# Particle number per cell and scaling factor effect on accuracy of DSMC simulation of micro flows

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Received December 2003
Revised October 2004
Accepted October 2004

## Abstract

**Purpose** – This paper aims to give some guidance on the selection of particle numbers per cell and the number of molecules per particle in the micro flow simulation by using DSMC method.

**Design/methodology/approach** – The numerical investigation is performed to study the effects of particle number per cell and the scaling factor of real molecules to a simulated particle on accuracy of DSMC simulation of two-dimensional micro channel flows in the "slip flow" and "transition flow" regimes.

**Findings** – Numerical results show that both the particle number per cell and the scaling factor have effect on the accuracy of the DSMC results from the statistical error and the physical aspects. In the "slip flow" regime, a larger value of scaling factor can be used to obtain accurate results as compared to the "transition flow" regime. However, in the "transition flow" regime, much less number of particles in each cell can be used to generate accurate DSMC results as compared to the "slip flow" regime.

**Research limitations/implications** – The present work is limited to the two-dimensional case.

**Practical implications** – The results of this paper are very useful for the two-dimensional micro flow simulation by DSMC.

**Originality/value** – The work in this paper is original and provides guidance on micro flow simulation.

**Keywords** Flow, Channel flow, Numerical analysis, Monte Carlo simulation

**Paper type** Research paper

## Introduction

As development of micro-electro-mechanical-systems (MEMS), there is an increasing demand for predicting and optimizing their functionalities and features before they are manufactured. Fluid effect plays an important role in determining the features of MEMS. Since the size of most micro devices is in the micron level, the flow in MEMS is usually called micro flow. For this case, the mean free path of molecules approaches the characteristic length of the device, and the continuum assumption of flow may not be valid. In general, the rarefaction of a fluid can be classified by Knudsen number, $Kn = \lambda/L$, where $\lambda$ is the mean free path of molecules, $L$ is the characteristic length of the device. When $Kn < 0.01$, the flow is considered to be in the "continuum" regime, and the continuum assumption of fluid is valid. As $Kn$ increases, the flow enters in the "slip flow" ($0.01 < Kn < 0.1$) and "transition flow" ($0.1 < Kn < 3$) regimes. When $Kn > 3$, the flow enters the free molecular dynamics. It should be indicated that the conventional CFD (computational fluid dynamics) techniques can only be applied in the "continuum" regime. Since most micro flows in MEMS are in the "slip flow" or

International Journal of Numerical Methods for Heat & Fluid Flow
Vol. 15 No. 8, 2005
pp. 827-841

0961-5539
DOI 10.1108/09615530510625101

"transition flow" regime, the conventional CFD methods cannot properly predict the unique features of MEMS. Thus, some new methods are needed to solve micro flows in MEMS.

Obviously, the ideal method for micro flow simulation is molecular dynamics (MD) (Bird, 1976). In this method, each molecule is independent. So, the number of unknowns in the computation is proportional to the number of molecules in the flow field. Although the size of MEMS is very small, the flow field still contains a large number of molecules. For example, the air in $1\,mm^3$ contains about $2.7 \times 10^{16}$ molecules. Currently, it is still impractical to apply the MD method for simulation of micro flows. In fact, even using the most powerful supercomputer, the MD method is still limited to the nano size of flow field. To solve the micro flow with reasonable computational effort, some simplified methods are presented by various researchers.

Among all the simplified approaches, the direct simulation Monte Carlo method (DSMC) is the most popular model for simulation of micro flows. DSMC is a particle-based method, which was pioneered by Bird (1994). DSMC method was initially applied to hypersonic flow problems related to re-entry vehicles at high-altitude where the rarefaction effect is important. Due to similarity of rarefaction, DSMC method becomes an efficient tool in simulating the micro flow since the early of 1990s (Arkilic *et al.*, 1997; Beskok and Karniadakis, 1999, Pan *et al.*, 2000, 2001, 2002; Ho and Tai, 1998, Oran *et al.*, 1998; Xue and Fan, 2000; and Xue and Chen, 2003). Unlike MD method which takes each individual molecule into consideration, DSMC method assumes that a group of molecules have the same properties such as velocity and temperature. Among the group of molecules, there is no need to consider each individual molecule. In other words, the group of molecules is taken as one independent variable, which is usually termed as simulated particle. The number of real molecules per simulated particle is called scaling factor. In actual DSMC computation, the gas is represented by many simulated particles distributed in cells and all the macro properties of the flow field are obtained by statistical analysis. The inter-molecular collision is still considered in the DSMC method. According to probability of collision, a pair of particles can be selected for collision from two particles within a cell. Then after collision, the change of properties of collided molecules will be assigned to their respective particle. Using this way, the computational effort can be greatly reduced.

