DSMC Simulation of Heat Transfer in Subsonic Rarefied Gas Flows through Micro/Nanochannels Imposing a Constant Inflow/Wall Temperature Difference

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We use the direct simulation Monte Carlo (DSMC) method and investigate the subsonic rarefied gas flow through micro/nanochannels, imposing a constant pressure ratio and a constant temperature difference between the inflow and wall temperature. We further study the heat transfer characteristics of subsonic nitrogen gas flow under this imposed temperature difference. We show that, specifying a higher temperature magnitude would lead to more rarefactions even imposing a fixed temperature difference. This consequently results in a higher wall heat flux rate for a fixed inflow-wall temperature difference. Our investigating shows that the number of simulated particles need to increase suitably if one wishes to avoid statistical fluctuations on the wall heat flux values.

I. Introduction

As demand on NEMS and MEMS devices increase s, more understanding of the heat transfer characteristics through such devices becomes very crucial. Indeed, the miniaturization of MEMS and NEMS devices requires advanced understanding of micro and nanoscale flows and heat transfer physics. This is due to the fact that the fluid flow behavior in tiny scales is fundamentally different than that of the macroscopic scales; mainly because the characteristic length scales of micro-devices can be very close to the mean-free path of the flowing gas (λ) [1]. In most microchannel systems, the mean free path of molecules is within the same order of the microchannel height (H). The ratio λ/H is commonly referred as the Knudsen number. Using higher value of this number, the flow should be treated from the molecular point of view, as opposed to that from the continuum point of view [2]. In micro/nanoflows, the Reynolds number is very low (in the order of 10) and this means that the viscous forces may dominate the inertial force and the viscous transports of momentum and heat can be regarded as the important aspects of such flows [3]. Literature shows that the DSMC has been used numerously to solve the rarefied gas flow problems, i.e., where the continuum assumption breaks down. The DSMC is a numerical tool, which can be applied to simulate flow in a rather physical way using molecular model concepts. In this model, the state of flow is determined by the positions of the representative molecules and their velocity components [4]. Several studies have been performed to elaborate the heat transfer characteristics in the rarefied gas flows. Liou and Fang [3] studied the effects of Knudsen number on heat transfer characteristics of supersonic flows in microchannels using the DSMC method. In this regard, they changed the inlet Knudsen number from 0.031 to 0.186 while the inlet Mach number was 4.15, the wall temperature was 323 K, and the incoming gas flow temperature was 300 K and constants in all cases. Their results showed that the magnitude of the temperature jump would increase at the wall with increasing Kn. Additionally, it was found that the heat transfer value to the isothermal wall would increase significantly as Kn

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increased. The results also showed that the enhanced wall heat transfer rate would mainly cause by the increased number of molecules that incident the wall. Ye et al. [5] studied the heat and mass transfer characteristics of the rarefied subsonic nitrogen gas flow through microchannels using the DSMC method. In order to study the effects of wall temperature on the mass flux and the wall heat flux rates, they changed the wall temperature $T_w$ from 200K to 800K while the temperature of the incoming gas flow $T_{in}$ was constant at 300 K. In all the simulated cases, the majority of wall heat flux transfer occurred close to the channel entrance region. The heat transfer decreases to nearly zero when it approached the middle part of channel. Their results show that, sudden jumps in the heat transfer flux and the temperature distribution are clearly observed at the exit region of the channel in cases where $T_w$ is greater than $T_{in}$. Darbandi, et al. [6] studied the effects of outlet boundary conditions on the wall heat fluxes. They simulated the supersonic rarefied gas flow through micro/nanochannels and showed that, the wall heat flux rates increase as the back pressure increases. Darbandi, et al. [7], also investigated the effects of wall temperature on the wall heat flux rates and showed that the wall heat flux rates would decrease as the wall temperature increased. In this study, we apply a constant temperature difference between the wall and incoming flow and examine the effects of various wall and inflow temperatures on the heat transfer phenomena and the flow configuration for subsonic rarefied gas flows through 2D channels.

