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DSMC SIMULATIONS OF GASEOUS FLOWS IN MICROCHANNELS

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ABSTRACT

The direct simulation Monte Carlo (DSMC) method is a particle-based numerical modeling technique. Recently it is used for simulating airflow in micro-electro-mechanical-systems (MEMS) where micron-scale features become important and cause the traditional continuum based CFD to fail, even at standard conditions. However, DSMC, as a traditional tool to study rarefied gas dynamics, faces many problems when it is applied to micron-scale geometries related to MEMS devices. For example, DSMC consumes huge memories and long CPU time that can easily be beyond the capacity of latest workstations and supercomputers. It is of significance for a successful DSMC simulation to adjust some critical parameters not only to control the consummation of computational resources in reasonable limitation but also to keep the output accurate.

In this paper, DSMC is used to simulate gaseous flow in a microchannel. The Bird's No Time Counter (NTC) scheme is adopted to determine particle collisions. The Cercignani-Lampis-Lord (CLL) gas-surface model is employed for the interaction between the walls of microchannel and computational particles. Meanwhile a unique method is employed to reproduce the pressure-driven process and to avoid the poor interface treatment. The interactive relationship among some important parameters, such as weight factor, cell sizes, and time step, is discussed. All of them are contributed to the total number of particles that affect the quantities of computational resources consumed. To keep the simulation efficient, a scheme is developed to optimize the parameters.

The gaseous microchannel flow in the slip-flow regime, for which the Knudsen number is less than 0.1, is compared to an analytical solution using the Navier-Stocks equations with slip-velocity boundary condition. In the region near the inlet and outlet, microchannel flow is developing. There is a significant discrepancy on the average velocity and the contour of streamwise velocity between DSMC and the analytical solution. Since the effects of inlet and outlet are not included in the analytical solution, the simulation result should be validated against analytical solution in the computational domain where the effects from the inlet and outlet can be neglected. After the flow is fully developed, the simulation output agrees with analytical result well. The streamwise velocities in microchannel in fully developed region are a function of the distance from inlet unlike the result of traditional macrochannel flow.

Simulations are also carried out under different Knudsen numbers and compared with analytical solution. The deflection of simulation from the analytical data becomes generally clear with the increase of Knudsen number due to the effects of rarefaction. The non-linear pressure distribution along the direction of microchannel is observed. However, the non-linearity becomes less pronounced when the Knudsen number is increased. The results show that for the pressure-driven microflows, the gradient of the pressure along the direction of microchannel dominates the motion of gas in a microchannel.

INTRODUCTION

Studies on Micro-Electro-Mechanical-Systems (MEMS) become more prevalent both in scientific inquiry and commercial applications, such as airbag triggers, micromotors, micro pressure sensors etc. With the increasing demand of micron size mechanical devices, it is of great important to understand the behavior of flows in micro devices.

Precise simulations can predict the fluid effects in micro devices and evaluate the performance of a new micro device before hardware fabrication. Traditionally, the majority of computational and analytical methods for studying fluid flow are based on the Euler or Navier-Stokes equations. For example, computational fluid dynamics (CFD), as the most common simulation method used in macro-scale flowfields, is under the critical assumption that the fluid is treated as a continuum. Unfortunately, the traditional continuum based CFD becomes inaccurate when it simulates the flows around the devices with micron-size features because of the breakdown of the continuum assumption. Such fluid should be treated as a collection of discrete particles rather than as a continuum when the scale length (L) of the flow gradient approaches the average distance traveled by a particle between collisions (the mean free path λ).

The direct simulation Monte Carlo (DSMC) method is a particle-based numerical modeling technique pioneered by G. A. Bird (1994). DSMC models the flow as it physically exists: a collection of discrete particles each with a position, a velocity, and an internal energy etc. These particles are moved and allowed to interact with the surfaces of boundaries, and intermolecular collisions are performed on possibility in small time steps. As the result, DSMC can solve the problems in which the degree of rarefaction in flowfields is high or the characteristic length of scale is small.

