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GAS PROPERTIES EFFECTS IN MICROCHANNEL STUDIES USING DIRECT SIMULATION MONTE CARLO

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ABSTRACT

This paper concern is to study the gas properties effect in flow and heat transfer behaviors through microchannels using the direct simulation Monte Carlo method. The flow is rarefied and supersonic. The channels are investigated at two different inlet boundary conditions. The collision process is modeled using the NTC (no-time-counter) scheme. The VHS model is chosen to simulate collision between particle pairs. The study is provided for many different gases including nitrogen, helium, and oxygen. The Knudsen number is chosen in a manner to provide slip flow through the channel. The results show that the heat transfer from the wall is lower for heavier gases. A comparative study among the monatomic, diatomic, polyatomic gases shows that the heat transfer rate is lower for the polyatomic gases. The result shows that, the heat transfer from the wall is lower for the heavier gases than that for the lighter gas. For a fixed Mach number, the heat transfer from the wall decreases as the molecular diameter increases.

INTRODUCTION

Micro electrical mechanical systems MEMS are a new emerging technology with sufficient potential for a steady growth in future. Attention to microdevices is increasing due to their advantages over macro counterparts, e.g., low costs, small sizes and masses, and rapid response times [1]. Microchannels can be considered as one of the most important parts in MEMS device. Since the flow and heat transfer play important roles in those conduits, their simulations provide important information for their design and construction [2-3]. Gas flows through microchannels are mostly in rarefied regime. As is known, the rarefied gas flow should be treated different from the continuum flow.

The rarefied gas flow regimes are categorized by their Knudsen number (Kn) value, which is defined as the ratio of the mean free path (λ) of fluid to a characteristic dimension of the channel (H). For the flows with small Knudsen number, $Kn<0.01$, a continuum assumption is justifiable. In continuum flow regime, the Navier-Stokes equations govern the flow filed as long as the flow can be assumed infinity divisible. A higher Knudsen number can result in slip flow regime first and a transition flow next ($0.01<Kn<1$). For flows with Knudsen number between ($0.01<Kn<0.1$), the non-equilibrium effects dominate in the flow near the wall surfaces. Therefore, it needs applying the slip boundary conditions if we wish to solve the Navier-Stokes equations. If flow becomes more rarefied, the linear stress-strain relation in the Navier-Stokes equation is not valid and that the kinetic effects should be reconsidered [4].

The Boltzmann equation governs the rarefied flow regimes. However, the exact solutions for the Boltzmann equation can the provided for a limited number of simple geometries. Therefore, complexity in the Boltzmann equation promotes the researchers to use the direct simulation Monte Carlo (DSMC) method in solving the rarefied flow regimes. The DSMC method is not only a technique for simulating the real gas flows but also a rather definite solution method for the kinetic equation. Brid [3] used the DSMC method to solve the dynamic equation governing a full physically model of rarefied gas at molecular level. Indeed, DSMC is one of the most successful

particle simulation methods and has been used largely for analyzing the rarefied gas flows. Different applications of DSMC have been reported by Oh, et al. [5] for simulating supersonic microflows. Unlike the MD (the deterministic molecular dynamics method), the DSMC is a statistical-based method, with its own statistical fluctuation behavior.

Past investigations show that the research concentration in DSMC has been mostly in studying the gas rarefaction level and geometry effects on flow configuration and heat transfer characteristics considering one or two specific gases as the working fluid [1, 4, 6-7]. In the present study, we use the DSMC method to study the supersonic slip flow considering different gas properties. However, to expand our study suitably, we examine the effects of molecular diameter, molecular mass, molecular degree of freedom on the wall heat transfer rate distribution. Additionally, we study the effects of inlet Mach number and velocity inlet boundary conditions on the achievable results. We treat the Knudsen number, the flow direction, and the free stream temperature as the independent variables. To the knowledge of the authors, similar study has not been presented previously. Furthermore, this paper specially focuses on the effect of gas properties on the flow and heat transfer behaviors.

