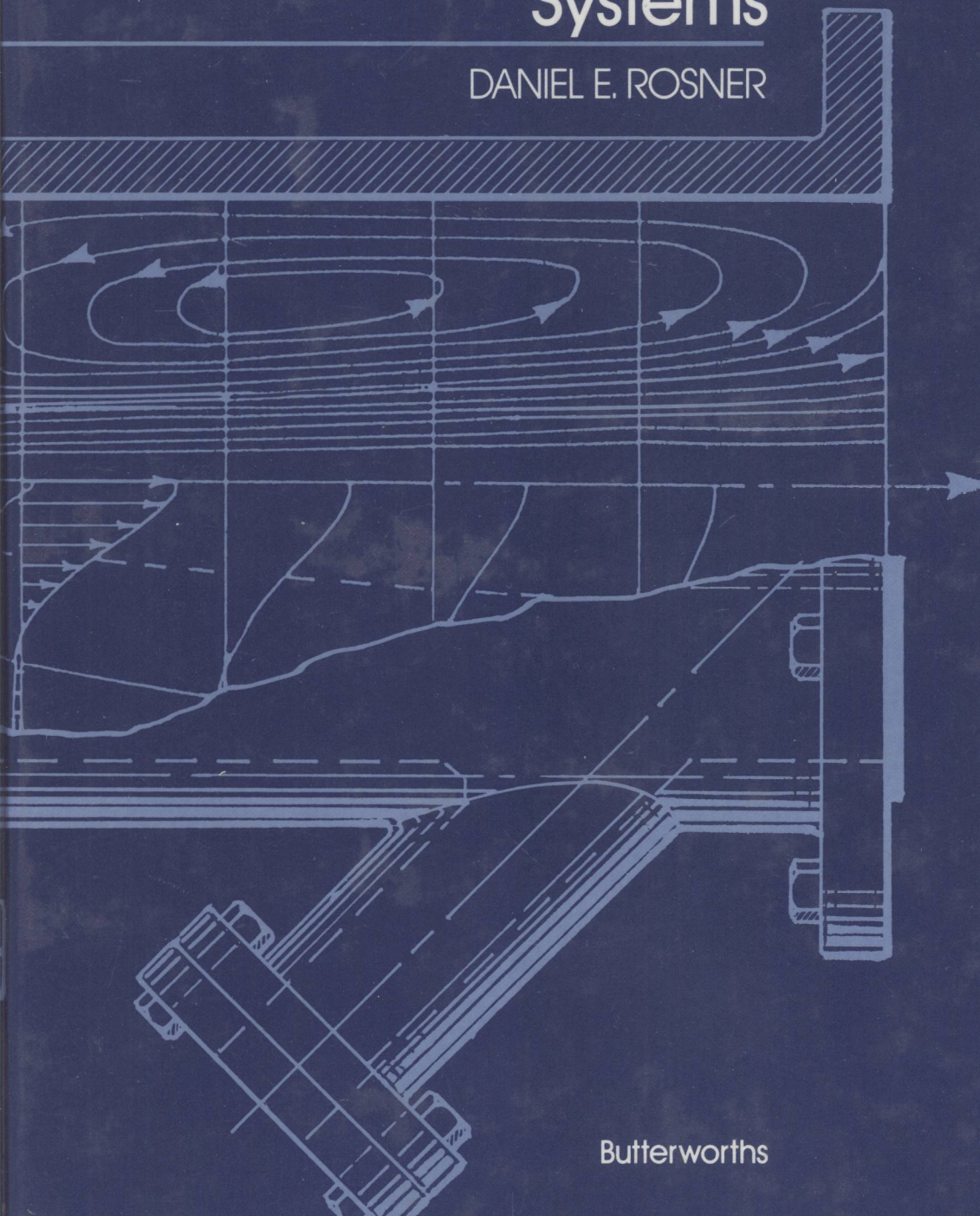


Transport Processes in Chemically Reacting Flow Systems

DANIEL E. ROSNER



Butterworths

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Transport Processes in Chemically Reacting Flow Systems

