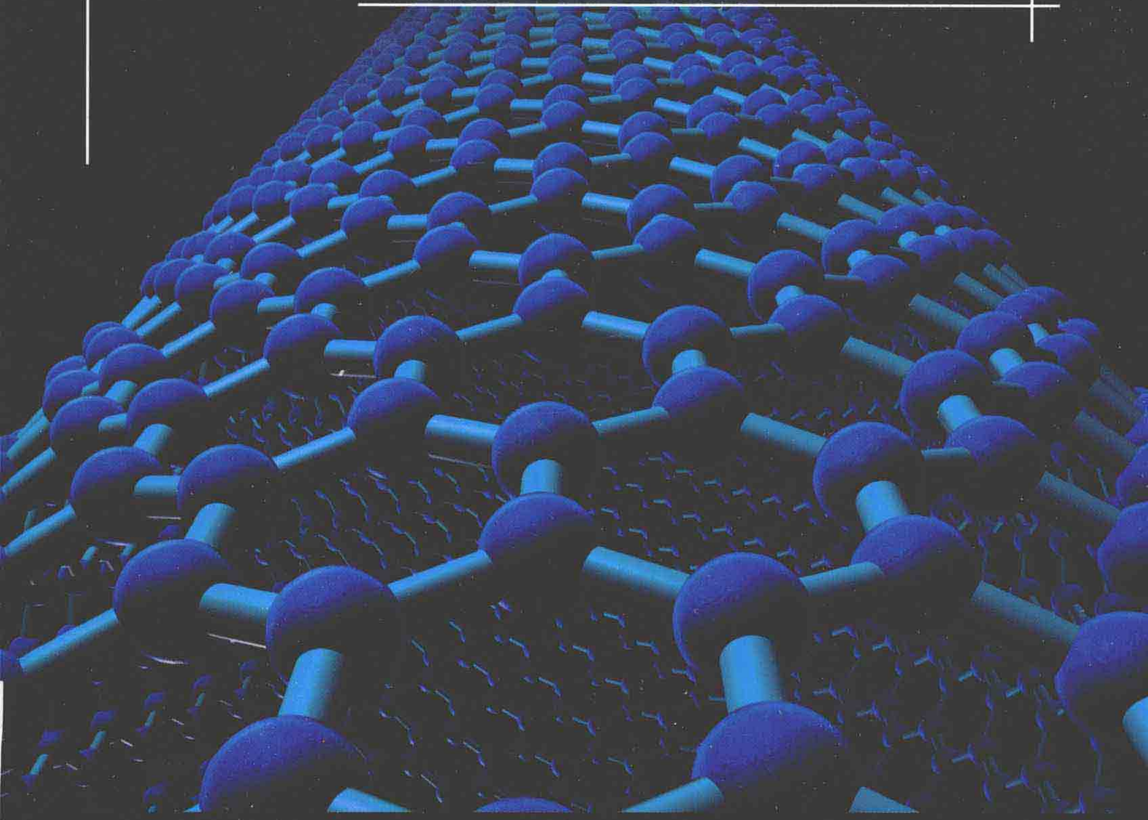
McGraw-Hill Nanoscience and Technology Series

MICROFLUID MECHANICS

PRINCIPLES AND MODELING



WILLIAM W. LIOU AND YICHUAN FANG

Microfluid Mechanics

Principles and Modeling

William W. Liou

Yichuan Fang

Department of Mechanical and Aeronautical Engineering
Western Michigan University
Kalamazoo, Michigan

McGraw-Hill

New York Chicago San Francisco Lisbon London Madrid
Mexico City Milan New Delhi San Juan Seoul
Singapore Sydney Toronto

The McGraw-Hill Companies

Library of Congress Cataloging-in-Publication Data

Liou, William W.
Microfluid mechanics / William W. Liou, Yichuan Fang.
p. cm.
Includes index.
ISBN 0-07-144322-3
1. Fluid dynamics. I. Fang, Yichuan. II. Title.
TA357.L567 2005
620.1'06—dc22
2005048383

1 2 3 4 5 6 7 8 9 0 DOC/DOC 0 1 0 9 8 7 6 5

ISBN 0-07-144322-3

The sponsoring editor for this book was Kenneth P. McCombs and the production supervisors were Richard Ruzycka and Sherri Souffrance. It was set in Century Schoolbook by International Typesetting and Composition. The art director for the cover was Margaret Webster-Shapiro.