THE DSMC SCHEME

The DSMC method is a particle method for the simulation of non-equilibrium gas flows [3]. The gas is modeled at microscopic level using particles in which each particle represents a large number of physical molecules. DSMC is based on moving particles and considers binary collision between particle pairs. We use variable hard sphere (VHS) model [3] to simulate the collisions between molecules. For the finite total cross-section, the hard sphere HS model has an advantage because of providing an easily calculated collision mechanics and that it has a disadvantage, because the scattering law is not realistic and that the cross-section is independent of the relative translational energy in the collision [3]. This model treats the particle as a solid sphere with variable diameter, which is scattered isotropically. The particle diameter is given by

$$d = d_{ref}\left(\frac{C_{r,ref}}{C_r}\right)^{\vartheta} \qquad (1)$$

where the subscript *ref* denotes the reference values, C_r is the relative velocity and υ is the relative speed exponent in the VHS model.

DSMC ALGORITHM

At the beginning of calculation, the particles are uniformly distributed in the cells. At each time step, all particles move according to their individual velocities. They may interact with the boundaries, and finally indexed.

Figure 1 shows a typical flowchart for the DSMC simulation. As is observed, there are essentially five important steps including: 1. move particle, 2. check boundary interaction, 3. sort the particles in different cells, 4. perform intermolecular collisions, and 5. sample macroscopic properties of interest.

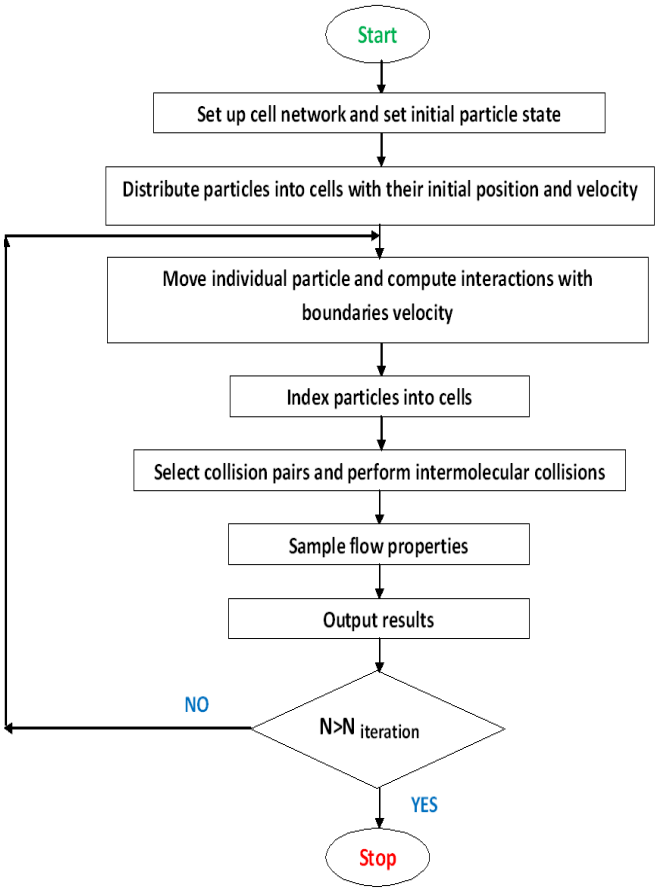
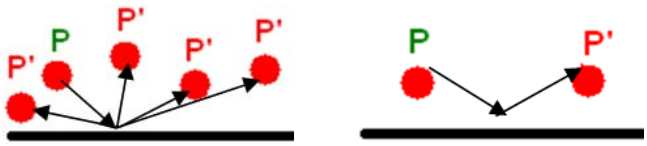


Figure 1 A typical DSMC flowchart.

WALL BOUNDARY INTERACTION

Figure 2 shows two types of wall boundary conditions, which are generally used in DSMC. One is the specular reflection of particles, and another one is the diffuse reflection of particles. The specular reflection is a mirror-like reflection, where the angle of reflection is equal to the angle of incidence. In a specular reflection, the normal velocity of particle is reversed, the tangential velocity is retained, and the energy is preserved. The specularly reflecting wall represent a "smooth" wall and it does not cause any resistance to the flow. This is equivalent to an inviscid wall boundary condition treatment in conventional CFD schemes.