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To my wife, Susan

List of Primary Figures

Figure 2.1-2 Coordinate surfaces in the cylindrical polar coordinate system. Here the position of each point in space is defined by the three numbers: r, θ, z . The volume element about this point is $(\Delta r) \cdot (r \Delta \theta) \cdot (\Delta z) \equiv \Delta V$. (See, also, Figure 2.5-4(a).) Each local vector (say, the velocity \mathbf{v}) can, appropriately, be resolved into its r, θ, z components (v_r, v_θ, v_z , respectively).

Figure 2.5-1 “Absolute” molar enthalpies for several important ideal gases containing the chemical elements C, H, O, and N.

Figure 2.5-3 Summary of friction-loss factors ($Re > 10^5$) for common fluid-filled system components (after Beek and Muttzall (1975)).

Figure 2.5-4 Orthogonal polar coordinate systems: (a) cylindrical (r, θ, z); (b) spherical (r, θ, ϕ).

Figure 3.2-2 Temperature dependence of the dynamic viscosity, μ , of selected liquids (near atmospheric pressure).

Figure 3.2-3 Corresponding states correlation for the viscosity of simple fluids; based primarily on data for group VIIIA elements (after Bird, *et al.* (1960)).

Figure 3.3-1 Thermal conductivities of various substances (adapted from Rohsenow and Choi (1961)).

Figure 3.3-2 Corresponding-states correlation for the thermal conductivity of simple fluids; based primarily on data for group VIIIA elements (after Bird, *et al.* (1960)).

Figure 3.4-1 Predicted small-particle Schmidt number (ν/D_p) for SiO_2 particles in 1500 K air; transition between free-molecule (Eq. (3.4-8)) and continuum (Eq. (3.4-14)) behavior (Rosner and Fernandez de la Mora (1982)).

Figure 4.3-2 Steady one-dimensional isentropic flow of a perfect gas with $\gamma = 1.3$ (adapted from Shapiro (1953)).

Figure 4.3-3 Steady one-dimensional flow of a perfect gas (with $\gamma = 1.3$) in a constant-area duct; frictionless flow with heat addition (adapted from Shapiro (1953)).

Figure 4.3-4 Steady one-dimensional flow of a perfect gas (with $\gamma = 1.3$) in a constant-area duct; adiabatic flow with friction (adapted from Shapiro (1953)).

Figure 4.3-8 Normal shock property ratios as a function of upstream (normal) Mach number Ma (for $\gamma = 1.3$).

Figure 4.4-3 Experimental values for the overall drag coefficient (dimensionless total drag) for a cylinder (in cross-flow), over the Reynolds' number range $10^{-1} \leq Re < 10^6$ (adapted from Schlichting (1979)).

Figure 4.4-4 Experimental values for the overall drag coefficient (dimensionless total drag) for a sphere over the Reynolds' number range $10^{-1} \leq Re \leq 10^6$ (adapted from Schlichting (1979)).

Figure 4.4-5 “Road map” of common methods of solution to problems in transport (convection/diffusion) theory.

Figure 4.5-3 Experimental and theoretical friction coefficients for incompressible Newtonian fluid flow in a straight smooth-walled circular duct of constant cross section (after Denn (1980)).

Figure 4.5-6 Tangential velocity profile within the laminar BL on a flat plate at zero incidence (after Blasius [1908] and Schlichting (1979)).

Figure 4.7-1 Experimentally determined dependence of fixed bed friction factor f_{bed} on the bed Reynolds’ number (adapted from Ergun (1952)).

Figure 5.3-3 Experimentally determined *local* Nusselt numbers for cross-flow of a Newtonian fluid ($Pr = 0.7$) about a circular cylinder at various Reynolds’ numbers (adapted from Giedt, W. H. *Trans. ASME* **71**, 378 (1949) and Van Meel (1962)).

