DSMC Modeling of Rarefied Flow through Micro/Nano Backward-Facing Steps

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Abstract
In this study we use direct simulation Monte Carlo (DSMC) method to simulate subsonic nitrogen flow through micro/nanoscale backward-facing step. This paper investigates the effect of Knudsen number on the fluid and thermal behavior of the step geometry. We observed that increasing the Knudsen number makes remarkable variations in flow behavior such as decreasing in average flow Mach number and increasing in average flow temperature. Our results showed that variations in flow and thermal field properties are more sensible at low Knudsen number. Also the results show that increasing Knudsen number decrease the length of separation zone behind the step. Additionally, gas flow becomes more uniform at higher flow Knudsen number.
Keywords: *Direct simulation of Mont Carlo, rarefied gas flow, step flow, Knudsen number*

Introduction

Over the last several decades the improvements in performance and shrinkage of device size have been dominant driving forces in micro/nano electronics to promote scientific and economic progress. There has been significant progress in the developments of gaseous micro/nano electro mechanical systems (MEMS / NEMS) for measurement and manipulation at the molecular and atomic levels [1]. Consequently, a true understanding of the thermal behavior of rarefied micro/nano gas flows is crucial for an optimal design, fabrication, and operation of MEMS/NEMS. Rarefied gas condition usually occurs in aerospace and micro-nano scales applications. The aerospace application occurs at high altitudes. Alternative application is the usage in micro and nano scales devices such as micro-nano systems. Fast progress in micro/nanoscale devices has drawn the attention of many workers to extend suitable numerical tools to analyze nanoscale flows through basic geometries, e.g., channels, backward-facing steps, and nozzles, more accurately. However, the flow in such scales can be rarefied.

The flow and heat transfer in such narrow channels usually cannot be dealt with continuum models because the molecular mean free path is not negligible compared with the characteristic lengths. Accordingly, they must be treated as rarefied-gas flows and heat transfer should be modeled based on kinetic theory.

One of the most important parameter in rarified gas is Knudsen number. Knudsen number, defined as the ratio of gas mean free path to the characteristic length of the geometry, $Kn=\lambda/L$, is the main parameter indicating gas flow rarefaction. Hypersonic flows fall into rarefied flow regimes due to small mean free path while micro/nano systems belongs to rarefied condition due to the small size of the geometry. The flow is considered as a continuum one when $Kn < 0.001$. For large $Kn > 10$, the molecular density is low and there are very few collisions between gas molecules. Most collisions occur only at the boundaries of the geometry. This regime is called as free-molecular regime. The continuum flow is governed by the Navier-Stokes equations (NS), whereas the free molecular flow is governed by the collisionless Boltzmann equation. Between the free molecule regime and the continuum regime, in the range $0.001<Kn<10$, there are the two regime called the slip and transition regime where both kinds of collisions occur, i.e. wall-molecule and inter-molecule interactions. Slip regime occurs at $0.001<Kn<0.1$ while transition regime occurs at $0.1<Kn<10$. The classification of flow regime based on Kn number is shown in Fig 1.

For a dilute gas there exist more efficient particle-based simulation algorithms. A popular method is direct simulation Mont Carlo (DSMC), introduced by Bird in early 1970s [2]. DSMC uses a stochastic algorithm to evaluate collision probabilities and scattering distributions in accordance with kinetic theory.

One of the conventional geometry in microscale is step geometry. This geometry is conventional in micro fluidic devices and medical instruments. Nowadays lab-on-chip is one of the important applications of MEMS which consists of microchannels. Micro/nano steps are especially appear where microchannels with various diameter should be connected to each other.

Some researcher had investigated step geometry. Lee et al [3] investigated a microchannel with a 90 degree turn at the channel centre. These channels are very similar to step geometry in separation zone. They tried to survey the effect of geometry on separation zone. They found that the largest separation zone occurs at miter bend. Raju et al. [4] investigated microscale flow in a channel with two 90 deg bends. They surveyed the effect of considering slip velocity on the wall. They found that slip velocity reduces

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separation zone and increase mass flow. Bao et al. [5] surveyed similar microscale backward facing step flow in transition regime. They used continuum based Burnett equations. These equations are limited with the Knudsen number and they are not useful at very high Knudsen numbers. Also Oztop et al [6] investigated the effect of Reynolds number on double step geometry. Although these results are so worthy, but their work was not a complete study which investigates Knudsen number effect on the separation zone and flow parameters.