a) diffusive reflection b) specular reflection

Figure 2 Two types of particle reflection from wall

COLLISION PAIR SELECTION

In a rectangular cell, the probability P of collision between two simulated molecules over time step (Δt) is given by [3]

$$P = \frac{F_n.\sigma_T.C_r.\Delta t}{V_c} \quad (2)$$

and the maximum probabilities of collision between two simulation particles are calculated from

$$P_{max} = \frac{F_n.(\sigma_T.C_r)_{max}.\Delta_t}{V_c} \quad (3)$$

where F_n is the number of real molecules represented by one simulated particle, $C_r.\sigma_T$ is the total collision cross-section, and V_c is the cell volume. In no-time-counter (NTC) scheme, the probability changes to pairs are selected from the cells at the time step.

$$P_{max} = \frac{0.5.N.\overline{N}.F_n.(\sigma_T.C_r)_{max}.\Delta t}{V_c} \quad (4)$$

where $\overline{N}$ is the time ensemble average of particles occupied a cell. For each possible pair of collision, the method picks up a random particle and finds its corresponding sub-cell. Within this sub-cell, it picks up another random particle so that these two particles form a collision pair. The collision is now computed with the probability using.

$$P_{chek} = \frac{\sigma_T.C_r}{(\sigma_T.C_r)_{max}} \quad (5)$$

This essentially means that a random number is compared with the value at Eq. (5). If it is larger than it, we should consider a collision, otherwise nothing. Then, the molecule moves to the next step to calculate the post-collision velocity. The velocity components (u, v, w) of the reflected molecules for the diffusive wall reflection are determined from

$$\begin{aligned} u &= \sqrt{-\log(Rf(0))}V_{vmp}\sin(2\pi.Rf(0)) \\ v &= \pm\sqrt{-\log(Rf(0))}V_{vmp} \\ w &= \sqrt{-\log(Rf(0))}V_{vmp}\cos(2\pi.Rf(0)) \end{aligned} \quad (6)$$

where V_{vmp} is the most probable speed of the molecules at the wall temperature and $Rf(0)$ is a uniformly distributed random fraction between 0 and 1. The positive and negative symbols correspond to the lower and upper walls, respectively. Reflection from the symmetry boundary is considered specular, i.e., the normal velocity component is being reversed while the tangential component remains unchanged.

SAMPLING OF MACROSCOPIC PROPERTIES

Sampling of microscopic data is used to compute macroscopic flow properties such as density, velocity, temperature, pressure, etc., locally within each cell. All quantities are calculated at the geometric center of each cell. They are the mean values of all the individual values located in a cell. The calculations of smooth flow properties require a large sample size to accurately model the distribution function. The magnitude of statistical fluctuation is proportional to the inverse square root of the sample size. The sample size used in the present study has an order of 10^7. Our study showed that this choice would guarantee the required accuracy the present calculation.

SETTING THE CELL WIDTH

Although particles are allowed to cross the cells faces, individual collisions may occur with neighbors in the same cells. More specifically, the DSMC uses the sub-cell approach, where local collision rates are based on the individual cells, but the possible collision pairs are restricted to sub cells. A rule of thumb is that the cell width should be ($\Delta x \approx \lambda/3$), where again λ is the mean free path.

SETTING THE TIME STEP

In the DSMC, there is no stability limit for choosing the time step. However, from a physical point of view, there is some limitation caused by the mean collision time. The time step should be sufficiently small in order to uncouple the molecular motions and collisions. An estimate can be calculated from

$$\Delta t = 0.25.\frac{\Delta x}{\grave{C}_{vmp}} \quad (7)$$

where Δx is cell width and $\grave{C}_{vmp}$ is the most probable molecular speed, which is determined by free stream temperature [1].

