DSMC simulation of the gas flow through a bend and a short microchannel

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Abstract. The present work is related to the study of the gas flows through micro-channels with 90° bend, and short straight channels. The direct simulation Monte Carlo (DSMC) method has been used to study the flow. The DSMC simulations of the gas flow through micro-channels of real dimensions, which are used in the laboratory or in industry, are computationally very expensive, requiring large amounts of the computer resources and time. This fact places a limit on the applicability of the DSMC method while considering the real channel dimensions. It is a good practice to approximate the three dimensional micro-channel into two dimensions, and to study the flow characteristics, when the channel width is essentially large in comparison with their heights. However, the simulation of gas flows in more complicated channels with rectangular cross-section having comparable height and width unavoidably requires a 3D consideration. In the present paper, the 3D flow through a bend and short straight channels are presented, and the flow characteristics studied using the DSMC method. The complete 3D simulations were carried out for the case the height H at 19.83e-6m considering to the same as the one used in the laboratory (without taking similarity of the flow into consideration for the reduction of the actual dimensions of the channel). However, the other dimensions (length and width) were chosen different from the real channel due to the computational requirements. Two types of pressure boundary treatment have been implemented in three dimensions using the DSMC method.

1. Introduction
Micro-channel is the one of the basic elements of many micromechanical systems; in recent years, the gas flows through straight and uniform micro-channels have been extensively studied. However, the most applications involve more complex geometries including elements such as channel junctions, bends, sudden expansions and contractions, etc. [15, 16]. The numerical modelling plays an important role in understanding the gas flow behaviour inside the micro-channel systems. The dimensions of the micro-channel systems are such that it is necessary to consider rarefaction, which often requires an application of both continuum and kinetic numerical approaches. Particularly, this is important for micro scale gas flows in micro devices with a complex geometry, which are, in general, non-equilibrium and cannot be well described by using only equations and models of the classical fluid dynamic theory [17]. Typical examples for such flows are the gas flows through different micro-junction combinations [4, 5, 13, 14].

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Several researchers have studied [3-6, 19] the gas flow through the 90\(^\circ\) bend micro-channel, at relatively high pressures, of the order of atmospheric pressure, and a very little work has been done for a lower pressure. It is a usual practice to approximate a three dimensional micro-channel into a 2D one assuming the flow to be uniform in the third direction. However, this approximation will be valid when the sidewalls are far apart, and do not influence the flow in the middle of the channel. In the present study a three dimensional flow is simulated.

One of the main objectives of this paper is a numerical study of the behaviour of the gas flows [3-6, 19] through 90\(^\circ\) bend micro-channel using the DSMC method [1, 2, 9-12] applying a pressure difference between the inlet and outlet of the channel. To simulate such flows a given pressure is applied at the open ends of the micro-channel.

Two types of approaches have been considered for maintaining a given pressure at the pressure boundaries [8], and the flow evolution through the micro-channel has been computed for various Knudsen numbers in a range from 0.043 to 0.087. The simulations are carried out in three dimensions considering short micro-channels and 90\(^\circ\) bend micro-channels (for the sake of simplicity hereafter referred to as bend micro-channel). The height of micro-channel is taken to be the same as the one that were used in the laboratory (UP/IUSTI) [20]. However, the computational time and memory requirements have placed a limit on choosing the other dimensions (length and width) to be the same as the real micro-channel. The results of the DSMC based code are first compared for validation with the finite volume method SIMPLE-TS [7] results provided by Shterev K and Stefanov S, allowing for a successful assessment of the accuracy of the results. The details of the flow structure near the corner are analyzed for some selected cases, and a comparison of the pressure boundary treatment considering the straight channel is presented. The investigation has a preliminary character.

