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Heat transfer and fluid characteristics of rarefied flow in thermal cavities

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ABSTRACT

In the present study, we investigate the characteristics of thermal cavities in the rarefied flow regime using the Direct Simulation Monte Carlo (DSMC). We use a recently developed iterative technique to impose a desired wall heat flux boundary condition in the DSMC algorithm. Fluid mechanics and heat transfer behavior are studied over the walls and in the domain of the thermal cavity over a wide range of Knudsen number in the slip and transition regimes. The vortice behavior is described at different Knudsen numbers in detail. We numerically justify unconventional flow movement from the cold region to the hot region. Finally, we consider the effects of molecular structural parameters such as molecular mass and degree of freedom on the thermal behavior of the thermal cavity flows.

1. Introduction

In recent years, small-scale electromechanical systems have been widely employed in many practical applications including mechanical and engineering biomedical devices. In this regards, a true understanding of the hydrothermal behavior of rarefied flow is required for an optimal design, operation, and manufacturing of these devices [1]. Advances in the development of high density power electronics, heat recovery and high temperature power has led to the development of high temperature heat exchangers (HTHE) with temperatures as high as 2500 K [2]. Investigating thermal conditions in small-scale systems due to high power densities requires the application of efficient techniques to predict allowable performance limits of these systems [3]. As the gas density reduces, Knudsen number (Kn), defined as the ratio of the mean free path of gas molecules to the characteristic length of the flow domain, $Kn = \lambda/L$, increases and the flow analysis must be performed using accurate approaches based on gas kinetic theory [4]. A well-established classification of the gas flow regimes exists according to Kn range [5]: continuum regime ($Kn < 0.001$), slip flow regime ($0.001 < Kn < 0.1$), transition flow regime ($0.1 < Kn < 10$), and free molecular regime ($Kn \geq 10$). Direct simulation Monte Carlo (DSMC) is widely employed to model flow fields in all degrees of flow rarefaction [6].

The aim of this study is to simulate rarefied flow in thermal cavity geometries with an imposed heat flux on the bottom wall. This small-scale thermal cavity represents devices such as a Pirani gauge [7] or a cantilever heater [8]. The rarefied gas flow behaviors in the thermal cavity with constant wall temperature have been studied in the literature. For example, Papadopoulos et al. [9] used direct simulation Monte-Carlo method to study characteristics of thermal creep convective motion in a rectangular geometry at $Kn = 0.05$. They found that a vortex is formed by thermal creep at the non-isothermal boundaries; vortex formation was also observed in the absence of gravity. Aoki et al. [10] used kinetic theory to investigate the flow of a rarefied gas caused by a discontinuous wall temperature in a two-dimensional square container. The steady flow in the container was numerically analyzed using the Bhatnagar–Gross–Krook (BGK) model of the Boltzmann equation. They showed that, as the rarefaction effect decreases, the maximum flow speed tends to approach a finite value, but the region with appreciable flow shrinks to the points of discontinuity. Therefore, the overall flow in the container vanishes non-uniformly in the continuum limit. Sone et al. [11] introduced

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various kinds of flows induced by the temperature effects and discussed their physical mechanisms in rarefied gases. They demonstrated that a tangential temperature gradient along the surface could induce the flow movement from the cold to the hot region. This behavior was known as thermal creep that vanishes in the continuum limit. Liu et al. [12] considered heat transfer in the continuum and early transition regimes (Kn = 0.2) in the vacuum package Micro-Electro-Mechanical-Systems (MEMS) devices with constant wall temperature. They concluded that, if the bottom plate temperature partially increases, the gas temperature near the bottom surface would be greater in comparison with the case where the bottom plate temperature is increased uniformly. In addition, they indicated that gravity in low-pressure MEMS packaged devices has little effect on heat transfer. Cia et al. [13] analyzed heat transfer effects in a vacuum package in the free molecular and near continuum regimes. They simulated a square cavity where the bottom plate represents a hot chip and the other plates were set at room temperature. In the free molecular flow regime, the density and temperature were surveyed with a proposed model. They especially concentrated on the free molecular flow and proposed a model that links the number densities reflected on and traveling away from the walls. Rana et al. [14] studied the effects of rarefaction on the heat transfer behavior of square cavity using the regularized 13 moments (R-13) equations. The heat transfer was compared between the classical Navier–Stokes (NS) and R-13 equation with specified wall temperature (SWT) boundary condition at Kn $\leq$ 0.5. They showed that the classical NS equations overestimate the heat transfer in the MEMS packaged device.

