , is constant at  $3 \text{ dm}^3/\text{s}$ . What is the corresponding reactor volume?

Solution

1. Mole Balance

$$V = \frac{F_{A0} - F_A}{-r_A}$$

2. Rate Law (second order)

$$-r_A = kC_A^2$$

3. Combine

$$V = \frac{F_{A0} - F_A}{kC_A^2}$$

$$4. F_{A0} = \nu_0 C_{A0} = \frac{3 \text{ dm}^3}{\text{s}} \cdot \frac{2 \text{ molA}}{\text{dm}^3} = \frac{6 \text{ molA}}{\text{s}}$$

$$5. F_A = \nu_o C_A = \frac{3 \text{ dm}^3}{\text{s}} \cdot \frac{0.1 \text{ molA}}{\text{dm}^3} = \frac{0.3 \text{ molA}}{\text{s}}$$

$$6. V = \frac{(6 - 0.3) \frac{\text{mol}}{\text{s}}}{\left(0.03 \frac{\text{dm}^3}{\text{mol} \cdot \text{s}}\right) \left(2 \frac{\text{mol}}{\text{dm}^3}\right)^2} = 47.5 \text{ dm}^3$$

If you like the **Puzzle Problems** in “What is wrong with the solutions”† you can find more for later chapters on the Web site under **Additional Material** for that chapter.

For more puzzles on what’s “wrong with this solution,” see additional material for each chapter on the CRE Web site home page, under “Expanded Material.”



Solved Problems

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

## SUPPLEMENTARY READING

- For further elaboration of the development of the general balance equation, see not only the Web site [www.umich.edu/~elements/6e/index.html](http://www.umich.edu/~elements/6e/index.html) but also
  - R. M. FELDER and R. W. ROUSSEAU, *Elementary Principles of Chemical Processes*, 3rd ed. New York: Wiley, 2000, Chap. 4.
  - R. J. SANDERS, *The Anatomy of Skiing*. Denver, CO: Golden Bell Press, 1976.
- A detailed explanation of a number of topics in this chapter can be found in the tutorials.
  - B. L. CRYNES and H. S. FOGLER, eds., *AIChE Modular Instruction Series E: Kinetics*, Vols. 1 and 2. New York: AIChE, 1981.
- A discussion of some of the most important industrial processes is presented by
  - G. T. AUSTIN, *Shreve's Chemical Process Industries*, 5th ed. New York: McGraw-Hill, 1984.
- Short instructional videos (6–9 minutes) that correspond to the topics in this book can be found at <http://www.learncheme.com/>.
- See the Web site, “Process Safety Across the Chemical Engineering Curriculum,” (<http://umich.edu/~safeche/index.html>).

† **Puzzle Problems** for each chapter can be found on the CRE Web site under Expanded Material.

# 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, former head 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 S1-1 in Chapter 1. In Chapter 2, we will show how to size and arrange these reactors *conceptually*, so that the reader may see the structure of chemical reaction engineering (CRE) design and will not get lost in the mathematical details.

In this chapter, we

- Define conversion
- Rewrite all balance equations for the four types of industrial reactors in Chapter 1 in terms of the conversion,  $X$
- Show how to size (i.e., determine the reactor volume) these reactors once the relationship between the reaction rate and conversion is known that is given, i.e.,  $-r_A = f(X)$
- Show how to compare CSTR and PFR sizes
- Show how to decide the best arrangements for reactors in series, a most important principle

In addition to being able to determine CSTR and PFR sizes given the rate of reaction as a function of conversion, you will be able to calculate the overall conversion and reactor volumes for reactors arranged in series.

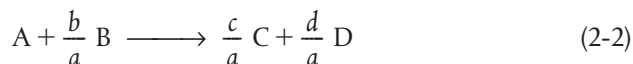
## 2.1 Definition of Conversion

Conversion helps us measure how far a reaction has progressed. 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, we *must* choose the limiting reactant as the basis of calculation. For single reactions, we can use conversion to 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. We shall choose species A as our limiting reactant and, thus, our *basis of calculation*. The limiting reactant is the reactant that will be completely consumed first after the reactants have been mixed. We next divide the reaction expression through by the stoichiometric coefficient of the limiting reactant, that is, of species A, in order to arrange the reaction stoichiometry in the form

“A” is our basis  
of calculation



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 of 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, that is, complete conversion. For *reversible reactions*, the maximum conversion is the equilibrium conversion  $X_e$  (i.e.,  $X_{\max} = X_e$ ). We will take a closer look at equilibrium conversion in Section 4.3.

## 2.2 Batch Reactor Design Equations

In most batch reactors (BRs), 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 present in the reactor (i.e.,  $t = 0$ ), then the total number of moles of A that have reacted (i.e., have been consumed) after a time  $t$  is  $[N_{A0}X]$ .

$$[\text{Moles of A reacted (consumed)}] = [\text{Moles of A fed}] \cdot \left[ \frac{\text{Moles of A reacted}}{\text{Moles of A fed}} \right]$$

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

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  $X$ :

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

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

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

Moles of A in the reactor at a time  $t$

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

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 in the reactor 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

**Batch reactor (BR)**  
design equation

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

We call Equation (2-6) the differential form of the BR mole balance and it is often referred to as the **design equation** for a 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 7) and for reactors with heat effects (Chapters 11–13), 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. 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.

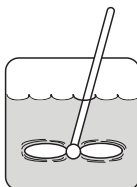
Uses of a BR

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

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

Batch time  $t$   
to achieve a  
conversion  $X$

Next, this equation is integrated with the limits that the reaction begins at time equals zero where there is no conversion initially (i.e., when  $t = 0$ ,  $X = 0$ ) and ends at time  $t$  when a conversion  $X$  is achieved (i.e., when  $t = t$ , then  $X = X$ ). Carrying out the integration, we obtain the time  $t$  necessary to achieve a conversion  $X$  in a batch reactor



Batch Reactor  
Design Equation

$$t = N_{A0} \int_0^X \frac{dX}{-r_A V} \quad (2-7)$$

The longer the reactants are left in the reactor, the greater the conversion will be. Equation (2-6) is the differential form of the design equation, and Equation (2-7) 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; for example, 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  $F_{A0}X$ .

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

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

The molar flow rate of A leaving the system  $F_A$  equals the molar feed rate of A into the system  $F_{A0}$  minus the rate of reaction of A within the system ( $F_{A0}X$ ). The preceding sentence can be expressed mathematically as

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

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

Rearranging gives

$$\boxed{F_A = F_{A0}(1 - X)} \quad (2-8)$$

The entering molar flow rate of species A,  $F_{A0}$  (mol/s), is just the product of the entering concentration,  $C_{A0}$  (mol/dm<sup>3</sup>), and the entering volumetric flow rate,  $v_0$  (dm<sup>3</sup>/s).

$$\boxed{F_{A0} = C_{A0} v_0} \quad (2-9)$$

Liquid phase *For liquid systems*, the volumetric flow rate,  $v$ , is constant and equal to  $v_0$ , and  $C_{A0}$  is commonly given in terms of molarity, for example,  $C_{A0} = 2$  mol/dm<sup>3</sup>.

*For gas systems*,  $C_{A0}$  can be calculated from the entering mole fraction,  $y_{A0}$ , the temperature,  $T_0$ , and pressure,  $P_0$ , using the ideal gas law or some other gas law. For an ideal gas (see Appendix B):

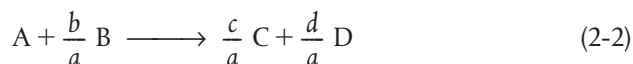
Gas phase

$$C_{A0} = \frac{P_{A0}}{RT_0} = \frac{y_{A0}P_0}{RT_0} \quad (2-10)$$

Now that we have a relationship [Equation (2-8)] 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 a Vat)

Recall that the CSTR is modeled as being well mixed such that there are no spatial variations in the reactor. For the general reaction



the CSTR mole balance Equation (1-7) 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  $X$

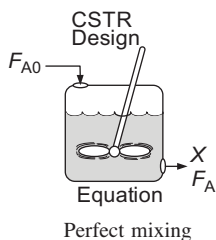
$$F_A = F_{A0} - F_{A0}X \quad (2-12)$$

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

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

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

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



Evaluate  $-r_A$  at the CSTR exit conditions!!

Because the reactor is *perfectly mixed*, the exit composition from the reactor is identical to the composition inside the reactor, and, therefore, the rate of reaction,  $-r_A$ , 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—that is, no radial gradients in concentration, temperature, or reaction rate.<sup>1</sup> As the reactants enter and flow axially down the reactor, they are consumed and the

<sup>1</sup> This constraint will be removed when we extend our analysis to nonideal (industrial) reactors in Chapters 16–18.

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 given in Chapter 1, 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  $X$

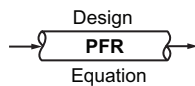
$$F_A = F_{A0} - F_{A0}X \quad (2-12)$$

Differentiating

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

and substituting into Equation (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 (2-7) 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.

### 2.3.3 Packed-Bed Reactor (PBR)

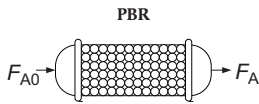
*Packed-bed reactors* are tubular reactors filled with catalyst particles. In PBRs, it is the weight of catalyst  $W$  that is important, rather than the reactor volume. The derivation of the differential and integral forms of the design equations for packed-bed reactors are analogous to those for a 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 5.<sup>†</sup>

In the *absence* of pressure drop, that is,  $\Delta P = 0$ , we can integrate Equation (2-17) with limits  $X = 0$  at  $W = 0$ , and when  $W = W$  then  $X = X$  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  $W$  (i.e., mass) necessary to achieve a conversion  $X$  when the total pressure remains constant.

