Physical Aspects of Rarefied Gas Flow in Micro to Nano Scale Geometries Using DSMC

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Rarefied gas flow in micro/nano electro mechanical systems (MEMS/NEMS) does not perform exactly as that in macro-scale devices. The main goal in this study is to investigate mixed subsonic-supersonic flows in micro/nano channels and nozzles and to provide physical descriptions on their behaviors. We use DSMC method as a reliable numerical tool to extend our simulation. It is because the DSMC provides accurate solution for the Boltzmann equations over the entire range of rarefied flow regime or Knudsen numbers. As is known, the appearance of oblique/normal shocks at the inlet of a channel or a nozzle adds to the complexity of internal flow field analyses. We found some very unique physical aspects of micro/nano flows including mixed supersonic-subsonic flow regimes in constant area ducts and the attenuation of emitted shocks, which are attributed to the strong viscous forces and dominant rarefaction effects in micro/nano scales. We simulated nozzle flow under different flow conditions including different Knudsen and Reynolds numbers and inlet-outlet pressure ratios. It was observed that as the Knudsen number increases, the viscous dissipation forces increase and the flow in nozzle would not be choked at its throat and no supersonic flow is observed in the divergent part. Contrary to the classical gas dynamics, no shock stands in the divergent part despite specifying a back pressure at the outlet. Alternatively, we observed that multiple expansion-compression waves would be generated and amplified as the back pressure was decreased.

I. Introduction

Micro and nano channels are widely used in Microelectromechanical and Nanoelectromechanical Systems (MEMS and NEMS). In order to enhance the design and performance of such systems, it is mandatory to achieve a deeper understanding of flow and heat transfer behavior through them. The magnitude of gas rarefaction is known as a main parameter to assess such systems if the Knudsen number is sufficiently high [1-2]. In such conditions, the solutions have to be established based on the kinetic principles such as those in treating the Boltzmann equation. However, the exact solution of the Boltzmann equation can be derived for a limited number of free-molecular flows and simple geometries. Thus, the non-equilibrium gas flow problems occurring in complex geometries need the numerical treatments of the Boltzmann equation. However, the complexity in Boltzmann equation promotes the use of alternative tools such as direct simulation Monte Carlo (DSMC). It is claimed that the DSMC is one of the most successful particle simulation methods in treating rarefied gas flows [3].

The DSMC method has been widely used to simulate both supersonic and subsonic micro flows. Oh et al. [4] coupled DSMC with monotonic Lagrangian grid (MLG) to study the supersonic flow behavior in microchannels. They specified the back pressure at the outlet benefiting from a virtual region outside the channel. They applied the variable hard sphere (VHS) model [3] to simulate the molecular collision and simulated the flow at three Knudsen numbers of 0.07, 0.14, and 0.19. Their results showed that the downstream variable magnitudes would qualitatively agree with those of Fanno theory. They also found that the velocity slip and temperature jump would increase at the

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channel entrance as Kn increases. Le et al. [5-6] studied the flow and heat transfer in high speed gas flows through 2-D microchannels imposing zero and non-zero back pressures. They observed that the subsonic flow would appear near the outlet region if the applied back pressure was lower than the ordinary exit pressure in a full supersonic flow case. Additionally, the flow temperature and wall heat transfer rate showed rapid increase at the channel outlet due to energy conversion from the kinetic form to the internal one. Titove and Levin [7] used a collision limiter method called equilibrium direct simulation Monte Carlo (eDSMC) to simulate high pressure flows in nozzle and embedded-channels. Providing sufficient number of collisions, the eDSMC method predicted the simple inviscid compressible flow field behavior properly. They concluded that eDSMC would be an alternative tool to solve the Euler equations and potentially the Navier-Stokes (NS) equations under high pressure gradients and small viscous conditions.

The development of DSMC was initially engaged with the simulation of high speed rarefied gas flows. The extension of DSMC algorithm to solve low speed flows requires the proper boundary condition implementations at the outlet section and the inclusion of pressure impact on the velocity of molecules adjacent to the outlet section. Liou and Fang [8] used the characteristics theory to implement the back pressure condition. They simulated flow in simple and patterned microchannels with suitable accuracy [9]. Roohi et al. [10-11] simulated channel flows with different Mach regimes and discussed different possible choices to simulate the choked flow in micro/nano scale channels.

