ESSENTIALS OF MICRO- AND NANOFLUIDICS

This book introduces students to the basic physical principles needed to analyze fluid flow in micro- and nanosize devices. This is the first book to unify the thermal sciences with electrostatics, electrokinetics, and colloid science; electrochemistry; and molecular biology. The author discusses key concepts and principles, such as the essentials of viscous flows, electrochemistry, heat and mass transfer phenomena, elements of molecular and cell biology, and much more. This textbook presents state-of-the-art analytical and computational approaches to problems in all these areas, especially in electrokinetic flows, and gives examples of the use of these disciplines to design devices used for rapid molecular analysis, biochemical sensing, drug delivery, DNA analysis, the design of an artificial kidney, and other transport phenomena. This textbook includes exercise problems, modern examples of the applications of these sciences, and a solutions manual available to qualified instructors.

A. Terrence Conlisk is Professor of mechanical and aerospace engineering at The Ohio State University. He is an internationally recognized expert in the areas of micro- and nanofluidics, helicopter aerodynamics, and complex flows driven by vortices. He is the author of numerous publications and hundreds of technical presentations and seminars delivered throughout the world. After his PhD thesis (Purdue, 1978) on the prediction of the fluid dynamics and separation of isotopes in a gas centrifuge, he began his work on various aspects of the dynamics of two- and three-dimensional vortices, with a focus on helicopter aerodynamics. Since 1999, he has been involved in modeling ionic and biomolecular transport through micro- and nanochannels for the design of devices used for rapid molecular analysis, sensing, drug delivery, and other applications. Professor Conlisk's wide spectrum of research interests makes him uniquely qualified to write on the thoroughly interdisciplinary fields of micro- and nanofluidics.

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With Applications to the Biological and Chemical Sciences

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To my mother and father, Ginny and Terry, who first taught me the value of education.

To my brother and sisters, Virginia, Bill, Mary, and Elizabeth for friendship, love and support, and the many good times that so few families experience.

And to my wife, Paulette, and children, Terry and Katie, for their love and understanding; and for putting up with me over these many years. Without you this book would not have been possible.

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Preface

The book is meant to be used as a text for an interdisciplinary course in micro- and nanofluidics that includes the study of ionic and biomolecular transport at the advanced undergraduate and beginning graduate levels. The rationale for this book is that most, if not all, problems in the twenty-first century are interdisciplinary in nature, yet no textbooks address the topics required for investigating problems that cut across disciplines in engineering, the physical sciences, and mathematics. The closest approach to this concept is in the several texts that address the thermal sciences at a strictly undergraduate level (Moran *et al.*, 2003). Another set of texts addresses problems in applied mathematics applicable to engineering problems generally at the advanced graduate level (Bird *et al.*, 2002). Still another set of texts under the general area of biophysics links the mathematics and biological sciences, again most often at the advanced graduate level (Murray, 2001, 2003). In contrast, this book aims at the advanced undergraduate and beginning graduate student pool.

A number of other related books are on the market, but all are monographs directed at the senior graduate student (Karniadakis *et al.*, 2005; Masliyah and Bhattacharjee, 2006; Tabeling, 2005; Liou & Fang, 2006; Nguyen & Wereley, 2002; Bruus, 2008; Kirby, 2010; Chang and Yeo, 2010). All these texts emphasize the unique features of transport at the micro- and nanoscale, of which there are many. In contrast, while the reader will be exposed to many of these unique features, it is my contention that transport at the micro- and nanoscale actually unifies all the thermal sciences, fluid dynamics, heat and mass transfer, and thermodynamics; it also, sometimes by necessity, unifies the thermal sciences with electrostatics, electrokinetics, and colloid science; electrochemistry; and molecular biology. This book is the first to show how all these fields are interrelated at the micro- and nanoscale and show how it is essential for a researcher, student, or faculty to acquire an understanding at some level of all these fields. The fundamental concepts within these fields are supported by addressing the continuum and molecular computation techniques that may be employed to solve these problems.