In this paper, we present the results of our DSMC simulations for the rarefied step flow and investigate the effect of Knudsen number on the flow/thermal field inside the step geometry. We investigate the effect of Knudsen number on two essential parameters: temperature and Mach number variations. Also we survey the effect of Knudsen number on the separation zone and the length of this region. We tried to investigate a wide range of Knudsen number (Kn=0.01 up to Kn=10).

DSMC method

The direct simulation Monte Carlo DSMC is a numerical tool to solve the Boltzmann equation based on the direct statistical simulation of the molecular processes described by the kinetic theory. The primary principle of the DSMC is decoupling of the stages of motion and collisions for all simulated particles. DSMC is considered as a particle method in which one particle represents a large number of real gas molecules. After fulfilling all molecular movements, collisions between molecules are simulated separately in each cell of the grid covering the computational domain.

For decades DSMC technique has been regarded as a powerful numerical method for studying rarefied gas dynamics problems. The DSMC technique uses a finite set of model particles denoted by their positions and velocities, $\{xi , \xi i\}$, $i = 1, \ldots ,N$ that move and collide in a computational domain to perform a stochastic simulation of the real molecular gas dynamics. The basic concept of the method is built on a discretization in time and space of the real gas dynamics process and splitting the motion into two successive stages of free molecular motion and binary intermolecular collisions within the grid cells in each time step. DSMC method is a direct simulation algorithm for rarefied flow based on kinetic theory. It simulates gas flow as a collision of discrete particles with various position, velocities, and energies.

In DSMC each simulated particle represents a large number of real molecules with the same properties. During the simulation, the molecular motions and intermolecular collisions are performed over small time intervals which are smaller than the mean collision time. The macroscopic quantities such as flow velocities, densities, and temperatures are calculated through sampling the microscopic quantities of all the particles in the computational domain.

The macroscopic quantities such as flow velocities, densities, and temperatures are calculated through sampling the microscopic quantities of all the particles in the computational domain. In Figure 2, one can see the flowchart of DSMC method.

All of the results presented in this section are for a micro/nano step geometry which has a length to height ratio equal to 5, and an step ratio equal to 2. Our geometry is single step geometry. It is a pressure driven channel and pressure ratio is equal to 2. The gas moving through the channel is rarefied. Temperatures of all of walls are constant and they are equal to 300 K. The gas which moves through the channel is nitrogen. Figure 3 shows the convergence of mass flow rate at the inlet and outlet of nanochannel for case1. In this case Knudsen number is 0.01. We continued our simulation even after meeting convergence criterion. This helps to suppress the statistical DSMC errors more effectively. We also performed a grid independency activity to finalize the suitable grid sizes in our simulations. Figure 4 shows the pressure distributions on the lower wall of the geometry achieved using Grid 1 (100×60 cells), Grid 2 (200×120 cells), and Grid 3 (300×180 cells). It is observed that Grid 2 and Grid 3 provide similar pressure distributions. Therefore, we continue our study using Grid 2.

We study different test cases in order to elaborate the micro/nano flow behavior in subsonic regimes. This paper investigated the effect of the Knudsen number on the flow parameters of the micro/nano step flow.

Results and discussion

We consider four test cases. These cases are different in Knudsen number. They are named case1, 2, 3and 4 for Kn=0.01, 0.1, 1 and 10. Figure 5 shows the effect of Kn number on mach number of channel at the end of channel(X/L=1). In this figure, horizontal vertex shows Y/H that H is the height of nano step geometry, and vertical vertex shows Mach number at this section.