The non-dimensional number directing the degree of rarefaction is Knudsen number ($Kn=\lambda/L$). The Kn domain is often divided into four flow regimes (Schaff and Chambre,1958): For $Kn < 0.01$, the traditional continuum assumption is valid, and the Navier-Stokes equations are applicable in their common form. For $0.01 < Kn < 0.1$, known as 'slip-flow' regime, the Navier-stokes equations are applied with the usual no-slip wall boundary condition replaced by a slip-flow boundary condition (Arkilic et al., 1994). DSMC is an attractive method to simulate the flows in this regime due to the distinct effects of rarefaction; For $0.1 < Kn < 3$, known as 'transition' regime, the behavior of flows deflect far from the Navier-Stokes-based analysis. DSMC is an effective tool to study the fluid effects in the flowfield; For $Kn > 3$, known as 'free molecular' regime, the flow is sufficiently rarefied to neglect molecular collisions to be neglected. The collisionless Baltzmann equation is therefore applied.

DESCRIPTION OF DSMC

The computational approximations associated with DSMC method are the ratio of the number of simulated molecules to the number of real molecules and the time step over which the molecular motion and collisions are uncoupled, and the finite cell and sub-cell sizes in physical space. The fundamental requirements are that the linear dimensions of the cells should be small in comparison with the scale length of the macroscopic flow gradients in the streamwise direction, which generally means that the cell dimensions should be of the order of the local mean free path, and the time step should be much less than the local mean collision time. Theoretically, the DSMC becomes more exact when the cell size and the time step tend to zero.

Mean free path

The conventional method to define the mean free path is through recourse using the unrealistic hard sphere model which has as a fixed diameter d and cross section $\sigma = \pi d^2$. The mean free path in an equilibrium gas of number density n is then

$$\lambda = \left(2^{1/2} n\sigma\right)^{-1} \quad (1)$$

The Chapman-Enskog result for the coefficient of viscosity in a had sphere gas at temperature T is

$$\mu = (5m/16)(\pi RT)^{1/2} / \sigma \quad (2)$$

where m is the molecular mass and R is the gas constant. The cross section may be eliminated from Eqs. (1) and (2) to give the standard result

$$\lambda = (16\mu/5)(2\pi RT)^{-1/2} / \rho \quad (3)$$

where ρ is the gas density.

The inconsistency in the above procedure is that the coefficient of viscosity has a fixed temperature exponent of $1/2$, while the real gas coefficient of viscosity

$$\mu \propto T^{\omega} \quad (4)$$

where ω is generally in the range 0.6 to 0.9. Therefore, as an alternative scheme, a consistent definition of the means free path, obtained through the variable cross-section hard sphere (VHS), was introduced by Bird (1983). The mean free path in a VHS is

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

which can account for the real gas temperature exponent of the coefficient of viscosity.

Collision frequency

The mean free path is defined in a frame of reference moving with the stream speed of the gas and is therefore equal to the mean thermal speed $\bar{c}'$ of the molecular divided by the collision frequency, ν i.e.

$$\lambda = \bar{c}'/\nu \qquad (6)$$

The mean thermal speed $\bar{c}'$ in an equilibrium gas at temperature T is given by

$$\bar{c}' = 2/\left(\pi^{1/2}\beta\right) \qquad (7)$$

where $\beta=(2RT)^{-1/2}$ is the reciprocal of the most probable molecular speed.

The combination of Eqs. (6) and (7) gives an expression of the collision frequency at temperature T, i.e.:

$$\nu = \frac{2}{\lambda}\sqrt{\frac{2RT}{\pi}} \qquad (8)$$

Computational time step and total simulated particle numbers

For one of the fundamental requirements, the computational time step (Δt) can be roughly estimated by Δt <<1/ν, i.e., the time step should be much smaller than the mean collision time.