## 2.4 Sizing Continuous-Flow Reactors

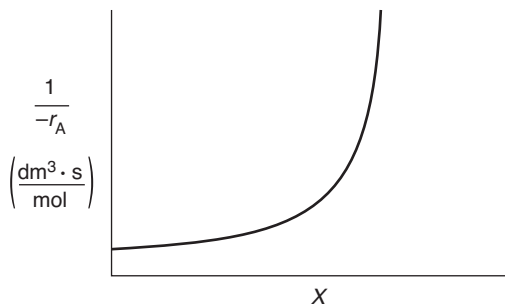
In this section, we are going to show how we can size CSTRs and PFRs (i.e., determine their reactor volumes) using the appropriate mole balance in terms of conversion and knowledge of the rate of reaction,  $-r_A$ , as a function of conversion,  $X$  (i.e.,  $-r_A = f(X)$ ). The rate of disappearance of A,  $-r_A$ , is almost always a function of the concentrations of the various species present (see Chapter 3). When only one reaction is occurring, each of the concentrations can be expressed as a function of the conversion  $X$  (see Chapter 4); consequently,  $-r_A$  can be expressed as a function of  $X$ .

As an example, we shall choose a particularly simple functional dependence on concentration, that is, first-order.

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

Here,  $k$  is the specific reaction rate and is a function of temperature only, and  $C_{A0}$  is the entering concentration of A. We note in Equations (2-13) and (2-16) that the reactor volume is 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

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



**Figure 2-1** Typical curve of the reciprocal rate as a function of conversion.

<sup>†</sup> Be sure to watch the YouTube video (<https://www.youtube.com/watch?v=S9mUAXmNqxs>).

We can use Figure 2-1 to size CSTRs and PFRs for different entering flow rates. By *sizing* we mean either determine the reactor volume for a specified conversion *or* determine the conversion for a specified reactor volume. Before sizing flow reactors, let's consider some insights. If a 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, the reciprocal rate ( $1/-r_A$ ) 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, the reciprocal rate ( $1/-r_A$ ) 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, that is,  $X = 1$ , the reciprocal rate approaches infinity as does the reactor volume, that is,

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

“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,  $X = X_e$ . We will discuss  $X_e$  further in Chapter 4.

### Examples of Reactor Design and Staging Given $-r_A = f(X)$

To illustrate the design of continuous-flow reactors (i.e., CSTRs and PFRs), we consider the irreversible isothermal gas-phase isomerization



Researchers at the Central Lab performed experiments to determine the rate of chemical reaction as a function of the conversion of reactant A and the results are shown in Table 2-1. The temperature was constant at 500 K (440°F), the total pressure was constant at 830 kPa (8.2 atm), and the initial charge to the reactor was pure A. The entering molar flow of reactant A is  $F_{A0} = 0.4$  mol/s.

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

TABLE 2-1 RAW DATA<sup>†</sup>

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

<sup>†</sup>Proprietary coded data courtesy of Jofostan Central Research Laboratory, Çölow, Jofostan, and published in *Jofostan Journal of Chemical Engineering Research*, Volume 21, page 73 (2023).

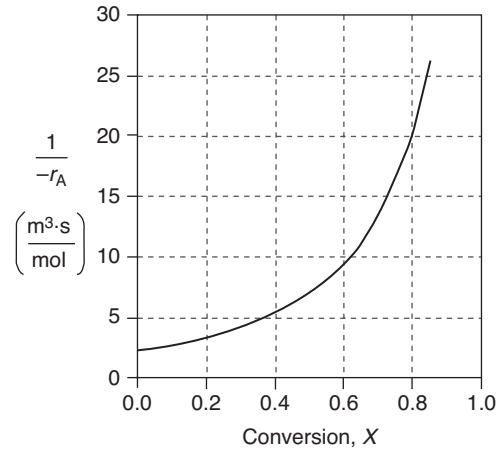
Recalling the CSTR and PFR design equations, (2-13) and (2-16), we see that the reactor volume varies directly with the molar flow rate  $F_{A0}$  and with the reciprocal of  $-r_A$ ,  $\left(\frac{1}{-r_A}\right)$ , for example,  $V = \left(\frac{F_{A0}}{-r_A}\right)X$ . Consequently, to size reactors, we first convert the raw data in Table 2-1, which gives  $-r_A$  as a function of  $X$  first to  $\left(\frac{1}{-r_A}\right)$  as a function of  $X$ . Next, we multiply by the entering molar flow rate,  $F_{A0}$ , to obtain  $\left(\frac{F_{A0}}{-r_A}\right)$  as a function of  $X$  as shown in Table 2-2 of the processed data for  $F_{A0} = 0.4$  mol/s.

TABLE 2-2 PROCESSED DATA

$X$	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.

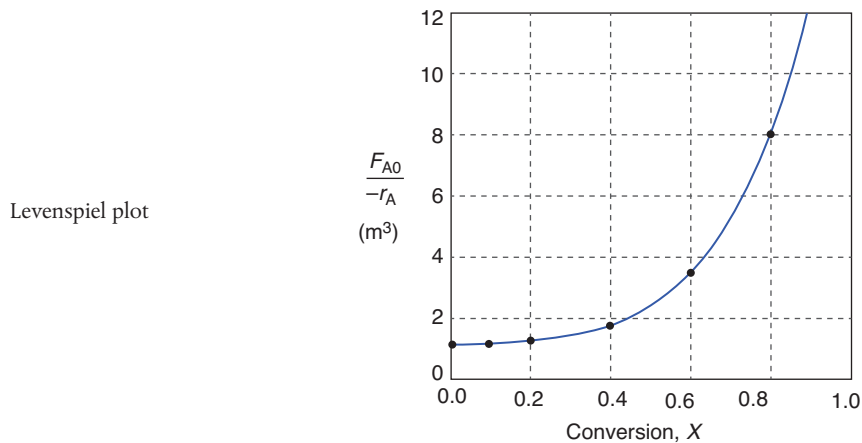
To size reactors for different entering molar flow rates,  $F_{A0}$ , we would use rows 1 and 4, as shown by the arrows in Table 2-2 to construct the following figure:



**Figure 2-2(a)** Levenspiel plot of processed data 1 in Table 2-2.

However, for a given  $F_{A0}$ , rather than using Figure 2-2(a) to size reactors, it is often more advantageous to plot  $\left(\frac{F_{A0}}{-r_A}\right)$  as a function of  $X$ , which is called a Levenspiel plot.<sup>†</sup> We are now going to carry out a number of examples where we have specified the flow rate  $F_{A0}$  to be 0.4 mol A/s.

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



**Figure 2-2(b)** Levenspiel plot of processed data 2 in Table 2-2.

We are now going to use the Levenspiel plot of the processed data (Figure 2-2(b)) to size a CSTR and a PFR.

<sup>†</sup> After Professor Octave Levenspiel (1/1/1926–3/5/2017), Oregon State University, Corvallis, OR.

**Example 2-1 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  $F_{A0} = 0.4 \frac{\text{mol}}{\text{s}}$ , which is the flow rate used to construct the Levenspiel plot in Figure 2-2(b).

- (a) Using the data in either Table 2-2 or Figure 2-2(b), calculate the volume necessary to achieve 80% conversion in a CSTR.
- (b) Shade the area in Figure 2-2(b) 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 2-2(a), 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

$$V = 0.4 \frac{\text{mol}}{\text{s}} \left( \frac{20 \text{ m}^3 \cdot \text{s}}{\text{mol}} \right) (0.8) = 6.4 \text{ m}^3 \quad (\text{E2-1.1})$$

$$V = 6.4 \text{ m}^3 = 6400 \text{ dm}^3 = 6400 \text{ liters} \quad \text{Answer}$$

- (b) Shade the area in Figure 2-2(b) that yields the CSTR volume to achieve 80% conversion. Rearranging Equation (2-13) gives

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

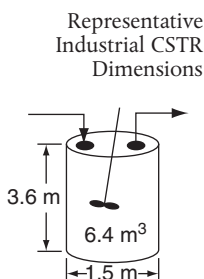
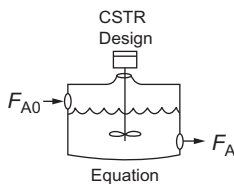
In Figure E2-1.1, the volume is equal to the area of a rectangle with a height ( $F_{A0}/-r_A = 8 \text{ m}^3$ ) and a base ( $X = 0.8$ ). This rectangle is shaded in the figure.

$$V = \left[ \frac{F_{A0}}{-r_A} \right]_{X=0.8} (0.8) \quad (\text{E2-1.2})$$

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

$$V = [8 \text{ m}^3][0.8] = 6.4 \text{ m}^3 = 6400 \text{ dm}^3 = 6400 \text{ L} \quad \text{Answer}$$

The CSTR volume necessary to achieve 80% conversion is 6.4 m<sup>3</sup> 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. Oops!

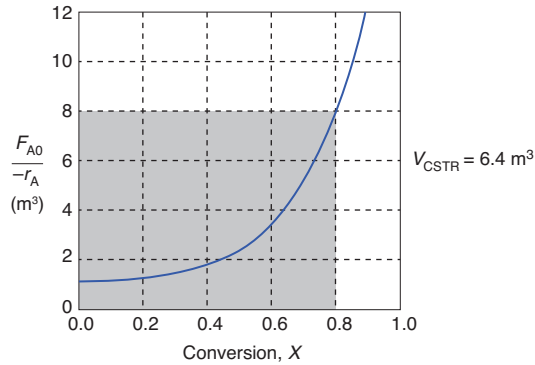


Figure E2-1.1 Levenspiel CSTR plot.

