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Analytical Heat and Fluid Flow in Microchannels and Microsystems



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Nondum Deducta Deducendi, Nondum Probata Probandi

To our families

Preface

In 2013 I had the unique opportunity of being an invited keynote speaker at the ASME Summer Heat Transfer Conference, held from July 14–19 in Minneapolis, Minnesota, which marked the 75th Anniversary of the founding of the Heat Transfer Division of ASME. Prof. S.A. Sherif from the University of Florida at Gainesville, who was the General Conference Chair and a long time friend, kindly introduced me to Prof. Francis A. Kulacki from the University of Minnesota, Chair of the 75th Anniversary Steering Committee, whom I knew from his many publications and achievements, but never had the chance to meet until then. Prof. Kulacki gave me the honor of attending the lecture, demonstrating his vivid interest and motivation on analytical heat and mass transfer, and afterwards brought to me the very kind invitation for contributing with a publication on integral transforms in heat and mass transfer, based on that lecture, to the Springer Brief Series under his coordination.

The lecture title was "75 Years of Integral Transforms in Heat and Mass Transfer: From an Analytical to a Hybrid Numerical-Analytical-Experimental Approach", aimed at reviewing the last 75 years on integral transforms in heat and mass transfer, with special emphasis on showing its extension to various classes of a priori non-transformable problems, as the flexible hybrid numerical-analytical version of the integral transform method, well known as the Generalized Integral Transform Technique (GITT) (Cotta 1990, 1993, 1994a, b). However, at the same conference, a second paper from our group was presented (Knupp et al. 2013), with the title "Conjugated Heat Transfer in Heat Spreaders with Micro-Channels" that also dealt with the application of the Generalized Integral Transform Technique (GITT), combined with a single domain reformulation strategy, to analyze conjugated heat transfer within a complex configuration formed of multiple microchannels within a polymeric substrate. The interest raised by this second work was beyond our expectations, attracting both audiences on computational methods and on micro-scale heat transfer. Therefore, the concept of the present book, with focus on integral transforms application in heat and fluid flow analysis of microchannels and microsystems, was then proposed to Prof. Kulacki. The proposal was written down by the end of October 2013, and the first versions of the Chapters were viii Preface

assembled by May 2014, before they were tested in a graduate level course as supplementary material, during the second semester of 2014. At that time I had already invited Prof. Carolina Naveira-Cotta, my wife and collaborator, and Prof. Diego C. Knupp, the first graduated DSc jointly advised by myself and Carolina, also a close collaborator, to contribute on this project as my co-authors. I could not be more fortunate in these invitations, since both became very enthusiastic about the project and were very helpful in all the stages of the book preparation. Prof. Naveira-Cotta heads the Nano and Microfluidics and Microsystems Lab at COPPE, Federal University of Rio de Janeiro, and Prof. Knupp works in the Heat and Mass Transfer Lab at the State University of Rio de Janeiro, UERJ, Nova Friburgo, both in Brazil. In lack of a more logical criterion, we have decided to list our names in the cover page following the alphabetical order of our citation names.

