

# Gaseous Flows and Heat Transfer through Micro- and Nano-channels

Hongwei Sun\*, Pengtao Wang\*, Sai Liu\*, Minghao Song\* and Mohammad Faghri\*\*

\*University of Massachusetts-Lowell, Lowell, MA 01854, [Hongwei\\_Sun@uml.edu](mailto:Hongwei_Sun@uml.edu)

\*\* University of Rhode Island, Kingston, RI 01880

## ABSTRACT

The overall object of this paper is a systematic study of gaseous flows and thermal transport in two-dimensional micro- and nano-channels using direct simulation Monte Carlo (DSMC) method. In the flow study, a validation of DSMC code was conducted by simulating a continuum flow in microchannel and the results show that the discrepancy of friction coefficient from theoretical prediction is well below 5%. Then, the effects of compressibility and rarefaction on the flows were investigated through simulating flows with (a) same outlet Knudsen number (Kn) but different pressure drop ratios (=1.3 and 4.5) and (b) low pressure drop ratio (=1.9) but different Kn numbers (=0.043 and 0.083), respectively. For the situation (a), it was found that the high pressure drop flow (pressure ratio: 4.5) show a 15% higher friction coefficient than that of a fully developed flow while the low pressure drop flow (pressure ratio: 1.5) is consistent with incompressible flow prediction. The inspection for the velocity profile development shows that when pressures drop increase along the channel, the center-line velocity become flatten and the velocity gradients near the wall are higher compared with parabolic velocity profile. However, for the situation (b), the rarefactions actually reduce the friction coefficients by 22% (Kn: 0.083) and 36% (Kn: 0.043). An apparent velocity slips along the channel wall exist for both flows. We also studied gaseous flows in microchannels with different surface roughness. The DSMC results show that both relative surface roughness and roughness distribution play very important roles in microchannel flows. High magnitude and densely distributed surface roughness induce higher friction coefficient than that of smooth channels.

In the thermal transport study, we simulated gaseous flows in micro/nano channels under uniform wall temperature (500K) boundary condition. Both temperature distribution and the effects of rarefaction on Nusselt number (Nu) are discussed by comparing with those of fully developed flows.

**Keywords:** DSMC, thermal transport, gaseous

## 1 INTRODUCTION

The rapidly emerging Microelectromechanical Systems (MEMS), Nanoelectromechanical Systems (NEMS), and other microscale devices with applications in diverse fields such as molecular biology, space propulsion, particle physics, require a fully understanding of flows in micro- and nano- scales to achieve desired performance. The governing equations based on continuum assumption may become inaccurate to describe their flow behaviors and the simulation technologies based on molecular or atomic interactions like Molecular Dynamics (MD), DSMC etc. become very powerful. The flow chart in Fig.1 clearly illustrates their relationships between these technologies [1].

The Knudsen number (Kn), which is the ratio of the mean free path to the characteristics length of a system, is commonly used to define different gas states. When Kn is in the range of 0.01 to 0.1, the flow is in the slip flow regime where the continuum-based equations with the slip flow boundary condition are valid. For Kn in the range of 0.1 to 3, the flow is in the transition regime where the continuum flow theory is not valid. For Kn >3, the flow is in the free molecular regime where the collisionless Boltzmann equation can be used to predict the flow behavior.

The DSMC method of Bird [2] is a well-developed technology. This technique models thousands or millions of “simulated molecules” activities to obtain a description of gas flows. A detail description is followed. Researchers have been using DSMC to simulate flows in microscale devices and acquire a large amount of valuable results [3-8]. In these simulations, the molecules were reflected either specularly or diffusely from the wall surface depending on the assumption of surface conditions. However, research by Davis [9], on a rarefied gaseous flow in channels with one corrugated wall show lower values of flow rate than if the wall were diffusely reflected. Another study by Usamo et. [10] reported a large reduction of flow conductivity caused by surface roughness in the transient region using DSMC. Our experiment also shows that not just inter-molecular behaviors are important, physical situations of microchannel surface play an important role [11]. Therefore, the overall object of this paper is a systematic study of gaseous flows in two-dimensional micro- and nano-channels in terms of the effects of compressibility, rarefaction, and surface roughness which are usually

neglected in conventional flow analysis, using direct simulation Monte Carlo (DSMC) method.