As it shown, increasing Knudsen number decrease average Mach number at this section. It is obvious that increasing Knudsen number makes less variation at this section and so the flow is more uniformly with increasing Mach number. The variation of Mach number is more sensible at low Knudsen number (For example Kn=0.01). At case 3 and 4 (Kn=1 and 10) there are similar Mach number and so Knudsen number does not effect on flow behavior at high Knudsen number. Also this trend is shown in figure 6 which shows the Mach number at whole of the nano step geometry. The other lengths in this figure are non dimensionalized with the BF step height. As is seen, the maximum separation length is for the slip flow Case with Kn=0.01. However, it is observed that the length of separation region slightly decreases as the flow Kn number increases from the top limit of slip flow regime (Kn=0.10) to the low limit of free-molecular regime (Kn=10.0). The first reason for this phenomenon is the decrease of Reynolds (Re) number with the increase of Kn number. As the Re number decreases, the viscous forces become more dominant

and consequently the length of separated region would decrease. The second reason is attributed to the rarefaction effects, which causes the velocity slip at the walls. Therefore, the flow adjacent to wall gets a lower chance of separation.

Figure 7 shows the velocity profile on the lower wall of the geometry where separation zone occurs. The separation zone is where velocity profile is negative and one can see that increasing Knudsen number, decrease the length of separation region.

Figure 8 shows the temperature contour at X/L=0.3. As it shown at high Knudsen number the flow regime is more uniform and it is obvious that high Knudsen number can not affect temperature profile. We does not show Kn=1 in this figure, because the result for Kn=1 is really similar to Kn=0.1 and Kn=10. Figure 9 also shows the temperature profile at whole of the channel. Although in figure 8 we speak about a special section (X/L=0.3), but one can see the same behavior at all of the geometry in the figure 9.

Conclusion

As it shown the simulations of micro/nano BF step flow demonstrate that the length of separation region considerably decreases as the flow influences more in the transition regime. However, the variations in the flow properties are much slower in the mid-transition and free-molecular regimes compared with the slip and early transition regimes.

Additionally in this paper we survey the effect of the Knudsen number in other specifications of the flow such as the velocity and temperature contours. These effects are not so sensible at high Knudsen number. Our results showed that increasing Knudsen number cause nitrogen gas more uniformly and there are not a really big gradient at high Knudsen number.