The speed of sound is different for each gas due to having different R, γ, and T_∞ values. For example, the universal gas constant is a function of molecular mass, i.e., the values for lighter gas are greater than the heavier ones. Also, γ is a function of molecule degree of freedom therefore γ has the maximum value for a monatomic gas. Then, for the lighter gases the inlet velocity is greater than the heavier ones. The wall heat flux can be calculated from the energy flux differences between incident and reflection molecules as follows:

$$q = \frac{[(\sum_{i=1}^{n}\varepsilon_{tr} + \sum_{i=1}^{n}\varepsilon_{rot})_i - (\sum_{i=1}^{n}\varepsilon_{tr} + \sum_{i=1}^{n}\varepsilon_{rot})_r].F_n}{\Delta t.\Delta x} \quad (8)$$

where n is the total number of simulated molecules, which strike the wall during the sampling, F_n is the number of real gaseous molecules represented by one computational molecule, and Δt is the time period of sampling. Additionally ε_{tr} and ε_{rot} are the molecular translational and rotational energies, respectively. Furthermore indexes i and r represents incident and reflected molecules, respectively.

PROBLEM DESCRIPTION

In this study, we consider a supersonic flow passing through a channel with two different inlet boundary conditions including a free stream Mach number M_∞ (or the free stream velocity) and a constant free stream temperature. The channel height and length are 1.2 μm and 6 μm, respectively. The channel geometry is schematically shown in Fig. 3. We only simulate

one half of the channel height due to the flow symmetry. This reduces the computational time efficiently while the results are not affected.

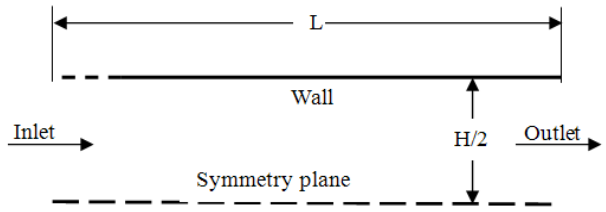


Figure 3 The geometry of microchannel and the important boundary conditions.

In order to generate adequate inlet velocity profile, we assume that a part of the wall at the entrance region have specular reflection status it is by dashed line. We use rectangular cells to discrete the solution domain. Each cell is divided into 4 sub-cells, in other words, each cell is divided into two sub-cells in each direction. The time step is chosen to be less than the averaging mean collision time. Initially 10 to 20 particles are set in each cell. Table 1 provides the details of chosen test cases in the current study. In all cases, the inlet Knudsen number and Mach number are set to 0.062 and 4.15, respectively. The inlet number density is 1.74×10^{25} and the wall temperature is 323K. The computational domain is broken into a 100×60 grid. Also the inlet velocity is set to 1500(m/s).

We study different gases in our test cases. The test cases are classified in four groups. In this table we used "Yes" to denote the employed working gas, the inlet conditions, and the effects, which were investigated.

Table 1 Details of chosen test cases

Group	1	2	3	4	
Gas species	1-7	8-11	12-18	11-22	
N_2	Yes	Yes	____	____	
O_2	Yes	Yes	Yes	____	
H_2	Yes	Yes	____	____	
He	Yes	Yes	____	____	
Ar	Yes	____	Yes	Yes	
NH_3	Yes	____	____	____	
CH_4	Yes	____	____	____	
Fixed inlet Mach	Yes	____	Yes	Yes	
Fixed inlet velocity	____	Yes	____	____	
The effect of diameter	____	____	Yes	____	
Mass effect	____	____	____	____	Yes
DOF effect	____	____	____	Yes	____

STUDY OF SUPERSONIC FLOW IMPOSING DIFFERENT INLET BOUNDARY CONDITIONS

Figure 4 shows the distribution of wall heat transfer rate along the microchannel. Since helium is the lightest gas; its heat transfer rate is greater than other gases it is because its free stream velocity increase. Alternatively CO_2 is the heaviest gas and it normally performs a minimum heat transfer rate from the wall.