Plots of  $(F_{A0}/-r_A)$  versus  $X$  are often referred to as Levenspiel plots (after Prof. Octave Levenspiel).

**Analysis:** Given the conversion, the rate of reaction as a function of conversion along with the molar flow of the species A, we saw how to calculate the volume of a CSTR. From the data and information given, we calculated the volume to be  $6.4 \text{ m}^3$  for 80% conversion. We showed how to carry out this calculation using the design equation (2-13) and also using a Levenspiel plot.

**Example 2-2 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 again,  $F_{A0} = 0.4 \text{ mol/s}$ .

- (a) First, use one of the integration formulas given in Appendix A.4 to determine the PFR reactor volume necessary to achieve 80% conversion.
- (b) Next, shade the area in Figure 2-2(b) that would give the PFR volume necessary to achieve 80% conversion.
- (c) 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 2-2 to produce the results shown in Table 2-3.

TABLE 2-3 PROCESSED DATA 2

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

(a) **Numerically evaluate PFR volume.** For the PFR, the differential form of the mole balance is

$$F_{A0} \frac{dX}{dV} = -r_A \tag{2-15}$$

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 (Equation (A-23)) given in Appendix A.4 to numerically evaluate Equation (2-16). The five-point formula with a final conversion of 0.8 gives 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  $X = 0.8$ .

$$V = \frac{\Delta X}{3} \left[ \frac{F_{A0}}{-r_A(X=0)} + \frac{4F_{A0}}{-r_A(X=0.2)} + \frac{2F_{A0}}{-r_A(X=0.4)} + \frac{4F_{A0}}{-r_A(X=0.6)} + \frac{F_{A0}}{-r_A(X=0.8)} \right] \quad (E2-2.1)$$

Using values of  $[F_{A0}/(-r_A)]$  corresponding to the different conversions in Table 2-3 yields

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

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

The PFR reactor volume necessary to achieve 80% conversion is 2165 dm<sup>3</sup>. This volume could be achieved by using a bank of 100 PFRs that are each 0.1 m in diameter with a length of 2.8 m (e.g., see margin figure or Figures 1-8(a) and (b)). Note: As we proceed through later chapters and have analytical formulas for  $-r_A$ , we will use integration tables or software packages (e.g., Polymath, rather than quadrature formulas, such as Equation (E2-2.1)).

**(b) The PFR volume, that is, 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  $X$ .**

$$V = \int_0^{0.8} \frac{F_{A0}}{-r_A} dX = \text{Area under the curve between } X = 0 \text{ and } X = 0.8 \quad (\text{see shaded area in Figure E2-2.1})$$

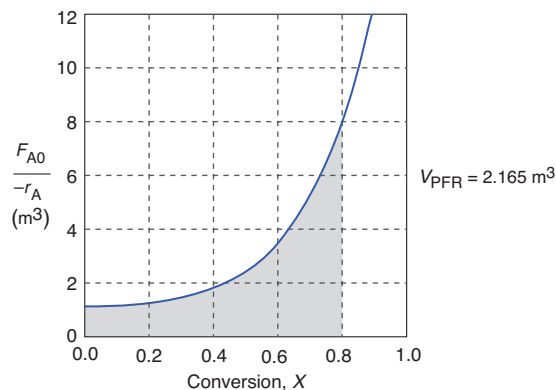
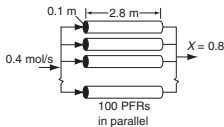


Figure E2-2.1 Levenspiel PFR plot.



PFR

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 dm<sup>3</sup> (2.165 m<sup>3</sup>).

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

We know that as we proceed down the reactor, the conversion increases as more and more reactant is converted to product. Consequently, as the reactant is consumed, the concentration of reactant decreases, as does the rate of disappearance of A for isothermal reactions.

(i) For  $X = 0.2$ , we calculate the corresponding reactor volume using Simpson's rule (given in Appendix A.4 as Equation (A-21)) with increment  $\Delta X = 0.1$  and the data in rows 1 and 4 in Table 2-2.

$$V = F_{A0} \int_0^{0.2} \frac{dX}{-r_A} = \frac{\Delta X}{3} \left[ \frac{F_{A0}}{-r_A(X=0)} + \frac{4F_{A0}}{-r_A(X=0.1)} + \frac{F_{A0}}{-r_A(X=0.2)} \right] \quad (\text{E2-2.2})$$

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

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

This volume (218 dm<sup>3</sup>) is the volume at which  $X = 0.2$ . From Table 2-2, we see the corresponding rate of reaction at  $X = 0.2$  is  $-r_A = 0.3 \frac{\text{mol}}{\text{m}^3 \cdot \text{s}}$ .

Therefore at  $X = 0.2$ , then  $-r_A = 0.3 \text{ mol/m}^3 \cdot \text{s}$  and  $V = 218 \text{ dm}^3$ .

(ii) For  $X = 0.4$ , we can again use Table 2-3 and Simpson's rule with  $\Delta X = 0.2$  to find the reactor volume necessary for a conversion of 40%.

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

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

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

From Table 2-2 we see that at  $X = 0.4$ ,  $-r_A = 0.195 \text{ mol/m}^3 \cdot \text{s}$  and  $V = 551 \text{ dm}^3$ .

We can continue in this manner to arrive at Table E2-2.1.

TABLE E2-2.1 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 (dm <sup>3</sup> )	0	218	551	1093	2165

The data in Table E2-2.1 are plotted in Figures E2-2.2(a) and (b).

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

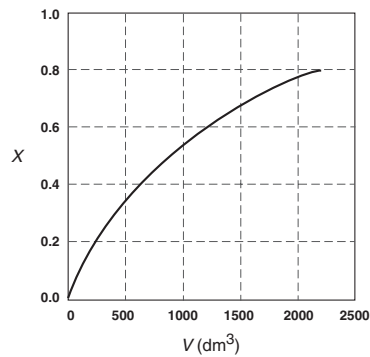


Figure E2-2.2(a) Conversion profile.

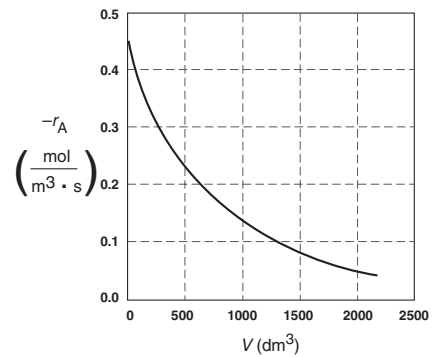


Figure E2-2.2(b) Reaction rate profile.

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

### Example 2-3 Comparing CSTR and PFR Sizes

Compare the volumes of a CSTR and a PFR required for the same conversion using the data in Figure 2-2(b). Which reactor would require the smaller volume to achieve a conversion of 80%: a CSTR or a PFR? The entering molar flow rate and the feed conditions are the same in both cases.

#### Solution

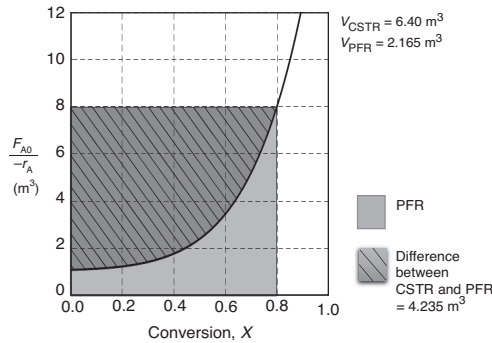
We will again use the data in Table 2-3.

TABLE 2-3 PROCESSED DATA 2

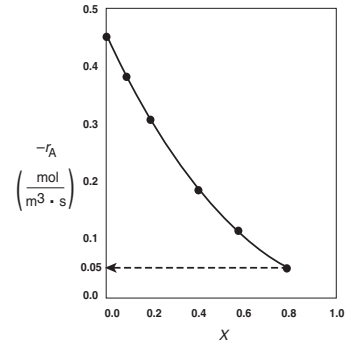
X	0.0	0.1	0.2	0.4	0.6	0.7	0.8
$(F_{A0}/-r_A)(\text{m}^3)$	0.89	1.08	1.33	2.05	3.54	5.06	8.0

The CSTR volume was 6.4 m<sup>3</sup> and the PFR volume was 2.165 m<sup>3</sup>. When we combine Figures E2-1.1 and E2-2.1 on the same graph, Figure 2-3.1(a), we see that the crosshatched area above the curve is the difference in the CSTR and PFR reactor volumes. Figure E2-3.1(b) shows the rate of reaction,  $-r_A$ , as a function of conversion. We note that at 80% conversion the rate is approximately one-tenth the initial rate.

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



**Figure E2-3.1(a)** Comparison of CSTR and PFR reactor sizes for  $X = 0.8$ .



**Figure E2-3.1(b)**  $-r_A$  as a function of  $X$  obtained from Table 2-2.

**Analysis:** 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.,  $-r_A = 0.05 \text{ mol/m}^3 \cdot \text{s}$  in Figure E2-3.1(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, there are exceptions such as autocatalytic reactions, product-inhibited reactions, and nonisothermal exothermic reactions; these trends will not always be the case, as we will see in Chapters 9 and 11.

## 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 the moles of A fed to the first reactor, minus all the moles of A reacted up to point  $i$ .

$$F_{A_i} = F_{A_0} - F_{A_0}X_i$$

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.

