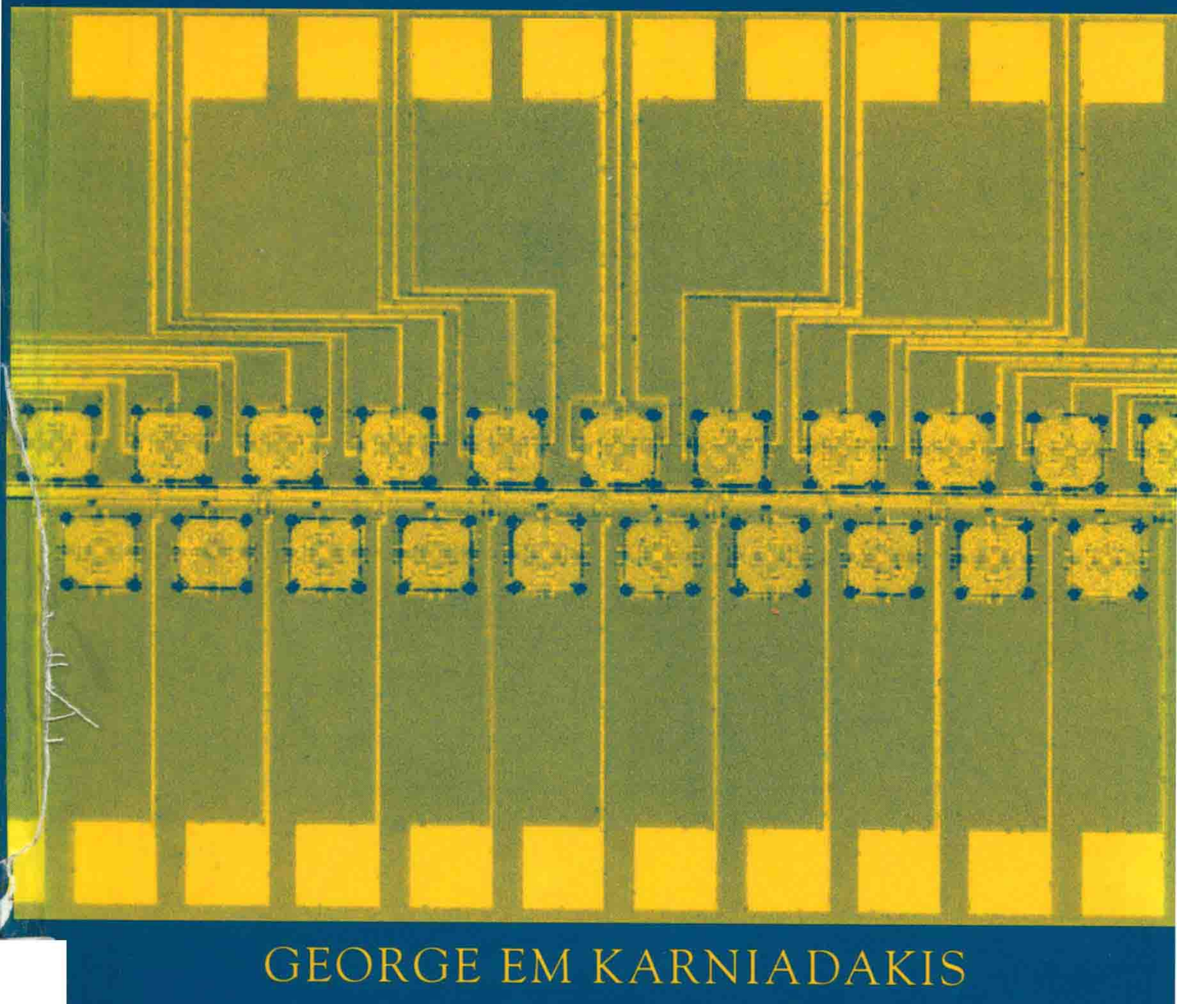
MICRO FLOWS

Fundamentals and Simulation



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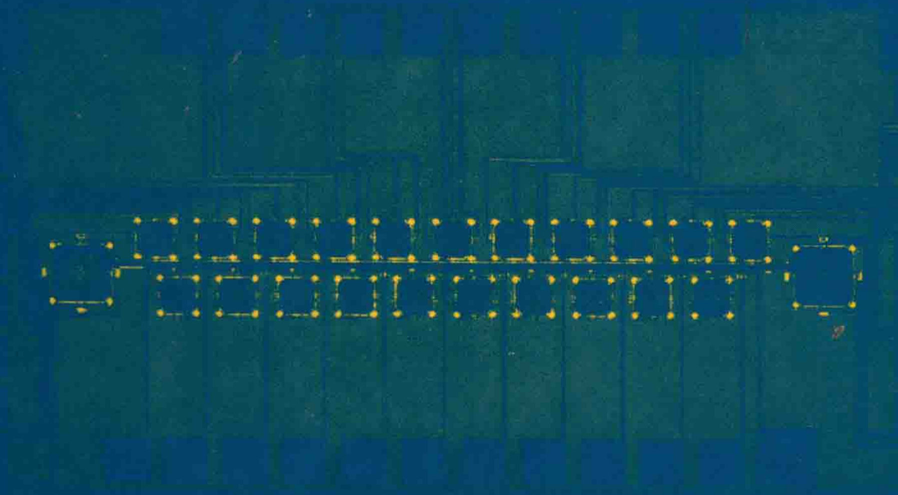

This book addresses flow and heat transfer in micro scales and MEMS devices. It includes gas and liquid flows as well as particulate micro flows, and presents a comprehensive study of fundamental concepts and simulation methods as well as prototype applications such as micro accelerometers, electrostatic comb drives, micro nozzles, and micro fluidic control via electric fields.

New material is included here along with a compilation of published material in this rapidly developing field. The book develops working engineering models, that is, macro models that can be easily employed in applications, while providing a rigorous mathematical and numerical framework for deeper understanding and effective treatment of phenomena encountered in micro scales.

This book is appropriate for graduate students and researchers in fluid mechanics and in electrical, mechanical, and chemical engineering or for physicists who work on other aspects of MEMS and need to incorporate flow modeling in their work.

COVER ART: Prototype micro channel with integrated pressure sensors (*courtesy of C.M. Ho and Y.C. Tai*).

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Micro Flows

Fundamentals and Simulation

With 193 Illustrations

Springer

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Preface

Our work in micro scale fluid mechanics started in 1989, after being prompted by interesting discussions with Dan Cho and William Trimmer, who were among the first to address the multidisciplinary research aspects in micro electro mechanical systems (MEMS). Although neither of the two had worked in fluid mechanics before, they foresaw the need to understand fluid flow in micro scales in early applications of MEMS, such as the squeezed film damping effects in the wobble motor. Such a recognition is also evident in the 1988 influential report on "Small Machines, Large Opportunities" by the National Science Foundation (Gabriel et al., 1988).