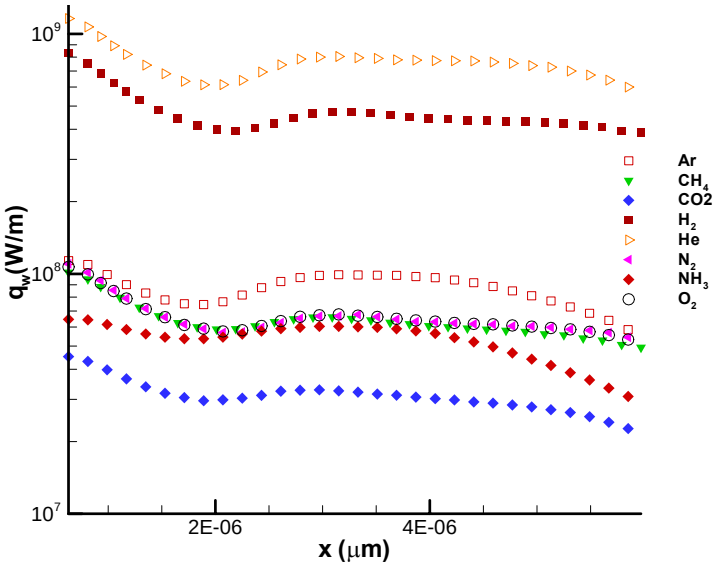


Figure 4 Wall heat flux rate in the microchannel with a fixed inlet Mach number, Group1

Figure 5 shows the effect of gas choices on the Mach number contours. It can be seen that different gasses perform different positions of their peaks. Consistent with Figure 4, the heat fluxes initially decrease and keep relatively unchanged, because most of heat has been transferred to the bulk flow and the thermal layer becomes developed throughout the rest of the microchannel. Thus, it can be concluded that the flow deceleration near the wall and the development of thermal boundary layer govern the wall heat flux magnitude in the microchannel. Specifying the inlet velocity instead of the inlet Mach number, the role of molecular mass can be removed. However, a fixed inlet velocity would cause different inlet Mach numbers conditions for the different investigated cases and this would result in different wall heat flux behaviors in the microchannel.

Figure 6 shows the distribution of wall heat transfer rate along the microchannel for Group 2. Two of the profiles perform similarly with no peak at all and the two others perform major peaks near in the microchannel. The heat transfer rate steadily decreases after that. Figure 7 shows Mach contours for cases with a fixed inlet velocity of 1500 m/s for Group 2. The gases with lighter molecular masses do not reach supersonic condition. It is because there is no bow shock in the channel and that the heat is uniformly transferred from the wall along the microchannel.

EFFECT OF MOLECULAR MASS

Figure 5 shows Mach contours of different gases together. However, to quantify various gas properties, we study the effects of each gas separately. So, we need investigating the effect of each property separately on the heat transfer rate through the microchannel. At the first step, we concentrate on the molecular mass effect on the flow and heat behaviors of two types of monatomic and diatomic gas, i.e. Argon (as a monatomic gas) and oxygen (as a diatomic gas). Figure 8 shows the distribution of wall heat flux along channel for argon at three different conditions. As before, increasing the molecular mass would lead to a change in the inlet velocity if the inlet Mach number is fixed. This affects the momentum near the walls. Since the molecular velocity is a function of inlet properties, an increase in molecular mass, for a fixed inlet Mach number, would cause a decrease in the inlet velocity.