Printed and bound by RR Donnelley.

This book was printed on recycled, acid-free paper containing a minimum of 50% recycled, de-inked fiber.

Microfluid Mechanics

Nanoscience and Technology Series
Omar Manasreh, Series Editor

MICHAEL H. PETERS • *Molecular Thermodynamics and Transport*
KENNETH GILLEO • *MEMS / MOEM Packaging*
NICOLAE O. LOBONTIU • *Mechanical Design of Microresonators*
ROBERTO PAIELLA • *Intersubband Transitions in Quantum Structures*
JOSEPH H. KOO • *Polymer Nanocomposites*
JENS W. TOMM AND JUAN JIMENEZ • *Quantum-Well High-Power Laser Arrays*

Preface

This book is written as a textbook for an analytical-oriented microfluid flow course with graduate students who, preferably, have already taken an advanced fluid mechanics course. The derivations of the equations are presented, whenever possible, in a fairly detailed manner. The intent is that, even without the help of an instructor, students can self-navigate through the materials with confidence and come away with a successful learning experience. Similarly, practicing engineers who are interested in the subject should also be able to pick up the book and follow the flow of the contents without much difficulty. Some background in modern numerical computation tools will help the readers getting the full benefit of the two computer programs, NB2D and DSMC-IP, associated with the book. In fact, it is highly recommended that readers do make use of these Fortran programs.

The book begins with an introduction to the kinetic theory of gas and the Boltzmann equation to build the foundation to the later mathematical modeling approaches. With the dilute gas assumption, the nature of the micro gas flows allows the direct application of the Chapman-Enskog theory, which then brings in the modeling equations at the various orders of the Knudsen number in Chapter 4. The direct simulation Monte Carlo (DSMC) method and the information preservation (IP) method are described as the numerical tools to provide solutions to the Boltzmann equation when the Knudsen number is high. The later chapters cover the hybrid approaches and the important surface mechanisms. Some examples of micro gas flows at high and low speeds are shown. One interesting aspect of micro gas flows that is yet to see extensive examination in the literature is the characteristics of the flow disturbances at microscales. Chapter 11 provides a detailed description of some of our preliminary studies in this area.

Although a part of the content of the book has been used in a one-semester graduate level microfluid dynamics course at Western Michigan University, the book is best used as a textbook for a two-semester course. Chapters 1 to 4 provide the introductory content for the basic mathematical and the physical aspects of micro gas flows. The computer program NB2D may be used, for example, as project exercises. The second part would emphasize the DSMC and the IP solution methods, and their parallelization. The computer program DSMC-IP can be used for term project type of assignments. In the situation where the analytical microfluid course is preceded by another experiment-oriented course on microfabrication or microengineering, and the students have already had somewhat extensive knowledge of micro gas flows, the instructor may wish to concentrate on Chapters 2, 4, and 5 in the lectures and leave the rest as reading assignments. When the book is used in a 16-to-20-hour short-course setting, the instructor may wish to highlight the materials from Chapters 2, 4, 5, and 7. It might be a good idea to provide opportunities to run at least one of the two computer programs onsite. Chapters 1, 3, and 10 can be assigned as overnight reading materials.

The book does not contain extensive updates and details on the current engineering microfluidic devices. We feel that the book's focus is on the fundamental aspects of mirofluid flows and there is a myriad of readily available information on the technologies and the many different microfluidic device applications that have been cleverly designed and painstakingly manufactured by experts in the field. Also, since new devices are being brought to light almost daily, we feel that what is current at the time of this writing may become outdated within a few years.