The interest on micro-scale heat transfer within our group at COPPE/UFRJ started back in 1997 (Mikhailov and Cotta 1997), after Prof. Mikhail D. Mikhailov from Sofia, Bulgaria, moved to work with us in Rio de Janeiro, at that specific occasion mainly motivated by contributing to the work of (Barron et al. 1996), improving their analytical solution through a more robust computation of the associated eigenvalues employing the *Mathematica* system. The interest raised by this initial effort was markedly increased along the years by the close interactions with Prof. Sadik Kakac. University of Miami, USA, and later on TOBB University, Ankara, Turkey, Prof. Dimos Poulikakos, ETH, Zurich, Prof. Patrick Tabeling, ESPCI, Paris, Profs. Jacques Padet, Mohammed Lachi and Mourad Rebay, Université de Reims, Prof. Yildiz Bayazitoglu, Rice University, Houston, Prof. Olivier Fudym, École des Mines, Albi, Prof. Manish Tiwari, ETH/Zurich, presently at UCL, London, UK, Profs. Jean Christophe Batsale and Christophe Pradère, from ENSAM/Bordeaux, France, Prof. Luiz Otávio Saraiva Ferreira, UNICAMP, Brazil, and Prof. John Rose, Queen's Mary College, London. The first two MSc thesis were then concluded in 2003/2004 (Castilho 2003; Castellões 2004), the first one advised by Profs. Rodrigo Guedes and Francesco Scofano, at the Military Institute of Engineering, in Rio de Janeiro, and the first sponsored research project was initiated in 2004 (CNPq, Brazil). The participation as invited lecturer in the NATO Advanced Studies Institutes in 2004 (Cotta et al. 2004a, b) and 2009 (Cotta et al. 2009a, b), organized and coordinated by Prof. Sadik Kakaç, was crucial for the exchange of ideas with worldwide leaders in this area and for the maturity of this line of research within our group. Then, parallel to the advancement of the theoretical research on heat and fluid flow in microsystems, aimed at progressively exploring more complex modeling at the micro-scale, an experimental infrastructure was established, based on non-intrusive measurement techthermography with as infrared microscopic micro-PIV/micro-LIF, so as to allow for a complete and critical effort on the comparison of theoretical and experimental results for different microsystems and physical situations. In addition, along the last few years, the theoretical approach has been further developed and employed in close collaboration with our co-worker and closest collaborator, Prof. Helcio R.B. Orlande, of COPPE/UFRJ, Brazil, towards the solution of computationally intensive inverse problem analysis, in combination with Bayesian Inference and non-intrusive experimental techniques, when the analytic Preface

nature of the method brings up the possibility of working on the integral transformed experimental domain, with marked reduction on computation effort through data collapsing (Naveira-Cotta et al. 2011; Knupp et al. 2012). Such initiatives have then induced the creation, in 2011, of the Nano and Microfluidics and Microsystems Lab (LabMEMS), at COPPE/UFRJ, which now concentrates the essential infrastructure for design, fabrication, characterization, and testing of microsystems in different platforms and for various applications. This laboratory is part of the infrastructure complex offered by the establishment of the Interdisciplinary Nucleus of Fluid Dynamics (NIDF) also recently created at COPPE/UFRJ.

This book is then built on top of this background, being an attempt of consolidating part of this line of research into a single volume of the Mechanical Engineering Series. The first chapter brings an introduction and motivation to the analysis of heat and fluid flow in microchannels and microsystems, and the important aspects to be considered when modeling at this microscale. It also presents a brief review and a melt pot of new ideas on the GITT approach, discussing different aspects of interest to the micro-scale heat and fluid flow analysis, reviewed in recent invited lectures (Cotta et al. 2012, 2013, 2014a, b), besides the unpublished one presented at the ASME Minnesota heat transfer conference in 2013. The second chapter is devoted to the integral transform analysis of heat and fluid flow in single microchannels. It is arranged in a sequence of increasing complexity, dealing with transient and periodic states, slip flow, viscous dissipation, axial diffusion effects, electrosmotic flow, inverse problem analysis, rough and corrugated walls, conjugated problems, and channels with irregular cross sections. The third chapter has a focus on actually built microsystems, with multichannel configurations that have also been experimentally analyzed. The analysis deals with comparing the obtained GITT solutions with those from the experimental runs, and also against numerical results from commercial CFD codes. In light of the markedly different length and time scales present in actual microsystems simulations, it is expected that the computational effort on the implementation of purely discrete approaches can be particularly critical. Therefore, the hybrid numerical—analytical nature of the present methodology provides an interesting alternative to the fully numerical approaches.

This Preface would not be complete without giving credit to the students and ex-students, now our colleagues, whose articles and theses are part of a coherent and collaborative development of this research line. A special word is dedicated to Ms. Patricia Oliva Soares, whose MSc dissertation is summarized in section 2.3, and who left us very early and very young, before having the chance to fulfil her dreams. I wish to particularly express my gratitude to Prof. Luiz Bevilacqua, Prof. Átila Silva Freire, and Prof. Fernando Duda, who have closely supported the creation and establishment of this research area and its laboratory at COPPE/UFRJ. Finally, we are thankful and dedicate this effort to our families, for once more accepting our partial absence in critical moments for completion of this mission.

