Rarefied Gas Dynamics

The aim of this book is to present the concepts, methods, and applications of kinetic theory to rarefied gas dynamics. After introducing the basic tools, problems in plane geometry are treated using approximation techniques (perturbation and numerical methods). These same techniques are later used to deal with two- and three-dimensional problems. The models include not only monatomic but also polyatomic gases, mixtures, and chemical reactions. A special chapter is devoted to evaporation and condensation phenomena.

Each section is accompanied by problems that are mainly intended to demonstrate the use of the material in the text and to outline additional subjects, results, and equations. This will help ensure that the book can be used for a range of graduate courses in aerospace engineering or applied mathematics.

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Rarefied Gas Dynamics
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Rarefied Gas Dynamics
From Basic Concepts to Actual Calculations

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Preface

The present volume is intended to cover the present status of the theoretical tools of rarefied gas dynamics. The meaning and usefulness of the subject, and the extent to which it is covered in the book, are discussed in some detail in the introduction. In short, I tried to present the basic concepts and the techniques used in probing difficult, and partly unsolved, questions and in attacking difficult problems posed by aerospace research, environmental sciences, aerosol reactors, micromachines, and vacuum technology. For the book to be up-to-date without being excessively large, it was necessary to omit some topics, which are treated elsewhere, as indicated in the introduction. Their omission does not alter the aim of the book: to provide a working understanding of the essentials of rarefied gas dynamics and to form the foundation and give the background for a study of the original literature.

The tables and figures should not be considered as a complete collection of the information required to attack practical problems or as a substitute for the calculations that must be carried out in each specific instance. They rather illustrate the kind of results to be expected when using a particular method. General principles and essentials can be given in a book such as the present one, but the coverage of different applications must be left to the scientist or engineer dealing with that application.

The problems that are given at the end of the various sections are mainly intended to demonstrate the use of the material in the text and to outline additional subjects, results, and equations.

The general prerequisites of the book are such that it can also be used in a graduate course in engineering or applied mathematics.

Although I have tried to provide a rather complete bibliography, the choice of the topics and of the references certainly reflects a personal bias and I apologize in advance for any omission.

During the work on the manuscript, I have benefited from personal and electronic contacts with many colleagues. Since any list would be incomplete, I restrict my acknowledgment here to those who have helped me with the figures: K. Aoki, M. S. Ivanov, and K. Koura, who gave me permission to reproduce pictures from some of their papers in Chapter 7 and provided the relevant files, and L. Valdettaro, who helped me in the preparation of the software required to produce the remaining pictures.

Introduction

The subject of rarefied gas dynamics can be conveniently defined as the study of gas flows in which the average value of the distance between two subsequent collisions of a molecule (the so-called mean free path) is not negligible in comparison with a length typical of the structure of the flow being considered (e.g., the radius of a pipe or the radius of curvature of the nose of a space shuttle). The field is thus seen to be one that intrinsically requires the use of statistical ideas typical of the kinetic theory of gases as embodied in the integro-differential equation proposed by Boltzmann in 1872 and bearing his name.

Limiting cases of the Boltzmann equation yield the continuum description, commonly based on the Euler or Navier–Stokes equations, at the extreme of small mean free paths, and the collisionless (or free-molecular) flow, at the extreme of large mean free paths. Although most problems in rarefied gas dynamics involve the central region between these two limiting behaviors, commonly called the transition regime, there are interesting problems at the two extremes as well.

In addition to the description based on the Boltzmann equation, the study of rarefied flows requires an additional piece of information concerning the interaction of the gas molecules with the solid (or, possibly, liquid) surfaces that bound the gas expanse. It is to this interaction that one can trace the origin of the drag and lift exerted by the gas on the body and the heat transfer between the gas and the solid boundary.

