

Influence of molecular structure on thermal behavior in vacuum packaged MEMS/NEMS using DSMC

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Abstract: In the present study, we investigate the characteristics of micro/nano thermal cavity in rarefied flow regime using direct simulation Monte Carlo (DSMC) method. We use a recently developed iterative technique to impose a desired wall heat flux boundary condition in the DSMC solver. Hydrothermal and heat transfer behaviors are studied over the walls and inside the domain of the thermal cavity over a wide range of Knudsen number in the slip and transition regimes. Finally, we consider the effects of molecular structural parameters on the hydrodynamics and thermal behaviors in micro/nano thermal cavity flows.

Keywords: “Heat flux; Rarefied flow; DSMC; Micro/Nano thermal cavity; MEMS/NEMS”

Introduction

Micro/Nano electromechanical systems (MEMS/NEMS) have been widely employed in many practical applications including mechanical and engineering biomedical devices

Direct simulation Monte Carlo (DSMC) is used as a crucial tool to model flow field in all degrees of rarefaction. This thermal cavity represents micro/nano devices such as micro-Pirani gauge or micro-cantilever heater. In contrast to the NS equations, there is no classical way to implement a specified heat flux distribution on the wall using DSMC method; especially some MEMS/NEMS require the specified wall heat (SWH) boundary condition.

The rarefied gas flow behaviors in the thermal cavity with constant wall temperature have been studied in the literature. For example, Liu et al. [1] considered the heat transfer at the continuum regime and early transition regime ($Kn=0.2$) in the vacuum package MEMS devices with constant wall temperature. They concluded that if the bottom plate temperature was partly enhanced, the gas temperature near the bottom surface was greater than when the bottom plate temperature is increased uniformly. Rana et al. [2] studied the effects of rarefaction on the heat transfer behavior of square cavity using R13 equation. The heat transfer was compared between the classical Navier-Stokes (NS) and the R13 equation with specified wall temperature (SWT) boundaries condition at $Kn \leq 0.5$.

Previous simulations of rarefied thermal cavity were based on the specified wall temperatures (SWT) boundaries. For the first time, simulation of cavity with SWH boundary condition reports in this paper.

DSMC approach

The DSMC is a particle method based on the kinetic theory for simulation of the rarefied gases. The method is carried out by modelling the gas flow using many

independent simulating particles. The DSMC algorithm includes four primary steps: moving the particles, indexing them, collision simulation, and sampling.

Iterative technique

Iterative technique is one of the recently developed methods for imposing wall heat flux in the DSMC method. The wall temperature can be obtained [3]

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

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

In the DSMC method, the heat transfer flux q is the sum of the translational and rotational energies of both the incident and the reflected molecules per unit time and per unit area of the wall, i.e.,

$$q_w = \frac{[(\sum_{i=1}^n \varepsilon_{tr} + \sum_{i=1}^n \varepsilon_{rot})_{inc} - (\sum_{i=1}^n \varepsilon_{tr} - \sum_{i=1}^n \varepsilon_{rot})_{ref}] N_0}{\Delta t \Delta x} \quad (3)$$

where the subscripts *inc* and *ref* are the incident and reflected molecular, respectively, n is the total number of simulated molecules that strike the wall during the sampling, Δt is the time period of the sampling, and N_0 is the number of gaseous molecules related with a computational molecule.

Results and Discussion

We analyzed monatomic argon and diatomic nitrogen molecules. The heat flux (positive/negative) is imposed on the bottom wall, and thermal condition of the three other walls are set as constant temperature, $T_s=300K$. The square cavity length is $L=1nm$. Heating and cooling processes are performed over a wide range of Knudsen number in the slip and transition regimes, i.e., $Kn=0.05, 0.2, 0.5, 1$ and 3 .

As one test case, figure. 2 shows the nondimensional heat flux and the temperature contours at $Kn=0.05$. Figure. 3

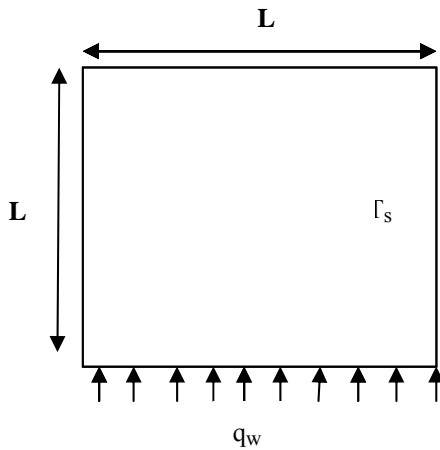


Fig. 1. Geometrical configuration of the micro/nanocavity

Table. 1. Properties of gases [4]