In the early 1990s, micro channel flow experiments at the University of Pennsylvania by the groups of H. Bau and J. Zemel revealed intriguing results for both liquids and gases that sparked excitement and new interest in the study of low Reynolds number flows in micro scales. Another influential development at about the same time was the fabrication of the first micro channel with integrated pressure sensors by the groups of C.M. Ho and Y.C. Tai. While the experimental results obtained at the University of Pennsylvania indicated global deviations of micro flows from canonical flows, pointwise measurements for gas flows with pressure sensors, and later with temperature sensors, revealed a new flow behavior at micro scales not captured by the familiar continuum theory. In micro geometries the flow is *granular* for liquids and *rarefied* for gases, and the walls "move." In addition, other phenomena such as thermal creep, electrokinetics, viscous heating, anomalous diffusion, and even quantum and chemical effects may become important. Most importantly, the material of the wall and the quality of its surface play a very important role in the momentum and energy exchange.

One could argue that at least for gases the situation is similar to low-pressure high-altitude aeronautical flows, which were studied extensively more than 30 years ago. Indeed, there is a similarity in a certain regime of the Knudsen number. However, most gas micro flows correspond to a low Reynolds number and low Mach number in contrast to their aeronautical counterparts. Moreover, the typical micro geometries are of very large aspect ratio and this poses more challenges for numerical modeling, but also creates opportunities for obtaining semi-analytical results.