II. Modeling

The DSMC method was first introduced by Bird [6] to study rarefied gaseous flows. This method consists of indexing molecules into the cells, tracking the movements of molecules, selecting collision pairs, and calculating post collision properties. Computational domain is divided into a number of cells and each cell is divided into four subcells to be used for selecting collision pair purposes. The DSMC method has two distinct characteristics. The first is that, each simulated particle is a representative of a large number of real molecules in this method. Another one is uncoupling of molecular motion and molecular collision by a computational time step. This time step is smaller than the physical collision time and is set such that a typical molecule moves about one third of the cell dimension at each time step.

![Figure 1. The geometry of micro/nanochannel and the imposed boundary conditions.](image)

As is seen in Fig. 1, we investigate the subsonic rarefied nitrogen gas flow with an inlet pressure of $P_{in}$ and a temperature of $T_{in}$ moving through a two-dimensional microchannel. In the present simulations, the time step is chosen in a manner to result in a typical molecule moves about one fourth of the cell dimension in each computational time step. The variable hard sphere (VHS) is applied as a collision model in all the simulations. By this model, the intermolecular potential between collision pairs are simulated and post-collision velocities are calculated. For the equilibrium gases, the temperature can be calculated from [2] the

$$T = \left( 3T_{tr} + \zeta_r T_{rot} \right) \left/ \left( 3 + \zeta_r \right) \right.$$  \hspace{1cm} (1)

which the molecular vibrational energy is neglected. $T_{tr}$ and $T_{rot}$ are translational and rotational temperatures, respectively. They can be determined using a number of related parameters such as the Boltzmann constant $k$, molecular mass $m$, molecular velocity $c$, mean velocity of simulated molecules $c_\text{ms}$, the number of rotational degrees of freedom $\zeta_r$, and the rotational energy of an individual molecule. They yield

$$\frac{3}{2} k T_{tr} = \bar{m}c^2 - \bar{m}c_0^2$$  \hspace{1cm} (2)

$$T_{rot} = \left( 2/k \right) \left( \bar{e}_{rot} / \zeta_r \right)$$  \hspace{1cm} (3)

The bar over variables represented the sample averaging values. According to the above equations, the temperature of gas depends on the velocity magnitude and the rotational energy of particles. The net heat flux on a wall can be calculated from

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where \( n \) is the total number of simulated molecules that strike the wall during the sampling, \( N_0 \) is the number of gaseous molecules associated with one computational molecule, and \( \Delta t \) is the time period of sampling. In fact, the wall heat flux rate is determined by the difference of energy in incident and reflected molecules.

### III. Boundary Conditions

All the boundary conditions in DSMC can be divided in two main classes. First, those boundaries in which the molecules enter or exit from the domain. Second, the boundaries in which no molecule is permitted to cross that, i.e., the solid boundaries.

**A. Inlet/Outlet Subsonic Condition**

In the DSMC method, all three flow parameters, i.e., density, temperature and velocity must be specified for the incoming molecules at the inlet/outlet boundaries. In high speed flow cases, such as those of hypersonic flows, the thermal velocity can be smaller in magnitude compared with the mean velocity. In the DSMC simulation of high-speed gas flow, the conventional approach is to impose a “vacuum” condition at the exit boundary, where no molecule is permitted to enter the computational domain from the region external to the flow domain. In case of low-speed flows, the thermal motion can be of the same order of magnitude as the mean molecular motion. It then becomes inappropriate to neglect the mass influxes at a flow boundary [8]. Liou and Fang [9] proposed an implicit boundary treatment for low speed MEMS flow simulations. In their method, the number of molecules entering the computational domain and their corresponding internal energy and velocity components are determined in an implicit manner using the local mean flow velocity, temperature, and number density magnitudes.