Figure 5.3-4 Polar plot of experimentally determined local $St_h Pr^{2/3}$, C_f and C_p -distributions for cross-flow of a Newtonian fluid about a circular cylinder at $Re = 1.7 \times 10^5$ (adapted from Fage and Falkner (1931) and Giedt (1959)).

Figure 5.5-1 Nusselt number distribution in a straight circular duct with fully developed viscous (Newtonian) fluid flow.

Figure 5.5-2 Experimentally determined dependence of packed-bed Nusselt number, $Nu_{h,bed}$, on the bed Reynolds’ number, Re_{bed} , and fluid Prandtl number, Pr (adapted from Whittaker (1972)).

Figure 5.6-1 Area-averaged natural convective heat-transfer data for vertical flat surfaces in an otherwise quiescent Newtonian fluid. Note transition to turbulence (within the thermal BL) at Ra_h -values (based on plate length) above *ca.* 10^9 (adapted from Eckert and Jackson (1950)).

Figure 5.7-1 Constant velocity and temperature contours for a turbulent round jet in a co-flowing stream of velocity, U_s , and temperature T_s (adapted from Forstall and Shapiro (1950)).

Figure 5.7-2 Universal velocity profile near the wall for fully developed turbulent pipe flow of a Newtonian fluid.

Figure 5.8E Chart for predicting the centerline temperature of an infinitely long cylinder (adapted from Heisler (1947)).

Figure 5.9-1 Dependence of total hemispheric emittance on surface temperature for several refractory materials (log-log scale) (adapted from Rosner (1964)).

Figure 5.9-2 Predicted view-factors between two parallel coaxial disks (adapted from Sparrow and Cess (1978)).

Figure 5.9-3 Predicted view-factors for the concentric cylinder geometry: (a) outer cylinder to inner cylinder; (b) outer cylinder to itself.

Figure 5.9-4 Total effective emissivity of water vapor as a function of “optical depth” $p_{H_2O} \cdot L$ (adapted from Eckert (1937)).

Figure 6.4-3 Transfer-coefficient reduction factor due to Stefan flow “blowing” ($B_m > 0$) and enhancement factor due to Stefan “suction” ($-1 \leq B_m < 0$) (after Bird, Stewart, and Lightfoot (1960)).

Figure 6.4-4 Catalyst effectiveness factor for first-order chemical reaction in a porous solid sphere (adapted from Weisz and Hicks (1962)).

Figure 6.4-5 Catalyst effectiveness factor *vs.* experimentally observable (modified) Thiele modulus (adapted from Weisz and Hicks (1962)).

Figure 6.4E Fraction, f , of initial solute content which has escaped *vs.* the dimensionless time $\tau \equiv Dt/R_p^2$ for an isothermal sphere.

Figure 6.5-2 Possible diffusion flame shapes for a coaxial fuel jet discharging into a duct surrounded by an equal-velocity, uniform oxidizer stream (adapted from Burke and Schumann (1928)).

Figure 6.6-1 Particle capture fraction correlation for ideal ($Re \rightarrow \infty$) flow past a transverse circular cylinder (Israel and Rosner (1983)). Here $t_{\text{flow}} \equiv (d/2)/U$.

Figure 7.1-2 “Corresponding states” correlation for the compressibility $pV/(RT)$ of ten vapors (after G.-J. Su (1946)).

Figure 7.2-1 Correlation of perimeter-averaged “natural convection” heat transfer from/to a horizontal circular cylinder in a Newtonian fluid (adapted from McAdams (1954)).

Figure 7.2-2 Pressure dependence of methane/air laminar flame speed (adapted from Diedrichsen and Wolfhard (1956)).

Figure 7.2-3 Dependence of laminar flame speed on burned gas temperature for several ($\Phi = 0.8$) fuel/air mixtures (adapted from Kaskan (1951)).

Figure 7.2-6 Correlation for the GT combustor efficiency *vs.* parameter proportional to (inverse) Damköhler number (adapted from S. Way (1956)).