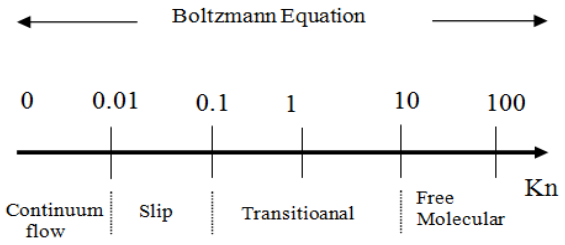

Fig. 1: Classification of flow regime based on Knudsen number

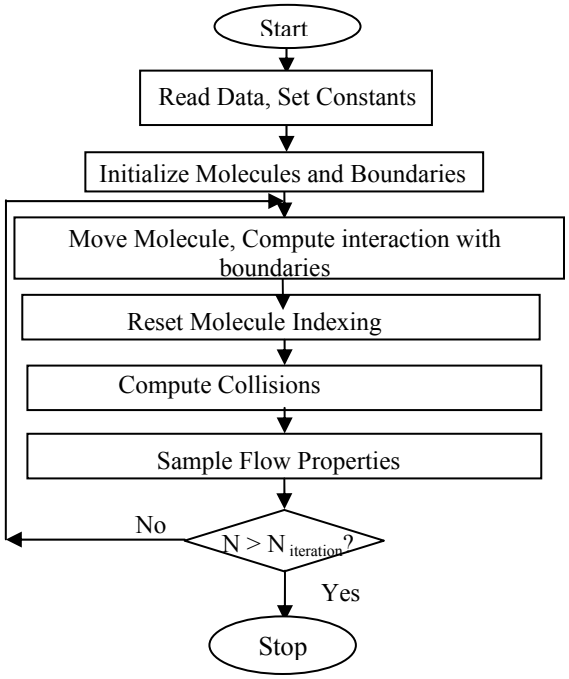

Fig.2: Flowchart of DSMC

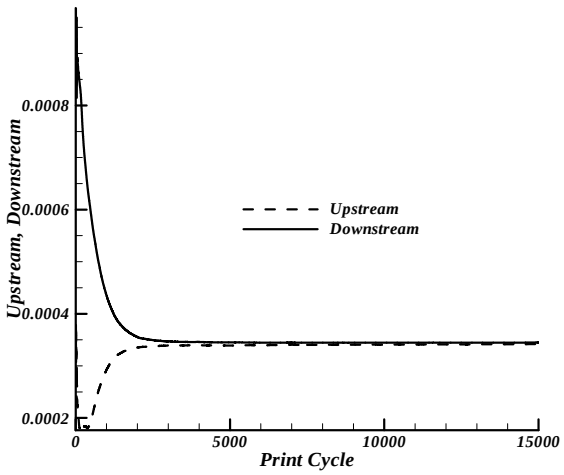

Fig.3: Convergence of mass flow rate

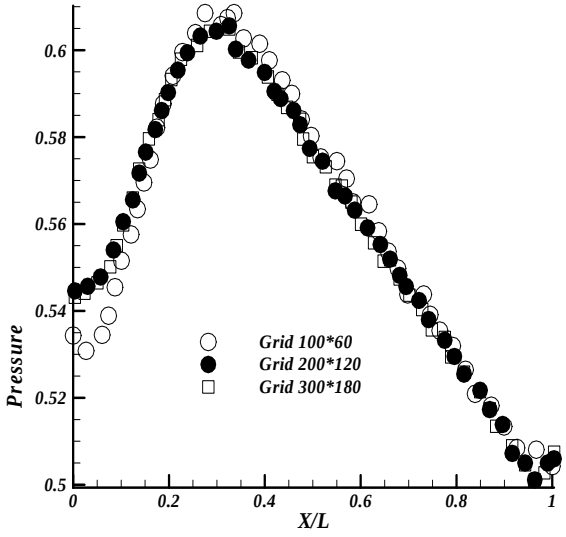

Fig.4: Grid study effect