2. Problem formulation

We consider a pressure driven isothermal monatomic rarefied gas flow through the micro-channel with 90\(^\circ\) bend. The Knudsen number (\(Kn\)), which is the ratio of the mean free path to the characteristic length [1, 2], determines the rarefaction of the gas: \(Kn = \frac{\lambda}{H}\), \(\lambda\) is the gas mean free path and \(H\) is characteristic length (the minimum of the distances between the opposite side walls). The DSMC simulations were carried out for a steady state of nearly isothermal rarefied gas flow through the micro-channels with 90\(^\circ\) bend, and straight channels with different aspect ratios 1/36, and 1/60. Macroscopic field variables have been studied. All the simulations were carried out in three dimensions. In the present study is related to the flows of pressures about 1000Pa to 5000Pa. The particles were treated using the hard sphere model.

In defining Knudsen number, the mean free path is defined as \(\lambda = \frac{1}{\sqrt{2\pi n d^2}}\), where \(d\) is the diameter of the molecule, and \(n\) is the reference number density. In the paper all macroscopic variables are given in non-dimensional form by using the scales: mean free path of gas molecules for length, thermal velocity \(V_{th}\) for velocity, and \(T_w\) for temperature and the time values are scaled by the ratio of mean free path and molecular thermal velocity \(\lambda / V_{th}\).

Two types of boundary conditions were considered for maintaining the pressure at the inlet and outlets. The first is by injecting the model particles at a constant rate with a semi-Maxwellian distribution of velocity with zero bulk velocity [18, 19], and the second approach as described below under the subsection approach 2. Several methods of the pressure boundary treatments for the DSMC simulation of microchannel pressure driven flow are discussed in the literature [1, 6, 8, 18]. In the present work, two types of approaches have been implemented corresponding to a given pressure at the open boundaries.
2.1. Approach 1
At the open boundaries, the particles are injected according to a ‘semi-Maxwellian velocity distribution with zero bulk velocity for particle flux at a constant’ as [18, 1]:

\[
\frac{\dot{N}}{A} = n V_{mp} \frac{\exp(-q^2) + \sqrt{\pi} q[1 + \text{erf}(q)]}{2\sqrt{\pi}}
\]  

Where, \(q = \frac{V - \bar{V}}{V_{mp}}\), \(V_{mp}\) is the most probable velocity, \(A\) is the area of an element. A particle would be removed from the list of particles whenever it is supposed to leave the computational domain via open boundaries.

2.2. Approach 2
In this approach the treatment of the upstream boundary is different from the downstream boundary. The first Monte Carlo (MC) sweep in approach 2 is the same as approach 1, and for all subsequent MC sweeps the rate of the incoming particles is calculated using equation 1 using an updated speed of the flow.

2.2.1. Upstream boundary. It is based on the first-order extrapolation to determine the inlet mean velocity from the flow inside the computational domain [21, 8]. At the upstream boundary, the pressure \(p_{in}\) and temperature \(T_{in}\) are the given parameters to the flow and the number density \(n_{in}\) could be obtained from the equation of state as following:

\[
n_{in} = \frac{p_{in}}{k T_{in}}
\]  

The velocity components are updated after every MC sweep as:

\[
(u_{in})_m = u_m
\]
\[
(v_{in})_m = v_m
\]
\[
(w_{in})_m = w_m
\]

Where the subscript \(m\) denotes average cell values and the subscript ‘\(in\)’ signifies the inlet boundary.

2.2.2. Downstream boundary. At the downstream boundary, the approach is similar to the one developed by Wang and Li [8], based on the given flow parameter, pressure \(p_e\) at the exit. The other mean properties of the flow are to be determined from the preceding calculations, using the following equations

\[
(p_e)_m = \rho_m + \frac{p_e - p_m}{\rho_m \sigma_m^2}
\]
\[
(u_e)_m = u_m + \frac{p_e - p_m}{\rho_m \sigma_m}
\]
\[
(v_e)_m = v_m
\]
\begin{align*}
\left( w_s \right)_m &= w_m \\
T_s &= \frac{p_s}{(\rho u)_m R}
\end{align*} \tag{9, 10}

\( a_m \) is the local sound speed, and \( \rho \) is the density. The equations 6, 7, 8, and 10 are similar to the one developed by Wang and Li \[8\].

The first approach of treatment of boundaries with a ‘semi-Maxwellian velocity distribution with zero bulk velocity for incoming particle flux at a constant rate’ has been one of the simplest for implementation. However, the flow properties predicted by it are less accurate at the boundaries when used with the short channels, however, for an aspect ratio of 1/60 and of lower value they give an acceptable result as shown in figures 1, 2 and 3.