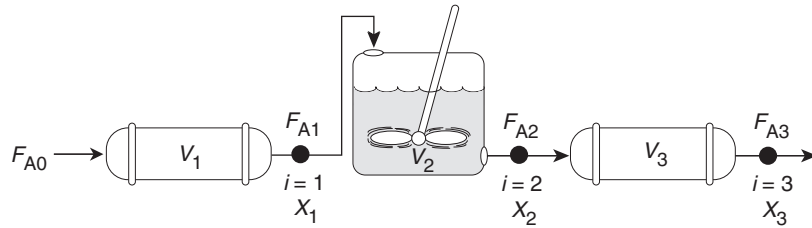


Figure 2-3 Reactors in series.

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 the impeccable data in Table 2-1 from Jofostan Central Research laboratories 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.

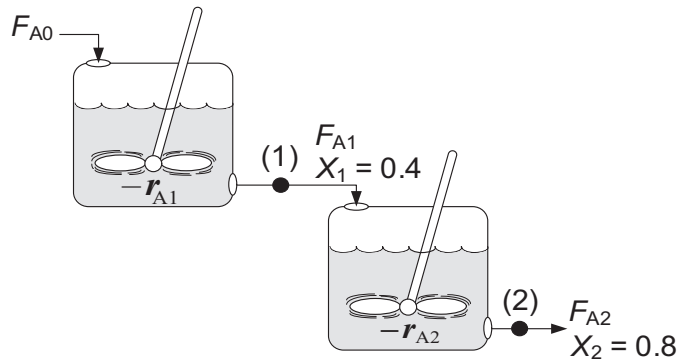


Figure 2-4 Two CSTRs in series.

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

A mole balance on reactor 1 gives

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

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

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), and rearranging

$$\text{Reactor 1} \quad \boxed{V_1 = \frac{F_{A0}X_1}{-r_{A1}}} \quad (2-21)$$

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 steady-state mole balance on the second reactor is

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

$$\mathbf{Reactor 2:} \quad F_{A1} - F_{A2} + r_{A2}V_2 = 0 \quad (2-22)$$

The molar flow rate of A at point 2 is

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

combining Equations (2-22) and (2-23) and rearranging

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

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

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

In the examples that follow, we shall again use the molar flow rate of A used in Example 2-1 (i.e.,  $F_{A0} = 0.4$  mol A/s) and the reaction conditions given in Table 2-3 in Example 2-3 processed data 2.

#### Example 2-4 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? (See Table 2-3.)

TABLE 2-3 PROCESSED DATA 2

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

*Solution*

**For Reactor 1**, we observe from either Table 2-3 or Figure 2-2(b) that when  $X = 0.4$ , then

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

Then, using Equation (2-13)

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

$$V_1 = 820 \text{ dm}^3 \text{ (liters)} \quad \underline{\text{Answer}}$$

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

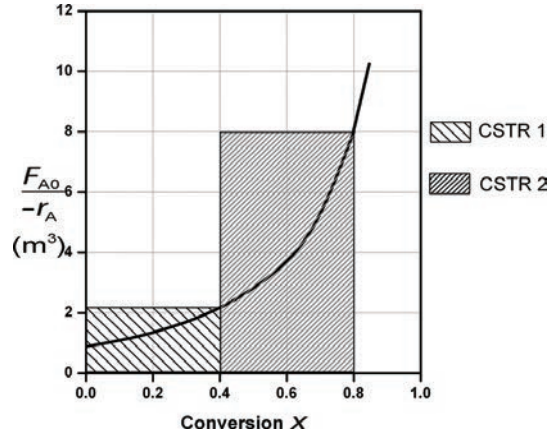
Using Equation (2-24)

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

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

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

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



**Figure E2-4.1** Two CSTRs in series.

The shaded areas in Figure E2-4.1 could also have been used to determine volumes of CSTR 1 and CSTR 2.

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

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

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

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

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

Notice in Example 2-4 that the sum of the two CSTR reactor volumes ( $4.02 \text{ m}^3$ ) in series is less than the volume of one CSTR ( $6.4 \text{ m}^3$ ) to achieve the same overall conversion.

**Analysis:** When we have reactors in series, we can speed our analysis and calculations by defining an overall conversion at a point in the series, rather than the conversion of each individual reactor. In this example, we saw that 40% was achieved at point 1, the exit to the first reactor, and that a total of 80% conversion was achieved by the time we exit the second reactor. Using two CSTRs in series will give a smaller total volume than one CSTR 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 these CSTRs in series with the volume of one plug-flow reactor for the same conversion, say 80%.

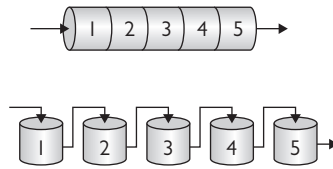


Figure 2-5 Modeling a PFR with CSTRs in series.

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

Useful Concept!

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

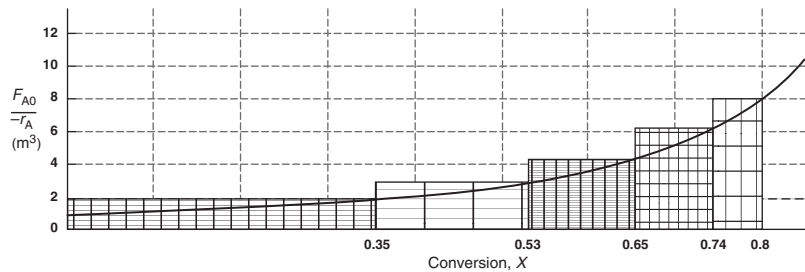


Figure 2-6 Levenspiel plot showing comparison of CSTRs in series with one PFR.

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.

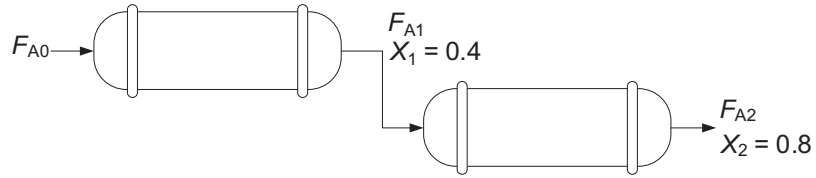


Figure 2-7 Two PFRs in series.

PFRs 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 PFRs in series is the same as one PFR with the same total volume.

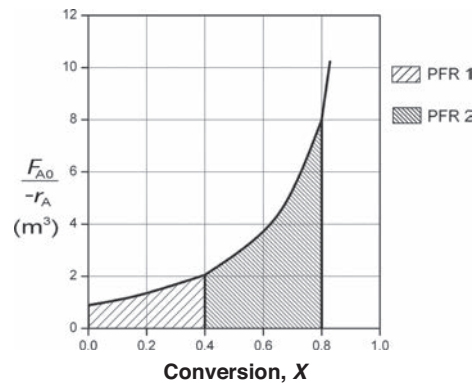
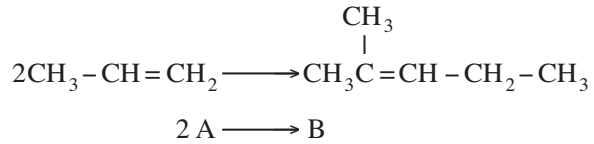


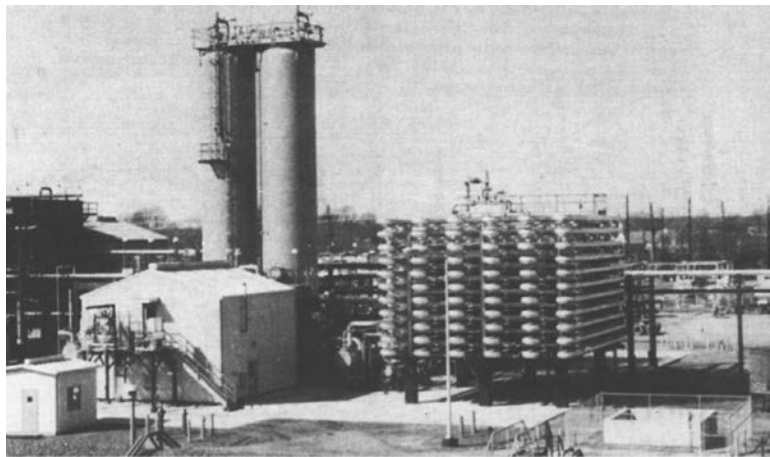
Figure 2-8 Levenspiel plot for two PFRs in series.

2.5.3 Combinations of CSTRs and PFRs in Series

The final sequences we shall consider in this chapter are combinations of CSTRs and PFRs in series. An industrial example of reactors in series is shown in the photo in Figure 2-9 where two CSTRs in series are followed by a PFR. This sequence is used to dimerize propylene (A) into isohexanes (B), for example,

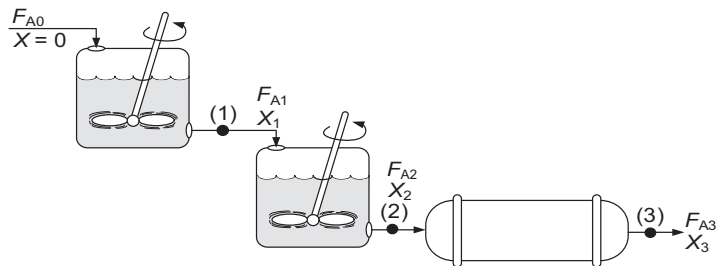


Not sure whether the size of these CSTRs is in the Guinness Book of World Records.



**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 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 that the reaction carried out in the reactors in Figure 2-10 follows the same  $\left(\frac{F_{A0}}{-r_A}\right)$  versus  $X$  curve given by Table 2-3.