The number flux of molecules entering the computational domain is described using the Maxwellian distribution function as follows[8]:

\[
F_j = \frac{n_j}{2\sqrt{\pi} \beta_j} \left[ \exp \left(-s_j^2 \cos^2 \nu \right) + \sqrt{\pi} s_j \cos \nu \left\{ 1 + \text{erf} \left( s_j \cos \nu \right) \right\} \right]
\]

where

\[
S_j = U_j \beta_j
\]

\[
\beta_j = 1/\sqrt{2RT_j}
\]

where \( F_j \) represents the number flux through a cell face of the boundary cell \( j \), “erf” denotes the error function, \( R \) the gas constant, and \( n_j \) the number density of molecules in the \( j \)th cell. \( T_j \) and \( U_j \) denote the local temperature and the streamwise mean velocity component, respectively. The value of \( \nu \) is zero for the upstream boundary and \( \pi \) for the downstream exit boundary.

The velocity components of the entering molecule are determined using the acceptance-rejection method [2] and the Maxwellian distribution function. At the upstream inlet boundary, the streamwise velocity \( u \) and the cross-stream velocities, \( v \) and \( w \), of the molecules entering to the computational domain through the cell face of a boundary cell \( j \) can be written as

\[
u = A \cos(\phi) + V_{j,in}
\]

\[
w = A \sin(\phi)
\]

where...
where $R_j$ represents a random fraction number, and $C_{mp}$ the local most probable thermal speed of molecules. At the downstream, the velocity components for the molecule entering the computational domain through the exit flow boundary are obtained from

$$u = \left( U_{j,\text{out}} - 3C_{mp} \right) R_j$$
$$v = A \cos(\varphi) + V_{j,\text{out}}$$
$$w = A \sin(\varphi)$$

where $V_{j,\text{out}}$ denotes the exit local transverse mean velocity. If the vibrational energy is neglected, the internal energy of the entering equilibrium gases of diatomic molecule consists of the translational energy, $e_{tr}$, and the rotational energy $e_{rot}$, as follows:

$$e_{tr} = mc^2/2$$
$$e_{rot} = -\ln \left( R_j \right) kT_j$$

where $c$ is the speed of an entering molecule, $m$ the mass of simulated gas, and $k$ the Boltzmann constant.

To apply Eqs. (5) to (11), we need the number density, temperature, and mean velocity at the flow boundaries. At the upstream boundary, the pressure, $P_{in}$, and density, $\rho_{in}$, are the given parameters of flow. The temperature, $T_{in}$, can be obtained according to the equation of state as follows:

$$\rho_{in} = \frac{P_{in}}{(T_{in}R)}$$
$$n_{in} = \frac{\rho_{in}}{m}$$

Liou and Fang [9] used the first-order extrapolation to determine the streamwise mean velocity, $U_{j,\text{in}}$, from that of the computed for cell $j$. It is given by:

$$U_{j,\text{in}} = U_j$$

The transverse mean velocity, $V_{j,\text{in}}$, is set zero. This method is easy to use. However, Wang and Li [10] showed that it would take a long time to converge because the velocity of coming particles does not embody the pressure information. It also shows that this treatment has some difficulties when the wall temperature is quite different from the gas temperature. They proposed another treatment for the upstream pressure boundary based on the theory of characteristics. It yields [10]

$$U_{j,\text{in}} = U_j + \left( P_{in} - P_j \right) / (\rho_j a_i)$$
$$V_{j,\text{in}} = V_j$$

where $a_i$ is the local inlet speed of sound. At the downstream boundary, the only given flow parameter is the outlet pressure, $P_{out}$. The other mean properties of the flow are to be determined implicitly as the calculation proceeds. In the implicit boundary treatment, the flow variables are first computed using the characteristics-theory-based equations as follows [8]:

\begin{align*}
A &= \sqrt{-\ln(R_j)C_{mp}} \\
\varphi &= 2\pi R_j \\
C_{mp} &= \sqrt{2RT_j}
\end{align*}
\[
\rho_{j,\text{out}} = \rho_j + \left( P_{\text{out}} - P_j \right) a_j^2
\]

\[
U_{j,\text{out}} = U_j + \left( P_j - P_{\text{out}} \right) \left( \rho_j a_j \right)
\]

\[
V_{j,\text{out}} = V_j
\]

\[
T_{j,\text{out}} = P_{\text{out}} \left( \rho_{j,\text{out}} R \right)
\]

The subscript \(\text{out}\) denotes the exit boundary.