Figure 7.2-7 Correlation of GT combustor stability limits *vs.* parameter proportional to (inverse) Damköhler number (after D. Stewart (1956)).

Figure 7.2-8 Correlation of flashback limits for premixed combustible gases in tubes (after Putnam and Jensen (1949)).

Figure 7.2-10 Test of proposed correlation of the dimensionless “blow-off” velocity, $U_{\text{bo}}L/\alpha_u$ *vs.* S_uL/α_u for a flame stabilized by a bluff body of transverse dimension L in a uniform, premixed gas stream (adapted from Spalding (1955)).

Figure 7.2-11 Correlation of laminar jet diffusion flame lengths (adapted from Altenkirch *et al.* (1977)).

Figure 7.2-12 Approximate correlation of fuel-droplet burning rate constants at elevated pressures (based on data of Kadota and Hiroyasu (1981)).

Figure 8.1-1 Correlation of heat loss/gain by circular cylinder in a steady cross-flow of air (after McAdams (1954)).

Figure 8.2-1 Correlation of inertial capture of particles by a circular cylinder in cross-flow (Israel and Rosner (1983)).

List of Primary Tables

- Table 2.5-1** Scale factors for the three most commonly used orthogonal coordinate systems.
- Table 3.2-1** Lennard-Jones potential parameters (after Svehla (1962)).
- Table 3.2-2** Correlation between Lennard-Jones parameters and accessible macroscopic parameters.
- Table 3.4-1** Power-law curve-fit to available $D_{ij}(T)$ data for some low-density binary gas mixtures.
- Table 3.13E** Ion diffusion coefficients in 25°C water.
- Table 5.4-1** Steady-state, source-free energy diffusion in one dimension.
- Table 5.5-1** Heat transfer and friction for fully developed laminar Newtonian flow through straight ducts of specified cross-section (after Shah and London (1978)).
- Table 5.9-1** Black body radiant emission from surfaces at various temperatures.
- Table 5.9-2** Approximate temperature dependence of total radiant-energy flux from heated solid surfaces (cf. Rosner (1964)).
- Table 6.4-1** Representative parameter values for some heterogeneous catalytic reactions (after Hlavacek *et al.* (1969)).
- Table 6.5-1** Physical and combustion properties of selected fuels in air (after NACA 1300 and Fristrom and Westenberg (1965)).
- Table 6.6-1** Critical Stokes' numbers for "pure" inertial impaction.
- Table 6.7-1** Some estimates of overall combustion kinetics parameters (after Kanury (1975)).
- Table 8.1-1** Thermodynamic and transport properties of air at 20 atm (after Poferl and Svehla (1973)).

Preface

I have succumbed to the temptation to write the book for which I searched in vain while I was a student and young lecturer! This text has evolved from my teaching of Yale University undergraduate and graduate courses dealing with the transport of energy, mass, and momentum in chemically reacting fluids, to students of engineering (chemical, mechanical, aeronautical, etc.) and applied science (e.g., materials, geophysics/geochemistry, medicine). The manuscript was put into its present form with the partial support of EXXON Research and Engineering Co., in connection with my teaching of the short course: "Introduction to the Fluid Mechanics of Combustion" (part of the EXXON R & E—Technical Education Program) and Olin Corporation (in connection with a short course presenting chemical engineering concepts to chemists). Accordingly, it is written in such a way as to be accessible to students and practicing scientists whose background has until now been confined to physical chemistry, classical physics, and/or applied mathematics. Indeed, the basic principles of these underlying fields are here generalized and reformulated so as to be able to deal with chemically reacting flow systems of current and future engineering interest. It is not necessary that the student have a previous course in fluid mechanics (i.e., momentum transfer by convection and diffusion); however, in that case the material presented here should certainly be covered over a period of more than one semester. Reflecting my own interdisciplinary background and involvement in ME, AeroE, and ChE, a special effort has been made to write the book in such a way as to make accessible to engineers educated in one area (say, ME or AeroE) the fruitful approaches and results of engineers in adjacent disciplines (especially chemical engineering, as in my treatment of the topics of momentum/energy/mass transport in packed bed exchangers, and also residence-time distribution analysis). While this is undoubtedly not the first such attempt at unifying these engineering fields under one cover, it may be the first having some of the advantages associated with being written by a single author. Inevitably, portions of my notation will, at first, appear unfamiliar and, perhaps, downright cumbersome, but, in most cases, it possesses a certain logic and suggestiveness which does not tax one's memory. Thus, it will not take the reader long to identify a quantity like $\dot{m}'_3 \textcircled{2}$ as the convective mass flow rate per unit area (say, $\text{kg/m}^2\text{-s}$) of chemical species 3 evaluated at station (location) $\textcircled{2}$, etc. (see Nomenclature).