The volumes of the first two CSTRs in series (see Example 2-4) are:

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

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

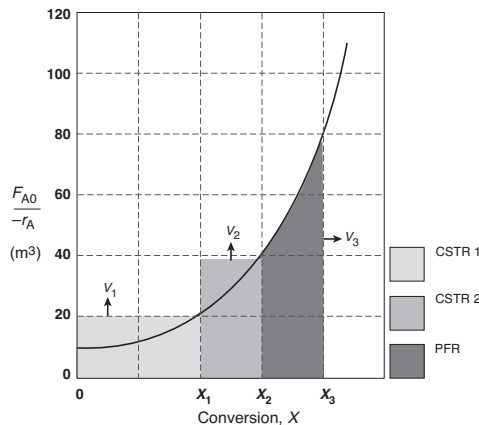
Starting with the differential form of the PFR design equation

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

rearranging and integrating between limits, when  $V = 0$ , then  $X = X_2$ , and when  $V = V_3$ , then  $X = X_3$  we obtain

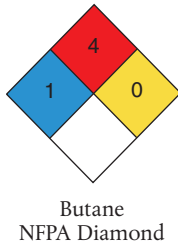
$$\text{Reactor 3:} \quad V_3 = \int_{X_2}^{X_3} \frac{F_{A0}}{-r_A} dX \quad (2-25)$$

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



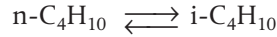
**Figure 2-11** Levenspiel plot to determine the reactor volumes  $V_1$ ,  $V_2$ , and  $V_3$ .

The  $(F_{A0}/-r_A)$  versus  $X$  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 5 and adiabatic systems in Chapter 11, where we will see that for adiabatic exothermic reactions the temperature increases with increasing conversion.



**Example 2-5 An Adiabatic Liquid-Phase Isomerization**

The isomerization of butane



was carried out adiabatically in the liquid phase. The data for this reversible reaction are given in Table E2-5.1. (Example 11.3 shows how the data in Table E2-5.1 were generated.)

TABLE E2-5.1 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 11, Example 11-3. It is *real data* for a *real reaction* carried out adiabatically, and the reactor scheme shown below in Figure E2-5.1 is used.

Real Data  
for a  
Real Reaction

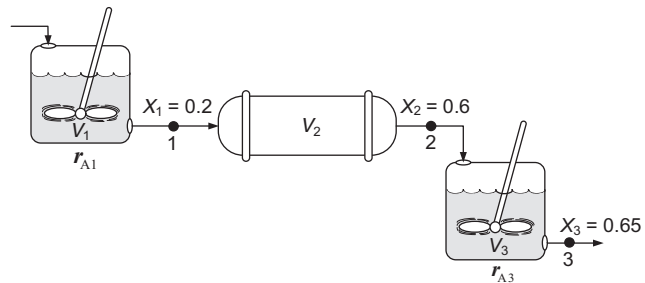


Figure E2-5.1 Reactors in series.

Calculate the volume of each of the reactors for an entering molar flow rate of n-butane of 50 kmol/hr, that is,  $F_{A0} = 50$  kmol/h.

*Solution*

Taking the reciprocal of  $-r_A$  and multiplying by  $F_{A0}$ , we obtain Table E2-5.2.

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

TABLE E2-5.2 PROCESSED DATA<sup>†</sup>

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

<sup>†</sup>Data from Table E11-3.1.

(a) For the first CSTR,

$$\text{when } X = 0.2, \text{ then } \frac{F_{A0}}{-r_A} = 0.94 \text{ m}^3$$

$$V_1 = \frac{F_{A0}}{-r_A} X_1 = (0.94 \text{ m}^3)(0.2) = 0.188 \text{ m}^3 \quad (\text{E2-5.1})$$

$$\boxed{V_1 = 0.188 \text{ m}^3 = 188 \text{ dm}^3} \quad (\text{E2-5.2})$$

(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  $X_1 = 0.2$ ,  $X_2 = 0.4$ , and  $X_3 = 0.6$

$$\begin{aligned} V_2 &= \int_{0.2}^{0.6} \frac{F_{A0}}{-r_A} dX = \frac{\Delta X}{3} \left[ \left( \frac{F_{A0}}{-r_A} \right)_{X=0.2} + 4 \left( \frac{F_{A0}}{-r_A} \right)_{X=0.4} + \left( \frac{F_{A0}}{-r_A} \right)_{X=0.6} \right] \\ &= \frac{0.2}{3} [0.94 + 4(0.85) + 1.32] \text{m}^3 \end{aligned} \quad (\text{E2-5.3})$$

$$\boxed{V_2 = 0.38 \text{ m}^3 = 380 \text{ dm}^3} \quad (\text{E2-5.4})$$

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

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

$$F_{A2} - F_{A3} + r_{A3}V_3 = 0 \quad (\text{E2-5.5})$$

Rearranging

$$V_3 = \frac{F_{A2} - F_{A3}}{-r_{A3}} \quad (\text{E2-5.6})$$

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

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

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

Simplifying

$$\boxed{V_3 = \left( \frac{F_{A0}}{-r_{A3}} \right) (X_3 - X_2)} \quad (\text{E2-5.7})$$

We find from Table E2-5.2 that at  $X_3 = 0.65$ , then  $\frac{F_{A0}}{-r_{A3}} = 2.0 \text{ m}^3$

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

$$\boxed{V_3 = 0.1 \text{ m}^3 = 100 \text{ dm}^3} \quad (\text{E2-5.8})$$

A Levenspiel plot of  $(F_{A0}/-r_A)$  versus  $X$  is shown in Figure E2-5.2.

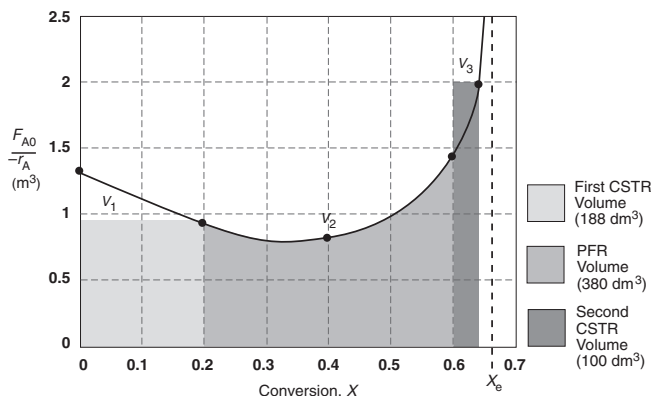


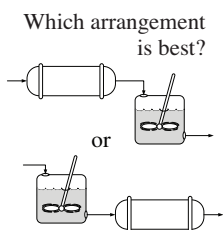
Figure E2-5.2 Levenspiel plot for adiabatic reactors in series.

For this adiabatic reaction, the three reactors in series resulted in an overall conversion of 65%. The maximum conversion we can achieve is the equilibrium conversion, which is 68%, and is shown by the dashed line in Figure E2-5.2. Recall that at equilibrium, the rate of reaction is zero and an infinite reactor volume is required to reach equilibrium ( $V \sim \frac{1}{-r_A} \sim \frac{1}{0} = \infty$ ).

**Analysis:** For exothermic reactions that are not carried out isothermally, the rate usually increases at the start of the reaction because reaction temperature increases. However, as the reaction proceeds the rate eventually decreases as the conversion increases because the reactants are consumed. These two competing effects give the bowed shape of the curve in Figure E2-5.2, which will be discussed in detail in Chapters 11 and 12. Under these circumstances, we saw that a CSTR will require a smaller volume than a PFR at low conversions.

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

If we look at Figure E2-5.2, 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, that is,  $V_{\text{PFR}} > V_{\text{CSTR}}$ . However, if we compare the areas under the curve between  $X = 0.6$  and  $X = 0.65$ , we see that the area under the curve (PFR volume) is smaller than the rectangular area corresponding to the CSTR volume, that is,  $V_{\text{CSTR}} > V_{\text{PFR}}$ . This result often occurs when the reaction is carried out adiabatically, which is discussed when we look at heat effects in Chapter 11.



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 plot  $(F_{A0}/-r_A)$  versus  $X$ , but

also on the relative reactor sizes. As an exercise, examine Figure E2-5.2 to learn if there is a better way to arrange the two CSTRs and one PFR. Suppose you were given a Levenspiel plot of  $(F_{A0}/-r_A)$  versus  $X$  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 were 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, and initial reactant concentrations). However, such circumstances are **seldom** encountered and we must revert to the methods we describe in Chapters 3 and 4 to obtain  $-r_A$  as a function of  $X$ .

**It is important to remember 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 and combinations of reactors.**

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, that is,  $-r_A = f(X)$ , different reactor schemes can readily be sized. In Chapters 3 and 4, 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,  $\tau$ , is obtained by dividing the reactor volume by the volumetric flow rate entering the reactor

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

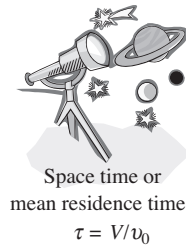
$\tau$  is an important quantity!

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

Given  $V$  and  
 $\left[ \begin{array}{l} F_{A0} \\ -r_A \end{array} \right]$  vs.  $X$  find  $X$

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

Chapter 3 shows  
 how to find  
 $-r_A = f(C_A)$   
 +  
 Chapter 4 shows  
 how to find  
 $C_A = g(X)$   
 ↓  
 Chapters 3 and 4  
 are combined to  
 get  $-r_A = f(X)$



it takes for this upstream fluid volume to enter the reactor completely is called the *space time*  $\tau$ . It is also called the *holding time* or *mean residence time*.