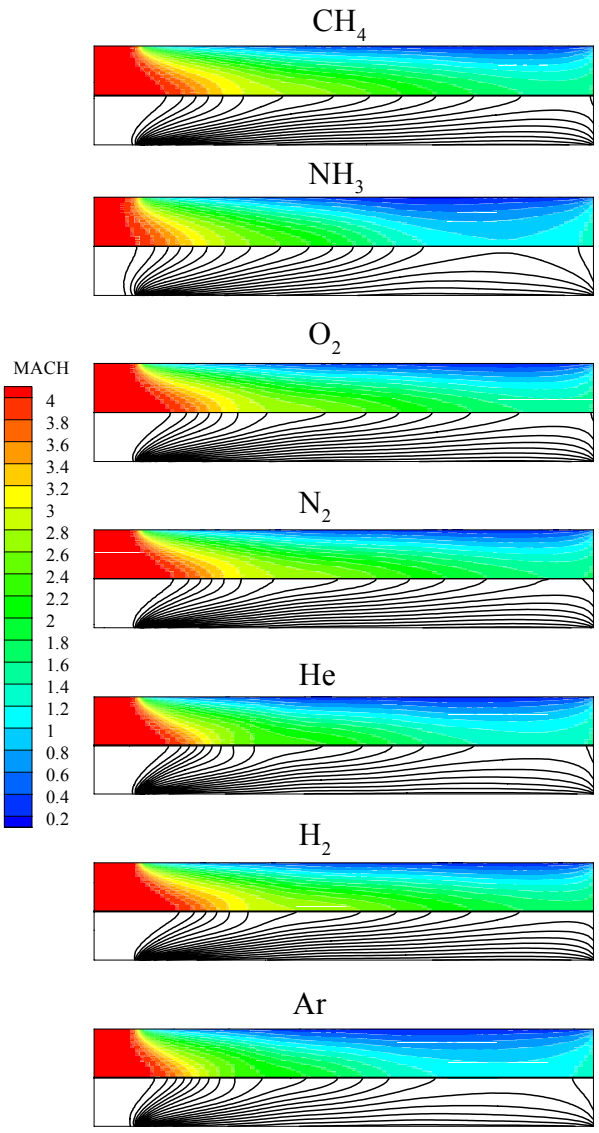


Figure 5 Mach number contours for different gas choices with M_{in}=4.15, Group 1

Although the fluid momentum is a function of molecular mass, the effect of mass increase is not sufficiently large compared with the gas molecular speed. Generally, the molecular velocity has dominated role on the wall heat flux rate. A heavier gas would have a lower heat transfer rate in comparison with the lighter gas at equivalent conditions.

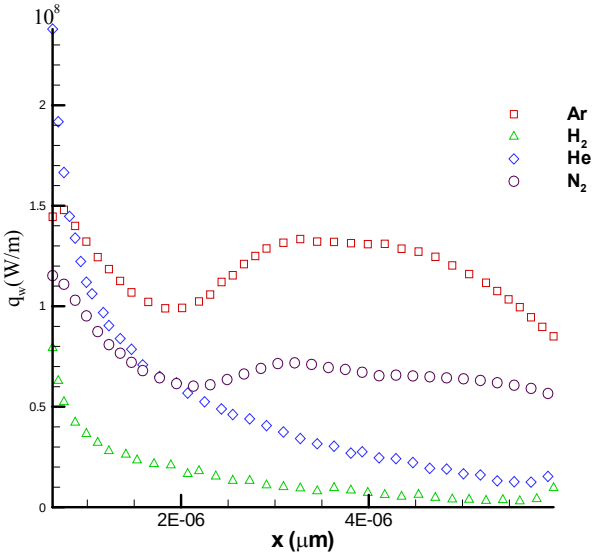


Figure 6. wall heat flux for different gases with a fixed inlet velocity magnitude, Group 2.

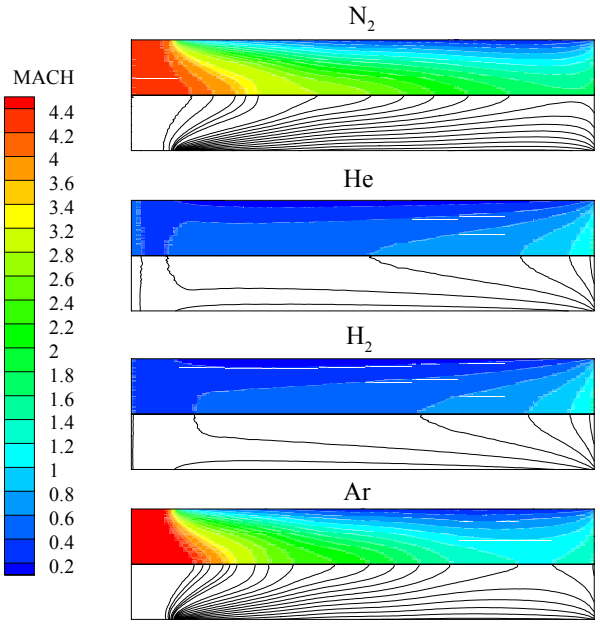


Figure 7 Mach number contours for different gas choices with V_{in}=1500 (m/s), Group 2.

Figure 9 shows the velocity distribution along the microchannel centerline. There is a two bow shock interactions around

2e-6 (μm), which decreases the velocity magnitude. The decrease in velocity magnitude continues for all cases; however, it plays differently for the three test cases. It is because they have different molecular mass magnitudes. Figure 10 shows the wall heat flux for oxygen as a diatomic gas. It exhibits very similar to a monatomic gas, i.e., argon.

