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# Book Review

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## *Chemically Reacting Flow: Theory and Practice*

Robert J. Kee, Michael E. Coltrin, and Peter Glarborg, Wiley, New York, 2003, 848 pp., $88.95

Written by acknowledged experts, this is a weighty tome in more ways than one. In a number of respects, it is the inverse of the tiny, attractive book on combustion by Warnatz, Maas, and Dibble. Beyond being simply large and heavy to transport, it also makes for heavy reading. Designed to assist engineers working on reacting flows, it covers the experience of the authors in over 20 years of research.

Perhaps it is best to begin with a description of what this book is not. Although there are anywhere from 5 to more than 20 "problems" at the end of each of the 16 chapters that follow the nine-page introductory chapter, this is not an undergraduate textbook. Although some of the presentation, such as the elementary kinetic theory of gases, statistical mechanics, and the introduction to transport coefficients, is at the beginning undergraduate level, most of the material is too advanced for undergraduates, and the problems seem too wide ranging, extending from a small number of simple calculations, to amplifications of the authors' interpretations of certain fundamental points, to long, multipart questions related to applications and involving extensive plotting of graphs and writing of Excel programs. Given sufficient time off from other pressing tasks, some practicing engineers may enjoy doing this, thereby benefiting from the intended "educational setting" of the book.

The book also is not an encyclopedic review. With only 449 reference citations in a book numbering 848 + xxxiii pages, the literature is not covered thoroughly on any one topic. The citations include mainly the publications of the authors and their colleagues, along with basic references with which the authors have familiarity. To become aware of the full extent of contributions to any of the subjects addressed, the reader will have to go beyond this volume, for example to review journals. The volume therefore fulfills the stated objective of providing "reference material" only with respect to various fundamental background subjects and the research of the authors. The book is not addressed to mathematicians, physicists, chemists, or neophytes but rather to seasoned chemical and mechanical engineers with a research bent.

What this book *is* is a chatty presentation of material leading up to Chemkin, codes for calculating certain laminar, chemically reacting flows. These codes have been immeasurably beneficial to research in combustion and related fields, and the lead author is one of the principal originators of Chemkin. The equations and numerics underlying the codes are finally given, in fewer than 100 pages, in the last two chapters, the culmination of the book, where the results of a few representative applications also are summarized. There is, however, a long road to get there, as may be gleaned from the observation that more that 600 pages precede these chapters. Those pages delve into various aspects of fluid mechanics, thermodynamics, statistical mechanics, kinetic theory of gases, molecular transport properties, chemical kinetics, and numerical methods—every subject that anyone might conceivably need to get started. There is even an appendix reproducing van Dyke's classic simple example of asymptotic matching, along with appendices summarizing vectors, tensors and matrices, conservation equations in various coordinate systems, and the use of Excel 98. One of the chapters along the way is actually part of the culmination, namely that entitled "Heterogeneous Chemistry," which starts right out with Surface Chemkin and then proceeds to present the background thereof, exhibiting the basis of the applications to surface catalysis.

It may be worthwhile to be a bit more specific about just what all this background material is, even though space certainly will not allow a complete enumeration here. It takes the authors six chapters to get through their presentation of fluid mechanics, despite no turbulence. The initial development is quite general, allowing for both variable density and compressibility, although suppression of acoustics is also addressed, termed "pressure filtering." Equations of many of the classical idealized flows are given and discussed, including Couette flow, Poiseuelle flow, duct-entrance flow, Jeffrey–Hamel flow, stagnation flow, opposed flow, von Kármán swirling flow, and boundary-layer flow, for example, including various transformations and finite difference approximations. There are elementary presentations of molecular energy levels, Boltzmann statistics, and partition functions, including sample calculations of thermodynamic properties. Considerably detailed descriptions are given of the law of mass action, chemical equilibrium, collision reaction-rate theory, transition-state theory, and unimolecular reactions, with indications of what RRK, QRRK, and RRKM theories are, as well as, in later chapters, one-step and detailed reaction mechanisms, chain reactions, explosion limits, fuel oxidation, NO production, sulfur oxidation, and chlorine chemistry. Molecular transport properties are addressed in a number of

places, including early "brief discussions" while conservation equations are derived and later summaries of Lennard–Jones and Stockmayer potentials, rules for estimating unknown cross sections and energies, the Boltzmann equation, Chapman–Enskog theory, and collision-integral formulas. Concerning numerical methods, first stiffness and then explicit and implicit methods, ODE solvers, Newton algorithms, hybrid methods, and sensitivity analysis all are covered. These abbreviated lists may impart some flavor of the scope of the volume.

To be honest, I must say that the style of presentation in this book does not appeal to me. In reading it, I became impatient at the seemingly excessive repetition of essentially the same statements and the lack of clarity of terms when first encountered and often of the later explanations as well. Already in the first equation in the book, the equation of state for a multicomponent ideal gas, all symbols are defined in the text immediately following the equation, except mysteriously for $T$, the temperature. Now most readers will know what $T$ means, but won't they also know that $p$ stands for pressure? And the complete list of nomenclature at the beginning of the book can always be consulted for the meaning of any symbol anyway, so it would seem to me to be most logical to define either all symbols or none. Various equations are written in forms that almost certainly are wrong; for example, an equation is written for the substantial derivative for a system that evidently equates a finite quantity on the left-hand side to an infinitesimal quantity on the right. Long and detailed derivations of stress relationships and conservation equations are presented from the continuum viewpoint specifically in cylindrical coordinate systems, rather than in the simpler Cartesian system used in many elementary fluids textbooks; one wonders how many true aficionados of cylindrical systems there are out there, as opposed, say, to aficionados of spherical systems, even though the authors devote one long paragraph to explaining why they chose to cast the developments into the cylindrical system. At one point, in a discussion of the dissipation function, the reader is told bluntly that the bulk viscosity can be negative, which of course it cannot be; the point that the authors are probably trying to make is that, for the dissipation rate to be never negative, the second viscosity coefficient must be nonnegative, a point that would have been much more transparent from the equation if Cartesian rather than cylindrical coordinates had been adopted.

The references listed at the end of the book are numbered alphabetically, and in the text each reference is cited only by number; I found myself perpetually turning back to the references and thumbing through them to find out who was being cited, a loss of time that would have been avoided if the more common practice had been used of citing by author when the list is alphabetical, or even if the numbering had been in the order of appearance, so that it would not be necessary to search through all reference pages each time. Although there may exist readers for whom the overall writing style will be attractive, this reader is not one of them. It would seem to me to have been preferable to rely on standard excellent texts for fluids, thermodynamics, statistical mechanics, kinetic theory, and chemical kinetics, to save a lot of time and get right to the culmination—the useful Chemkin formulations. Yet the authors have written this book with extreme patience and an evident love of their subject. The care in writing is exemplified by the attractiveness of most page layouts and the relative sparseness of typographical errors (which would be pointless to list here). Let us hope that there will be many readers, unlike me, with the patience and tenacity, like the authors, to wade carefully through this entire volume and thereby benefit from it.

Forman A. Williams
University of California, San Diego