Another basic component of micro/nano systems is the convergent-divergent nozzle. Micro/nano nozzle flow usually experiences different rarefaction regimes, i.e., it experiences continuum and slip regime at the convergent part while the transition and free molecular regimes may occur at the divergent part and the nozzle exit. The DSMC have been generally applied to simulate fluid flow in micro-nozzles with a wide range of rarefaction regimes. Indeed, DSMC has been largely used to predict the flow field inside micronozzles [12, 14-19].

Alexeenko et al. [12] applied DSMC to simulate continuum flow in axi-symmetric and three dimensional micronozzles flows. They observed that the viscous effects dominate the gas expansion and thrust reduction would occur due to significant wall shear stresses. They investigated the effect of tangential momentum accommodation coefficient magnitude on the flow behavior and showed that the flow would weakly depend on this coefficient when it was increased from 0.8 to 1. Louisos and Hitt [13] used the NS equations and studied the geometrical effects on the micronozzle performance. They reported a remarkable reduction in nozzle thrust as the angle of micronozzle divergent parts was increased over 30 degrees. They reported that the subsonic boundary layer would restrict the flow and would reduce the effective exit area. In another attempt, Alexeenko et al. [14] extended a coupled thermal-fluid analysis (finite element-DSMC) to study the performance of high temperature MEMS-based nozzles. They obtained the temporal variation of the nozzle temperature and gas flow fields. In addition, they reported the operational time limit for thermally insulated and convectively cooled nozzles. Liu et al. [15] used DSMC and NS equations with slip boundary conditions and simulated nozzle flows. They studied the effects of inlet pressures, Reynolds number and the micronozzle geometry and reported that the continuum-based results would show obvious deviations from the DSMC results once Kn exceeds 0.045. Xie [16] simulated low Knudsen number micronozzle flows using DSMC and NS equations solvers. He examined the dependence of mass flux on the pressure difference. He also reported the occurrence of multiple expansion-compression waves in the nozzle’s divergent section. Titove and Levin [17] proposed a collision-limiter method, i.e., equilibrium direct simulation Monte Carlo (eDSMC), to extend the DSMC to high pressure small-scale nozzle and channel flows. The eDSMC calculations captured the nozzle compression waves having suitable agreement with the high-order Euler flow solutions. Xu and Zhao [18] used the NS equations and the slip wall boundary conditions to simulate nozzle flow subject to a back pressure. They studied the structure of shocks at low Knudsen numbers. They found that the viscous effect would be the key parameter in shock wave formation and its structure within the micronozzles. Louisos et al. [19] reviewed the key findings obtained from the computational studies of supersonic micronozzle flows using either the continuum-based or kinetic-based techniques. They reported that the combination of viscous, thermal and rarefaction effects on the microscale flow would considerably affect the flow behavior in supersonic micronozzle flows. They described different aspects of rarefaction effects on the nozzle performance. They reported that the thermal non-equilibrium, i.e., the delay in the rotational and vibrational energy relaxations, would decrease the performance of micronozzle flows with low Reynolds numbers.

The objective of this work is to provide a deeper understanding of flow and heat behaviors in subsonic and mixed supersonic-subsonic regimes in micro/nanoscale channels and nozzles. We investigate the behavior of flow in micro/nanoscale channels under mixed supersonic-subsonic flow conditions. We also study the effects of wall temperature distribution on the flow field behavior in such circumstances. We also provide a deeper understanding of the flow fields in the convergent-divergent micronozzle geometries. We investigate the effects of back pressure, Knudsen number, and gas-surface interaction on the micronozzle behavior. We discuss the correct position, where
back pressure should be applied. We use DSMC method to simulate micro/nano flows over a wide range of rarefaction regimes confidently.