Gas	Diameter (d×10 ¹⁰ m)	Degrees of freedom (ζ)	Molecular mass (m×10 ²⁷ kg)	Viscosity index (ω)
Nitrogen	4.17	5	46.5	0.74
Argon	4.17	3	66.3	0.81

demonstrates by increasing the Kn number, range of heat flux variation between the bottom and the top region decreases, whereas the heat flux behavior affects on the temperature behavior directly. At a lower Kn number, in contrast to the heat flux distribution, the rang of temperature changes is smaller. At lower Kn numbers, intermolecular and surface- the molecules interactions are relatively high. Therefore, molecules rapidly transfer the

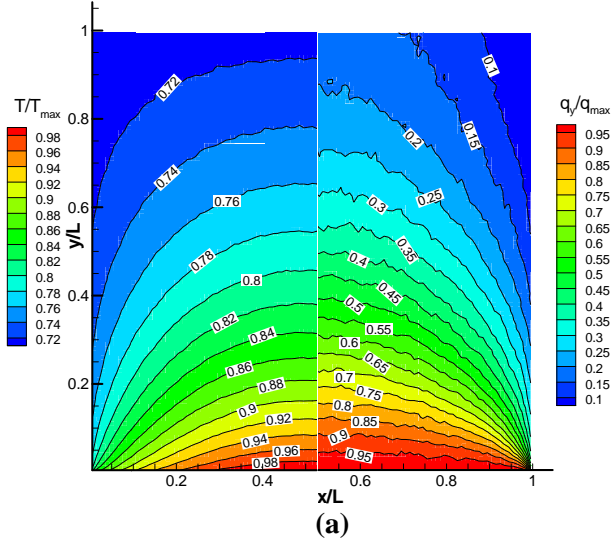


Fig. 2. The nondimensional heat flux and the temperature contours at Kn=0.05

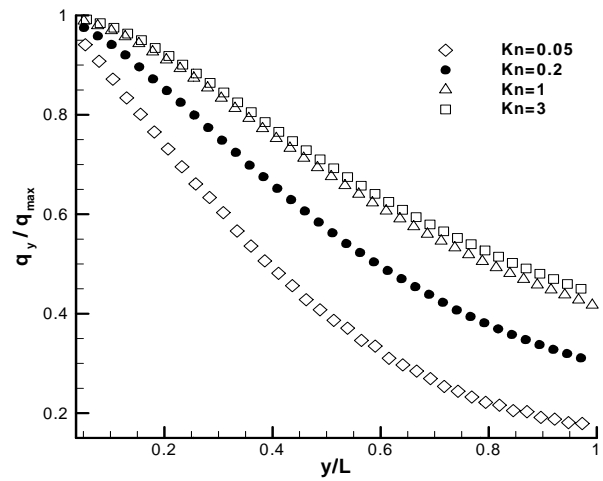


Fig. 3. The nondimensional heat flux distributions along y direction in the x=0.5

gained energy from the bottom wall to the side and top walls.

The relation between the specific heat capacity (C_p) and the degree of freedom (ζ) and gas constant (R) is [5]:

$$C_p = \left(\frac{\zeta}{2} + 1\right) R \quad (4)$$

the heat capacity depends on two factors: first, the number of degrees of freedom that are available to the particles in the gas to store thermal energy; second, molecular mass. The argon molecule can only store energy in three translational modes, but the nitrogen molecule possesses two additional rotational modes. On the other hand, the argon mass is larger than the nitrogen; therefore, the heat capacity of nitrogen is greater than argon. It means that if a constant level of energy is transferred to the argon and the nitrogen molecules, the argon temperature increases more than the nitrogen.

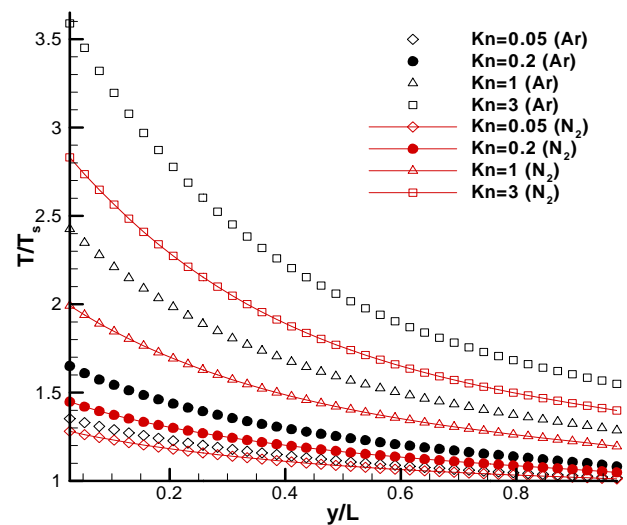


Fig.4. Comparison the nondimensional temperature between the argon and the nitrogen at different Kn