**B. Wall Condition**

We use the diffuse reflection model at the solid walls. In this model, the emission of impinging molecules is not correlated with the pre-impingement state of the molecules. The outgoing velocity of molecules is randomly assigned according to a half-range Maxwellian distribution determined by the wall temperature. This is also known as the full thermal and momentum accommodation coefficients. For a wall aligned in the y-direction, it yields

\[
u = \sqrt{-\ln(R_f)} C_{mp} \sin(2\pi R_f)\]

\[
v = \sqrt{-\ln(R_f)} C_{mp}\]

\[
w = \sqrt{-\ln(R_f)} C_{mp} \cos(2\pi R_f)\]

where the most probable speed is calculated using the wall temperature knowledge. It results in

\[
C_{mp} = \sqrt{2RT_w}\]

The temperature at the upper and lower walls of microchannel is uniform in this study.

**IV. Result and discussion**

We study different micro/nanoflows cases in order to elaborate the heat transfer characteristics in micro/nanochannel sizes. In these cases, the effects of inflow and wall temperature values and the number of simulated particles are examined properly. The details are summarized in Table 1. In all cases, nitrogen is considered as the working fluid. One-half of the geometry is simulated due to the symmetric flow conditions.

**Table 1. The details of chosen nine test cases in this study**

<table>
<thead>
<tr>
<th>Case</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
</tr>
</thead>
<tbody>
<tr>
<td>H((\mu m))</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>2.4</td>
<td>2.4</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>AR</td>
<td>8</td>
<td>8</td>
<td>8</td>
<td>5</td>
<td>5</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>PR ((P_{\text{in}}/P_{\text{out}}))</td>
<td>2.4</td>
<td>2.4</td>
<td>2.4</td>
<td>2</td>
<td>2</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(P_{\text{in}}) (atm)</td>
<td>1.2</td>
<td>0.6</td>
<td>0.12</td>
<td>2</td>
<td>2</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(T_{\text{in}}) (K)</td>
<td>300</td>
<td>300</td>
<td>300</td>
<td>350</td>
<td>400</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(K_{\text{in}})</td>
<td>0.0447</td>
<td>0.0894</td>
<td>0.447</td>
<td>0.0223</td>
<td>0.0261</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(T_{\text{w}}) (K)</td>
<td>300</td>
<td>300</td>
<td>300</td>
<td>200</td>
<td>300</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>No. of Mol.</td>
<td>21000</td>
<td>870000</td>
<td>87000</td>
<td>8700</td>
<td>48000</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>grid</td>
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<td>100×50</td>
<td>100×50</td>
<td>100×50</td>
<td>100×50</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

In order to validate our developed DSMC solver, we simulate the subsonic nitrogen gas flow through a microchannel under a constant pressure difference. While specifying a constant pressure ratio value, we change the inlet/outlet pressure values (Cases 1-3) to strengthen the rarefaction effects. The results are compared with the first/second-order analytical solutions [11]. In these cases, the pressure ratio value is equal to 2.4 but the inlet/outlet
pressure values is changed suitably. Case 3 has the lowest pressure value, and consequently is the most rarefied test case.

Figure 2 present the velocity profiles at the mid-channel for Cases 1 (a), 2 (b), and 3 (c). As is seen in this figure, as the flow becomes more rarefied, the achieved accuracy degrades and the results do not match suitable the first/second order solutions. The results of DSMC show great agreements with the second-order analytical solution. Figure 2(d) shows the velocity profiles for Case 3 in which the number of simulated particles is ten times larger than those used in Fig. 2(c). Comparing Figs. 2(c) with 2(d), it is obvious that the number of simulated particles has a great effect on the statistical fluctuation behaviors of the DSMC method. The comparison with the analytical solutions indicates that the current developed DSMC solver is reliable enough to be used in the test of this study.