The main differences between fluid mechanics at micro scales and in the macro domain can be broadly classified into four areas:

- Non-continuum effects,
- surface-dominated effects,
- low Reynolds number effects, and-
- multi-scale and multi physics effects.

Some of these effects can be simulated with relatively simple modifications of the standard simulation procedures of computational fluid dynamics. However, others require new simulation approaches not used in the macro domain. For gas micro flows, compressibility effects are very important because of relatively large density gradients, although the Mach number is typically low. Depending on the degree of rarefaction, corrections at the boundary or everywhere in the domain need to be incorporated. Increased rarefaction effects may make the constitutive models for the stress tensor and the heat flux vector in the Navier-Stokes equations invalid. On the other hand, working with the Boltzmann equation or with molecular dynamics implementation of Newton's law directly is computationally prohibitive for complex micro geometries. The same is true for liquids as atomistic simulation based on Newton's law for individual atoms is restricted to extremely small volumes. Therefore, hybrid atomistic-continuum methods need to be employed for both gas and liquid micro flows to deal effectively with deviations from the continuum and to provide a link with the large domain sizes. Most importantly, micro flows occur in MEMS devices which involve simultaneous action in the flow, electrical, mechanical, thermal, and other domains. This, in turn, implies that fast and flexible algorithms and low-dimensional modeling are required to make full-system simulation feasible, similar to the achievements in VLSI simulation.

The present book addresses gas and liquid micro flows as well as particulate flows. There is some emphasis on the gas flows for which most of the deviations from macro scales occur, but we also treat liquid-specific phenomena (e.g., electrokinetic effects and dielectrophoresis) and simulation methods (e.g., molecular dynamics). Particulate micro flows, that is, flows carrying macro molecules such as proteins or DNA molecules, are becoming increasingly more important in biofluidic applications. They involve moving domains and multiple length scales, and thus special methods are required to deal efficiently with their computational complexity. The original draft of this book was based in a large part on the Ph.D. thesis of Beskok on gas micro flows, which was supervised by Karniadakis. The current final version includes new work of our own as well as work by other researchers for general MEMS flows. The selection of material for a first monograph in a new and fast developing field is very difficult, so we have relied heavily on our own work and the very useful suggestions by our colleagues and anonymous reviewers.

The book addresses theoretical issues and develops semi-analytical models as well as numerical methods for simulating micro flows. It is appropriate for researchers in fluid mechanics who want to study this new flow field. It can be used as a textbook for a graduate level course in micro fluid mechanics or as a second textbook in a more general MEMS course, along with other references, e.g., (Cercignani, 2000; Allen and Tildesley, 1994; Gad-El-Hak, 2001; Madou, 1997). It is also suitable as a reference for electrical or mechanical engineers or physicists who work on other aspects of MEMS and need to incorporate flow modeling in their work. Our objective has been to develop working engineering models, i.e., macro models, that can be easily employed in applications rather than covering exhaustively all theoretical issues encountered in micro flows. To this end, we have included available experimental results that have been used to validate our models and that may be useful to other researchers in the MEMS field, e.g., the high-resolution mass flowrate measurements by Arkilic and Breuer. For the same purpose, we have also included theoretical results, e.g., tabulated accurate solutions of the Boltzmann equation by Cercignani, Loyalka, Sone and Aoki, and others, which can be used for interpreting experimental results and for developing numerical and semi-analytical models. It is this mix of material that we have attempted to include in the monograph that we believe may be most useful to a broader group of researchers in this interdisciplinary field.