A portion of the work the authors have accomplished at Western Michigan University has been performed under the support of NASA Langley Research Center. Near the completion of the manuscript, the second author moved to the Georgia Institute of Technology.

We appreciate the help of Dr. James Moss for reviewing a part of the manuscript. Thanks should go to those at McGraw Hill who worked on the book and to those who reviewed it. We should also thank Jin Su and Yang Yang for their work on the codes. The first author (WWL) would like to thank the unconditional support and patience of his wife, Shiou-Huey Lee, during this writing and the love from his children, Alex and Natalie.

William W. Liou
Kalamazoo, Michigan

Yichuan Fang
Atlanta, Georgia

Contents

Chapter

1

Introduction

Microelectromechanical systems (MEMS) are considered one of the major advances of industrial technologies in the past decades. MEMS technology was derived initially from the integrated circuit (IC) fabrication technologies. Now, microfabrication is a diverse spectrum of processing techniques that involve a wide range of disciplines from chemical sciences to plastic molding. As the name suggests, MEMS covers micron-sized, electrically and/or mechanically driven devices. Compared with the conventional mechanical or electrical systems, these MEMS devices are five to six orders of magnitude smaller in size. In fact, these dimensions are in the same range as the average diameter of human hair (about 50 μm, 50×10^{-6}m, or 50 μm). An MEMS device can be a single piece of hardware that produces outputs directly based on the inputs from external sources. The outputs can be mechanical and fluidic movement, electrical charges, analog signals, and digital signals. Often several microcomponents are integrated, such as the lab-on-a-chip device, which performs the multistage processing of the inputs and produces several different types of outputs, all in one single miniature device. The small sizes of MEMS make them portable and implantable. The manufacturing cost of MEMS is far from prohibitive because of the wide use of the batch-processing technologies that grow out of the well-developed IC industry. MEMS, therefore, offer opportunities to many areas of application, such as biomedical and information technology, that were thought not achievable using conventional devices. Estimates of the potential commercial market size were as high as billions of U.S. dollars by 2010.

Since the early work of Tai et al. (1989) and Mehregany et al. (1990) on the surface-machined micromotors, there has been an explosive growth of the number and the types of potential application of MEMS.

Accompanying this growth is the significant increase of new journals that are dedicated to reporting advances in the field. The universal use of the Internet also helps disseminate new MEMS knowledge quickly and hasten its development effectively. There are also a number of titles written by distinguished researchers in the field. [a sample of them would include Gad-el-Hak (2002), Karniadakis and Beskok (2002), Koch et al. (2000), Nguyen and Wereley (2002), and Li (2004)] MEMS related technologies, ranging from electrokinetics and microfabrication to applications, can be readily found in these and many other forms of publications and media.

As more new applications are proposed and new MEMS devices designed, it was often found that measured quantities could not be interpreted by using conventional correlations developed for macro scale devices. Electric power needed to drive a micromotor was extraordinarily high. The properties of MEMS materials, such as Young's modulus, have been found to differ from that of the bulk material. For MEMS that use fluid as the working media, or a microfluidic device, for instance, the surface mechanisms are more important than mechanisms that scale with the volume. Overcoming surface stiction was found to be important in the early work on micromotors. The surface tension is perhaps among the most challenging issues in microfluidic devices that involve the use of liquid for transporting, sensing, and control purposes. The mass flow rate of microchannels of gas and liquid flows in simple straight microchannels and pipes were found to transition to turbulence at a much lower Reynolds number than their counterparts at the macro scales. Due to the miniature size, there are uncertainties in measuring the various properties of MEMS, such as specimen dimensions, with sufficient accuracy. Nevertheless, it has become increasingly apparent that the physical mechanisms at work in these small-scale devices are different from what can be extrapolated from what is known from experience with macroscaled devices. There is a need to either reexamine or replace the phenomenological modeling tools developed from observations of macro scale devices.