## 2 METHODOLOGY

DSMC method was developed by Bird in earlier 1960s and is a particle-based simulation method that is based on molecular chaos of kinetic theory. In DSMC, a small number of simulated molecules, which represent a large number of real molecules, are used to reduce the computational requirement. Molecular movement and collisions are uncoupled by using a small time step on the order of a fraction of mean collision time. It consists of four primary processes: 1) particle movement, 2) particle indexing, 3) cross-referencing, and 4) collision simulation and sampling of the flow field. These are described in detail by Sayegh et al. [7].

In the process of particle movement, the distance traveled by a molecule is obtained by the product of the molecular velocity and the time step. The new position of a molecule determines if it passes to an adjacent cell, or reflects from the wall boundary, or collides with another molecule, or exits from the flow field. The molecules in the flow field are then indexed and cross-referenced prior to the modeling of the collisions and the sampling of the flow-field. The so-called No Time Counter (NTC) method is used to determine the number of the molecular pairs (NP) for the collisions as follow:

$$NP = \frac{1}{2} N_{smc} N_{smc} \bar{R}_{r,s} (\sigma_T c_r)_{\max} \frac{dt}{V_{cell}}$$

Where  $N_{smc}$  represents the number of simulated molecules in a cell and  $R_{r,s}$  is the ratio of real molecules to simulated ones.  $\bar{\sigma}_{\square}$  is the total collision cross section and  $c_r$  is the relative speed velocity. The interactions of the molecular pairs are described by the Variable Hard Sphere (VHS) model. The  $\bar{\sigma}_{\square}$  and  $c_r$  are calculated in this model by:

$$c_r = (u_r^2 + v_r^2 + w_r^2)^{1/2}$$

Where

$$u_r = (2Rf - 1) \cdot c_r$$

$$v_r = (1 - (2Rf - 1))^{1/2} \cos(2\pi Rf) \cdot c_r$$

$$w_r = (1 - (2Rf - 1))^{1/2} \sin(2\pi Rf) \cdot c_r$$

and

$$c_r \sigma_T = \left[ \frac{\{ 2kT_{ref} / (m_r c_r^2) \}^{\omega-1/2}}{\Gamma(5/2 - \omega)} \right]^{1/2}$$

$Rf$  is a random number.  $k$  is Boltzmann constant and  $T_{ref}$  reference temperature.  $m_r$  is the reduced mass of molecule.  $\square$  is an empirical constant. The collisions between molecules and the wall are modeled using the diffuse reflection model that assumes the molecules are reflected

from the wall surface according to the Maxwell distribution. Finally, the macroscopic variables such as pressure and temperature are calculated by sampling the microscopic variables such as molecular position and velocity.

### 2.1 Parameters Calculation

The pressure is calculated using an ideal gas equation that is based on the gas number density,  $n$ , and the absolute temperature,  $T$ , as:

$$P = nkT \quad (1)$$

The DSMC results revealed that the pressure is uniform over the depth of the channel when the flow is fully developed. Therefore, only the centerline pressure is presented in this research.

The friction coefficient is obtained by two different methods. In the first method, it is obtained from DSMC simulation results using the following expression:

$$f_D = \frac{D_H}{\Delta L} \frac{P_2 - P_1}{0.5 * (\rho_2 u_2^2)} \quad (2)$$

where the  $P_1$  and  $P_2$  are pressures at two points,  $\Delta L$  is the distance between these two points and  $\rho_2$  and  $u_2$  are density and average velocity at point 2. In the second method, the friction coefficient is calculated based on the slip flow theory for incompressible fully developed flow between parallel plates [12]. The Navier-Stokes equation is solved with slip boundary condition to obtain an expression for the friction coefficient. The momentum accommodation coefficient is assumed to be 1.0, which is reasonable for most engineering surfaces:

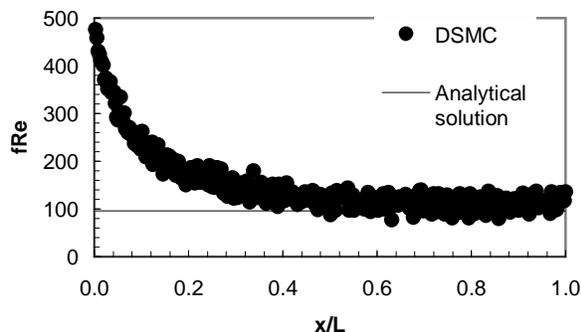
$$f_L = \frac{96}{(1 + 6Kn) Re} \quad (3)$$

## 3 SIMULATION AND DISCUSSION

The modeled microchannel with surface roughness is sketched in Fig. 2. The "surface roughness" is modeled by an array of rectangular blocks. The geometry is described by the "roughness" height ( $\epsilon$ ), the distance between "roughness" ( $s$ ), the channel height ( $H$ ), and the channel length ( $L$ ). The Kn number is defined as  $\lambda/H$  where  $\lambda$  is the mean free path of gas molecules. Relative surface roughness and roughness distribution are characterized by the ratios of  $\epsilon$  to  $D_h$  ( $D_h$  is hydraulic diameter,  $=2H$ ) and  $\epsilon$  to  $s$ , respectively.

In order to check the accuracy of the DSMC method, nitrogen continuum flow through a smooth channel with an aspect ratio ( $=L/H$ ) of 1.5 was simulated and the friction coefficient results are reported in Fig. 1. The solid line in this figure represents the value of  $fRe$  based on a fully

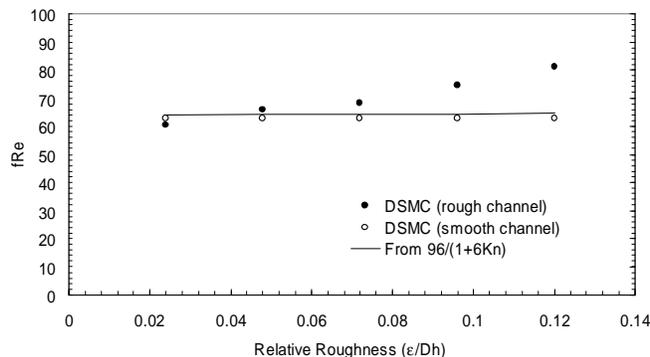
developed flow between parallel-plates. In spite of the fluctuation due to DSMC's statistical nature, there is a good agreement between the DSMC results and the continuum flow theory. The maximum average error is less than 5 percent.



**Fig. 1 Comparison of DSMC results with analytical results [12]**

### 3.1 Effects of Surface Roughness on Flows

To highlight the effect of surface roughness, several cases with low Mach number ( $Ma < 0.2$ ) and similar  $Kn$  ( $Kn \sim 0.08$ ) have been performed to minimize compressibility and rarefaction effect. It has been shown the effect of compressibility is negligible for a short microchannel when  $Ma$  is lower than 2.0 [12]. The DSMC results for the production of friction factor and Reynolds number ( $fRe$ ) versus relative surface roughness ( $\epsilon/D_h$ ) are plotted in Fig. 2. In the mean time, the prediction results from slip flow theory ( $f_D Re$ ) (Eq. 3) are also presented as a comparison. The value of  $\epsilon/D_h$  ranges from 2.4% to 12%. As seen in this figure, the slip flow theory accurately predicts the incompressible nitrogen flow in smooth microchannel and its results show good agreement with DSMC results.



**Fig.2 Friction coefficient results for nitrogen flow in smooth and rough channels**

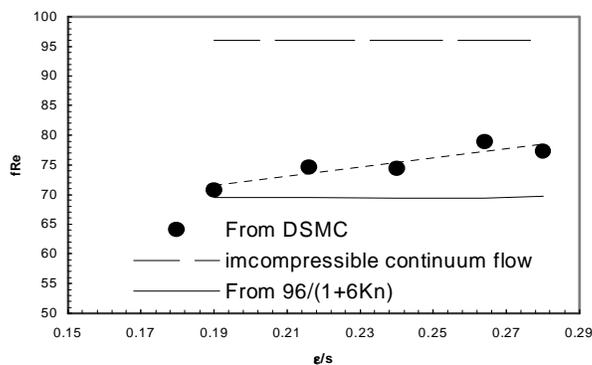
However, for nitrogen flows in rough channels under the similar conditions, the friction coefficient increase with