II. The DSMC Method

The DSMC method is a numerical tool to solve the Boltzmann equation based on direct statistical simulation of the molecular processes described by kinetic theory. This method is considered as a particle method. Each particle represents a large bulk of real gas molecules. The primary principle of the DSMC method is to decouple the motion and collision during a time step $\Delta t$ into two sequential stages of free-molecular movement and then collision. Implementation of the DSMC method requires to break down the computational domain into a collection of grid cells. The size of each cell should be sufficiently small to result in small variation in thermodynamic properties within each cell. The cells are divided into sub-cells in each direction. Sub-cells are then utilized to facilitate the selection of collision pairs [3]. After fulfilling all molecular movements, the collisions between molecules are simulated in each cell independently. In the current study, VHS collision model is used and the choice of collision pair is done based on the no-time counter (NTC) method [3]. The NTC scheme makes the computational time proportional to the number of simulated particles. The following procedure is followed to solve a stationary problem using DSMC. An arbitrary initial state of gas is specified in the entire computational domain and the desired boundary conditions are imposed. After achieving the steady flow condition, the sampling of molecular properties within each cell is fulfilled considering sufficient time period to avoid statistical scatterings. All thermodynamic parameters such as temperature, density, and pressure are then determined from the time-averaged data.

III. The Inlet and outlet boundary conditions

The one-dimensional wave theory indicates that there are three incoming characteristic waves responsible to propagate the information into a channel flow if the flow is supersonic at the inlet. Normally, the inlet Mach, temperature, and density magnitudes are specified there. However, the variables at the outlet are extrapolated from the interior domain. On the other hand, we need specifying one incoming characteristic wave at the outlet in the numerical simulation of channel flow with a specified pressure, say $p_e$, at its outlet. In DSMC, all the three flow parameters, i.e., density, temperature, and velocity must be specified for incoming molecules at the inlet/outlet boundaries. Therefore, the temperature and velocity must be computed using the information from the interior domain. In this regard, we can utilize the 1-D characteristic theory [8, 11]. For a backward-running wave, we consider $du/dx = dp/\rho$, where $\rho$ is density and $a = \sqrt{dp/\rho}$ is the speed of sound. Applying the definition of sound speed in the differential form to a boundary cell, it yields $(\rho_x)_j = \rho_j + (p_x - p_j)/a_j^2$. Using the ideal gas assumption, the temperature can be found from $(T_x)_j = p_j/(\rho_j)_R$ at the outlet. The subscripts $j$ represents the quantities at cell $j$ adjacent to the outlet boundary. Using the characteristic wave equation, the velocity is also computed from $(u_x)_j = u_j + (p_j - p_x)/(\rho_j a_j)$. For a subsonic pressure driven flow, the inlet velocity is also unknown and must be extrapolated from the interior domain. Following Wang and Li [13], the inlet velocity is calculated from $(u_{in})_j = u_j + (p_{in} - p_j)/(\rho_j a_j)$ and the density at the inlet is calculated from the equation of state $(\rho_{in})_j = p_{in} / (RT_{in})$.

IV. Wall and Symmetry boundary conditions

The channel walls are treated as diffuse reflectors using the full thermal accommodation coefficient, i.e., $\alpha=1$. The velocity of reflected molecules is randomly determined based on the one-half range Maxwellian distribution. It is determined using the wall temperature as it follows

$$
\begin{align*}
    u &= \sqrt{-\log(RF(0))} \ V_{mpf} \sin(2\pi \cdot RF(0)) \\
    v &= \pm \sqrt{-\log(RF(0))} \ V_{mpf} \\
    w &= \sqrt{-\log(RF(0))} \ V_{mpf} \cos(2\pi \cdot RF(0))
\end{align*}
$$

(2)

where $V_{mpf} = \sqrt{2RT}$ is the most probable speed of molecules at the wall temperature. The positive and negative symbols correspond to the lower and upper walls, respectively. Reflection from a symmetry boundary is considered specular, i.e., the normal velocity component is being reversed while the tangential component remains unchanged.
V. Results and Discussions

To implement more realistic inlet boundary conditions, we consider 10% of the wall at the entrance region of the channel as a specular reflector. Due to a symmetric flow condition, we only simulate one-half of the domain. We set 20–25 molecules in each cell at time zero. Each of them has a thermal velocity and a randomly defined location.