This book covers the fundamentals of microfluid flows. The somewhat limited scope, compared with other titles, allows a detailed examination of the physics of the microfluids from an *ab initio* point of view. Since the first principle theory is far less developed for liquids, the focus in this writing is the microfluid flows of gas. The Boltzmann equation will be introduced first as the mathematical model for micro gas flows. Analytical solutions of the Boltzmann equation can be found for a limited number of cases. The Chapman-Enskog theory assumes that the velocity distribution function of gas is a small perturbation of that in thermodynamic equilibrium. The velocity distribution function is expressed as a series expansion about the Knudsen number. The Chapman-Enskog theory is therefore adequate for micro gas flows where the Knudsen number and the departure from local equilibrium are small. It will be shown that the zeroth-order solution of the Chapman-Enskog theory leads to the Euler equations and the first-order solution results in the Navier-Stokes equations. The linear constitutive relations between the stress and strain, and that between the heat transfer and temperature gradient, which are used in the derivation of the Navier-Stokes equations from the continuum point of view of gas flow, are thus valid only for very small Knudsen number. The second-order solution of the Chapman-Enskog theory produces nonlinear closure models for the stresses and heat fluxes. The resulting equations were referred to as the Burnett equations. Two forms of the Burnett equations will be discussed. For micro gas flows of higher Knudsen number, the Boltzmann equation should be used to model the micro gas flow behavior.

The analytical solutions of these various mathematical model equations for micro gas flows can be found for simple geometry and for limited flow conditions, some of which are discussed in the appropriate chapters. For many of the complex design of microfluidic devices, the flow solutions can only be found by numerically solving the model equations. To this end, two computer programs are provided in the appendix section of the book. The programs are written using the standard FORTRAN language and can be compiled in any platforms. The NB2D code solves the Navier-Stokes equations as well as two forms of the Burnett equation. The all-speed numerical algorithm has been used in the numerical discretization. The density-based numerical method has been shown to be able to handle low-speed as well as high-speed flows, and is appropriate for gas flows commonly seen in microdevices. The DSMC/IP1D code uses the direct simulation Monte Carlo (DSMC) method and the information preservation (IP) method to provide simulations of the gas microflow at the large Knudsen number. The IP method has been shown to be exceptionally efficient in reducing the statistical scatter inherent in the particle-based DSMC-like methods when the flow speed is low. The two computer programs will provide the readers with numerical tools to study the basic properties of micro gas flows in a wide range of flow speeds and in a wide range of Knudsen number. Examples of low- and high-speed micro gas flow simulations are also presented in later chapters. One of the unsolved problems in conventional macro scale fluid dynamics is associated with the flow transition to turbulence. In Chap. 11, the behavior of the flow disturbances in two simulated micro gas flows is described.

The book is geared toward developing an appreciation of the basic physical properties of micro gas flows. The computer software, coupled with the necessary analytical background, enable the reader to develop a detailed understanding of the fundamentals of microfluidic flows and to further validate their findings using computer microflow simulations. The knowledge can then be used in either further studies of the microflows or in the practical design and control of microfludic devices.

References

Gad-el-Hak, M., *The MEMS Handbook*, Boca Raton, FL, CRC Press, 2002.

Karniadakis, G.E. and Beskok, A., *Microflows: Fundamentals and Simulation*, Springer, New York, 2002.

Koch, M., Evens, A., and Brunnshweiler, A., *Microfluidic Technology and Applications*, Research Studies Press, Hertfordshire, England, 2000.

Li, D., Electrokinetics in Microfluidics, *Interface Sciences and Technology*, Vol. 2, Elsevier Academic Press, London, UK, 2004.