J. W. Gibbs remarked that the role of theory in any science is to find the perspective from which the subject appears in its simplest form. My purpose is to present in a simple language but rather general form, principles and approaches that

have proven to be very fruitful, and that will doubtless remain so in solving the challenging problems still ahead of us. Thus, while our perspective and scope is broader than that found in many previous transport textbooks (especially those intended for undergraduates), the presentation here is deliberately concise and very selective, leaving many “details” for student exercises. I hope the result provides the dedicated reader with the fundamentally oriented yet up-to-date background needed to tackle more advanced, specialized topics. In any event, I am confident it will put the reader in a position to properly formulate and solve many important problems involving *rates* of energy, mass, or momentum transport in fluids that may be reacting chemically.

The pedagogical choice of *combustion* for many of the examples is not merely the result of my own research background. For the reasons outlined below I am convinced that combustion is an excellent “prototype” for presenting the important concepts of transport in chemically reacting fluid flows. First, it is perhaps the only area of chemically reacting flows not only common to chemical engineering, mechanical engineering, and aeronautical engineering, but also familiar in the daily experience of all applied scientists. Second, while avoiding the dazzling variety of phases, states, and chemical species encountered in present-day ChE reactor applications, combustors exhibit all of the important qualitative features of nonideal, transport-limited, nonisothermal reactors used to synthesize valuable chemicals—indeed, many chemicals (C_2H_2 , HCl, P_2O_5 , TiO_2 , etc.) *are* routinely produced in “flame” reactors. Finally, it should not be necessary to remind the reader of the economic importance of the efficient use of our remaining fossil fuels, and the prevention of combustion-related accidents. Since one of my primary objectives is to lay a proper foundation for subsequent study and R & D, in this introductory treatment I have deliberately avoided many topics, more heavily dependent on empiricism, associated with interacting multiphase transport (e.g., boiling, bubbling fluidized bed dynamics, etc.). However, as indicated in Section 2.6.4, the *macroscopic* conservation conditions (see the Introduction to Chapter 2) on which we systematically build our understanding of *single-phase* flow systems also provide the starting point for rational pseudo-continuum theories of dispersed *multiphase* situations. Therefore, it is appropriate that these underlying principles first be mastered in the context of either single-phase flows, or simple limiting cases of two-phase flows (e.g., steady flow through isothermal porous media) or packed beds (Sections 4.7, 5.5.5, and 6.5.1) and diffusion with chemical reaction in porous solid media (Section 6.4.4). [Study of Section 2.5 can be postponed without a loss in continuity; however, several of the derived forms of the conservation equations given here will prove useful in Chapters 4, 5, and 6.]

Also deliberately excluded is explicit material on what might be called the “systems” aspects of heat/mass exchangers, chemical reactors, and networks thereof. Thus, while we formulate and exploit the principles on which individual exchangers and chemical reactors are selected and designed (e.g., sized), explicit consideration of the economic optimization of specific devices, or the integration of many separate devices (as in multistage arrangements, or chemical “plants”) would take us too far from our central themes.