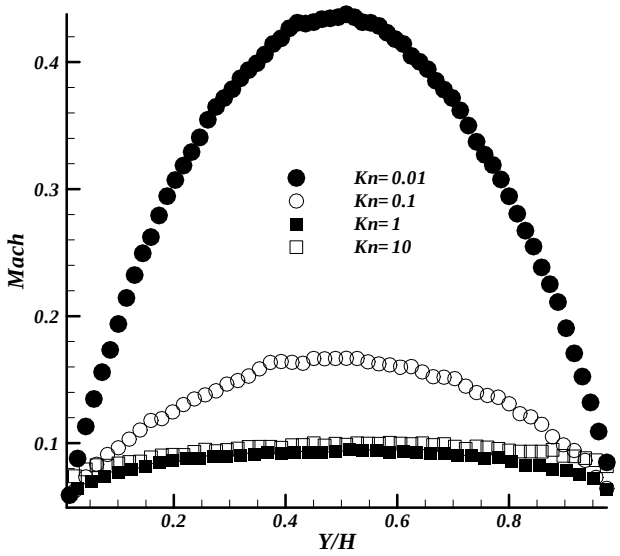

Fig.5: Mach number at X/L=1

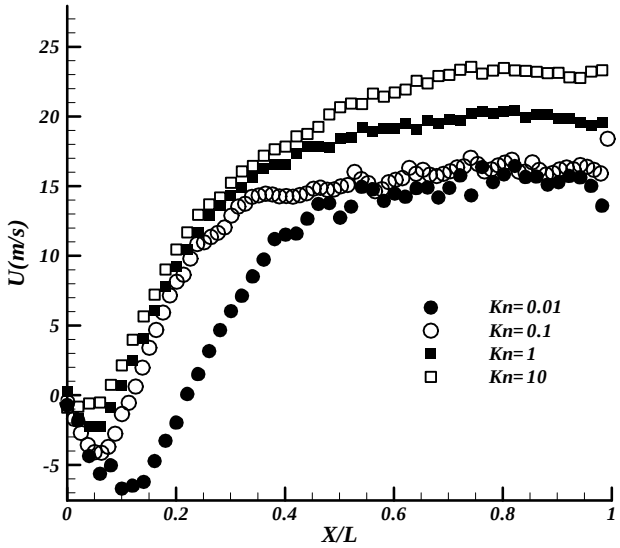

Fig.7: velocity profile over the lower wall

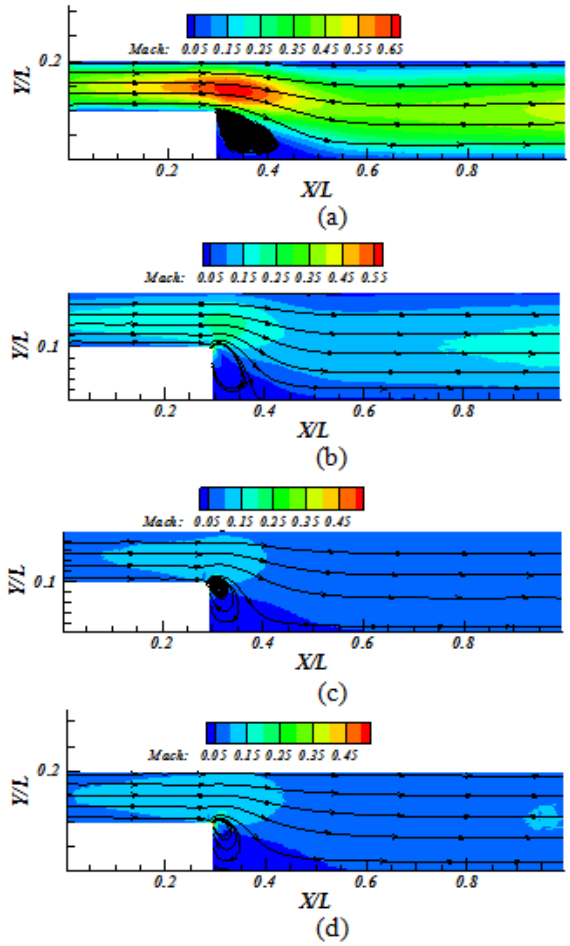

Fig.6: Mach number contours in step geometry at different Knudsen numbers a) Kn=0.01 b)Kn=0.1 c)Kn=1 d)Kn=10