A. Mixed supersonic-subsonic flow regime

In this case, we have nitrogen flow through a channel with an aspect ratio of 5 with transition regime status, Knin=0.43, Min=4.15, Tw=500 K, and a vacuum outlet condition. Figure 1 shows Mach, temperature, pressure, and normalized pressure gradient ($\frac{\mathbf{M}}{\nabla p}$) maps. Figure 2 shows the distributions of the above parameters along the channel centerline. Although the specified Mach at the channel inlet is 4.15, Figure 2(a) shows that the inlet Mach rapidly drops to 1.8 due to a series of normal/oblique shock waves at the channel inlet. The Mach reduction continues along the channel, becomes subsonic, and stays subsonic until around X/L=0.95. From Fanno theory, which corresponds to friction dominated flow in constant area ducts, it is known that if the channel becomes longer than a specific magnitude, which reflects the choking condition, the upstream condition changes from a supersonic condition to a subsonic one to meet the correct mass flow rate fed into the domain. Therefore, it is impossible to impose supersonic flow with an inlet Mach number of 4.15 for the current inlet Mach and Knudsen number specifications. It should be noted that the physics of flow in the channel is substantiated by the convective force, pressure gradient, shear stress, normal/oblique shocks and wall heat transfer. Figures 1(b) and 2(a) show that the temperature of the main flow increases over the temperature of its adjacent wall after passing through shocks and this causes gas cooling. From the basic Rayleigh theory, gas cooling can reduce the flow Mach number in subsonic regime. Meanwhile, the shear stress force, which accelerates the subsonic flow to choked flow condition, balances this effect and therefore there is low variation of Mach close to the entrance zone, i.e., around X/L=0.2-0.55. Figure 2(a) shows almost a symmetrical decrease and then increase in Mach from 0.65 to 0.55 and from 0.55 to 0.65, respectively. As the flow approaches the outlet, the flow temperature gradually decreases to the neighboring wall temperature and resulting in a gas cooling circumstances. Consequently, the shear stress increases the Mach number. Near the outlet, there is an expansion because of approaching vacuum pressure condition at the outlet. This expansion is followed by an increase in Mach and a decrease in temperature. The flow at the subsonic region near the wall is not affected by the expansion and therefore the wall temperature remains above the centerline temperature near the outlet, see Fig. 2(a).

Figure 2(b) shows that the pressure distribution performs an increase after the generated shocks. Once the viscous force starts accelerating the flow, the pressure decreases until the flow approaches to the outlet, where the expansion in flow causes further pressure reduction. The normalized pressure gradient contours shown in Fig. 1(d) and its centerline distribution illustrated in Fig. 2(b) clearly show that the normal/oblique shocks would occur at the entrance. Some unique aspects of the rarefied gas flows are clearly observed in this highly non-continuum flow. First, the change from supersonic to subsonic flow is attributed to the oblique shocks, which emanate from the boundary layer. In fact, the normal shocks forming at the entrance only reduce the Mach number from a supersonic one to another supersonic case. Second, the subsonic flow expands to weak supersonic flow at the outlet. These features can be attributed to the strong effects of viscosity in micro/nanoscale channels.

In order to study the effects of heat transfer to the channel on the flow behavior, we increase the wall temperature to Tw=1000 K while the other conditions are not changed. Figure shows Mach and temperature distributions along the channel for this case. Comparing with Fig. 2, there is no more peak in temperature profile near the inlet of channel and the inlet Mach number is subsonic due to stronger shocks at the inlet (Min=0.6). The variation of Mach along the channel centerline shows a decrease up to X/L=0.2 and a region of constant Mach around X/L=0.2-0.4. Next, there is an accelerating region, where the flow becomes supersonic at the channel outlet. It is concluded that the increase of wall temperature from 500 K to 1000 K decreases gas cooling. This can be concluded readily by comparing the variation of flow temperatures near the wall for the two investigated cases with each other. The heat transfer from the subsonic flow rapidly decelerates the flow until the flow temperature adjacent to the wall approaches the wall temperature from X/L=0.4, and the friction force starts accelerating the flow. The flow is accelerated further once the flow reaches the outlet vacuumed section. Figure 3-(b) shows the distributions of pressure and normalized pressure gradient for this test case. It is seen that the inlet pressure increases to 0.18 MPa, while it was 0.054 MPa in the preceding case. This indicates that the inlet shocks are much stronger in the new circumstances.
Fig. 1 Different contour maps in the channel imposing $K_{n_m}=0.43$, $M_{in}=4.15$, and vacuum outlet boundary conditions.
B. Nozzle Flow