While Chapters 4, 5, and 6 deal successively with momentum, energy, and mass transport, we clearly develop, state, and exploit useful quantitative “analogies” between these transport phenomena, including interrelationships that remain valid even in the presence of homogeneous or heterogeneous chemical reactions (Sections 6.5.3 and 6.5.5). Moreover, we include a separate chapter (7) on the use of transport theory in the systematization and generalization of experimental data on chemically reacting systems, emphasizing “similitude” methods that go far beyond ordinary “dimensional analysis.” Because of our present emphasis on the transport mechanisms of *convection* and *diffusion*, which operate for momentum, energy, and (species) mass, the somewhat “singular” subject of *radiative* energy transport (Section 5.9) is only briefly included. While some chemical reactors are *intended* to produce photons (e.g., combustion-driven furnaces or chemical lasers), radiation is often an incidental “by-product.” These factors, together with the “one-way” nature of the fluid dynamics–radiative energy coupling in most engineering devices (i.e., the fluid-momentum, energy, and species “density” fields are needed to predict the radiative behavior, but not vice versa), account for the brevity of this section. Nevertheless, what little is included is intended to indicate the nature of the radiative transport problem, and to suggest fruitful alternative approaches to deal with it.

Following a concise “overview” (Chapter 7, Summary) of the main points of each chapter, many of these principles and methods are then brought together in a comprehensive numerical example (Chapter 8) intended to also serve as a prototype (see Appendix 8.1, Recommendations on Problem-Solving) for student solutions to the novel problems posed at the end of each chapter. These “exercises,” which are an extremely important part of this textbook from the viewpoint of a student’s education, have been designed to bring out important qualitative and quantitative engineering implications of the topics treated in each chapter. Unless otherwise specified they were developed by the author in connection with his previous teaching, research, and consulting; however, in some cases (clearly cited), they are elaborations or revisions of similar problems included in earlier textbooks or treatises. Several complete solutions are provided to demonstrate the specific use of seemingly “abstract” concepts, mathematical formulae, and/or graphical or tabular data provided in each chapter. While our preference is for metric units (m–kg–s, or cm–g–s), some examples are deliberately included in other commonly used engineering unit systems (for conversion factors, see Appendix 8.6). Most equations derived or quoted herein are either dimensionless or, if dimensional, stated in a form in which they are valid in any self-consistent unit set.

In summary, the principles developed and often illustrated here for combustion systems are important not only for the rational design and development of engineering equipment (e.g., chemical reactors, heat exchangers, mass exchangers) but also for scientific research involving coupled transport processes and chemical reaction in flow systems. Moreover, the groundwork is laid for the systematic further study of more specialized topics (chemical reactor analysis/design, separation processes, multiphase transport, radiative energy transport, computational fluid mechanics, combustion science and technology, etc.). Indeed, while developed primarily for use as a graduate (and undergraduate) textbook in transport processes

(energy, mass, and momentum), our emphasis on fluids containing molecules capable of undergoing chemical reaction (e.g., combustion) should make this book useful in more specialized engineering courses, especially chemical reaction engineering and combustion fundamentals. Specific sequences of topics in each of these possible courses are identified in Tables P1 and P2. In each case it is assumed that the relevant background in the underlying sciences of chemical thermodynamics and chemical kinetics can be provided *via* readily available texts in these classical areas.

By this time the reader will have noted that this text is concerned with the *principles* underlying the development of comprehensive rational computer models of chemically reacting flow systems, rather than the description of recently developed computer aids to engineering design. Thus, our emphasis is on the use of fundamental laws in the clever exploitation of a judicious blend of experiment, analysis, and numerical methods to first develop the requisite understanding, and, ultimately, to develop mathematical models for the essential portions of engineering problems involving energy, mass, and/or momentum exchange. In this respect, the particular problems and solutions I have chosen to explicitly include here should be regarded merely as instructive “prototypes” for dealing with the challenging new engineering problems that face us.