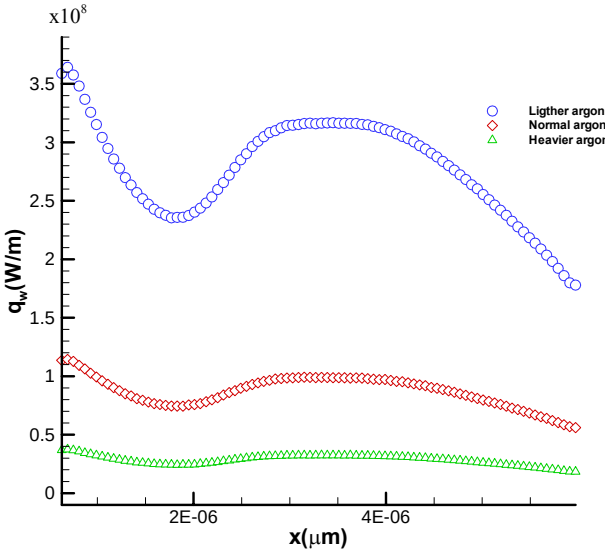


Figure 8 Wall Heat flux for three types of argon

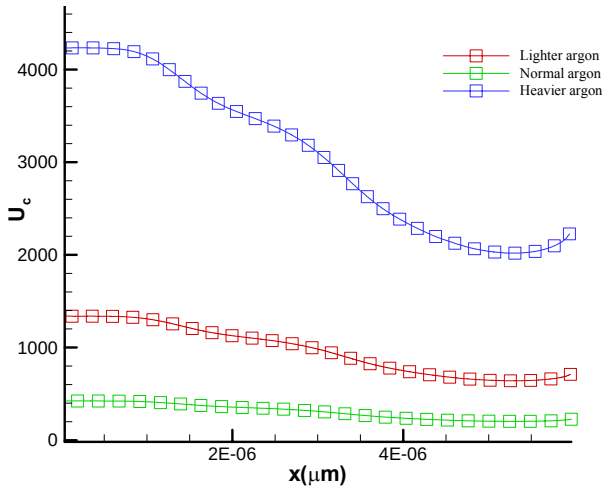


Figure 9 The effect of molecular mass on the centerline velocity distribution

EFFECT OF MOLECULAR DIAMETER

Figure 11 shows that the wall heat flux rate can be related to the molecular diameter. Smaller argon with a diameter smaller than the normal argon diameter perform two orders of magnitude more wall heat flux rate. Additionally, as the argon diameter increases, the wall heat transfer rate decreases two orders of magnitude. It is because the molecular diameter is related to the collision cross-section and the collision is accepted if the random number is less than$CVR/(\sigma_T.C_r)_{max}$. For a smaller molecular diameter, $(\sigma_T.C_r)_{max}$ decreases and $CVR/(\sigma_T.C_r)_{max}$ increases. Thus, the number of accepted collision pairs increases, and consequently the momentum and heat transfer rates increase. Similarly, this is applicable to diatomic and polyatomic gases.