The mean free path is another parameter which is function of the gas structure. The variable hard sphere (VHS) relation between the viscosity and the mean free path (λ) is defined according to [5]:

$$\lambda = (2\mu/15)(7 - 2\omega)(5 - 2\omega)(2\pi RT)^{-1/2}/\rho \quad (5)$$

Also the relation between the viscosity and the temperature according to the Chapman-Enskog expansion is defined as below:

$$\mu = \mu_{\infty} \left(\frac{T}{T_{\infty}} \right)^{\omega} \quad (6)$$

Equations (5) and (6) indicate that increase of ω , increase μ and therefore λ , so the mean free path of the argon is larger than the nitrogen. Increase of λ is equivalent to using a more rarefied gas, i.e., the constant energy is distributed to a lower number of molecules; consequently, increase of the nitrogen temperature is smaller than the argon for a specified energy.

Figure.4 illustrates the mean free path and the specific heat capacity coefficient cause the variation of argon temperature to be larger than nitrogen at specified Kn. Figure. 5 shows heat flux behaviour is similar to temperature behaviour. Heat flux of argon is considerable higher than nitrogen at each specified Kn.

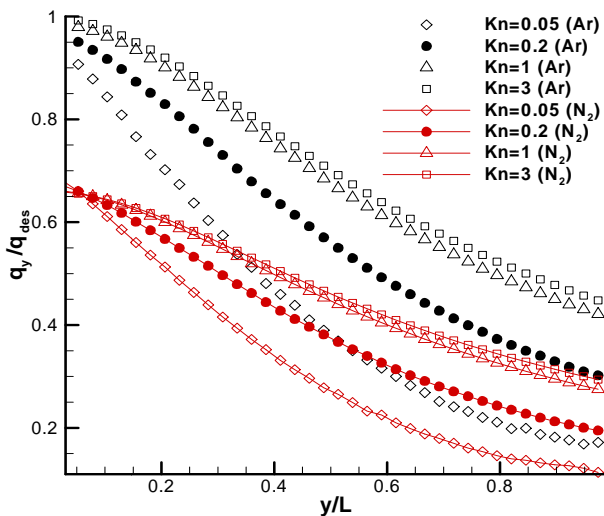


Fig.5. Comparison the nondimensional heat flux between the argon and the nitrogen at different Kn

Fig. 6 demonstrates that the Nu number variation of nitrogen on the bottom wall is larger than the argon at specified Kn number. The variation of Nu number between the argon and the nitrogen is remarkable at Kn=0.05 and 0.2, but this variation reduces by increasing Kn so that we observe the minor difference between Nu number at Kn=1 and 3.

Conclusions

The current work investigated hydrothermal behaviour of rarefied flow through micro/nano cavities using DSMC technique. We observed that the increase of the Kn

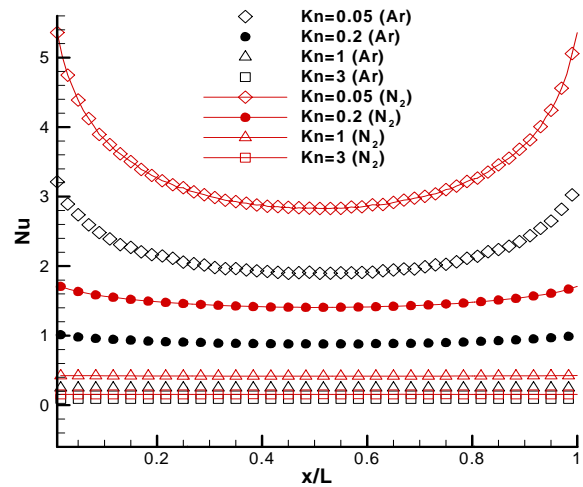


Fig. 6. Comparison the Nu number between the argon and the nitrogen at different Kn

number decreased the intermolecular and molecule-surface interactions; therefore, the penetration of the heat transfer inside the cavity weakened and the range of heat flux variation decreased. Our analysis indicated that the increase of the Kn number caused the Nu number on the bottom wall to decrease so that the conductive behavior dominates over the convective behavior beyond Kn=0.2. The effects of the molecular structures, i.e., mass, degree of freedom and viscosity-temperature index, was investigated on the hydrodynamics and thermal behavior in thermal micro/nano cavity. We observed the increase of ζ and ω , and the decrease of mass result in the increase of the temperature and the heat flux in the domain. We observed that molecular structure influences on the variation of the Nu number over the bottom wall at the lower Kn, but this variation is quite negligible by increasing the flow rarefaction.

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