Rio de Janeiro February 2015 Renato M. Cotta Professor, POLI & COPPE/UFRJ, Executive Committee Brazilian Academy of Sciences—ABC

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Chapter 1 Fundamentals and Methodologies

1.1 Introduction

A systematic research effort in micromechanics in the context of MEMS (Microelectromechanical Systems) devices, mainly on fabrication and operation, began in the late 1980s. However, the beginning of micro- and nanotechnologies is commonly and arguably attributed to the year of 1959, when the renowned theoretical physicist Richard Phillips Feynman gave the prophetic lecture entitled "There is plenty of room at the bottom," during the American Physical Society meeting at Caltech (Feynman 1960). Although the conceptual idea of Feynman was to go further by creating technology at the microscale, even anticipating some of today's standard MEMS technologies, some fundamental work in Microfluidics started much earlier. According to Karniadakis et al. (2005), in 1846 Poiseuille published the first paper describing flow in tubes with diameters from 30 to 150 μm, in 1909 Knudsen studied gas flows through glass capillaries in the transition and free molecular flow regimen, and in 1913 Gaede performed the first known experiment of flow in a microchannel, placing two parallel plates 4 μm apart.

Since then, many efforts and advancements have been made in miniaturization processes, allowing for the development of diversified miniaturized systems, employing, in many applications, liquid or gas streams. According to (Joyce 1983), the technology of using fluid controlled devices, known as Fluidics, dates back to 1959 or earlier, however, the intense application of this idea at the microscale is more associated with the 1990s and led to the creation of the scientific research area now known as Microfluidics (Tabeling 2005). In this context, microsystems featuring fluid flows started to be conceived, especially for chemical, biological, and biomedical applications, including chromatography, electrophoretic separation systems, the development of electroosmotic pumping systems, micromixers, microreactors, and DNA analysis, among others. Within such applications, the direct advantages of miniaturizing the laboratory setups include the remarkable reduction in the amount of the required sample, in addition to allowing for more

efficient, faster and safer analysis, besides the development of compact and portable systems, some of them leading to the so-called lab-on-a-chip and point-of-care diagnostic devices.

One potential consequence of paramount importance in microfluidics is the possibility of integration of various microsystems, leading to compact systems that should be able to perform all processes required in those analyses, such as detection, mixing, and characterization. The idea of integrating microreactors also leads to the possibility of development of microsystems for performing industrial processes, where the immediate question that arises is about the production volume that could be possibly tackled with a massive parallelism of the production system. A typical example is the biodiesel synthesis process, while following the research effort in designing, fabricating, testing, and optimizing the individual microreactors for the transesterification reaction of the specific set of vegetable oil, alcohol, and catalyst (Al-Dhubabian 2005; Han et al. 2011; Martinez et al. 2012; Pontes et al. 2015). The final goal is to have a portable and compact system that produces biodiesel in commercially viable volumetric rates with significant gains in energy consumption and production time in comparison to the traditional industrial batch processes (Salic and Zelic 2011; Billo et al. 2014).

In parallel to the advancements of microfluidics in chemical, biological, and biomedical applications, there has been ever growing developments in microelectronics, allowing for the conception of smaller integrated circuits with improved computational power, but with the penalty of markedly increased heat dissipation demands. The restriction associated with the electronics cooling needs, once conventional strategies are no longer effective in dissipating the heat generated in such devices, may lead to increased operation temperatures, affecting reliability and performance. Hence, new cooling strategies such as the employment of micro-heat sinks, since the pioneering work of (Tuckerman and Pease 1981), have remained very appealing (Kandlikar and Grande 2003; Yarin et al. 2009; Sharma et al. 2012; Renfer et al. 2013; Ohadi et al. 2013). With respect to high cooling/heating needs and the appeal for employing microthermal systems, it should also be mentioned the development of high concentration photovoltaic (HCPV) systems for electricity production, which permits reducing the investment cost and have the potential to make solar energy competitive with other electricity generation technologies. One issue of concern, however, is the fact that the PV cell efficiency is drastically reduced with the temperature increase, and therefore this technology has also the potential to benefit from cooling systems with microchannel passages (Royne et al. 2005). In fact, the use of micro-heat exchangers for both heat removal from HCPV systems and waste heat reuse in combined processes, such as water desalination, is a topic of major interest in the recent literature (Kasten et al. 2010; Guerrieri and Naveira-Cotta 2014).