We would like to thank our many colleagues who have generously provided their results to be included in this monograph, in some cases even unpublished results. In particular, we acknowledge Texas Instruments and also the following colleagues N. Aluru, K. Aoki, J. Banavar, H. Bau, R. Bayt, I.D. Boyd, K. Breuer, S. Chen, E. Cummings, G. Dent, G. Doolen, D. Freeman, R. Gale, P. Gascoyne, Y. Gogotsi, N.G. Hadjiconstantinou, C.M. Ho, M. Ivanov, A. Ketsdever, J. Koplik, P. Koumoutsakos, C. Liu, S. Lomholt, C. Megaridis, C. Meinhart, X. Nie, E. Oran, S. Quake, Y.C. Tai, S. Tison, S. Troian, T. Veijola, X. Wang, J. White and W. Ye. We also acknowledge very helpful discussions with G. Bird, D. Cho, N. Gatsonis, M. Gad-el-Hak, H. Lam, M. Maxey, K. Mayaram, and W. Trimmer. We are grateful to K. Sreenivasan, who originally suggested this project on behalf of Springer and provided a thorough review of an earlier version; also to Li-Shi Lou, J. M. Khodadadi, and M. Maxey, who read and corrected our manuscript. We would like to thank our students and collaborators P. Dutta, M. Kirby, D. Liu, Ma Xia, T. Warburton, and also Madeline Brewster for their help with figures and formatting of the book. We also acknowledge the sponsorship of NSF, NIST, and DARPA during various stages of our work on micro fluidics in the last ten years.

Finally, we would like to acknowledge the support of our families. The first author (G.K.) would like to thank his wife, Helen, and his son, Paris, for their love and support, and especially his mother-in-law, Koulla A. Christou, for her tremendous help in every day's real life obligations. The second author (A.B.) would like to thank Carolyn, Sarah Aylin, Sinan Martin, and Gungor Beskok for their continuous love, support, and patience.

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Nomenclature

Constants and Parameters

C_f	Fanning skin friction coefficient
C_D	Drag coefficient, mass discharge coefficient
k	Spring constant
k_B	Boltzmann constant
I_{sp}	Specific impulse
n	Number density
Q	Quality factor
R	Ideal gas constant
α	Volume fraction
γ	Adiabatic index
ϵ	Energy scale in Lennard-Jones potential
σ_v	Momentum accommodation coefficient
σ_T	Thermal accommodation coefficient

Non-Dimensional Numbers

Ec	Eckert number
Kn	Knudsen number
M	Mach number
Nu	Nusselt number
Po	Poiseuille number

Pr	Prandtl number
Re	Reynolds number
S	Squeeze number
Λ	Bearing number

Length Scales

A_c	Collisional cross-sectional area
h, H	Channel height
L	Channel length, characteristic dimension
D_H	Hydraulic diameter
d	Molecular diameter
δ	Mean molecular spacing
λ	Mean free path
λ_D	Debye length
σ	Length parameter in Lennard-Jones potential

Numerical Parameters

Ω	Solution domain
$\partial\Omega$	Boundary of Ω
$\boldsymbol{n}$	Unit outward normal
Δt	Time step
Δx	Spacing

Electric Parameters

F_e	Electric force
V	Voltage
α	Ionic energy parameter
ϵ	Permittivity
σ	Electric conductivity
ψ	Electroosmotic potential
ζ	Zeta potential

Differential Operators

∇^2	Laplacian
$\nabla\cdot$	Divergence
$\nabla\times$	Curl

Fluid and Thermal Variables

$\bar{c}$	Mean-square molecular speed
c_s	Sound speed
C_p, C_v	Specific heats
E	Total energy
E_{ij}	Strain tensor
f_0	Maxwellian distribution function
k	Thermal conductivity
$\dot{Q}$	Volumetric flowrate
$\dot{M}$	Mass flowrate
p, P	Pressure
$\mathbf{q}$	Heat flux vector
$\mathbf{v}, u_i, U$	Velocity $[u, v, w]^T$
$\bar{v}$	Average thermal speed
v_m	Maximum (most-probable) thermal speed
V_p	Particle volume
ΔP	Pressure difference
ΔT	Temperature difference
μ, ν	Dynamic, kinematic viscosities
μ_{ef}	Effective dynamic viscosity
Π	Pressure ratio
ρ	Density
σ_{ij}	Stress tensor
τ_w	Wall shear stress, non-dimensional wall temperature
ω	Vorticity

Contents