surface roughness. The increase in friction coefficient reaches as high as 26.5% while the  $\epsilon/D_h$  increasing from 2.4% to 12%. The velocity fields for  $\epsilon/D_h$  of 2.4%, 7.2% and 12.5% are also presented in Fig. 5. When the  $\epsilon/D_h$  is small (2.4%), the nitrogen flows smoothly through the roughness except for two small recirculation zones behind and in front of the “roughness” block. With the increases in  $\epsilon/D_h$ , one large recirculation zone is formed as the replacement of two small ones, as shown in case (b) and (c). It is believed that the increase of 26.5% in  $fRe$  is mainly due to the formation of recirculation zone when the  $\epsilon/D_h$  increase up to 12%.

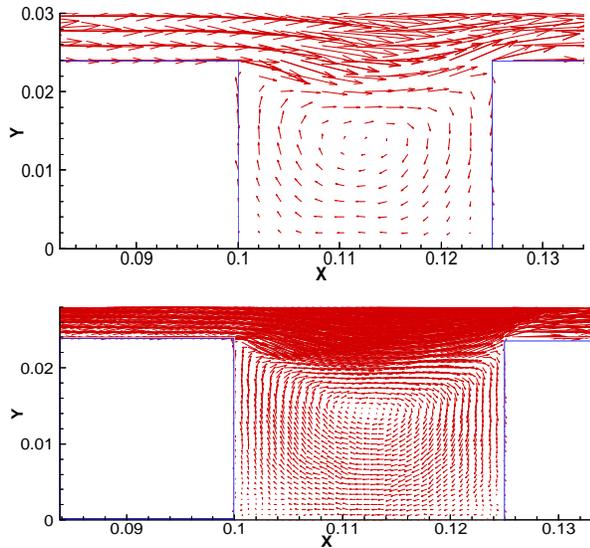
### 3.2 Effects of Rarefaction on Flows

When the characteristic length in the channel is comparable to gas molecular mean free path, which is characterized by an appreciable value of  $Kn$ , the interaction between molecules and wall become important. This change can be reflected on the change in  $fRe$ . A microchannel with relative surface roughness of  $\epsilon/D_h = 12\%$  and distribution of  $\epsilon/s = 0.48$  was chosen for studying the effect of rarefaction while  $Kn$  change from 0.02 to 0.08.

The inlet velocities are adjusted to reduce compressibility effect so that  $Ma$  is below 0.02 for all cases. The  $fRe$  versus  $Kn$  is shown in Fig. 3 which shows that  $fRe$  decrease as  $Kn$  increase. It means that surface roughness effect become less important for high  $Kn$  flows. The main reason may be that the interactions between gas molecules and channel walls are reduced for high  $Kn$  flows. At the same time, the momentum transport between molecules is also smaller for rarefied gas than gas under normal condition. The Fig. 4 is the amplified flow fields for cases of  $Kn=0.02$  and  $Kn=0.08$ . It is apparent that a large recirculation zone existed between roughness blocks. The recirculation zone causes the additional pressure loss and further increases the value of friction coefficient.



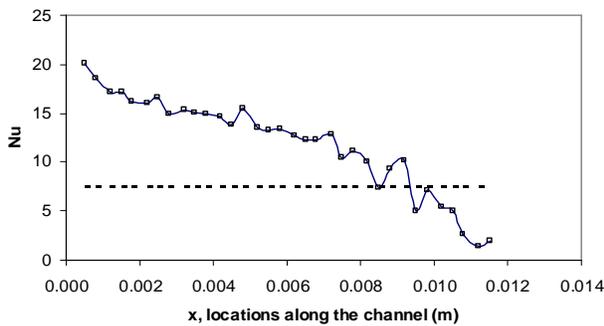
**Fig.3 Friction coefficient vs  $Kn$  in rough channel**