The no-time-counter (NTC) proposed by Bird (1994) for DSMC is a generalized scheme, in which the number of collision pairs (N_p) considered in a given cell is computed through the equation:

$$N_p \propto \Delta t \frac{N_c^2}{n_{ref} V_c} \qquad (9)$$

where V_c is the volume of a cell, N_c is the number of computational particles in the cell, n_{ref} is the simulated number density (the total simulated particles divided by the total simulated volume). NTC can overcome the defects of other generalized schems, such as the time-counter scheme (TC) by Bird and the null-collision scheme (NC) by Koura. The sensitive tests of the schemes for the evaluation of the lower limit of the mean molecular number per cell ($N_{c,min}$) were carried out by Koura (1990) and Kaburaki et al. (1994). The recommended $N_{c,min}$ is between 4 to 30.Considering a DSMC cell of volume V_c in which each simulated molecule represents F_n real molecules, the average number of simulated molecules per cell is:

$$N_c = \frac{nV_c}{F_n} \qquad (10)$$

where n is the number density in the real gas. Therefore the total number of the simulated particles (N_{tot}) is equal to the product of the average number of simulated molecules per cell and the total number of cells in flow field (C_{tot}), i.e.

$$N_{tot} = N_c C_{tot} \qquad (11)$$

One of the aforementioned requirements is that the cell dimension is of the order of the local mean free path. According to above expression, the N_{tot} is restricted by the capability of computational resource. As the linear dimension of the microchannels increases, it becomes computationally impractical to continue to maintain the two requirements: the cell size should be of the order of the mean free path and there should be enough particles in the cell. This means the possible scales of microchannels in which the simulations will be carried out are limited by the capability of the modern workstations or supercomputers. For example, the computational region (30μm×1.12μm) is divided into 300×20×1 sampling cells of which each consists of 2 collision subcells. The total number of simulated particles is about 2.4×10^5, which means nearly 20 particles in a collision subcell. The present calculation is performed on the Cray

J196 supercomputer. When the total number of samplings is 1.3×10^4, the CPU time and memories are approximate 7.12 hours and 100 MB respectively.

Boundary conditions

Modeling the interaction of gas molecules with solid surface plays an important role in the DSMC simulation. But there is no model of gas-surface interaction that is adequate over a wide range of factors for all combinations of gases and surfaces. Some analytical and numerical simulations are based on the assumption of diffuse reflections with full thermal and momentum accommodation (Piekos et al. 1995). Recently, the Cercignani_Lampis_Lord (CLL) gas-surface model (Lord 1990) has been generally accepted in the DSMC simulations

At inlet and outlet, considering the flow 'characteristics' (Piekos et al., 1996), the physical states of particles should be determined to avoid poor interface treatment. This means that some variables at both inlet and outlet should be specified from the states of particles inside the flowfield. For example, to reproduce the pressure-driven flow, the pressures at inlet and outlet should be specified. The most probable molecular thermal volecity of the introduced molecules can be determined in accordance with the temperature at inlet. The velocity components perpendicular to inlet and outlet are assigned to the incoming particles according to the thermal velocity component in the transverse direction. Finally, it is critical to determine the streamwise velocities of the incoming particles from the states of the particles inside the computational region. The optional method is to initialize them as zero at the beginning of the simulation and to specify them every iteration according to the average streamwise velocities of the particles in the cells along the inlet.

RESULT

Analytical and simulated results in slip flow regime

The characteristic length scales, as we know, in MEMS devices are typically on the order of microns. Even at standard conditions, the ratio of mean free path to the characteristic dimension cannot be negligible i.e., the effects of rarefaction is non-negligible.

The investigation of Harley et al (1995) demonstrated the existence of nonzero wall velocity in microchannels and showed the contribution of the nonzero slip velocity on the mass-flow pressure drop relationship. In the investigation of Arkilic et al. (1994), It was assumed that the flow in microchannle was compressible, isothermal, fully developed, and two-dimensional flow. Therefore, the Navier-Stokes equations were solved analytically for a long, isothermal channel in the slip flow regime when the common boundary conditions of non-slip wall are replaced by a Kn-dependent slip-wall velocity condition, given by:

$$u_{wall} = \frac{2-F}{F} Kn \left.\frac{\mathrm{d}u}{\mathrm{d}y}\right|_{wall} \tag{12}$$

where u is the streamwise velocity, Kn is the local Knudsen number, y is the transverse coordinate which is zero at the centerline of the channel, F is the tangential momentum accommodation coefficient which is assumed to vary between zero (specular reflection) and unit (diffuse reflection). In his further analysis, the pressure distribution along the length of the microchannel was expressed as a function of location in the microchannel direction and overall pressure ratio:

$$P_x = -6\sigma Kn_o + \sqrt{(6\sigma Kn_o)^2 + \left(P_i^2 + 12\sigma Kn_o P_i\right)\left(1-\frac{x}{L}\right) + (1+12\sigma Kn_o)\frac{x}{L}} \tag{13}$$

where $P_x = \frac{p(x)}{p_o}$ is the ratio of the local pressure and the outlet pressure, $\sigma = \frac{2-F}{F}$ represents the streamwise momentum accommodation, Kn_o is the outlet Knudsen number, x is the coordination in the channel direction, and L is the channel length. Meanwhile a theoretical streamwise velocity distribution was developed:

$$u = \frac{1}{2\mu}\frac{\mathrm{d}p}{\mathrm{d}x}\left(y^2 - \frac{H^2}{4} - \sigma H^2 Kn\right) \tag{14}$$

where μ is the coefficient of viscosity, and H is the channel height.

After the velocities are normalized by the area-averaged streamwise velocity at the channel exit, the Eqs. (14) is plotted in Figure 1. Several unique features are obvious: For maintance of a constant mass flow, the mean streamwise velocity increase to make up the density drop caused by the decrease of the pressure in the channel direction, which is different from the Pioseuille result at common conditions. And the velocities at walls are nonzero and increase in the streamwise direction.

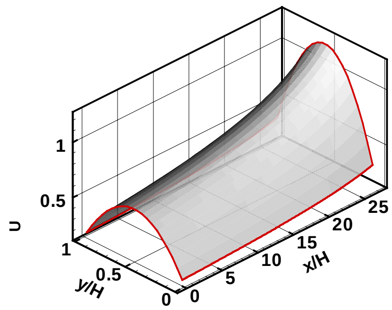

Figure 1 Plot of nondimensional streamwise velocity distribution in microchannel from Eqs. (14). The Knudsen number is 0.06, and the pressure ratio is 2.5

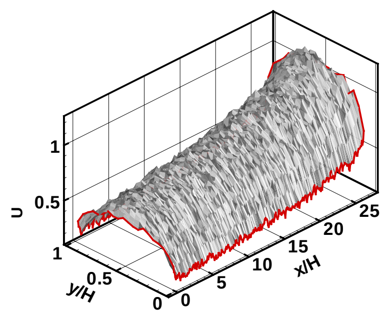

Figure 2 Computed streamwise velocity distribution in microchannel. The Knudsen number is 0.06 and the pressure ratio is 2.5

The DSMC result is presented in Figure 2. Compared with the analytical solution of Arkilic et al, the simulation reproduces the mean flow acceleration and the slip flow predicted by the theory successfully.However, in further comparisons, it is obvious that profiles of the velocity distributions near inlet and outlet are different from above analytical solution in Figure 3 and Figure 4. Considering the Navier-Stokes model's assumptions, there are pressure losses associated with the constriction and expansion of the flow. By stating that the flow is fully developed, it is implied that the entrance length is small enough to be negligible. However, in DSMC simulation, the effects of the inlet and outlet cannot be neglected because the streamwise velocities of the particles that are introduced into the computational region from inlet are uniform. And the quantities are equal to the aforementioned mean streamwise velocities of the particles in the cells along the entrance. This means that the microchannel flow in DSMC begins with a uniform flow. Therefore, the DSMC output shows the effects of inward flow are non-negligible at the entrance region and the assumption of fully developed flow used in Arkilic et al solution is invalid. In Figure 3, the clear deflection of simulated velocity distribution in comparison with the analytical result can be found. Fortunately, the discrepancy between the velocity distributions becomes less when the fluid moves down the channel. After the non-dimensional distance (the x-coordinate is normalized by the channel height H) is greater than 10, the microflow is supposed to be in fully developed region. Good quantitative agreement is obtained between the computational and analytical result as shown in Figure 5 and Figure 6. This agreement can last up to the non-dimensional