3. Validation: comparison with the SIMPLE-TS

First the DSMC simulations were performed using the approach 1, maintaining the pressure by injecting the model particles at a constant rate with a semi-Maxwellian distribution of velocity with zero bulk velocity at both the inlet and outlet. The DSMC simulations were carried out for a case of straight channel for an outlet pressure of 5025.547 Pa, and for inlet pressure of 15784.7 Pa (chosen from an experimental measurement) giving rise to the ratio of pressures as 3.1409 \[20\]. The corresponding outlet mean free path was used (by K Shterev et al) in the finite volume based SIMPLE-TS calculations, for an inlet to an outlet pressure ratio of 3. The DSMC simulations were carried out with the temperature of the walls and I/O boundaries at 297.15 K.

Figure 1.a shows the comparison of the pressure profile along the channel and along the normal directions in the middle section, for an aspect ratio of 1/60, the slightly higher value of the pressure predicted by the DSMC could be due to the higher pressure applied at the inlet. Figure 1.b shows a zoom of the comparison of the pressures obtained from both the methods near the inlet.

Figure 2 shows the comparison of the \( u \), the x-component of velocity along the centreline of the channel along the flow direction. The value predicted by approach 1 for the pressure boundary treatment slightly differs from the SIMPLE-TS calculations near the outlet. It falls short to predict the same level of gain in the velocity component \( u \) as that of the SIMPLE-TS by some observable an amount. However, a more careful investigation is required to quantize this deviation.

Figure 3 shows the temperature profiles obtained using the DSMC method for an aspect ratio 1/60, applying semi-Maxwellian boundary condition with zero bulk velocity. The temperature was largely the same along the channel.
Figure 1.a: A three dimensional DSMC based code validation with finite volume SIMPLE-TS method with pressure boundary with semi Maxwellian velocity distribution with zero bulk velocity, for straight channel of aspect ratio 1/60, comparison of pressure profiles.

Figure 1.b: A zoom of the figure 1.a near the inlet, comparison of the non-dimensional pressures along the channel, obtained from three dimensional DSMC simulations with finite volume SIMPLE-TS method; DSMC results using boundaries with semi Maxwellian velocity distribution with zero bulk velocity, for straight channel of aspect ratio 1/60
Figure 2: comparison of centerline $u$, the $x$-component of velocity obtained using DSMC and SIMPLE-TS methods, and $v$, $w$ ($y$ and $z$ components of velocity) for straight channel of aspect ratio 1/60, using semi-Maxwellian boundary condition with zero bulk velocity.

Figure 3: Temperature profiles obtained using the DSMC method for aspect ratio 1/60, semi-Maxwellian boundary condition with zero bulk velocity.
4. Application of approach 1 to the bend micro-channel

We apply the approach 1 (a semi-Maxwellian distribution of velocity with zero bulk velocity for injection of particles at both the inlet and outlet, and injecting the particles at a constant rate) to a 90 degree bend micro-channel with the length of each leg of the channel equal to the height 19.83e-6m and also the width equal to the height. In this case the centreline distance between the inlet and outlet is 3 times the height of the micro-channel. The pressure applied at the outlet $p_{out}$ is equal to 1e4 Pa and the pressure applied at the inlet $p_{in}$ is 3e4 Pa.

The figure 5.a shows the streamlines obtained from the gas flow through the bend micro-channel, applying outlet pressure 1e4 Pa, and inlet pressure 3e4 Pa, using the height of the micro-channel at 19.83e-6 m and with the centreline length of 3 times of the height, and width equal to the height. The stream is branching out means the flow is expanding and is compressible. Figure 5.b shows the corresponding cone plot. It also shows that the flow has the highest value of speed at the outlet.
Figure 6: $u$, $v$, $w$ (x, y and z components of velocity) for the gas flow through sharp 90 degrees bend micro-channel, at mid section along the z direction;

For $p_{out}=1e4Pa$, $p_{in}:p_{out}=3$,

$H=19.83e-6m$, the colour bar shows values in m/sec.

