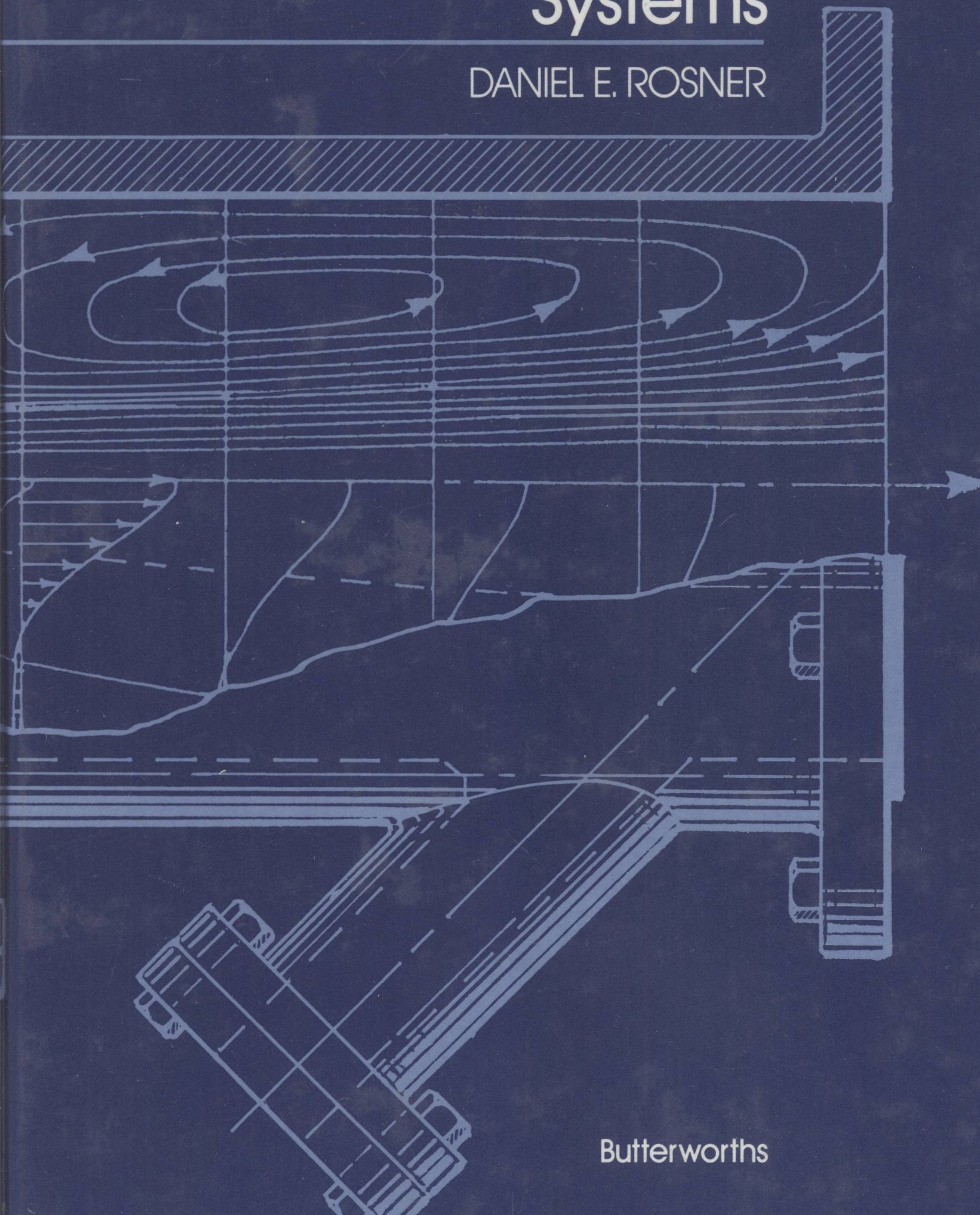
Transport Processes in Chemically Reacting Flow Systems

DANIEL E. ROSNER



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To my wife, Susan

List of Primary Figures

List of Primary Tables

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 $\dot{m}''_{3\,②}$ as the convective *mass* flow rate per unit area (say, kg/m^2-s) of chemical species 3 evaluated at station (location) 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

Topic(s)	*Textbook Section(s)*
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

Topic(s)	*Textbook Section(s)*
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

2 Governing Conservation Principles 27