With so many potential applications, and the need for understanding the physical phenomena and developing new models, correlations and solution methodologies, it has been observed an ever increasing interest of the scientific community in the field of microscale heat and fluid flow, which is characterized by the increasing number of high level reference books and textbooks, such as (Karniadakis et al.

1.1 Introduction 3

2005; Tabeling 2005; Kandlikar et al. 2005; Nguyen and Wereley 2006; Sobhan and Peterson 2008: Bruus 2008: Zhang 2007: Kockman 2008: Yarin et al. 2009: Kirby 2010), to name a few. Besides, as demonstrated in a number of comparative review works, the plain extension to the microscale of available experimental correlations and analytical expressions derived in the context of macroscale devices, could lead to significant deviations in predictions of relevant parameters for analysis and design purposes, such as friction factors and heat or mass transfer coefficients (Morini 2004; Yener et al. 2005; Rosa et al. 2009). It should be highlighted that much of the continuum theory developed for macroscale fluid flow and heat transfer is still applicable in the analysis at the microscales here considered, because although small, the systems considered may still be large enough to obey the continuum hypotheses, even though model extensions are eventually required, such as at the interface of a gas flow and the bounding walls. Nonetheless, the interplay between the various acting transport phenomena mechanisms and their relative importance may change remarkably in microscale, in comparison to what occurs for the same application in macroscale. Therefore, classical modeling assumptions and simplifications must frequently be reconsidered at microscale, as well as many correlations established for the macroscale, which rely upon these assumptions, must be employed with care.

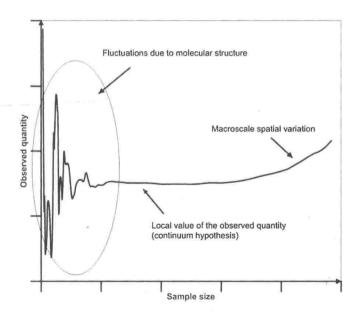
In the context of computational heat and fluid flow, analytic-based approaches for purely diffusive and convection-diffusion problems, despite the extensive progress achieved by discrete numerical methods, have been progressively advanced, unified and further formalized by a few research groups, in part motivated by offering benchmark results for validation and calibration of numerical schemes. In addition, a number of hybrid analytical-numerical methodologies have appeared in the open literature, which attempt to combine classical analytical methods with modern computational tools, in the search for more accurate, robust, and economical options to the nowadays well-established discrete solution methods. For instance, a hybrid method for solving diffusion and convection-diffusion problems that has been advanced along three decades is the so-called Generalized Integral Transform Technique (GITT) (Cotta 1990, 1993, 1994, 1998; Cotta and Mikhailov 1997, 2006; Cotta et al. 2013, 2014), based on the classical integral transform method for linear transformable diffusion problems (Koshlyakov 1936; Mikhailov and Ozisik 1984). This method was initially proposed as an approximate analytical solution approach to overcome barriers posed by a class of diffusion problems involving time-dependent boundary condition coefficients, that were before supposed to be tractable solely by discrete-type methods (Ozisik and Murray 1974; Mikhailov 1975), later on extended to include situations involving nonlinear physical properties, moving boundaries, irregular geometries, and nonlinear convective terms, to name a few, within a much broader hybrid numerical-analytical framework. The relative merits of this approach over purely numerical procedures include the automatic global error control and the mild increase in computational effort for multidimensional situations. The GITT hence complements the well known numerical methods for partial differential equations, either as a companion in code verification tasks or as an alternative analytically based approach. In particular, for heat and fluid flow analysis of microsystems, in light of the inherent multiscale nature of the posed problems, the purely discrete approaches may lead to significant computational costs, and the hybrid approach advantages can become more evident. This work is thus aimed at illustrating applications of integral transforms to the analysis of heat and fluid flow at microscale. In the following sections, microscale effects on heat and fluid flow are briefly discussed, and then starting from a fundamental convection—diffusion problem formulation, the formal solution procedure of the Generalized Integral Transform Technique (GITT) is described. Chapter 2 presents specific aspects of the methodology as applied to slip-flow analysis, electrosmotic flows, inverse analysis of convection with slip flow, microchannels with corrugated walls and irregular shapes, and conjugated heat transfer in microchannels. Then, Chap. 3 demonstrates the developed theory in the theoretical—experimental analysis of micro-heat spreaders and micro-heat exchangers.