On the other hand, it should be indicated that the accuracy of DSMC results is mainly affected by two aspects of error. One is from the statistical error. Since all the macroscopic properties of flow field are obtained by sampling all the particles within a cell, the number of particles per cell must be sufficient to minimize the statistical error. Clearly, the larger the particle number per cell, the less the statistical error. However, the increase of particle number per cell would considerably increase the computational effort. Thus, one has to balance these two in selecting the proper number of particles per cell. Another aspect of error is from the scaling factor per simulated particle. As mentioned above, the scaling factor represents a group of real molecules having the same properties. When $Kn$ number is very small, the molecular motion of many individual molecules is similar. Thus, they can be grouped as a simulated particle. As $Kn$ number increases, the individuality of molecular motion enhances, and less and less molecules can be grouped into a particle. We can expect that the small value of scaling factor would reduce the error from DSMC assumption. If the scaling factor is taken as 1,

that is, one simulated particle representing one real molecule, the DSMC method becomes a kind of MD methods. On the other hand, we can see that the total number of molecules in a flow field is fixed for a given problem. So, the choice of small value of scaling factor implies the use of a large number of simulated particles in the flow field. This means that the scaling factor is directly related to the total number of particles in the flow field. If the scaling factor is very small, the error from DSMC assumption is small. But the number of particles for this case is very large, and the required computational effort is very large. If the scaling factor is too large which may be impractical, the error from the DSMC assumption could be large. However, for this case, the total number of particles is small, and as a consequence, the required computational effort is small. Therefore, to balance the computational effort and the error from DSMC assumption, one also needs to select the proper value of scaling factor.

The effect of statistical error on accuracy of DSMC results has been studied by some researchers (Piekos and Breuer, 1996; Huang and Bogy, 1997; Axelander and Garcia, 1997; Mackowski *et al.*, 1999; Stefanov and Cercignani, 1993; Mavriplis *et al.*, 1997; Fallavollita *et al.*, 1993; and Chen and Boyd, 1996). In contrast, the analysis of error from the scaling factor per simulated particle receives very little attention. Bird (1994) only gives a rough guidance for selection of scaling factor. He indicated that the scaling factor range from $10^{10}$ to $10^{12}$ can provide reasonable DSMC results for a two-dimensional problem. We feel that this range is still too big. In addition, we believe that the scaling factor in the "slip flow" regime is different from that in the "transition flow" regime since the extent of molecular collision free motion in these two regimes is different. The objective of this study is to systematically investigate effect of the scaling factor per simulated particle and the particle number per cell on accuracy of DSMC results. Through this work, we are trying to give a guidance in selecting the scaling factor and particle number per cell for accurate DSMC results. It is indicated that the present study also gives a guidance for distribution of cells in the flow field. As discussed earlier on, the scaling factor is related to the total number of particles in the field. So, if the particle number per cell is fixed, the scaling factor is related to the number of cells in the field. This means that, to obtain accurate DSMC results, the number of cells cannot be chosen arbitrarily. It must be above the certain value. We wish that the present study is helpful to minimize the computational effort, and in the meantime, to make the DSMC results more accurate. We will take the two-dimensional micro channel flow in the "slip flow" and "transition flow" regimes to illustrate our study.

