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Extended Thermodynamic Approach for Non-Equilibrium Gas Flow

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Abstract. Gases in microfluidic structures or devices are often in a non-equilibrium state. The conventional thermodynamic models for fluids and heat transfer break down and the Navier-Stokes-Fourier equations are no longer accurate or valid. In this paper, the extended thermodynamic approach is employed to study the rarefied gas flow in microstructures, including the heat transfer between a parallel channel and pressure-driven Poiseuille flows through a parallel microchannel and circular microtube. The gas flow characteristics are studied and it is shown that the heat transfer in the non-equilibrium state no longer obeys the Fourier gradient transport law. In addition, the bimodal distribution of streamwise and spanwise velocity and temperature through a long circular microtube is captured for the first time.

AMS subject classifications: 76P05, 82B40

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1 Introduction

Due to the rapid development in fabrication technology for constructing micro-electro-mechanical systems (MEMS), fluid flow at the micro- and nano-scale has received considerable attention. A basic understanding of the nature of flow and heat transfer in these devices or structures is considered essential for efficient design and control of MEMS. Gas flows in micro-scale devices suffer from non-equilibrium effects when the gas molecular mean free path is the same order as the characteristic length of the device. The degree of

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non-equilibrium of a gas is generally expressed through the Knudsen number ($Kn=\lambda/L$) which is the ratio of the molecular mean free path, λ, to a typical dimension of the flow field, L. The different rarefaction regimes can be summarised according to the value of the Knudsen number [1]: (i) no slip ($Kn\leq 10^{-3}$); (ii) slip ($10^{-3}<Kn\leq 10^{-1}$); (iii) transition ($10^{-1}<Kn\leq 10$); and (iv) free molecular flow $Kn>10$, respectively. Most MEMS operate at the slip and early transition regime ($Kn<1$) [2]. Different approaches have been employed by various researchers to capture and describe the non-equilibrium phenomena that arise due to an insufficient number of molecular collisions occurring under rarefied conditions. Microscopically, the Boltzmann equation [3] provides an accurate description of a dilute gas at all degrees of rarefaction and describes its state through a molecular distribution function that treats the gas as a large number of interacting molecules, colliding and rebounding according to prescribed laws. However, solutions of the Boltzmann equation, either directly or through the direct simulation Monte Carlo (DSMC) method [4], entail significant mathematical complexity and are computationally expensive, particularly for low-speed, low Knudsen number flows in the slip and transition regime in microchannels.

Due to the difficulties associated with solving the Boltzmann equation, there is significant effort being made to construct alternative solution strategies that can provide an accurate description of a gas with Knudsen numbers that extend into the early transition regime, such as the lattice Boltzmann method (LBM) [5, 6], the discrete-velocity method (DVM) [7–9], the Boltzmann kinetic equation, and the unified gas-kinetic scheme (UGKS) [10]. Among these methods, the extended thermodynamic equations developed with the method of moments, which have been used to predict the hydrodynamic quantities successfully [11–15], is being paid more and more attention.

Grad [16] introduced the moment method for an approximate solution procedure for the Boltzmann equation. He expanded the phase-density distribution function in Hermite polynomials, the coefficients of which are linear combinations of the moments of the molecular distribution function. The 13 moment equations (G13) was first proposed by Grad via truncated distribution function at the third order in Hermite polynomials, which include the five lowest moments of the collision invariants, and stress and heat fluxes proposed by Stokes and Fourier. Struchtrup [17,18] regularized the G13 equations by using a Chapman-Enskog-like expansion for the closure conditions. The R13 method, which can capture Knudsen layers close to the solid surfaces, is an improvement over the G13 method for some problems [19, 20]. However, the R13 equations cannot capture the Knudsen-layer velocity profile accurately, and overpredict the mass flow rate sometimes [21]. In the present study, a set of 26 moment equations, which are based on the regularizing procedure of Struchtrup for R13 method, are employed by truncating the Hermite polynomials at the fourth order. It is proved to overcome many of the limitations in the R13 method [11]. The R26 method also has limitations. One of the problems by using the regularized moment method is that the equation set, which is a mixed system of the first- and second-order partial differential equations (PDEs), is more complicated. Another problem is that moments higher than second-order have no clear intuitive phys-