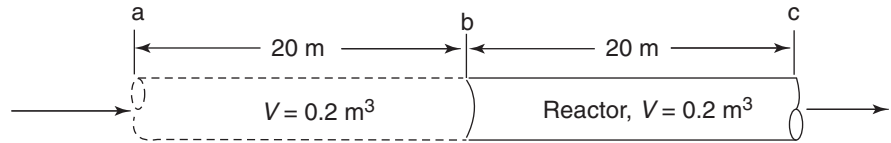


Figure 2-12 Tubular reactor showing identical volume upstream.

For example, if the reactor volume is  $0.2 \text{ m}^3$  and the inlet volumetric flow rate is  $0.01 \text{ m}^3/\text{s}$ , it would take the upstream equivalent reactor volume ( $V = 0.2 \text{ m}^3$ ), shown by the dashed lines, a time  $\tau$  equal to

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

to enter the reactor ( $V = 0.2 \text{ m}^3$ ). In other words, it would take 20 s for the fluid molecules at point **a** to move to point **b**, which corresponds to a space time of 20 s. We can substitute for  $F_{A0} = v_0 C_{A0}$  in Equations (2-13) and (2-16) and then divide both sides by  $v_0$  to write our mole balance in the following forms:

$$\text{For a PFR} \quad \tau_p = \left( \frac{V_p}{v_0} \right) = C_{A0} \int_0^X \frac{dX}{-r_A}$$

and

$$\text{For a CSTR} \quad \tau_{\text{CSTR}} = \left( \frac{V_{\text{CSTR}}}{v_0} \right) = \frac{C_{A0} X}{-r_A}$$

For plug flow, the space time is equal to the mean residence time in the reactor,  $t_m$  (see Chapter 16). This time is the average time that 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>

Practical guidelines	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	

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

Table 2-5 shows an order of magnitude of the space times for six industrial reactions and associated reactors.

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

	Reaction	Reactor	Temperature	Pressure atm	Space Time
(1)	$C_2H_6 \rightarrow C_2H_4 + H_2$	PFR <sup>†</sup>	860°C	2	1 s
(2)	$CH_3CH_2OH + HCH_3COOH \rightarrow$ $CH_3CH_2COOCH_3 + H_2O$	CSTR	100°C	1	2 h
(3)	Catalytic cracking	PBR	490°C	20	1 s < $\tau$ < 400 s
(4)	$C_6H_5CH_2CH_3 \rightarrow C_6H_5CH = CH_2 + H_2$	PBR	600°C	1	0.2 s
(5)	$CO + H_2O \rightarrow CO_2 + H_2$	PBR	300°C	26	4.5 s
(6)	$C_6H_6 + HNO_3 \rightarrow$ $C_6H_5NO_2 + H_2O$	CSTR	50°C	1	20 min

Typical industrial  
reaction space  
times

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

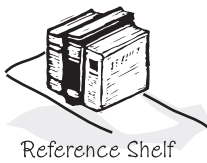
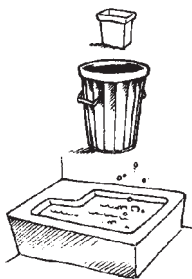


Table 2-6 gives typical sizes for batch and CSTR reactors (along with the comparable size of a familiar object) and the costs associated with those sizes. All reactors are glass lined and the prices include heating/cooling jacket, motor, mixer, and baffles. The reactors can be operated at temperatures between 20°F and 450°F, and at pressures up to 100 psi.

TABLE 2-6 REPRESENTATIVE PFAUDLER CSTR/BATCH REACTOR SIZES AND PRICES<sup>†</sup>

Volume	Price
20 dm <sup>3</sup> (Waste Basket)	\$30,000
200 dm <sup>3</sup> (Garbage Can)	\$40,000
2000 dm <sup>3</sup> (Jacuzzi)	\$75,000
30000 dm <sup>3</sup> (Gasoline Tanker)	\$300,000

<sup>†</sup>Doesn't include instrumentation costs.



## 2.6.2 Space Velocity

The space velocity (SV) is another term used by reaction engineers and is defined as

$$SV \equiv \frac{v_0}{V} \quad SV = \frac{1}{\tau} \quad (2-27)$$

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

Slight differences  
in space velocities

The space velocity 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.

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

The gas volumetric flow rate,  $v_0$ , in the GHSV is normally reported at standard temperature and pressure (STP).

$$\text{GHSV} = \frac{v_0|_{\text{STP}}}{V} \quad (2-29)$$

### Example 2-6 Reactor Space Times and Space Velocities

Calculate the space time,  $\tau$ , and space velocities for the reactor in Examples 2-1 and 2-2 for an entering volumetric flow rate of 2 dm<sup>3</sup>/s.

#### Solution

The entering volumetric flow rate is 2 dm<sup>3</sup>/s (0.002 m<sup>3</sup>/s).

From Example 2-1, the CSTR volume was 6.4 m<sup>3</sup> and the corresponding space time,  $\tau$ , and space velocity, SV are

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

It takes 0.89 h to put 6.4 m<sup>3</sup> into the reactor and the corresponding space velocity, SV, is

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

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

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

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

**Analysis:** This example gives an *important industrial concept*. These space times are the times for each of the reactors to take the volume of fluid equivalent to one reactor volume and put it into the reactor.

## Summary

In 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–conversion data  $-r_A = f(X)$  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. By combining the information in Chapters 3 and 4, 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 (Table 3-1) and in Step 2, we will find the concentrations as a function of conversion (Figure 4-3). Combining Steps 1 and 2 in Chapters 3 and 4, 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.

Coming attractions  
in Chapters 3 and 4

## 2.7 And Now... A Word from Our Sponsor—Safety 2 (AWFOS–S2 The NFPA Diamond)

In this AWFOS–S, we describe the National Fire Protection Agency (NFPA) Diamond which quickly identifies risks of hazardous materials. This identification is extremely important to first responders in an emergency. Each color in the diamond represents a different type of hazard, while the numbers in the hazard refer to a degree of concern one should have about the material. The different types of hazards and levels of concern of the NFPA diamond are shown in Figure 2-13.

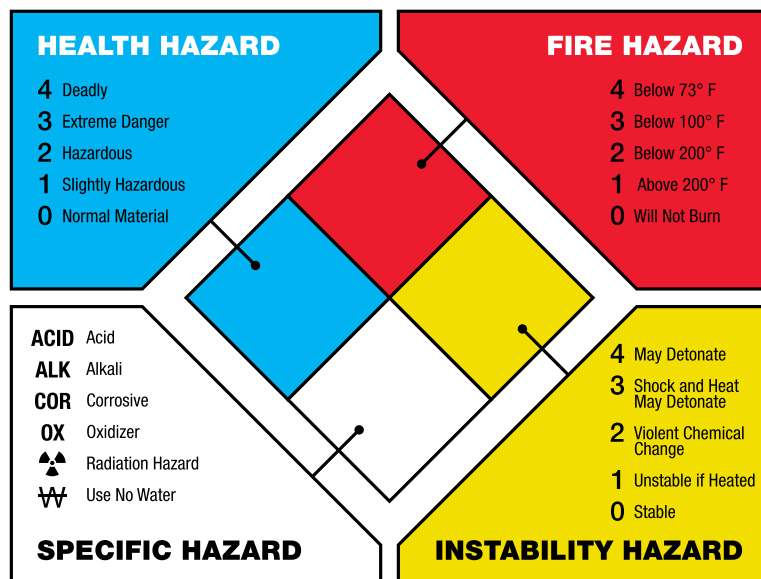


Figure 2-13 Components of each color of the NFPA Diamond. (Image: Dmitry Kovalchuk/Shutterstock)

A tutorial on how to fill in the numbers in the diamond for the insecticide dichlorodiphenyltrichloroethane (DDT) using the CAMEO Chemicals Website (<https://cameochemicals.noaa.gov>) is given in the NFPA Diamond tutorial on the safety Website (<http://umich.edu/~safeche/nfpa.html>, <http://umich.edu/~safeche/assets/pdf/CAMEO.pdf>). The NFPA Diamond for the chemical DDT discussed in Example 1-1, DDT, is shown in Figure 2-14.



**Figure 2-14** NFPA Diamond Levels of Concern for DDT. (Image: Idea.s/Shutterstock)

We see that the number two in the red (top-most) diamond indicates DDT has a flash point below 200°F, the zero in the yellow (far-right) diamond indicates it is stable, the blank in the white (bottom-most) diamond indicates no specific hazard, and the two in the blue (far-left) diamond indicates DDT is hazardous to one's health.

The following photographs show two examples of how the NFPA Diamond is used in industry.