## Direct simulation Monte Carlo (DSMC) method

DSMC is a particle-based method. The basic idea of this method is to simulate the evolution of a large number of simulated particles that represent real molecules in the flow field. The primary approximation of DSMC method is to uncouple the molecular motion and the intermolecular collision over a small time interval. In the DSMC method, the computational domain is divided into many cells, which contain several sub-cells. Then a set of particles are randomly distributed in each cell. Each particle represents a large number of real molecules, which is called the scaling factor. Every particle posses a position, velocity components and energy, etc. In general, DSMC algorithm consists of four procedures: moving of particles, indexing of particles,

inter-molecular collision of particles and sampling of particles in each cell. The particle evolution has two distinct stages in a very small time interval during the simulation: movement stage and collision stage. In the "movement stage", the particles move according to their velocity. The new position of particles can be determined by

$$\vec{x}_i^{n+1} = \vec{x}_i^n + \vec{V}_i^n \Delta t \tag{1}$$

where $\vec{x}_i^{n+1}, \vec{x}_i^n$ are positions of the $i$th particle respectively at the time level $n + 1$ and $n$, $\vec{V}_i^n$ is the velocity vector of the $i$th particle at the time level $n$, $\Delta t$ is the time step size. When the particles reach the solid boundary, they will reflect from the surface according to different reflection models, which will be addressed in the section of boundary conditions.

In the "collision stage", inter-molecular collisions occur on the base of probability. Different collision models such as the variable hard sphere (VHS) and the variable soft sphere (VSS) models can be applied to approximate the inter-molecular collisions. After movement and collision, the macroscopic quantities in the flow field, such as velocity, density and temperature are obtained by sampling the microscopic quantities of all the particles in each cell. In the DSMC computation of a steady flow problem, the four procedures are repeated until the flow reaches its steady state. In the following, we will give some brief description about the scaling factor of simulated particle, the inter-molecular collision model, the probability of collision between molecule pairs, the implementation of boundary conditions, and the sampling of particles in a cell.

*Scaling factor of simulated particle*

As mentioned in the introduction, DSMC method assumes that a group of molecules have the same properties, and they can be grouped into a simulated particle. So, in the DSMC computation, we only distribute the particles instead of real molecules. The computation of probability of collision between particle pairs is based on the number of particles in a cell. As a result, the computational effort of DSMC method is greatly reduced. The number of real molecules per simulated particle is called the scaling factor, $F_N$. It is noted that the scaling factor is not the direct input parameter in the DSMC computation. Due to this fact, the effect of scaling factor is often ignored by the user. In the DSMC computation, people usually input the number of cells first. Then in each cell, sufficient number of particles are distributed in order to minimize the statistical error. As will be shown in the next section, this way may not guarantee that accurate DSMC results can be obtained. The reason is that the pre-given number of cells may not be appropriate. Suppose that the total number of gas molecules in a flow field is $N_m$, the number of particles required in a cell for minimizing the statistical error is $N_p$, and the scaling factor is $F_N$. Then the number of cells required in the flow field should be $N_c = N_m/(F_N \cdot N_p)$. In general, $N_m$ is fixed for a given problem. If $N_p$ is given, $F_N$ uniquely determines $N_c$. Alternatively, if $F_N$ is given, $N_p$ uniquely determines $N_c$. When both $F_N$ and $N_p$ are changed, $N_c$ value may not be unique. Since $F_N$ and $N_p$ have effect on the accuracy of DSMC results, the value of $N_c$ also has effect on the accuracy of DSMC results, which cannot be chosen arbitrarily.

*Inter-molecular collision model*

In DSMC computation, the inter-molecular collision model is very important. It determines the status of molecules after collision. For an unrealistic hard sphere model,

in which the gas molecule has a fixed diameter $d$ and cross section $\sigma = \pi d^2$, the molecular mean free path in an equilibrium gas with number density $n$ is

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

Bird introduced a more reasonable variable hard sphere (VHS) model. The mean free path of this model is

$$\lambda = \frac{2\mu}{15} \frac{(7 - 2\omega)(5 - 2\omega)(2\pi RT)^{-1/2}}{\rho} \tag{3}$$

where $\omega$ is the viscosity index, $\rho$ is the molecular mass. $R$ is gas constant and $T$ is gas temperature. In the present DSMC computation, the VHS model is employed.