The objective of this book is to introduce students in the physical and mathematical sciences and engineering to the basic physical principles appropriate to analyzing fluid flow in micro- and nanoscale devices. The book will emphasize the fundamental principles involved in the formulation and solution of problems in fluid mechanics and mass transfer for pressure-driven and electrically driven motion of biofluids and electrolyte solutions at the micro- and nanoscale. It will introduce the student to a variety of subject matter spanning the physical sciences, thermal engineering, and applied numerical methods to enable the student to solve problems of an interdisciplinary nature. On completion of the book, the student should be able to extract from a raw physical situation the essential principles from which a useful model for thermal, ionic, and biomolecular transport may be developed.

The primary target audience of this text is the advanced undergraduate and beginning graduate engineering student; however, it is hoped that the book will be accessible to some advanced undergraduate students in physics and the chemical and biological sciences with the appropriate mathematics background.

In writing this book, I have been greatly influenced by the style and format of White (2006), which is aimed at a similar audience and contains exercises at the end of each chapter. White uses canonical problems in the field to illustrate basic fluid dynamic phenomena, and I have followed this style, expanding into heat and mass transfer, electrostatics, electrochemistry, electrokinetics, and molecular biology.

As with any book project, many people have contributed. I am thankful for Dr. David Mott, who read, with a keen eye, an advanced draft of the book, and to Professor Shaurya Prakash, who read a nearly final version of the manuscript. I am very thankful to Professor Susan Olesik, who read an early draft of the electrochemistry chapter, and to Dr. Arfaan Rampersaud, who reviewed the chapter on molecular biology. I am also thankful to Professor Minami Yoda, with whom I have worked over the past seven or so years. We have cut our teeth on micro- and nanofluidics together over that time. I am grateful to my colleagues Professor Shuvo Roy, Dr. Bill Fissell, and Professor Andrew Zydney, who introduced me to the fluid dynamics of the kidney. Professor Sherwin Singer read the molecular simulation chapter and made many suggestions and corrections that have been incorporated. Dr. Harvey Zambrano also helped me greatly with that chapter. I am also grateful to Professors Narayan Aluru and Ron Larson and Dr. Dirk Gillespie for their contributions.

And thanks to those researchers who have contributed the boxed vignettes that are about their work or some aspect of micro- and nanofluidics for which I did not have room. They are acknowledged at the end of the presentation.

I am particularly grateful for all the discussions I have had with faculty at the nanoscale science and engineering center, called the Center for the Affordable Nanoengineering of Polymeric Biomedical Devices (CANPBD).

Thanks go to my present and former students, Prashanth Ramesh, Ankan Kumar, Pradeep Gnanaprakasam, and Devi Pulla, some of whose work appears in the book; to Mike Stubblebine, who helped catalog the figures; and to Professor Subhra Datta and Dr. Lei Chen, who both have done much in the way of research that appears in this book. Subhra wrote first drafts of several sections, and Lei produced many of the figures that appear in the book. Both have

read the manuscript, portions more than once. Thanks also to Dan Hoying, an undergraduate physics student who read a nearly final version of the book, and Zhizi Peng and Cong Zhang, who produced several figures; Cong was a significant contributor to the solutions manual; and to Harvey Zambrano who helped me write a section in the molecular dynamics chapter; and to Kevin Disotell who read the final proofs; and to Jim Marcicki who taught me about batteries.

I am grateful to my "Introduction to Micro- and Nanofluidics" class in the Autumn quarter of 2010, who used the book and had many suggestions that were heartily received and implemented. Thanks also go to graduate student Martin Kearney-Fisher, who read the entire manuscript and gave me pages of corrections and suggestions, almost all of which I have incorporated. Martin's suggestions have made the manuscript much better.

Thanks also to my editor, Peter Gordon, who kept me on task and made a number of suggestions on how to write the book, especially the early chapters. He also provided me with additional resources that allowed a more thorough treatment of this rapidly expanding field. And thanks go to Peggy Rote for her diligence in managing the production process.

If I have forgotten to thank someone, I apologize.

The book begins with an introduction and overview of micro- and nanofluidics in Chapter 1, followed by Chapter 2, "Preparatory Concepts." Chapter 2 is meant to unify concepts on two levels: discussing the fundamental roles of transport coefficients in fluid mechanics and heat and mass transfer and the relationship between thermodynamics, the equilibrium science, and heat transfer and fluid mechanics, the nonequilibrium thermal sciences. These two initial chapters are followed by a discussion of the governing equations and boundary conditions associated with micro- and nanofluidics. At the micro and nano levels, several new phenomena come into play:[1]

1. Because of the large surface-to-volume ratio, the characteristics of surfaces play a major role in fluid and mass transport.
2. Classical means of transporting fluids, such as pressure drop, may not be possible.
3. Noncontinuum effects arise when the length scale associated with the fluid transport becomes less than 10 nm.