![Velocity Profiles](image)

**Figure 2. Velocity profiles at the mid-channel, (a) case 1, (b) case 2, (c) case 3, and (d) case 3 with ten times higher in the number of simulated particles**

After code validation, we would like to lunch a statistical fluctuation study. As is seen in Table 1, the numbers of simulated particles for case 4 to 6 are 870,000, 87,000, and 8,700, respectively. The calculated wall heat flux rate distributions are showed in Fig 3 for these three cases. There are large statistical fluctuations in Case 6, which has the lowest number of simulated particles. However, the results for Cases 4 and 5 are approximately the same. It means that we can perform our simulations using 87,000 particles rather than 870,000 ones without losing the achieved accuracy. One of the most important parameters on the wall heat flux rates is the temperature difference between wall and the channel. In Case 5 and Cases 7 to 9, we fix the temperature difference equal to 100 K and investigate the effects of various inflow/wall temperature magnitudes on the flow heat transfer rates.
Figure 3. Wall heat flux rates for different number of simulated particles, Cases 4 to 6

Figure 4 shows the wall heat flux rates considering various inflow/wall temperatures. According to this figure, the wall heat flux rate would monotonically decrease as the inflow/wall temperature difference value increases. Also, the wall heat flux rate decreases exponentially along the channel. Liou and Fang [3] showed that the wall heat flux rates would increase as the Knudsen number increased. However, it performs a decrease in our study.

Figure 4. Effects of various inflow/wall temperature magnitudes on the wall heat flux distributions considering a constant temperature difference, Cases 5 and 7 to 9.

As are known, the rarefaction, velocity slip, and temperature jump are three important parameters, which govern the flow in micro/nanoscale studies [6, 7]. Specially, the rarefaction is one of the most important ones among them. It affects the micro/nanoscale heat transfer characteristics considerably [3, 6-7, 12]. Figure 5 shows the wall Knudsen number distributions for Cases 5 and 7 to 9. As is seen in this figure, Case 9 has the most rarefied condition among the others. In this case, the temperature has the highest value, which consequently leads to the lowest density value Case. The lowest density value means that the most rarefied flow performs the highest Knudsen number value.
Figure 5. Wall Knudsen number distributions for various inflow/wall temperatures considering a constant wall/inflow temperature difference, Cases 5 and 7 to 9.

Figure 6 shows the temperature jump distributions under constant inflow/wall temperature difference condition for Cases 5 and 7 to 9. The temperature jump on the wall depends on the amount of flow rarefaction and the temperature gradient magnitude at the wall face [11]. As is seen, Case 9 is the most rarefied flow case performing the lowest temperature jump at the wall. It is because of performing the lowest temperature gradient magnitude at the wall, see Fig. 7. It means that the temperature gradient at the wall performs a stronger effect than the Knudsen number on the flow and heat behaviors in nanoscales flows.

Figure 6. Temperature jump distributions for various inflow/wall temperatures considering a constant wall/inflow temperature difference, Cases 5 and 7 to 9.

Figure 8 illustrates the effects of different wall/inflow temperature magnitudes on the velocity slip distribution along the channel wall. According to this figure, the velocity slip at the wall increases as the rarefaction increases. Of course, this is one of the main cornerstones of the rarefied flow behaviors, which has been greatly elaborated in many different articles [8, 11].
Figure 7. Temperature gradient distributions on the wall for Cases 5 and 7 to 9

Figure 8. Effects of various inflow/wall temperature magnitudes on the wall velocity slip distributions considering a constant temperature difference, Cases 5 and 7 to 9.

V. Conclusion

We used DSMC to simulate the subsonic nitrogen gas flow through micro/nanochannels. We studied the effects of various inflow/wall temperature magnitudes on the flow/wall heat transfer rates imposing a constant temperature difference between the incoming flow temperature and the channel wall temperature. We studied the effect of various parameters such as the flow rarefaction, the temperature jump, and the velocity slip on the wall heat flux rate behavior. The results showed that the wall heat flux rates would increase as the inflow/wall temperature magnitude decreases. It is mainly due to receiving high temperature jump values at lower temperature conditions. The results also showed that, a high temperature gradient value at the wall face would result in a high temperature jump distribution in cold conditions.
References