*Probability of collision between molecule pairs*

The probability of a collision between two molecules is proportional to the product of their relative speed $C_r$ and total cross-section $\sigma_T$. The mean value and the maximum value of the product of $C_r$ and $\sigma_T$ can be computed in each cell at every time interval. By applying acceptance-rejection method, the collision pairs could be chosen. In this method, the computational time is proportional to the square of the number of molecules in the cell and will lead to large computational effort. The non-time-counter (NTC) scheme proposed by Bird (1994) for the DSMC method is an efficient scheme. In the NTC scheme, considering a cell of volume $V_C$ in which each simulated particle represents $F_N$ real molecules, the probability $P$ of collision between two simulated particles over the time internal $\Delta t$ is proportional to the product of their relative speed $C_r$ and total cross-section $\sigma_T$, that is

$$P = F_N \sigma_T C_r \Delta t / V_C \tag{4}$$

The average number of real molecules in the cell is $nV_C$ and averaged number of simulated particles is $N_p = nVc/F_N$. The total of collisions can be calculated by selecting all $N_p(N_p - 1)/2$ pairs in the cell and by computing the collisions with probability $P$. Only a fraction of the pairs are chosen in order to make the computation more efficient. The probability $P$ can be normalized by $P_{\max}$ given by

$$P_{\max} = F_N (\sigma_T C_r)_{\max} \Delta t / V_C \tag{5}$$

In the NTC method, $(1/2) N_p \bar{N}_p F_N (\sigma_T C_r)_{\max} \Delta t / V_C$ pairs are chosen from the cell in the time interval, where $N_p$ is a fluctuating quantity and $\overline{N}_p$ is an average value. The collision is then computed with probability $\sigma_T C_r / (\sigma_T C_r)_{\max}$ and the computational time is linear with $N_p$. In our DSMC computation, NTC scheme is applied to make our computation more efficiently.

*Implementation of boundary conditions*

The interaction between gas molecules and solid walls is an important boundary condition in DSMC computation. Generally, there are three models to describe the interaction: specular reflection model, diffuse reflection model and the diffuse scattering model with incomplete energy accommodation (Cercignani–Lampis-Lord's CLL model). In present DSMC computation, the diffuse reflection model is applied,

which means that the gas molecules reflect from the solid walls with full thermal and momentum accommodation. Another important boundary condition is the properties at the inlet and outlet of the flow field. Conventional DSMC application for hypersonic problems uses upstream and down stream velocities to implement the boundary conditions. For micro flows, which usually are subsonic, this method may not sustain the given pressure at the inlet and outlet and bring errors in DSMC computation. By directly controlling the particle numbers in the cells near the inlet and outlet, the given pressure ratio of inlet to outlet can be maintained. This kind of implementation for boundary conditions is adopted in the present study.

*Sampling of particles in a cell*

The DSMC method is inherently stochastic, so that most macroscopic properties are computed by averaging technique. For example, a DSMC cell contains $n$ molecules, the mass of each molecule is $m_i$ and the cell volume is $V_C$. So, the mass density $\rho$ of gas in the cell can be obtained by

$$\rho = \frac{1}{V_C} \sum_{i=1}^{n} m_i \tag{6}$$

These obtained macro properties from DSMC method usually are fluctuating values and contain statistical errors. If the number of molecules $n$ in the cell is very small, the statistical error will be significant. Theoretically, in the DSMC computation, each cell should contain as many molecules as possible. However, due to the limitation of computational effort, in practical application, only a certain number of molecules are employed. In fact, most DSMC applications only distribute dozens of simulated particles in each cell since each particle represents a large number of real molecules. To minimize the statistical error, it is important to put sufficient number of particles in each cell.

## Numerical investigation of scaling factor and particle number per cell effect

In this section, we will systematically investigate the effect of particle number per cell and scaling factor on the accuracy of DSMC results. To illustrate our study, we will take the two-dimensional micro channel flow as an example. Both the "slip flow" regime and the "transition flow" regime are considered. The effect of particle number per cell on the accuracy of DSMC results will be studied first. Then followed by the effect of scaling factor per simulated particle on the accuracy of DSMC results. The combined effects of scaling factor and particle number per cell will also be discussed.