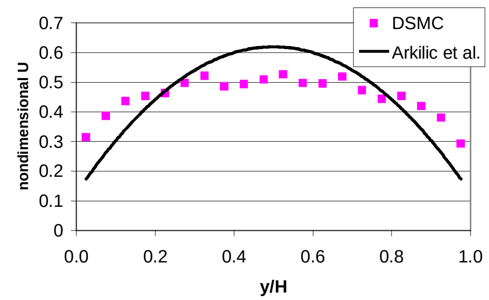

Figure 3 Comparison of simulated and analytical predicted velocity distribution at inlet

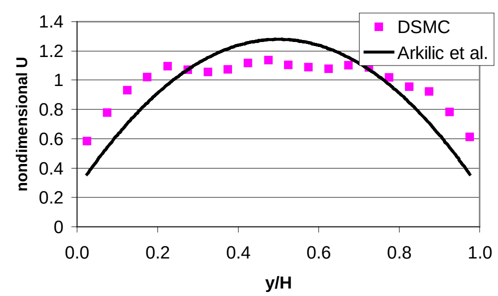

Figure 4 Comparison of simulated and analytical predicted velocity distribution at outlet

distance approximately equal to 25 and is broken again near the exit due to the non-negligible effects of outward flow. Compared with the entrance length, the exit length is short.

Overall, excellent agreement is obtained between the analytical solution of Arkilic et al and the DSMC result in fully developed flow region. The accuracy of DSMC technique is validated. In fact, DSMC provides a technique to study the velocity distributions near the inlet and the outlet where there are no reliable analytical solutions.

Simulated result in transition flow regime

Advantage can be taken of the fact that the DSMC method is valid in all Knudsen number regimes. DSMC is therefore an attractive tool for investigating the effects of rarefaction from slip flow regime (0.01<Kn<0.1) to transition flow regime (0.1<Kn<3). In transition regime, the mean free path is comparable to the characteristic dimension of the flow. The analytical solution of Navier-Stokes equations (even with the slip flow boundary condition) becomes inaccurate. On the other hand, the degree of rarefaction is not high enough to apply the collisionless Boltzmann equation. However, the lack of knowledge of the flow features in transition regime will block the development of MEMS devices which contain regions in both the slip flow and transition regimes.

Simulations are carried out under different Knudsen numbers that are specified as 0.174, 1, and 2.79 respectively.

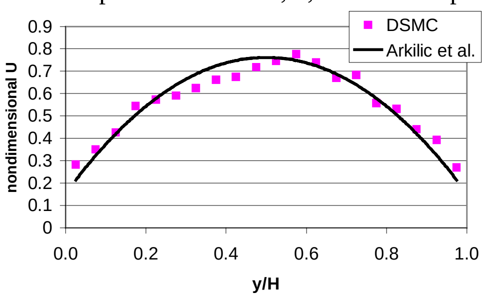

Figure 5 Comparison of simulated and analytical predicted velocity distribution at x/H=10

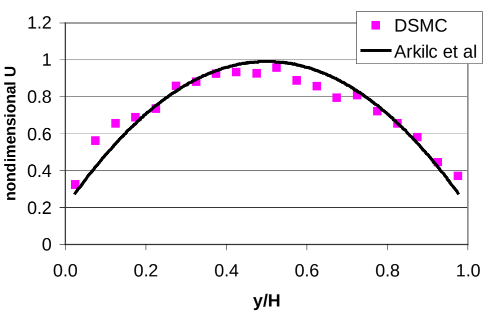

Figure 6 Comparison of simulated and analytical predicted velocity distribution at x/H=20

One of the DSMC results is plotted in Figure 7. To compare with the analytical prediction, the DSMC velocity distribution in the microchannel at x/H=20 is shown in Figure 8.

It is noted that the significant discrepancy between DSMC and analytical solution occurs even in fully developed region in transition regime. The Knudsen number has a stronger influence on the velocity distribution, which cannot be predicted precisely by the solution of the Navier-Stokes equations.

Another interesting result plotted in Figure 9 is the dependence of the velocity distributions upon the increase of the Knudsen number. It shows that the shapes of velocity distributions are much flatter when the Knudsen number is up. The contour of the velocity at Kn = 1 has lost the parabolic feature which can be found at Kn = 0.06. Meanwhile the local maximum velocity is down and the 'slip' velocity is up with the increase of the Knudsen number.

