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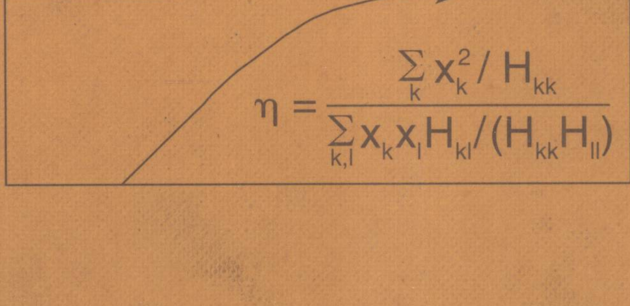

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Alexandre Ern Vincent Giovangigli

Multicomponent Transport Algorithms

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Preface

With the advent of sophisticated computer technology and the development of efficient computational algorithms, numerical modeling of complex multicomponent laminar reacting flows has emerged as an increasingly popular and firmly established area of scientific research. Progress in this area aims at obtaining better resolved and more accurate solutions of specific technological problems in less computer time. Therefore, it strongly relies upon the ability of evaluating fundamental parameters appearing in the physical models.

Transport properties constitute a typical example of the above characterization. Evaluating transport coefficients of dilute polyatomic gas mixtures is often critical in many engineering applications, including chemical reactors, hypersonic flows, combustion phenomena, and chemical vapor deposition. Using the kinetic theory of dilute polyatomic gas mixtures as a starting point, this book offers a systematic development of a mathematical and numerical theory for the evaluation of transport properties in dilute polyatomic gas mixtures. The present investigation is not specifically about the kinetic theory of gases, for which there are plenty of excellent and thoroughly documented textbooks; it is rather geared toward the development of new, efficient, and general algorithms with which to evaluate transport properties of dilute polyatomic gas mixtures at a reasonable computational cost.

In this book we compute the coefficients of the transport linear systems, i.e., the linear systems to be solved in order to obtain the transport coefficients, in their natural constrained singular symmetric form. New transport linear systems, corresponding to lower computational costs for practical applications, are also introduced. From a theoretical viewpoint, we extract the structural properties of the transport linear systems directly from the Boltzmann equation and use them systematically in order to derive a mathematical framework for iterative algorithms. As a result, we express all the transport coefficients as convergent series, and truncating these series then yields analytical approximate expressions for all the transport coefficients.

We hope that the present algorithms will be of extensive interest in theoretical calculations and numerical modeling for fluid mechanics, combustion, crystal growth, and other engineering applications. The material covered in this book is intended for people who are not familiar with multicomponent transport property evaluation as well as for experienced readers interested in the relevant areas of modern research. Readers need only be familiar with introductory linear algebra concepts and some basic ideas of the kinetic theory of dilute gases. The more elaborate sections of the book should still be readable at the same level since we restate the more sophisticated results as needed.

The logical ordering of the chapters closely follows the development of the present theory, from kinetic theory concepts, through the derivation of the transport linear system structure to convergence theorems for various iterative algorithms, followed by several numerical examples. Readers only interested in practical applications may consider a different reading path, which only includes the introductory parts of all chapters, Sections 2.1 and 2.2, the notation and the summaries of results presented in Section 2.3, the derivation of the transport linear systems described in Sections 2.4–2.8, the convergence theorems stated in Chapter 5, and the numerical results of Chapter 6. All the transport linear systems are treated explicitly, which contributes significantly to the length of the manuscript, but provides a complete source of reference for any transport coefficient that may be needed in a given application. A more detailed reading of the book includes the derivation of the transport linear system properties directly from the kinetic theory as detailed in Section 2.3, the mathematical framework of Chapter 4, the proofs of the theorems in Chapters 4 and 5, and the singular limit of zero concentrations treated in Chapter 3 and also considered in the subsequent chapters.

The authors owe their sincere thanks to many of their colleagues for several stimulating discussions. They are also grateful to Professor I. Kuščer, University of Ljubljana, for constructive remarks about chemically reacting flows, and to Professor M. D. Smooke and Doctor M. A. Tanoff, Yale University, and Professor V. Ern, University of Strasbourg, for numerous comments. The assistance of Mr. M. Multan from the Prêt Inter-Bibliothèques, Ecole Polytechnique, is also gratefully acknowledged.

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Paris, May 1994

Alexandre Ern
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