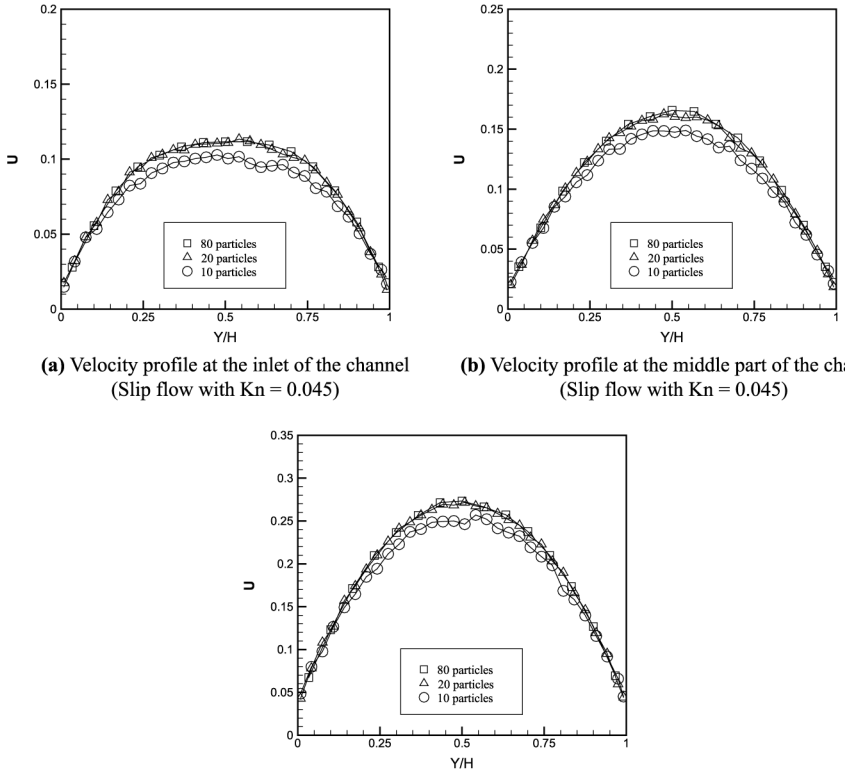
*Effect of particle number per cell*

In the micro channel flow, the pressure difference in the streamwise direction is the driven force for the flow. The intermolecular collisions are the mechanism to drive the fluid. It is very important to obtain sufficient collisions in the computation. In the DSMC method, the intermolecular collision is assumed to occur in each cell. This means that enough particles should be employed in each cell in order to obtain sufficient collisions. Meanwhile, sufficient particles in each cell are required to reduce the statistical error in the sampling. On the other hand, the use of a large number of particles in each cell will greatly increase the computational effort. Thus, one has to

balance the computational effort and the accuracy of DSMC results. What is the optimal number of particles in each cell is still an open question. From the literature, there is no certain solution to this question. It was found that many researchers (Piekos and Breuer, 1996; Huang and Bogy, 1997; Axelander and Garcia, 1997; Mackowski *et al.*, 1999; and Stefanov and Cercignani, 1993) applied 30-40 particles in each cell from their personal experiences. However, there are some DSMC computations (Mavriplis *et al.*, 1997; and Fallavollita *et al.*, 1993) which used as few as 10 particles in each cell, and some DSMC computations (Chen and Boyd, 1996) which employed as large as 50-120 particles in each cell. In the following, by simulating the two-dimensional micro channel flow in the "slip flow" and "transition flow" regimes, we attempt to find out the optimal (minimum) particle number in each cell, which can obtain accurate DSMC results, and in the meantime, requires small computational effort.

*"Slip flow" regime*. In this part, the effect of particle number per cell is studied when DSMC method is applied to simulate a micro channel flow in the "slip flow" regime with $Kn$ of 0.045 at outlet. The physical geometry is 1.32 $\mu m$ high and 20 $\mu m$ long. The pressure ratio of inlet to outlet is set to be 2.5 and the working gas is nitrogen. In total, about 240,000 simulated particles are employed to represent the real molecules in the physical domain and each particle represents about $3 \times 10^9$ real molecules. That is, the scaling factor is fixed as $3 \times 10^9$. As will be shown in the later part, this value of scaling factor is small enough to get accurate DSMC results. So, we can focus on the change of particle numbers in each cell. Since the total number of particles in the whole flow field is fixed as 240,000, the change of particle number in each cell is related to the change of cell number in the flow field. In this study, three cell numbers are selected as 3,000, 12,000 and 24,000 so that the particle numbers in each cell are 80, 20 and 10 respectively. Figure 1a, b, and c show the streamwise velocity distributions at the inlet, the middle part and outlet of the channel. The non-dimensional velocity U is normalized by the maximum velocity at the outlet of the channel. From these figures, it can be seen that when the particle number in each cell exceeds 20, the velocity profiles are almost the same. The results of particle number at 10 in each cell have relatively large deviation. The less accurate results may be caused by insufficient intermolecular collisions and statistical error for the sampling in each cell. From this study, we can say that in the "slip flow" regime, at least 20 particles in each cell are needed to obtain accurate DSMC results.