Much of my own learning occurs in the process of doing research in the general area of transport processes in chemically reacting systems. For this reason I wish to acknowledge the Office of Scientific Research of the U.S. Air Force and NASA–Lewis Research Laboratories for their financial support of research that has strongly influenced the orientation and content of this book. I am also indebted to

Table P1 Chemical Reaction Engineering

<i>Topic(s)</i>	<i>Textbook Section(s)</i>
Introduction	Ch. 1, Section 6.1
Conservation (Balance) Laws	Ch. 2
Transport (Diffusion) Laws	Ch. 3, Section 6.2
Ideal Plug-Flow Reactors: Empty and Packed (Fixed) Beds	Ex. 2.14, 5.11; Sections 6.1.3.1, 6.4.4, 6.7
Ideal (Well-) Stirred Tank Reactors	Sections 6.1.3.2, 6.7
Nonideal Reactors: PDE Models/Solution Methods	Section 7.4.3; Appendix 8.2
Modular Models of Real Flow Reactors; Stability and Parametric Sensitivity	Sections 6.7.4, 6.7.6, 6.7.7; Ex. 6.12
Diffusion and Chemical Reaction in Porous Media	Sections 3.4.4, 6.4.4; Ex. 6.6
Fixed-Bed Mass Transfer	Section 6.5.1; Ex. 6.10
Unpacked Duct Wall Reactors	Sections 6.1.3.1, 6.5.3; Ex. 6.9, 6.10
Similitude Methods in Systems with Chemical Reaction	Sections 6.4.4, 7.2.3.2, Ex. 6.8, 6.9
Chemical Reactor Scale Model Theory	Section 7.2.3
Summary	Section 7.4.2

Table P2 Combustion Fundamentals

<i>Topic(s)</i>	<i>Textbook Section(s)</i>
Introduction to Combustion: Scope, Importance	Ch. 1
Conservation (Balance) Laws	Ch. 2
Transport (Diffusion) Laws	Ch. 3
Thermodynamics of Combustion	Section 2.5.4; Ex. 2.9 (Solution)
Chemical Kinetics of Combustion	Sections 3.1.2, 6.7.6, 7.2.2.2
Premixed Flames (Deflagration Waves)	Sections 4.3.2, 6.5.5.8, 7.2.2.2
Detonation Waves	Section 4.3.2; Ex. 4.5
Flame Stabilization (Flashback, Blow-off)	Section 7.2.3.2; Ex. 7.4; Fig. 1.2-4
Ignition Energy	Section 1.1.1; Ex. 7.5
Diffusion Flames (Laminar and Turbulent)	Sections 1.1.2, 1.1.3, 6.5.5, 7.2.3.2c
Surface-Catalyzed Combustion/Incineration	Ex. 5.11; Section 6.9.1; Ex. 6.9; Section 6.5.3
Fuel Droplet Vaporization and Combustion Theory	Sections 1.1.3, 6.4.3.3, 6.5.5.7, 7.2.3.2d; Ex. 6.11
Stability and Parametric Sensitivity of Combustors	Sections 6.7.6, 7.2.3.1
Modular Mathematical Models of Combustor Performance	Sections 6.7.4, 6.7.6; Ex. 6.12
PDE Models of Combustion/Numerical Methods	Section 7.4.2; Appendix 8.2
Scale Model and Similitude Theory in Combustion Engineering	Section 7.2.3; Appendix 7.1
Heat and Mass Transfer from Combustion Gases	Sections 5.8, 5.9.3, 6.5.4; Ch. 8, Ex. 7.1, 7.6
Summary	Section 7.4.2

many colleagues at Yale University and EXXON Corporation for their helpful comments, and to the members of Technion–Israel Institute of Technology for their hospitality during the Fall of 1982, when this manuscript was essentially put into its present form. However, the author takes full responsibility for any errors of commission or omission associated with this first edition, and will welcome the written feedback of students, faculty, and practicing engineers and applied scientists who use this book.