The study of gas–surface interaction may be regarded as a bridge between the kinetic theory of gases and solid state physics and is an area of research by itself. The difficulties of a theoretical investigation are due, mainly, to our lack of knowledge of the structure of surface layers of solid bodies and hence of the effective interaction potential of the gas molecules with the wall. When a molecule impinges upon a surface, it is adsorbed and may form chemical bonds,

dissociate, become ionized, or displace surface molecules. Its interaction with the solid surface depends on the surface finish, the cleanliness of the surface, its temperature, etc. It may also vary with time because of outgassing from the surface. Preliminary heating of a surface also promotes purification of the surface through emission of adsorbed molecules. In general, adsorbed layers may be present; in this case, the interaction of a given molecule with the surface may also depend on the distribution of molecules impinging on a surface element.

This physical aspect has a mathematical counterpart: The Boltzmann equation must be accompanied by boundary conditions, which describe the aforementioned interaction of the gas molecules with the solid walls.

If we add the fact that polyatomic molecules (such as oxygen and nitrogen in the atmosphere) are far from being the hard spheres or centers of forces at distance commonly considered in elementary kinetic theory, it becomes clear that rarefied gas dynamics is a rather complex subject. Fortunately, there is a simplifying aspect, which has slowly been discovered and confirmed during forty years of research: It is possible to adopt simplified models that embody certain basic physical features and forget about other complexities, in order to obtain essentially accurate results for the purpose of engineering applications. Whereas modeling is more an art than a science, a long practice has repeatedly shown what should be embodied in a model and what can be forgotten: Basic physics, embodied in a certain number of general ideas and principles, should be respected; detailed information about interactions can be replaced by a qualitatively correct description that contains a few parameters to be adjusted so as to represent the behavior of real molecules within the accuracy required by applications.

Rarefied gas dynamics has existed, in principle, since the nineteenth century but came in the foreground with space exploration. One can even give a birthdate, July 1958, when the first international symposium on rarefied gas dynamics was held in Nice, France. Since then, these symposia have been held regularly every other year. The corresponding proceedings constitute a set of useful references as a whole and the list of them is given at the end of this introduction.

When glancing through the aforementioned volumes, one should not be surprised to find a shift of topics. The first few volumes contain a considerable amount of experimental papers, and the theoretical papers contain very general surveys on the Boltzmann equations but very few papers dealing with explicit solutions of some elementary problems. Also, the gas speeds in experiments were rather low, usually slightly supersonic. The first numerical solutions of some interest appear in 1962, but even in the late 1960s these were few in

number and not so accurate. Then one witnesses the reduction of experimental work and the increasing importance of numerical simulation. In the most recent issues, experiments regrettably occupy just a few pages of the proceedings. This is compensated for by the fact that numerical simulations have spread through all the subfields, indicating the maturity reached by our theoretical understanding of the subject. Increasingly complicated phenomena, such as reacting flows or evaporation and condensation, are the object of widespread interests.

Thus it is clear that the Boltzmann equation became a practical tool for the aerospace engineers, when they started to remark that flight in the upper atmosphere must face the problem of a decrease in the ambient density with increasing height. This density reduction would alleviate the aerodynamic forces and heat fluxes that a flying vehicle would have to withstand. However, for virtually all missions, the increase of altitude is accompanied by an increase in speed; thus it is not uncommon for a spacecraft to experience its peak heating at considerable altitudes (such as, e.g., 70 km).

In the area of environmental problems, rarefied gas dynamics is also required. Understanding and controlling the formation, motion, reactions, and evolution of particles of varying composition and shapes, ranging from a diameter of the order of .001 μm to 50 μm, as well as their space–time distribution under gradients of concentration, pressure, temperature, and the action of radiation, has grown in importance. This is because of the increasing awareness of the local and global problems related to the emission of particles from electric power plants, chemical plants, and vehicles as well as of the role played by small particles in the formation of fog and clouds, in the release of radioactivity from nuclear reactor accidents, and in the problems arising from the exhaust streams of aerosol reactors, such as those used to produce optical fibers, catalysts, ceramics, silicon chips, and carbon whiskers.