**Figure 2-15** NFPA Diamond in Action. (Photos: left, Gado Images/Getty; right, TFoxFoto/Shutterstock)

The NFPA Diamond along with its companion GHS Diamond (see AWFOS-S3) is shown on the *Process Safety Across the Chemical Engineering Curriculum* Web site. For tutorials and NFPA data sheets see

**NFPA Diamond Tutorial:** [https://cse.wvu.edu/files/safety-tutorials/Gen\\_Chem\\_Tutorial/HTML/GCST\\_10.htm](https://cse.wvu.edu/files/safety-tutorials/Gen_Chem_Tutorial/HTML/GCST_10.htm)

**CAMEO Chemicals Tutorial:** <http://umich.edu/~safeche/assets/pdf/CAMEO.pdf>

**Quick Card:** [https://www.nfpa.org/Assets/files/AboutTheCodes/704/NFPA704\\_HC2012\\_QCard.pdf](https://www.nfpa.org/Assets/files/AboutTheCodes/704/NFPA704_HC2012_QCard.pdf)

**Data Sheets:** <https://cameochemicals.noaa.gov/chemical/694>  
<https://cameochemicals.noaa.gov/chemical/4145>

**FAQs:** [https://www.nfpa.org/Assets/files/AboutTheCodes/704/704\\_FAQs.pdf](https://www.nfpa.org/Assets/files/AboutTheCodes/704/704_FAQs.pdf)

**The CRE Algorithm**

- Mole Balance, Ch 1
- Rate Law, Ch 3
- Stoichiometry, Ch 4
- Combine, Ch 5
- Evaluate, Ch 5
- Energy Balance, Ch 11

**Closure**

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

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

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

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

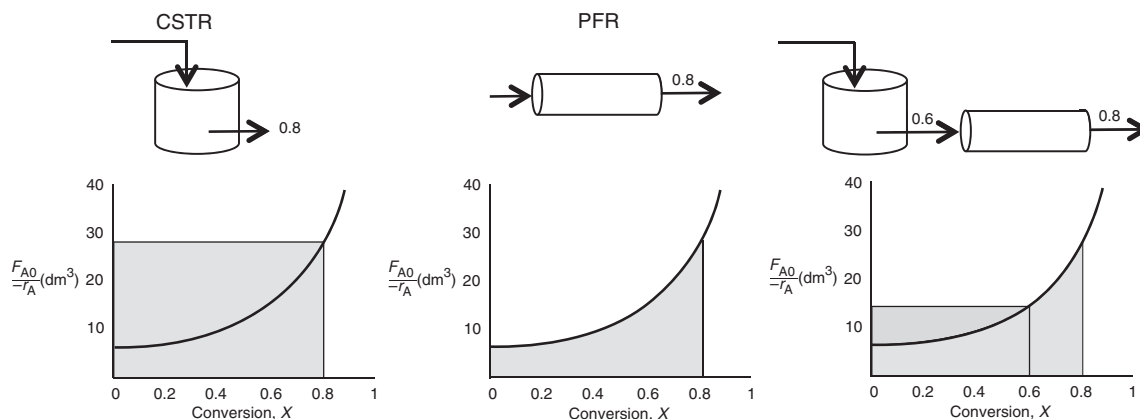
$$X_i = \frac{\text{Total moles of A reacted up to point } i}{\text{Moles A fed to the first reactor}} \quad (S2-3)$$

2. The differential and integral forms of the reactor design equations (i.e., GMBEs) are shown in Table S2-1.

TABLE S2-1 MOLE BALANCE FOR BR, CSTR, PFR, AND PBR IN TERMS OF CONVERSION

	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		$V = \frac{F_{A0}(X_{\text{out}} - X_{\text{in}})}{(-r_A)_{\text{out}}}$	
“Fluidized” CSTR		$W = \frac{F_{A0}(X_{\text{out}} - X_{\text{in}})}{(-r'_A)_{\text{out}}}$	
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 of A 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

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

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

## CRE WEB SITE MATERIALS

<http://www.umich.edu/~elements/6e/O2chap/obj.html>

### Useful Links

#### Living Example Problems

Polymath, Python, Matlab and Wolfram

#### Extra Help

Multiple Resources extra problems, screencasts and lecture notes

#### Additional Materials

New Technical Material, Detailed Derivations and Web Modules

#### Professional Reference Shelf

Material important to the practicing engineer that is not necessarily covered in all CRE courses.

#### YouTube Videos

Humorous videos covering topics varying from example problems to light hearted breaks from studying

### Evaluation

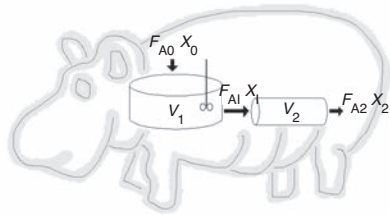
#### Self Tests

Interactive problems with solutions to provide extra practice of concepts

#### i>Clicker Questions

Interactive multiple choice questions to help access your understanding of the material

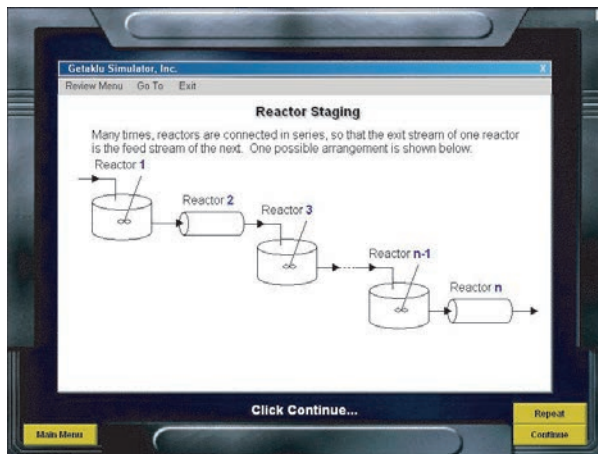
### Web Module Hippopotamus Digestive System



([http://umich.edu/~elements/6e/web\\_mod/hippo/index.htm](http://umich.edu/~elements/6e/web_mod/hippo/index.htm))

### Interactive Computer Games

Reactor Staging (<http://umich.edu/~elements/6e/icm/staging.html>)



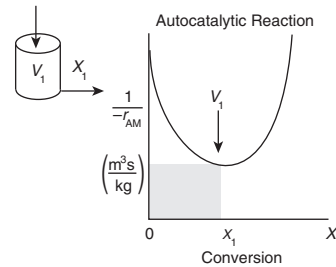
## QUESTIONS AND PROBLEMS

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

A = ● B = ■ C = ◆ D = ◆◆

### Questions

- Q2-1<sub>A</sub>** **QBR (Questions Before Reading).** Will or could there ever be a case where the CSTR volume is represented by something other than a square or rectangle on a Levenspiel plot?
- Q2-2<sub>A</sub>** **i>clicker.** Go to the Web site [http://www.umich.edu/~elements/6e/02chap/iclicker\\_ch2\\_q1.html](http://www.umich.edu/~elements/6e/02chap/iclicker_ch2_q1.html) and view at least five i>clicker questions. Choose one that could be used as is, or a variation thereof, to be included on the next exam. You also could consider the opposite case: explaining why the question should *not* be on the next exam. In either case, explain your reasoning.
- Q2-3<sub>A</sub>** (a) Without referring back, make a list of the most important items you learned in this chapter.  
 (b) Overall, what do you believe were the three major purposes of the chapter?



Levenspiel Plot for Autocatalytic Digestion in a CSTR

- Q2-4<sub>A</sub>** Go to the Web site [www.engr.ncsu.edu/learningstyles/ilsweb.html](http://www.engr.ncsu.edu/learningstyles/ilsweb.html). Take the Inventory of Learning Style test, and record your learning style according to the Soloman/Felder inventory, and then use Web Appendix I.3 to suggest two ways to facilitate your learning style in each of the four categories.  
 Global/Sequential \_\_\_\_\_  
 Active/Reflective \_\_\_\_\_  
 Visual/Verbal \_\_\_\_\_  
 Sensing/Intuitive \_\_\_\_\_
- Q2-5<sub>A</sub>** Go to the Chapter 2 Video Screencasts Web page (<http://www.umich.edu/~elements/6e/02chap/learn-cheme-videos.html>).  
 (a) View one or more of the screencast 5- to 6-minute videos and write a two-sentence evaluation.  
 (b) What did the speaker do well and what could be improved?
- Q2-6<sub>A</sub>** AWFOS-S2  
 (a) What is the NFPA diamond and why is it important?  
 (b) Go to Wikipedia and search ethylene oxide to find the NFPA diamond numbers.  
 (c) Draw the NFPA diamond for the chemicals propylene, isohexane, and isobutane that we discussed in Figure 2-6, and Example 2-5.

### Interactive Computer Games

- P2-1<sub>A</sub>** **ICG Staging.** Download the Interactive Computer Game (ICG) from the CRE Web site, <http://www.umich.edu/~elements/6e/icm/staging.html>. Play this game and then record your performance number, which indicates your mastery of the material. Your professor has the key to decode your performance number. *Note:* To play this game you *must* have Windows 2000 or a later version. Write the ICG Reactor Staging Performance here # \_\_\_\_\_.



### Problems

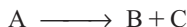
Before solving the problems, state or sketch qualitatively the expected results or trends.

- P2-2<sub>A</sub>** (a) Revisit the data in *Table 2-1 Raw Data* and calculate the batch reactor (BR) times to achieve 10%, 50%, and 80% conversion when 100 moles of A are charged to a 400 dm<sup>3</sup> reactor.  
 (b) 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? What conversion can be achieved in a 4.5 m<sup>3</sup> PFR and in a 4.5 m<sup>3</sup> CSTR?  
 (c) Revisit **Example 2-2**. Being a company about to go bankrupt, you can only afford a 2.5 m<sup>3</sup> CSTR. What conversion can you achieve?  
 (d) Revisit **Example 2-3**. What conversion could you achieve if you could convince your boss, Dr. Pennypincher, to spend more money to buy a 1.0 m<sup>3</sup> PFR to attach to a 2.40 m<sup>3</sup> CSTR?  
 (e) Revisit **Example 2-4**. How would your answers change if the two CSTRs (one 0.82 m<sup>3</sup> and the other 3.2 m<sup>3</sup>) were placed in parallel with the flow,  $F_{A0}$ , divided equally between the reactors?  
 (f) Revisit **Example 2-5**. (1) What is the worst possible way to arrange the two CSTRs and one PFR? (2) What would be the reactor volumes if the two intermediate conversions were changed to 20% and 50%, respectively? (3) What would be the conversions,  $X_1$ ,  $X_2$ , and  $X_3$ , if all the reactors had the same volume of 100 dm<sup>3</sup> and were placed in the same order?  
 (g) Revisit **Example 2-6**. If the term  $C_{A0} \int_0^X \frac{dX}{-r_A}$  is 2 seconds for 80% conversion, how much fluid (m<sup>3</sup>/min) can you process in a 3 m<sup>3</sup> reactor?
- P2-3<sub>B</sub>** You have two CSTRs and two PFRs, each with a volume of 1.0 m<sup>3</sup>. Use Figure 2-2(b) on page 45 to calculate the conversion for each of the reactors in the following arrangements.  
 (a) Two CSTRs in series. (**Ans:**  $X_1 = 0.435$ ,  $X_2 = 0.66$ )  
 (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 PFR followed by a CSTR.

