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Thermal and second-law analysis of a micro- or nanocavity using direct-simulation Monte Carlo

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In this study the direct-simulation Monte Carlo (DSMC) method is utilized to investigate thermal characteristics of micro- or nanocavity flow. The rarefied cavity flow shows unconventional behaviors which cannot be predicted by the Fourier law, the constitutive relation for the continuum heat transfer. Our analysis in this study confirms some recent observations and shows that the gaseous flow near the top-left corner of the cavity is in a strong nonequilibrium state even within the early slip regime, Kn = 0.005. As we obtained slip velocity and temperature jump on the driven lid of the cavity, we reported meaningful discrepancies between the direct and macroscopic sampling of rarefied flow properties in the DSMC method due to existence of nonequilibrium effects in the corners of cavity. The existence of unconventional nonequilibrium heat transfer mechanisms in the middle of slip regime, Kn = 0.05, results in the appearance of cold-to-hot heat transfer in the microcavity. In the current study we demonstrate that existence of such unconventional heat transfer is strongly dependent on the Reynolds number and it vanishes in the large values of the lid velocity. As we compared DSMC solution with the results of regularized 13 moments (R13) equations, we showed that the thermal characteristic of the microcavity obtained by the R13 method coincides with the DSMC prediction. Our investigation also includes the analysis of molecular entropy in the microcavity to explain the heat transfer mechanism with the aid of the second law of thermodynamics. To this aim, we obtained the two-dimensional velocity distribution functions to report the molecular-based entropy distribution, and show that the cold-to-hot heat transfer in the cavity is well in accordance with the second law of thermodynamics and takes place in the direction of increasing entropy. At the end we introduce the entropy density for the rarefied flow and show that it can accurately illustrate departure from the equilibrium state.

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I. INTRODUCTION

Micro- or nanoelectromechanical systems (MEMS/NEMS) are widely utilized in many practical applications including mechanical engineering and biomedical devices. The study of gaseous flow in micro- and nanoscales has been an interesting and appealing topic of research in recent years. It is well known that the traditional Navier-Stokes (NS) equations fail to predict the flow features as characteristic length enters microrange and beyond. Knudsen number, which is defined as the ratio of the mean free path in the gas to the characteristic length of the flow domain, $\mathrm{Kn} = \lambda/\mathrm{L}$, is a measure to determine degrees of gas rarefaction. A well-established classification of the gaseous flow regimes exists in microfluidics according to the Knudsen number range [1,2]. According to this classification, the state of a gaseous flow can be defined in four different regimes. Gaseous flow at $\mathrm{Kn} < 0.001$ is termed as continuum regime where the basic NS equations with no-slip/jump boundary conditions are valid in this regime. Gaseous flow with Knudsen number ranges of $0.001 < \mathrm{Kn} < 0.1$ is called slip flow. Special treatments such as applying velocity slip and temperature jump boundary conditions on the walls should be considered in the NS equations to capture slightly rarefied flow features in the slip regime. Transition regime is termed for gas flows within $0.1 < \mathrm{Kn} < 10$. In this regime, the NS equations lose validity and the well-known first-order shear stress and heat flux approximations fail to predict flow behavior. Flow is considered as free molecular if $\mathrm{Kn} > 10$. However, this classification is based mostly on data obtained from experiments and numerical studies of isothermal gaseous flows in long microchannels having simple one-dimensional (1D) geometries. For gaseous flows in 2D and 3D bounded domains with more complex geometries, the range of slip flow regime as defined above is questionable and should be reconsidered for each studied problem separately.

Different velocity slip models of varying complexity have been suggested to capture nonequilibrium effects in the slip regime [3–5]. Extending the lattice Boltzmann equations to the rarefaction regimes has been another appealing approach in modeling nonequilibrium phenomena [6–11]. In addition, high-order moment methods such as R13 and R26 are alternative powerful approaches in capturing nonequilibrium phenomena [12,13]. For example, it is reported that the predicted results of R13 and R26 methods for rarefied Couette and Poiseuille flows are accurate in early and midtransition regimes, respectively [13]. Despite the considerable efforts to

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