We study the effects of back pressure, Knudsen number, and gas-surface interaction on the micronozzle flow behavior. Table 1 provides a summary of the current test cases. Case 1 studies supersonic flow. Cases 2-5 consider the effects of back pressure. We simulate all 5 cases with viscous and inviscid wall boundary conditions. For all the cases, $L_t = 15\ \mu m$, $Kn_{in} = 4 \times 10^{-4}$, and $T_{wall} = T_{in} = 300\ K$. Two columns of data for $Kn_{in}$ are reported, i.e., the first one for viscous and the second one for the inviscid wall case. The Reynolds number, based on the throat height, is only reported for the viscous wall cases.
Table 1. Details of the chosen test cases for the nozzle

<table>
<thead>
<tr>
<th>Case</th>
<th>$P_{back}$ (KPa)</th>
<th>$K_n$ ($\times 10^{-}$)</th>
<th>$Re$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>---</td>
<td>8.01</td>
<td>9.67</td>
</tr>
<tr>
<td>2</td>
<td>7</td>
<td>3.24</td>
<td>6.92</td>
</tr>
<tr>
<td>3</td>
<td>15</td>
<td>1.95</td>
<td>1.63</td>
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<tr>
<td>4</td>
<td>25</td>
<td>1.93</td>
<td>1.13</td>
</tr>
<tr>
<td>5</td>
<td>35</td>
<td>1.01</td>
<td>0.914</td>
</tr>
</tbody>
</table>

C. Supersonic flow
Figure 4(a) shows Knudsen number contours for Case 1. The flow field obtained for this case is typical for supersonic micronozzles. The gas experiences one-order of magnitude rarefaction as it is expanded in the divergent part. The rarefaction is slightly stronger near the wall since the wall heat transfer decreases the density much stronger. In the vicinity of the nozzle exit, the impact of flow rarefaction is again significant. Figure 4-(b) shows the pressure contours. It is observed that the pressure distribution is non-uniform along the $y$-direction, i.e., $dp/dy>0$ in the convergent part and $dp/dy<0$ in the divergent part.

D. Effects of back pressure: Role of Boundary Layer
In this section, we study the effects of back pressure on the micronozzle behavior. The left plots in Fig. 5 show the nozzle Mach contours when back pressure decreases from 35 to 7KPa. For all cases, the flow is choked at the throat. In the divergent part, there are core regions of high Mach number. The number of these Mach cores increases as the back pressure decreases. However, their strengths decay and disappear as the flow approaches the nozzle outlet. Since the pressure at the exit region of nozzle is not uniform, it is mandatory to apply the back pressure at the end of an extended buffer zone. As the back pressure decreases, the first core moves farther from the throat. It is observed that the separated flow exists in a considerable part of the divergent region. The height of unseparated section is approximately equal for the three first cases. Therefore, the flow passes through a conduit with approximately constant rather than passing through a divergent section, see left plots in Fig. 5(a)-5(c). This causes an overall Mach number magnitude reduction at the nozzle exit and decreases the thrust generated. The Mach contours in case (d) are similar to full supersonic case, see Fig. 4, expect near the outlet. Xu and Zhao [18] studied the shock waves in micronozzle flows subject to back pressure at very low Knudsen numbers. In comparison with their results, we observe that the Mach cores are farther from the walls. This is due to a stronger influence of the viscosity/rarefaction at high Knudsen number flows presented here. The core regions disappear via forming a series of oblique/bow shocks. The strength of viscosity does not permit the shocks to approach the wall; therefore, closed high Mach number regions can appear there.

![Fig. 4](image-url) Knudsen number and pressure maps in the nozzle flow.