1.2 Microscale Effects on Heat and Fluid Flow

The classical heat and fluid flow theory is based upon the assumption that the fluid can be treated as a continuum instead of a collection of molecules, which allows for the classical modeling of the conservation equations: mass, momentum and energy. Nonetheless, it should be remembered that the fluids are in fact composed of a group of discrete molecules. For example, in a gas, the molecules are separated by distances which are much larger than the molecules themselves and even in a liquid, where the molecules are much more densely packed, all quantities such mass and velocity are very far from being continuous. In fact, even a very small quantity of a fluid, which may be regarded as a point from the macroscopic point of view, may be large enough to contain several thousands of molecules, which may be large enough for the observed quantity, taken as an average of the various individual molecules within that volume, not to be affected by fluctuations from different properties of the individual molecules. On the other hand, if the sample volume is made too small, the different number and different kinds of molecules present in the sample at each observation may result in irregular fluctuations from one observation to another at the same location, as illustrated in Fig. 1.1. In this case, the molecular structure starts affecting the measured property and it becomes evident that the fluid is, in reality, not a continuum. If one is interested in studying the fluid behavior at such a small scale, the continuum hypothesis is clearly no longer valid and a molecular approach should be used instead. It should be stressed, however, that even at microscopic fluid samples there may be several thousands of molecules, and the continuum hypothesis remains valid for most of the microfluidics applications with length scales of the order of at least 10 µm.

Momentum and energy transport in a fluid and convergence to a thermodynamic equilibrium state occur due to intermolecular collision. Hence, the time and length scales associated with the intermolecular collisions are important parameters for

Fig. 1.1 Qualitative representation of the influence of the size of the fluid sample in the local observation of a quantity



many applications. The distance traveled by the molecules between collisions is known as the mean free path, λ . In this context, a paramount important nondimensional parameter in fluid mechanics and heat transfer in microflows is the Knudsen number, which is defined as the ratio between the mean free path, λ , and a characteristic geometric length, L (Karniadakis et al. 2005). The Knudsen number is given by:

$$Kn \equiv \frac{\lambda}{L} \tag{1.1}$$

It is clear from Eq. (1.1) that lower Knudsen numbers indicate that the characteristic length of the flow is much larger than the average distances travelled between molecules collisions, similar to most macro applications under continuum hypotheses. Hence, the Knudsen number is one of the main tools used in order to analyze if a certain heat and fluid flow problem could still be modeled under the continuum hypotheses. In this sense, four different regimen of fluid flow are commonly adopted, depending on the range of the Knudsen number, given below and also illustrated in Fig. 1.2 (Gad-El-Hak 2005).

- Kn < 10⁻³ Continuum flow (classical continuum equations with no-slip and no-temperature jump boundary conditions)
- $10^{-3} < \text{Kn} < 10^{-1}$ Slip-flow (classical continuum equations with slip and temperature jump boundary conditions)
- 10⁻¹ < Kn < 10 Transition regime
- Kn > 10 Free molecular flow

In this text, the problem formulations to be considered shall be only within the continuum and slip-flow regimen, governed by the classical conservation equations of mass, momentum, and energy, with either the classical no-slip and