In contrast to the NS equations, there is no classical way to implement a specified heat flux distribution on the wall using the DSMC method; however, some MEMS require the specified wall heat flux boundary condition. In such engineering applications, a specified wall heat flux is more common than a specified wall temperature. For example, the Scienta Pirani gauge is divided into two types [7]: constant resistance, and constant current. The constant resistance type changes the supplied current to maintain the resistance of the filament constant. In fact, the temperature variation is calculated according to changing resistance; therefore, we can simulate this type with the SWT boundary condition. However, it should be noted that this requires more complicated electronics to be controlled. The other type, i.e., the constant current type, has a power supply that provides a constant current to the filament continuously. If we use a simple voltage control circuit, we will obtain a constant power Pirani gauge; therefore, this type could be simulated using the wall heat flux boundary condition.

To apply a specified wall heat in the DSMC method, Wang et al. [15,16] introduced an inverse temperature sampling (ITS) technique. More recently, Akhlaghi et al. [17] introduced an iterative technique to impose a desired (positive/negative) wall heat flux boundary condition in the DSMC method. They validated their technique for different sets of geometries. Our literature review shows that previous simulations of rarefied thermal cavities were based on specified wall temperature (SWT) boundaries [9–14]. Simulation of the cavity with wall heat flux boundary condition is not reported in the literature. Therefore, in the current work, we consider flow field and thermal behavior of a thermal cavity with the constant wall heat flux boundary condition over a wide range of Kn, i.e., from the slip to the mid transition regime, i.e., 0.05 < Kn < 3. The effects of the cavity walls on vortices behavior is discussed in detail. The heat flux and temperature distribution is connected to vortice behavior. The shear stress behavior on the walls and in the domain is considered with increasing Kn. We provide a physical description for the flow and thermal field behavior in the thermal cavity geometry. Finally, thermal analysis is presented for various gas molecular structural parameters.

2. Numerical method

2.1. DSMC approach

The DSMC is a particle method based on kinetic theory for simulation of rarefied gases. The method is carried out by modeling the gas flow using many independent simulator particles. More details about the DSMC algorithm were given in Ref. [18]. In the current study, we use and extend the previous codes of Roohi and co-workers [19–26] to simulate rarefied flow in small-scale cavities. More specifically, the numerical algorithm of the cavity solver from Ref. [19] is upgraded to include the iterative technique. The variable hard sphere (VHS) collision model is used as the collision model in all simulations. Collision pairs are chosen based on the no time counter (NTC) method, in which the computational time is proportional to the number of simulator particles [18]. We use the diffuse reflection model with full thermal accommodation for the walls. To satisfy the size limitation, the cell dimensions in both directions are 0.1λ (m), and we set the time step equal to 1×10^{-12} (s), smaller than the mean collision time. For a typical simulation, twenty particles are initially set in each cell to minimize the statistical scatter. In Table 1, cell size, number of particles in each cell, time step, number of time steps, and number of samples are reported.

2.2. The iterative technique

The Iterative technique is a newly-developed method for imposing a wall heat flux in the DSMC algorithm. This technique is based on the correction of the wall temperature during the DSMC simulation to obtain the desired wall heat flux. In this technique, the wall temperature can be obtained from Ref. [17]:

$$T_w(x)^{\text{new}} = T_w(x)^{\text{old}} + \Delta T_w(x) \tag{1}$$

$\Delta T_w(x)$ is defined as a correction value to the wall temperature such that the iterative algorithm converges and the final wall temperature distribution corresponding to the desired heat flux is established. A positive wall heat flux indicates heat being transferred from the gas to the wall, i.e., a cooling process. On the other hand, a negative value indicates that the wall is heating the gas. In the iterative technique, the corrected wall temperature is computed as follows:

$$T_w(x)^{\text{new}} = T_w(x)^{\text{old}} \left(1 + RF \frac{q_w(x) - q_{\text{des}}(x)}{|q_{\text{des}}(x) + \varepsilon_0|}\right) \tag{2}$$

In Eq. (2), q_w is the wall heat flux, computed according to Ref. [18], and ε_0 is a non-zero positive value that is negligible in comparison to the incident energy flux. ε_0 is typically considered a small non-zero value for adiabatic wall cases because Eq. (2) diverges if the desired heat flux (q_{des}) is set zero. RF is a relaxation factor used to avoid divergence during running the program. This amount is considered 0.03 in our simulations.

Table 1
Entry data for the numerical code.

	Cell size ($\text{m} \times 10^{-8}$)	Number of particles in each cell	Time step ($\text{s} \times 10^{-12}$)	Number of time steps to steady state condition ($\times 10^{+6}$)	Sample size ($\times 10^{+6}$)
Typical test cases	1.67	20	1	8	160