Daniel E. Rosner
New Haven

Contents

List of Primary Figures xvii

List of Primary Tables xxi

Preface xxiii

1 Introduction to Transport Processes in Chemically Reactive Systems 1

Introduction 1

1.1 Physical Factors Governing Reaction Rates and Pollutant Emission: Examples of Partial or Total “Mixing” Rate Limitations 3

1.1.1 Flame Spread across IC Engine Cylinder 3

1.1.2 Gaseous Fuel Jet 5

1.1.3 Single Fuel Droplet and Fuel Droplet Spray Combustion 6

1.2 Continuum (*vs.* Molecular) Viewpoint: Length and Time Scales of Fluid-Dynamic Interest 7

1.3 Types/Uses of “Control” Volumes 14

1.4 Notion of Conservation Principles and Their Application to Moving Continua 17

1.5 Notion of “Constitutive” Laws (and Coefficients) for Particular Substances 18

1.6 Uses of Conservation/Constitutive Principles in Science and Technology 19

1.6.1 Inference of Constitutive Laws/Coefficients Based on Analysis and Measurement of Simple (“Canonical”) Flow/Transport Situations 19

1.6.2 Solution of Simpler “Prototype” Problems Illustrating Effects of the Basic Interacting Phenomena 21

1.6.3 Guide Design of Small-Scale or Full-Scale Experiments, and the Interpretation and Generalization of Experimental Results 21

1.6.4 Comprehensive Exchanger/Reactor Design Predictions via Computer Modeling 22

1.6.5 Interpretation of Instrument Measurements Made in the Laboratory or Field 22

Summary 22

True/False Questions 23

References 24

Bibliography 24

2 Governing Conservation Principles 27

- Introduction 27
 - Approach 27
- 2.1 Conservation of Mass 31
 - 2.1.1 Total Mass Conservation 31
 - 2.1.2 Individual Species Mass Balance 33
 - 2.1.3 Individual Chemical Element Conservation 37
- 2.2 Conservation of Momentum (Mixture) 38
 - 2.2.1 Linear Momentum Conservation 38
 - 2.2.2 Angular Momentum Conservation 40
- 2.3 Conservation of Energy (First Law of Thermodynamics) 42
- 2.4 “Conservation” of Entropy (Second Law of Thermodynamics) 45
- 2.5 Alternative (“Derived”) Forms of the Conservation (Balance) Equations 47
 - 2.5.1 Introduction 47
 - 2.5.2 Origin of the “Accumulation Rate + Net Convective Outflow Rate” Structure of all Conservation Equations for a Fixed Control Volume 49
 - 2.5.3 Material Derivative Form of the Conservation PDEs 50
 - 2.5.4 Alternate Forms of the Energy Conservation PDE 52
 - 2.5.5 Macroscopic Mechanical Energy Equation (Generalized Bernoulli Equation) 56
 - 2.5.6 Explicit Form of the Differential Entropy Balance when $\dot{q}''' = 0$ 59
 - 2.5.7 Explicit Form of the Conservation PDEs in Alternate Orthogonal Coordinate Systems 61
- 2.6 Remarks on Important Generalizations 64
 - 2.6.1 Moving Control Volumes and “Jump” Conditions across Moving (or Fixed) Discontinuities (Shock Waves, Phase Boundaries, etc.) 64
 - 2.6.2 Conservation Equations Using an Accelerating (Noninertial) Coordinate Frame 67
 - 2.6.3 Approach (Reynolds’) to Treatment of Turbulence via Time-Averaging the Conservation Equations 69
 - 2.6.4 Approach to the Treatment of Multiphase Continua via Volume-Averaging the Conservation Equations 72
- 2.7 Comments on the Matrix of Fluid Mechanics 74
 - 2.7.1 Continuum/Molecular 74
 - 2.7.2 Compressible/Incompressible 75
 - 2.7.3 Viscous/Inviscid 75
 - 2.7.4 Newtonian/Non-Newtonian 76
 - 2.7.5 Steady/Unsteady 76
 - 2.7.6 Laminar/Turbulent 76
 - 2.7.7 Multidimensional/One-Dimensional 77
- Summary 77
- True/False Questions 78
- Exercises 80
- References 93
- Bibliography: Conservation Principles 94