- (f) A CSTR followed by a PFR. (**Ans:**  $X_{\text{CSTR}} = 0.435$ ,  $X_{\text{PFR}} = 0.71$ )  
 (g) A PFR followed by two CSTRs. Is this a good arrangement or is there a better one?  
 (h) **Caution:** Part (h) is a C level problem. A CSTR and a PFR in parallel with the flow equally divided. Calculate the overall conversion,  $X_{\text{ov}}$

$$X_{\text{ov}} = \frac{F_{\text{A0}} - F_{\text{ACSTR}} - F_{\text{APFR}}}{F_{\text{A0}}}, \text{ with } F_{\text{ACSTR}} = \frac{F_{\text{A0}}}{2} - \frac{F_{\text{A0}}}{2} X_{\text{CSTR}}, \text{ and } F_{\text{APFR}} = \frac{F_{\text{A0}}}{2} (1 - X_{\text{PFR}})$$

- P2-4<sub>B</sub>** The exothermic reaction of stilbene (A) to form the economically important tropophene (B) and methane (C), that is,

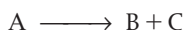


was carried out adiabatically and the following data recorded:

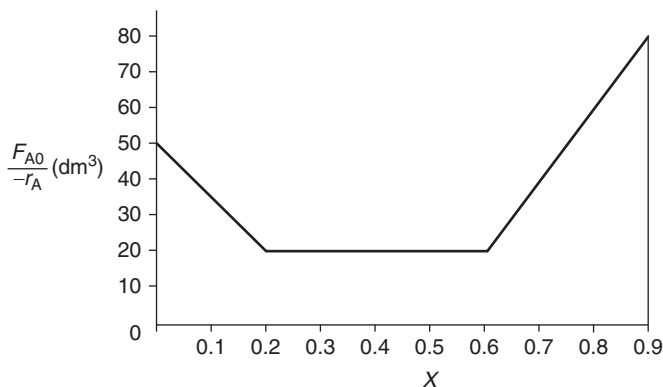
$X$	0	0.2	0.4	0.45	0.5	0.6	0.8	0.9
$-r_{\text{A}}$ (mol/dm <sup>3</sup> ·min)	1.0	1.67	5.0	5.0	5.0	5.0	1.25	0.91

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

- (a) Calculate the batch reactor (BR) times to achieve 40% and 80% conversion when 400 moles of A are charged to a 400 dm<sup>3</sup> reactor.  
 (b) What are the PFR and CSTR volumes necessary to achieve 40% conversion? ( $V_{\text{PFR}} = 72$  dm<sup>3</sup>,  $V_{\text{CSTR}} = 24$  dm<sup>3</sup>)  
 (c) Over what range of conversions would the CSTR and PFR reactor volumes be identical?  
 (d) What is the maximum conversion that can be achieved in a 105-dm<sup>3</sup> CSTR?  
 (e) 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?  
 (f) 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?  
 (g) Plot the conversion and rate of reaction as a function of PFR reactor volume up to a volume of 100 dm<sup>3</sup>.
- P2-5<sub>B</sub>** The financially important reaction to produce the valuable product B (not the real name) was carried out in Jesse Pinkman's garage (see *Breaking Bad* Season 3, Episode 7). This *Breaking Bad*, fly-by-night company, is on a shoestring budget and has very little money to purchase equipment. Fortunately, cousin Bernie has a reactor surplus company and you can get reactors from Bernie. The reaction



takes place in the liquid phase. Below is the Levenspiel plot for this reaction. You have up to \$10,000 to use to purchase reactors from those given below.



Cousin Bernie's Reactors

Reactor Type	Number	Volume (dm <sup>3</sup> )	Cost
CSTR	2	2	\$1,000
CSTR	1	4	\$2,000
PFR	2	4	\$2,000
CSTR	2	6	\$4,000
CSTR	3	12	\$8,000
PFR	2	12	\$6,000

What reactors do you choose, how do you arrange them, and what is the highest conversion you can get for \$10,000? Approximately what is the corresponding highest conversion with your arrangement of reactors?

Scheme and sketch your reactor volumes.



**P2-6<sub>B</sub>** Read the Web Module “Chemical Reaction Engineering of Hippopotamus Stomach” on the CRE Web site ([http://www.umich.edu/~elements/6e/web\\_mod/hippo/index.htm](http://www.umich.edu/~elements/6e/web_mod/hippo/index.htm)).

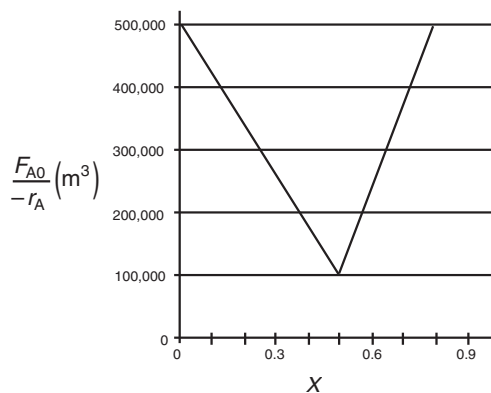


- Write five sentences summarizing what you learned from the Web Module.
- Work problems (1) and (2) in the Hippo Web Module.
- The hippo has picked up a river fungus, and now the effective volume of the CSTR stomach compartment is only  $0.2 \text{ m}^3$ . The hippo needs 30% conversion to survive. Will the hippo survive?
- 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>** **OEQ** (*Old Exam Question*). 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 P2-7<sub>B</sub>.



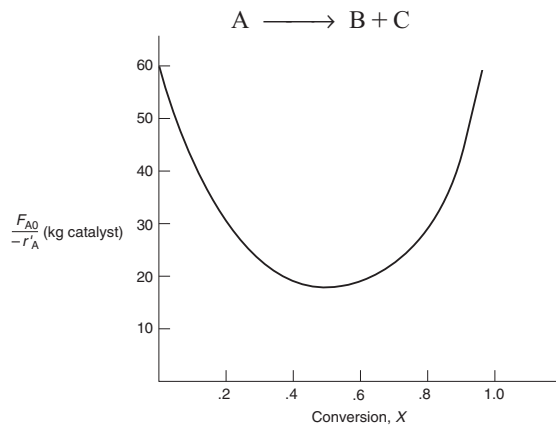
**Figure P2-7<sub>B</sub>** Levenspiel plot.

- 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%? (**Ans:**  $V_{\text{CSTR}} = 1.5 \times 10^5 \text{ m}^3$ )
- 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? In a  $6 \times 10^4 \text{ m}^3$  PFR?
- Think critically (cf. Introduction, Section H, page xxix) to critique the answers (numbers) to this problem.

**P2-8<sub>A</sub>** Estimate the reactor volumes of the two CSTRs and the PFR shown in the photo in Figure 2-9. *Hint:* Use the dimensions of the door as a scale.

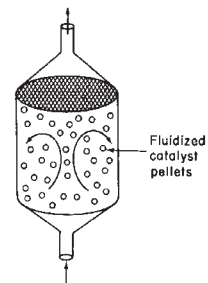
**P2-9<sub>D</sub>** Don't calculate anything. Just go home and relax.

**P2-10<sub>C</sub> OEQ** (Old Exam Question). The curve shown in Figure 2-1 is typical of a reaction carried out isothermally, and the curve shown in Figure P2-10<sub>C</sub> (see Example 11-3) is typical of a gas–solid catalytic exothermic reaction carried out adiabatically.



**Figure P2-10<sub>C</sub>** Levenspiel plot for an adiabatic exothermic heterogeneous 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? Use the smallest amount of catalyst weight to achieve 80% conversion of A.
- What is the catalyst weight necessary to achieve 80% conversion in a fluidized CSTR? (**Ans:**  $W = 23.2$  kg of catalyst)
- 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 catalyst weight,  $W$ .



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

**P2-11<sub>B</sub>** The experiments on reaction  $A \rightarrow B$  were carried out and the conversion-rate data is given in Table P2-11.

TABLE P2-11 CONVERSION-RATE DATA

$X$	0	0.2	0.4	0.6	0.8
$-r_A$ (mol/m <sup>3</sup> )	4	3	2.2	1.5	1.0

- What are the batch reactor times to achieve 10%, 50%, and 80% conversion for the reactor  $A \rightarrow B$  when the initial concentration is 2 molar?
  - Plot the reaction rate,  $-r_A$ , as a function of time up to a time necessary to achieve 80% conversion.
- Additional Homework Problems can be found on the CRE Web site under Chapter 2 **A. EXERCISES** hot button.

## SUPPLEMENTARY READING

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, *may or may not* be presented in

THORNTON W. BURGESS, *The Adventures of Poor Mrs. Quack*, New York: Dover Publications, Inc., 1917.

CHESTER L. KARRASS, *Effective Negotiating: Workbook and Discussion Guide*, Beverly Hills, CA: Karrass Ltd., 2004.

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