One cubic centimeter of atmospheric air at ground level contains approximately 2.5×10^{19} molecules. About a thousand of them may be charged (ions). A typical molecular diameter is 3×10^{-10} m (3×10^{-4} μm) and the average distance between the molecules is about ten times as much. The mean free path is of the order of 10^{-8} m, or 10^{-2} μm. In addition to molecules and ions one cubic centimeter of air also contains a significant number of particles varying in size, as indicated above. In relatively clean air, these particles, which include pollen, bacteria, dust, and industrial emissions, can number 10^5 or more. They can be both beneficial and detrimental, and they arise from a number of natural sources as well as from the activities of all living organisms, especially humans. The particles can have complex chemical compositions and shapes and may even be toxic or radioactive.

A suspension of particles in a gas is known as an aerosol. Atmospheric aerosols are of global interest and have important impact on our lives. Aerosols are also of great interest in numerous scientific and engineering applications.

A third area of application of rarefied gas dynamics has emerged in the past few years. Small machines, called micromachines, are being designed and built. Their typical sizes range from a few microns to a few millimeters. Rarefied flow phenomena that are more or less laboratory curiosities in machines of more usual size can form the basis of important systems in the micromechanical domain.

One should not forget the design and simulation of aerosol reactors, used to produce optical fibers, catalysts, ceramics, silicon chips, and carbon whiskers, which have been mentioned above as sources of air pollution.

A further area of interest occurs in the vacuum industry. Although this area existed for a long time, the expense of the early computations with kinetic theory precluded applications of numerical methods. The latter could develop only in the context of the aerospace industry, because until recently the big budgets required were available only there.

The present volume is an attempt to cover the theoretical aspects of rarefied gas dynamics. The most theoretical and mathematical aspects have been left out, and the aim is the understanding of the basic concepts and the computation techniques. Readers interested to the difficult but interesting rigorous mathematics concerning the Boltzmann equation are advised to consult the following book:

C. Cercignani, R. Illner, M. Pulvirenti, *The Mathematical Theory of Dilute Gases*, Springer-Verlag, New York (1994).

The analytical techniques used to obtain approximate solutions are dealt with in some detail, but only insofar as they are useful to introduce or illustrate important concepts or show properties of the solutions of the Boltzmann equation. For a more detailed study of these techniques as well as for a discussion of general properties of the Boltzmann equation and its models, two other books should be consulted:

C. Cercignani, *Mathematical Methods in Kinetic Theory*, Plenum Press, New York (1969; revised edition 1990),

C. Cercignani, *The Boltzmann Equation and Its Applications*, Springer-Verlag, New York (1988).

The former is a rather simple introduction to the theory of the Boltzmann equation; the latter is a rather complete monograph, written when a unified presentation of the mathematical and practical aspects of the theory of the Boltzmann equation looked feasible. Nowadays, with the great explosion of the subject in different directions, it seems appropriate to have a book aimed at

applications, leaving out the mathematical theory. In particular, computational methods such as the Direct Simulation Monte Carlo and important phenomena such as those related to polyatomic gases, chemical reactions, evaporation, and condensation were barely mentioned in the last reference and are treated here in detail.

Having defined more or less the general subject of the book and the main topics dealt with, it remains to say what is *not* treated here. Ionization phenomena, although discussed in Chapter 6, are only briefly touched upon and viewed as a neighboring topic. The great and important field of rarefied plasmas is left completely untouched. The same can be said for the interaction between gases and thermal radiation.

Finally, one should mention that the basic idea of a kinetic equation, having the Boltzmann equation as prototype, has spread to many other fields, not only to the two aforementioned areas, ionized gases and radiative transfer, and to the well-known area of neutron transport, but also to the behavior of electrons and holes in semiconductors, of dense gases, and of more sizable particles, such as those met in the theory of granular materials and car traffic. These topics are of great interest but are, of course, not dealt with here. Yet, the author hopes that people working in other areas of the growing field of kinetic equations can find suggestions and inspiration for problems in the aforementioned areas by consulting the present book.

List of the proceedings of the Symposia on Rarefied Gas Dynamics

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