As expected, the non-linear pressure distribution along the direction of microchannel is observed. The simulated pressure distributions are compared with the analytical prediction in Figure 10. With the reference of the continuum curve (Kn=0.0), the non-linearity becomes less pronounced when the Knudsen number is increased. For the pressure-driven microflows, the gradient of the pressure along the direction of microchannel dominates the motion of gas in microchannel. Comparing the velocity distribution in slip flow regime to that in transition flow regime, it is found that the different shapes of streamwise velocity distribution results from the different pressure gradient. So the tendency of increasing pressure curve linearity with increasing rarefaction results in the different shape of velocity distributions from slip flow to transition flow regime.

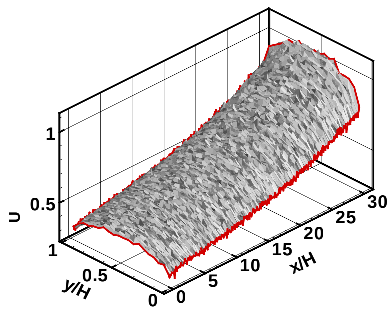

Figure 7 Computed streamwise velocity distribution in microchannel. The Knudsen number is 1.0 and the pressure ratio is 2.5

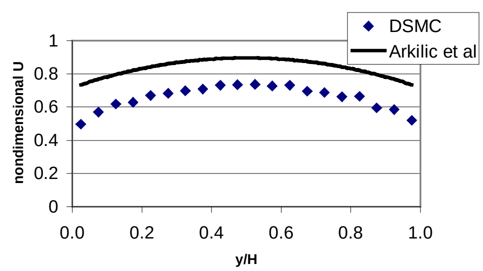

Figure 8 Comparison of the analytical prediction and DSMC computed velocity distributions at x/H=20. The Knudsen number is 1.0

CONCLUSION

The Direct Simulation Monte Carlo method is a powerful tool to investigate the behaviour of flows in microchannels in which some continuum-based fundamental assumptions might break down. A detail description of the DSMC application in microchannel has been presented in this paper.

The DSMC results for a slip flow regime microchannel were compared with the analytical solution of Navier-Stokes equations developed by Arkilic et al(1995). The DSMC result were divided into three regions, which are entrance region, fully developed region, and exit region. The agreement of the analytical prediction and simulated result can be found only in the fully developed region because the effects of inlet and outlet are not included in the analytical solution.

Simulations are also carried out under different Knudsen numbers and compared with

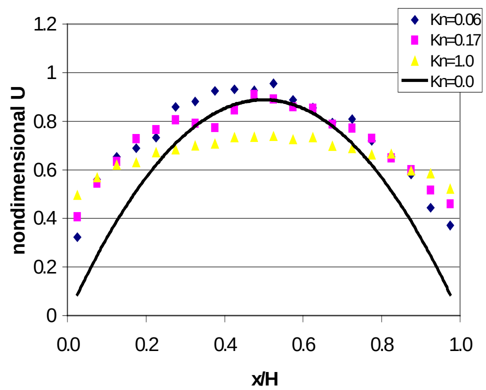

Figure 9 Comparison of the contours of velocity distributions with different Knudsen numbers at x/H=20

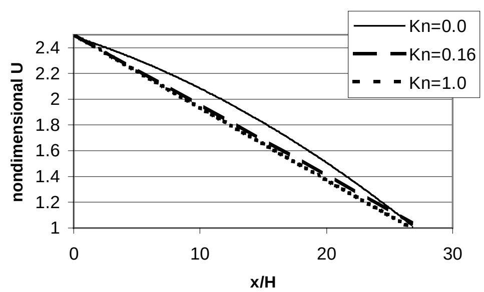

Figure 10 Comparison of pressure distributions with different Knudsen numbers

analytical solution to investigate the effects of rarefaction. The contours of velocity distribution become more flatter and the local maximum velocity is reduced but the 'slip' velocity is increased when the Knudsen different shapes of pressure distribution curves in slip flow regime and in transition flow regime, the velocity distribution shows the unique feature in each regime. It becomes evident that the gradient of the pressure along the direction of microchannel dominates the motion of gas.

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