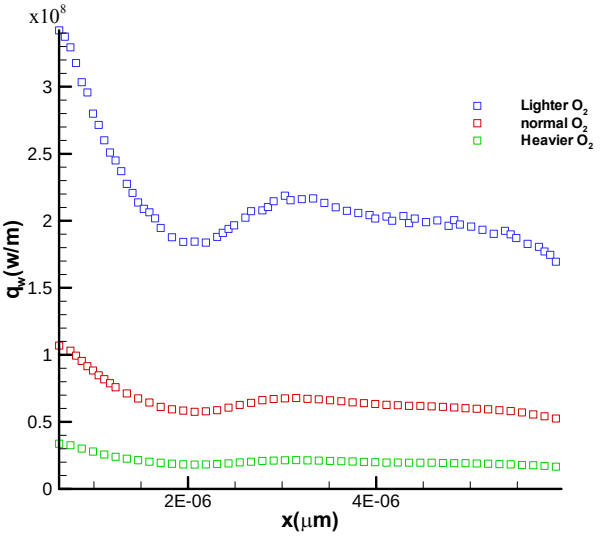


Figure 10 Wall Heat flux for three types of oxygen

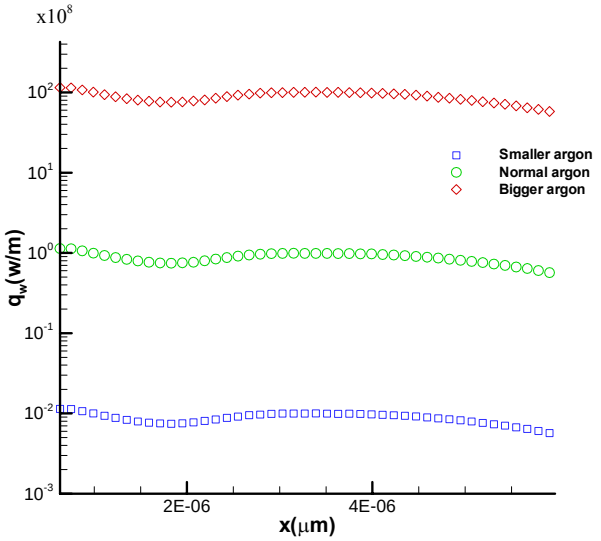


Figure 11. Wall Heat flux for argon with different diameters

EFFECT OF DEGREE OF FREEDOM

Figure 12 shows that the degree of freedom can affect the flow filed and heat flux rate from the wall. Gamma (γ) is a function of gas type. Gamma is maximum for the monatomic gases. Additionally, the speed of sound is a function of gamma. Therefore, gamma is maximum for a monatomic gas and consequently its speed of sound is maximum, while its other

properties remain unchanged. Increasing the speed of sound for a constant inlet Mach number, it requires to increase the velocity and the molecular velocity and momentum magnitudes. Considering this point, it is obvious that the heat transfer for the monatomic gases would be much greater than the diatomic and polyatomic gases.

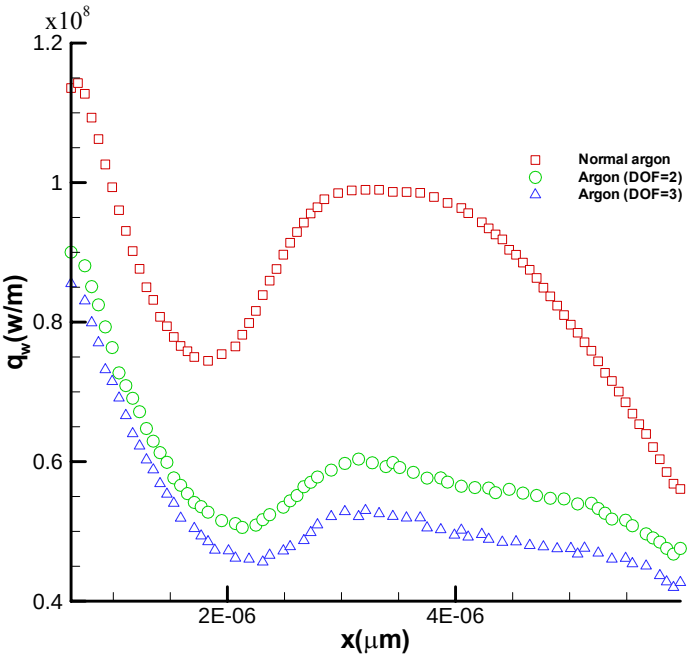


Figure .12 The effect of degree of freedom on the wall heat flux

CONCLUSION

Rarefied supersonic gas flow through the microchannel was simulated using the DSMC method. The molecular velocity has significant effect on the wall heat transfer for different gas choices. The flow decelerates after entering into a microchannel and eventually becomes fully developed due to strong viscous effects. We studied the effects of molecular mass and diameter variations on the heat transfer rate considering different real gases. For a fixed inlet Mach number that, the wall heat transfer rate for a heavier gas is lower than of a light gas. For gases with larger molecular diameters, the wall heat transfer rate decreases. A comparative study on monatomic, diatomic and polyatomic gases showed that the wall heat transfer rate is lower for the polyatomic gases. Using the conclusion of this work, we can choose appropriate gas to control the rate of heat transfer from a microchannel if the choice of gas does not affect the microdevice design and implantation.

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