Figure 6 shows the surface plots of $u$, $v$, $w$ (x, y and z components of velocity) for the gas flow through bend micro-channel, on the middle section along the z direction. It can be seen that the flow velocity is the highest at the outlet, which in the present case is about 0.6 mach. The surface plots for $u$ and $v$ show that the flow speeds up along the channel.

5. DSMC results using the approach 2 for the boundary conditions
The following are the results from the DSMC simulation using the approach 2 for a pressure boundary condition at the inlet and outlet.

Figure 7.a shows $u$, $v$, $w$ (x, y and z components of velocity), for the gas flow through straight channel of aspect ratio 1/36 for a ratio of inlet to outlet pressures 3,1409, there is an improvement of in the prediction of the velocity component $u$ at the outlet. The other components of velocity $v$, and $w$ are (fluctuating) around zero, along the channel as expected. The temperature (figure 7.b) was largely the same along the channel, but for some cooling near the outlet.
Figure 7.a: $u$, $v$, $w$ ($x$, $y$ and $z$ components of velocity) along the channel, for the gas flow through straight channel of aspect ratio 1/36 for a ratio of inlet to outlet pressures 3.1409

Figure 7.b: temperature along the channel, and normal to the flow direction at 90 percent of the channel length along both the normal directions, for the gas flow through straight channel of aspect ratio 1/36 for a ratio of inlet to outlet pressures 3.1409

Figure 8.a shows the $u$ ($x$ components of velocity) along the channel, for the gas flow through straight channel of aspect ratio 1/36 for a fixed ratio of inlet to outlet pressures 2.4, for various conditions of outlet $Kn$, the various $Kn$ were obtained by varying the pressure at the outlet. The figure 8.a shows that the flow velocity changes with the (outlet/inlet) rarefaction (or $Kn$) and it also shows the percentage gain in the velocity is along the channel is almost the same for the range of $Kn$ considered 0.043÷0.087. The figure 8.a shows that the flow velocity has a maximum around the $Kn$ 0.0553 in the range of $Kn$ considered.

Figure 8.b shows that the non-dimensional pressure along channel obtained, for the gas flow through straight channel of aspect ratio 1/36 for a fixed ratio of inlet to outlet pressures 2.4, for various conditions of outlet $Kn$, the pressure profile is similar for the range of $Kn$ considered.
Figure 8.a: $u$ along the channel, for the gas flow through straight channel of aspect ratio 1/36 for a fixed ratio of inlet to outlet pressures 2.4, for various conditions of outlet.

Figure 8.b: centerline pressure along the channel, for the gas flow through straight channel of aspect ratio 1/36 for a fixed ratio of inlet to outlet pressures 2.4, for various conditions of outlet.

6. Conclusions

DSMC simulations were carried out in three dimensions considering two basic elements: straight channel and 90 degrees bend micro-channel. The simulations were carried out for straight channel for various aspect ratios and for different inlet and outlet conditions.

A comparison of the results from the DSMC simulation with the results from the finite volume method SIMPLE-TS was performed, considering a short micro-channel of aspect ratio 1/60.

Two types of pressure boundary treatments were implemented using DSMC method in three dimensions. The first approach was using a ‘semi-Maxwellian velocity distribution with zero bulk velocity for the incoming particle flux’ with particles injected at a constant rate and the second approach was based on the mean properties of the incoming flow being determined from the preceding calculations inside the computational domain.

The flow structure around the bend was shown for a short bend micro-channel, the flow expansion and compressible behaviour was shown using the streamlines and cone plot.

It was shown that the flow velocity changes with the (outlet/inlet) rarefaction (or $Kn$) and it also shows the percentage gain in the velocity along the channel is almost the same for the range of $Kn$ considered 0.043÷0.087.

The flow velocity has a maximum around the $Kn$ 0.0553 in the range of $Kn$ considered 0.043÷0.087, for short micro-channels of aspect ratio 1/36, with the height of the micro-channel equal to width, for height equal to 19.83e-6m. The pressure profile along the channel was similar in the range of $Kn$ considered.
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