E. Inviscid walls
In DSMC, the viscosity of fluid is taken into account via simulating the intermolecular and gas-wall collisions. To study the effects of wall boundary layer on the shock waves structures, we consider the gas-wall interactions as an
specular one. Figure 5(right) shows Mach number contours for the back pressures considered in Fig. 5(left); however, imposing specular wall conditions, i.e., the normal velocity component of incident particles is being reversed while the tangential component remains unchanged. Frame (a) shows that slight bow shocks appear right after the nozzle throat. The shock is normal to the walls and to the flow direction. The flow is subsonic in the rest of nozzle. Again, the separation region near the wall is observed. This is due to the fact that the core flow is viscous. If we decrease the back pressure further, the shock moves closer to the outlet section and the separation region diminishes. As the back pressure is reduced further to 7 KPa, the shock waves move outside the nozzle and become oblique.

Figure 5 Mach number maps for different back pressures in nozzle flow with viscous (left) and inviscid (right) condition.
F. Effects of the Knudsen number

Our literature survey illustrates that the past references [6-12] have not investigated the physics of high Knudsen number flows in micronozzles. Figure 6 shows contours of Mach number for the chosen nozzle, however; we increase the inlet Knudsen number to Kn_{in}=0.025. The average outlet Knudsen number is Kn_{out}=0.521 for Fig. 6(a), 0.382 for Fig. 6(b), and 0.244 for Fig. 6(c). Figure 6(a) shows a unique behavior in the nozzle. It shows that the flow accelerates through the divergent region although it is not choked at the throat. Additionally, the Mach number reaches to unity at the exit of buffer zone. The acceleration of subsonic flow in the divergent section is quite unexpected. In fact, it is impossible to establish supersonic flow at this high inlet Knudsen number condition.

Following the increase of Knudsen number, the viscous force dominates in the flow field. Consequently, the dissipation of kinetic energy becomes so high that the flow neither chokes at the nozzle throat nor accelerates to supersonic condition in the divergent section. To confirm the role of viscosity, we simulated the same case; however, imposing inviscid wall conditions, see Fig. 6(b). It is observed that the flow is choked and it consequently accelerates in the divergent part. A series of bow shocks appear at the divergent part. They only change the supersonic flow condition to a lower supersonic flow magnitude.

Figure 6(c) shows Mach contours for the case with a back pressure of 20 KPa. The flow reaches to a maximum Mach number of 0.45 at the throat and is not choked. The subsonic flow decelerates in the divergent part, which is a quite physical behavior for subsonic flow. Therefore, we conclude that the thick viscous boundary layers prevent the formation of supersonic flow at higher inlet Knudsen numbers in the divergent part of nozzle. The observed physics implies that the flow must be subsonic in the nozzle and this requires applying a back pressure at the end of nozzle. It should be mentioned that similar results were observed for nozzle flow cases with higher inlet Knudsen numbers.

VI. Conclusion

Supersonic and subsonic flows in micro convergent-divergent nozzles were simulated using an extended unstructured DSMC solver. It was observed that the flow behavior in micronozzle can be characterized by a mixed impact of rarefaction, compressibility, and viscous forces parameters. The use of a buffer zone far from the nozzle exit allowed us to remove the possible occurrence of nonuniform pressure prediction at the nozzle exit. Applying a back pressure at the outlet, we observed that high viscous force effects would prevent the formation of any normal shock wave in the domain. Instead, we would capture some core regions of high Mach number magnitudes in the domain. These regions would diminish due to formation of bow shocks. In such case, the flow would virtually pass through an approximately constant height conduit rather than an actual divergent geometry/nozzle. It is because a significant part of the flow would separate near the wall. Eliminating the flow viscosity at the walls, we observed
that the thick bow shocks normal to the walls would appear. Meanwhile, the separated region would still stay in the divergent part because the main flow is still viscous. We observed that it is impossible to set up supersonic flow in micronozzles as soon as the inlet Knudsen number exceeds a moderate magnitude. This phenomenon is due to strong viscous forces in the flow field. Alternatively, to obtain a physical solution, it is required to apply a back pressure at the outlet so that a sound physical subsonic flow behavior can be captured in the micronozzle.

References