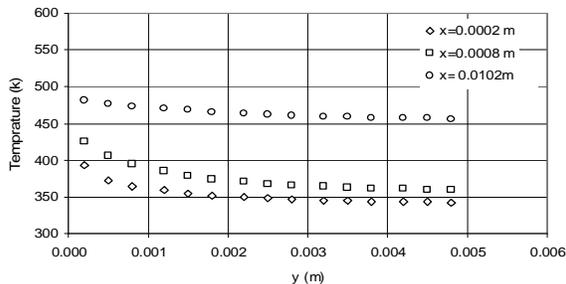
**Fig. 4** Flow velocity fields for  $\epsilon/D_h=12\%$  and  $\epsilon/s= 0.48$  for Kn of 0.02 (up) and 0.08 (down)

### 3.3 Effects of Rarefaction on Thermal Transport

To study rarefaction effect on thermal transport in micro- and nano- channels, we simulated nitrogen flow through a microchannel with constant wall temperature of 500K. The value of Kn is 0.11, which lies in slip flow region. The variation of local Nusselts number (Nu) and temperature profiles along the microchannel is shown in Figs. 5 and 6.



**Fig. 5** Local Nusselt number along microchannel



**Fig. 6** Temperature profiles at three locations

In the developing flow region, the Nu is high. But in fully developed region, instead of maintaining a value of 7.54 which is predicted by conventional continuum flow theory, the Nu continue decreasing until the gas temperature reach wall temperature, which is apparently the result from rarefaction. More cases are being simulated to quantify the Kn effect.

## FERENCES

- [1]Gag-el-Hak, "Flow Physics", MEMS handbook, CRC, 2001.
- [2]G. Bird, "Molecular Gas Dynamics and the Direct Simulation of Gas Flows, Oxford Science Publications, 1994.
- [3] E. S. Piekos and K. S. Breuer, Numerical Modeling of Micro-channel Devices Using the Direct Simulation Monte Carlo Method, *Journal of Fluid Engineering*, Vol. 118, pp. 464-469, 1996.
- [4] C. K. Oh, E. S. Oran, R. S. Sincovits, Computations of High-speed, High Knudsen Number Micro-channel Flows, *Journal of Thermophysics and Heat Transfer*, Vol. 11, No. 4, pp. 497-505, October-December 1997.
- [5] C. K. Oh, R. S. Sinkovits, B. Z. Cybyk, E. S. Oran, J. P. Boris, Parallelization of Direct Simulation Monte Carlo Method Combined with Monotonic Lagrangian Grid, *AIAA Journal*, pp. 1363-1370, 1996.
- [6] C. Mavriplis, J. C. Ahn and R. Goulard, Heat Transfer and Flow Fields in Short Micro-channels Using Direct Simulation Monte Carlo, *Journal of Thermophysics and Heat Transfer*, Vol. 11, No. 4, pp. 489-496, 1997.
- [7] R. Sayegh, M. Faghri, Y. Asako and B. Sundén, Direct Simulation Monte Carlo of Gaseous Flow in Micro-channel, *Proc. of the ASME National Heat Transfer Conference*, Albuquerque, NM, August 15-17, 1999.
- [8] W. Liou and Y. Fang, Heat Transfer in Microchannel Devices Using DSMC, *J. Microelectromech. Systm*, 10, pp. 274-279, 2001.
- [9] D. H. Davis, L. L. Levenson, and N. Milleron, Effect of "Rougher-than-Rough" Surfaces on Molecular Flow through Short Ducts, *Journal of Applied Physics*, Vol. 35, No.3, pp.529-532, March 1964.
- [10] M. Usami, T. Fujimoto, and S. Kato, Mass-flow Reduction of Rarefied Gas by Roughness of a Slit Surface, *Trans. Jpn. Soc. Mech. Eng.*, B, pp.1042-1050, 1988.
- [11] Stephen E. Turner, Hongwei Sun, Mohammad Faghri and Otto Gregory, Gas Flow Through Smooth and Rough Micro-channels, *Twelfth International Heat Transfer Conference*, Grenoble, France, August 18-23, 2002.
- [12] Hongwei Sun, Mohammad Faghri, Effects of Rarefaction and Compressibility of Gaseous Flow in Micro-channel Using DSMC, *Numerical Heat Transfer*, Part A, 38:153-168, 2000.