All these issues are discussed throughout the book, and the second point is the reason that electrokinetic transport methods become important.

The next three chapters cover the fundamentals of viscous flow, heat and mass transport, and electrostatics. While writing this book, I was astonished at how similar these fields are in the way of expressing basic transport phenomena. Many analogies between these three (or four, if mass transfer is considered separately) disciplines are discussed throughout.

[1] We are speaking here primarily of liquid flows. Gas flows are treated extensively by Liou and Fang (2006) and Karniadakis *et al.* (2005).

Following these three chapters are two chapters covering the fundamentals of electrochemistry and molecular and cell biology. These two chapters are meant to reintroduce engineering students to material they may have had in their first-year course work, although parts of each chapter are written at a higher level.

Following these two chapters, electrokinetic phenomena are discussed in Chapter 9. The two most important of these phenomena, electro-osmosis and electrophoresis, are discussed in great detail, and canonical problems of electro-osmosis are described in the spirit of the style of White (2006).

The next chapter covers the basics of numerical methods, from zero finding to the numerical solution of partial differential equations. The primary role of this chapter is to introduce the student to basic numerical methods that can be used to solve problems in micro- and nanofluidics. For some engineering students, this chapter is likely to be a review; however, physics and chemistry students may find this chapter valuable.

Next, the fundamental concepts involved in performing molecular simulations, specifically equilibrium molecular dynamics and nonequilibrium molecular dynamics, are presented along with examples of Poiseuille flow and electro-osmotic flow. It is surprising how different the philosophy and expectations of what is achievable in a simulation on the molecular level are from the continuum perspective. The reader need only compare the presentation of the numerical methods in this chapter with those presented in the previous chapter to see this. Note the differences in how the continuum and molecular results are verified and validated.

The book ends with a chapter devoted exclusively to applications. Applications are too numerous to mention, but I have chosen those applications with which I am familiar. Thus a simple model for DNA transport is presented, along with a section on biochemical sensing and the fluid mechanics and mass transfer involved in the design of a renal assist device.

Each chapter is followed by a set of exercises that range from simple calculations, such as determining the Debye length for a given set of parameters, to finding the solution of viscous flow through an annulus to the calculation of the numerical solution of the Poisson equation to completely open-ended exercises that require a written report. The exercises after Chapter 12 are all open ended. In these open-ended exercises, other applications not included in the book are introduced such as the use of nanoparticles to treat cancer. These exercises have been designed to make maximum use of the Web and emphasize the development of the technical writing skill of the student. A short introduction to technical writing is available from the author, on request.

Several appendices, giving a short introduction to the method of matched asymptotic expansions, the governing equations in cylindrical and spherical coordinates, a list of interesting and useful Web sites, and a prospective syllabus, are also included. Writing this book has been a tremendous learning experience, and I have bought several chemistry and biology dictionaries. I have also acquired more biology and chemistry textbooks in six years than I have in my entire life

(I have Cambridge University Press to thank for some of these). While all this about learning from books is true, I cannot tell you how many times I have been to Wikipedia or used the other Web sites that appear in Appendix B.

Much of the material in the book is gleaned from research papers, from those that are very old and classical to those published very recently. I have tried to be judicious in my choice of references, and to those whom I have overlooked, I apologize. I would be happy to be informed of the omission of a major paper that would contribute to a future manuscript. This has been quite a task, and I and my students, and several faculty, have read parts of the book, as noted earlier. Nevertheless, errors are inevitable, and I would be grateful if I could be informed of any errors that do appear in the book. For these errors, I take full responsibility.

The emphasis in this book has been the interdisciplinary nature of micro- and nanofluidics. This book is me speaking about what I think is important to know in micro- and nanofluidics. Thus I take responsibility for those many topics that are left out. For this, I do not apologize but merely say that tough choices were made. I hope that this book will be read by students with diverse backgrounds and that they will benefit from what I hope is a lucid presentation.