Mehregany, M., Nagarkar, P., Senturia, S., and Lang, J., Operation of microfavricated harmonic and ordinary side-drive motor, *IEEE Micro Electro Mechanical System Workshop*, Napa Valley, CA, 1990.

Nguyen, N.-T. and Wereley, S., *Fundamentals and Applications of Microfluidic*, Artech House, Norwood, MA, 2002.

Tai, Y., Fan, L., and Muller, R., IC-Processed micro-motors: Design, technology and testing, *IEEE Micro Electro Mechanical System Workshop*, Salt lake City, UT, 1989.

Chapter

2

Basic Kinetic Theory

2.1 Molecular Model

In kinetic theory, the composition of a gas is considered at the microscopic level. A gas is assumed to be made up of small individual molecules that are constantly in a state of motion. The name molecule can mean a single-atom molecule or a molecule with more than one atom. In each atom, a nucleus is surrounded by orbiting electrons. The internal structure of the molecule may change during an interaction with other molecules, such as collision. Collisions with other molecules occur continuously as the molecules move freely in their state of motion. Collision will also happen when a surface is present in its path. The intermolecular collision causes the magnitude and the direction of the velocity of the molecule to change, often in a discontinuous manner. If there is no collective, or macroscopic, movement, the motion of the molecule is completely random. This freedom of movement is not shared by liquid or solid molecules.

A molecular model for gas would then describe the nature of the molecule, such as the mass, the size, the velocity, and the internal state of each molecule. A measure for the number of molecules per unit volume, or number density n, would also be a parameter. The model also describes the force field acting between the molecules. The force field is normally assumed to be spherically symmetric. This is physically reasonable in light of the random nature of the large number of collisions in most cases. The force field is then a function of the distance between the molecules. Figure 2.1.1 shows a typical form of the force field $F(r)$ between two molecules with distance r. At a large distance, the weak attractive force approaches zero. The attractive force increases as the distance decreases. In close range, the force reverses to become repulsive

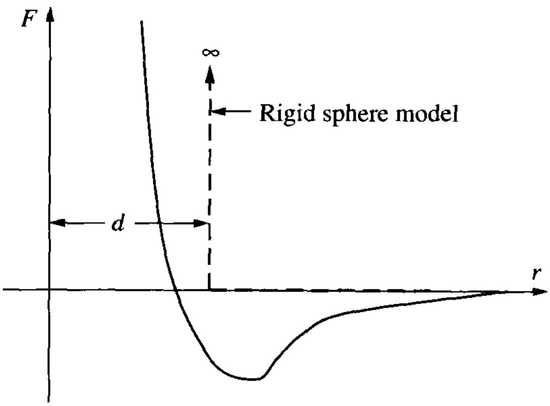


Figure 2.1.1 Sketch of spherically symmetric intermolecular force field.

as the orbiting electrons of the two molecules intermingle. Analyses with nonspherically symmetric force field are complicated. In fact, it is generally found that, the exact form of the force field is less important than other collision parameters. The force field of a simple rigid sphere model is shown in Fig. 2.1.1. The model assumes an infinitive repulsive force when the molecules are in contact and zero otherwise. The contact occurs when the distance between the centers of the molecules are the same as the assumed diameter of the sphere d. Use of the rigid sphere model can lead to accurate results if the diameter d is properly chosen according to some basic properties of the gas. The internal structure of the molecules affects the energy content of the gas. With the nuclei and the electrons in motion, the molecule can have, for instance, rotational and vibrational modes of energy in addition to the energy associated with the molecular translational motion.

These molecular quantities need to be related to macroscopic properties for analyses. This is especially true when there is a general macroscopic movement of the gas. As will be seen in the following section, a macroscopic property is merely the sample averaged value of the corresponding molecular quantity. The motion of the molecules is then not completely random when there is macroscopic motion.

2.2 Micro and Macroscopic Properties

In this section, we will use a simplified model to introduce the relations between the molecular behavior and the macroscopic properties of gases. We consider an equilibrium monatomic gas of single species