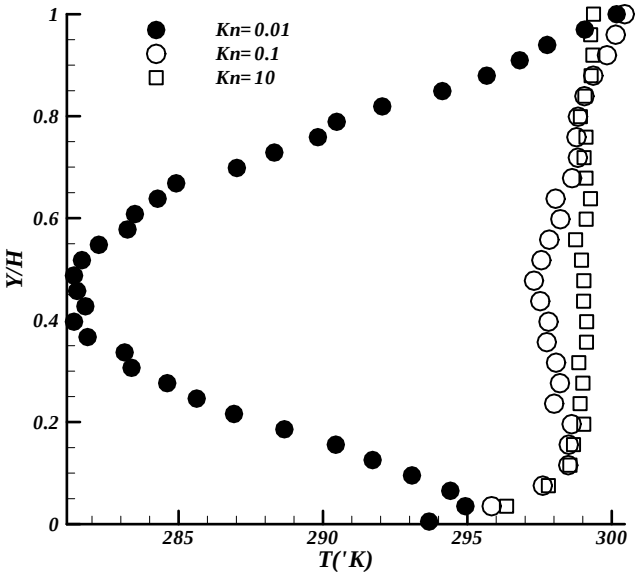

Fig.8: Temperature profile at X/L=0.3

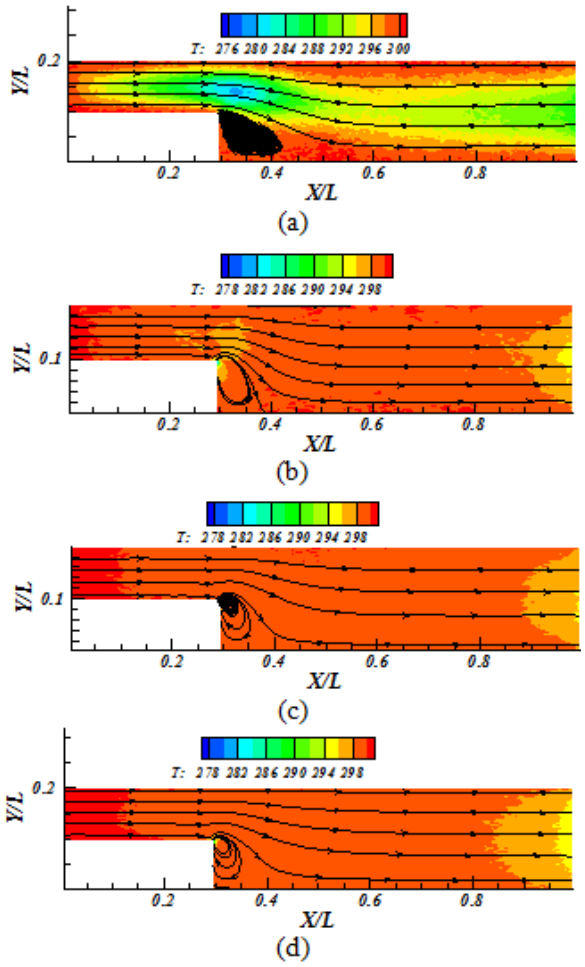

Fig.9: Temperature contours in step geometry at different Knudsen numbers a) Kn=0.01 b)Kn=0.1 c)Kn=1 d)Kn=10

References

1- Ho C. M. Tai Y. C., Micro-Electro-Mechanical Systems-and Fluid Flows, *Annu. Rev. Fluid Mech*., Vol. 30, 579–612, (1998).

2- Bird G.A., Molecular Gas Dynamics and the Direct Simulation of Gas Flows, *Oxford. U.K,* (1994)

3- Lee S. Wong M. Zohar Y., Gas flow in micro channels with bends. *J. Micromech. Microeng.* 11 (2001) 635–644

4- Raju R. and Roy S., Hydrodynamic Model for Microscale Flows in a Channel With Two 90 deg Bends. *Journal of Fluids Engineering.* (2004)vol 126.489-492

5- Bao F. and Lin J.Z., Continuum Simulation of the Microscale Backward-Facing Step Flow in a Transition Regime. *Numerical Heat Transfer*, (2011) Part A, 59: 616–632,

6- Oztop H. Mushatet K. Yilmaz I., Analysis of turbulent flow and heat transfer over a double forward facing step with obstacles. *International Communications in Heat and Mass Transfer* 39 (2012) 1395–1403

7- Huaang W. and Bogy D.B., Three-dimensional direct simulation of Mont Carlo method for slider air bearings. *Phys.Fluids*. (1997),9(6):1764-1769

8- Beskok A., "validation of a new velocity-slip model for separated gas microflows: *Numerical Heat transfer* (2011) Part B(40) 451-457

9- Sun H. Faghri M., "Effect of rarefactionand compressibility of gaseous flowin microchannel using DSMC" *Numerical Heat Transfer* (2000)153-168

10- Alexander F J. Garcia A L. Alder B J., "Direct simulation Mont Carlo For thin-film bearings". *Phys.Fluids*. (1994), 6(12):3854-3860

11- Darbandi M. Roohi E., "DSMC simulation of subsonic flow through nanochannel and Micro/Nano backward facing steps", *International communication in Heat and Mass transfer* (2011) pp:1-6

12- Wang M. Li Z. "Simulations for gas flows in Microgeometries using the direct simulation Monte Carlo method", *International Journal of Heat and Fluid Flow* 25 (2004) 975e985.

13- Kubotera H. Lmamura T., "Mont Carlo simulations of air shielding effect on lubricant transfer at the head disk interface" *American Institute of Physics*. (2009),94(24)

14- Akhlaghi H. Roohi E. Stefanov S. "A new iterative wall heat flux specifying technique in DSMC for heating/cooling simulation of MEMS/NEMS." *International journal of Thermal science* 59(2012) 111-125