*"Transition flow" regime*. For this case, the height of the micro channel is reduced so that the $Kn$ at outlet becomes 0.12, and the flow is in the "transition" flow regime. Since the size of flow field is reduced, the total number of real molecules is also reduced. The pressure ratio of inlet to outlet is also set to 2.5 and the working gas is nitrogen. As will be discussed in the following section, in the "transition flow" regime, the scaling factor of $9 \times 10^8$ is small enough to provide accurate DSMC results. Thus, in the following study, we fix the scaling factor as $9 \times 10^8$. This means that each particle in the "transition flow" regime represents about $9 \times 10^8$ real molecules. It is noted that the scaling factor in the "transition flow" regime is less than that in the "slip flow" regime. This is because in the "transition flow" regime, the molecular motion is much stronger than in the "slip flow" regime. Thus, less molecules in the "transition flow" regime can be grouped as a particle which has the same property. With the fixed scaling factor, the total number of particles in the flow field is still 240,000. In the study, four cell numbers of 3,000, 6,000, 12,000 and 24,000 are used respectively. This is equivalent to use 80, 40, 20 and 10 particles respectively in each cell. Figure 2a, b, c show the streamwise




**(a)** Velocity profile at the inlet of the channel (Slip flow with Kn = 0.045)

**(b)** Velocity profile at the middle part of the channel (Slip flow with Kn = 0.045)

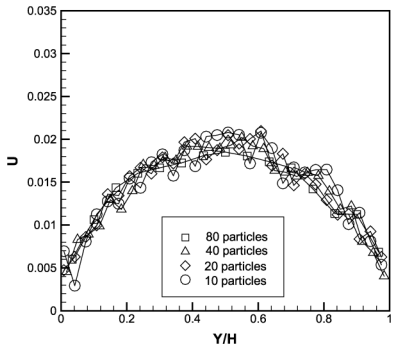
**(c)** Velocity profile at the outlet of the channel (Slip flow with Kn = 0.045)

**Figure 1.**

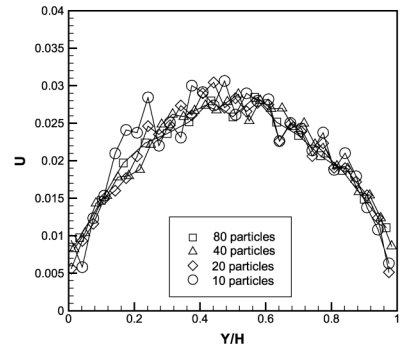
velocity distributions at the inlet, middle part and the outlet of the channel. It can be clearly observed from Figure 2 that besides some fluctuations, the four results have a good agreement. This means that with 10 particles in each cell, the DSMC results in the "transition flow" regime are still acceptable. This may be explained by such consideration: In the "transition flow" regime, the gas becomes more rarefied and the collision events occur less than that in the "slip flow" regime. With 10 particles in each cell, the collisions are sufficient so that the results are reasonable.

*Effect of scaling factor per simulated particle*

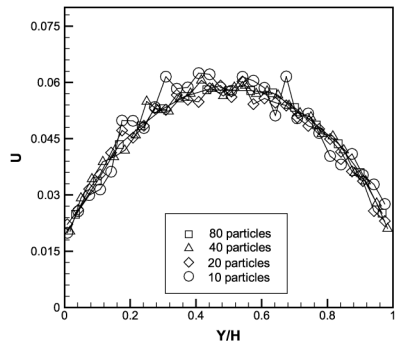
In the previous section, the effect of particle number per cell on the accuracy of DSMC results is studied in both the "slip flow" and "transition flow" regimes under fixed scaling factors. The scaling factor is very important in the DSMC computation. For a given physical problem, the number of real molecules is fixed. So, once the scaling factor is given, the total number of simulated particles in the flow field is roughly determined. In general, a small scaling factor will bring a large number of simulated particles in DSMC computation and the DSMC results would be accurate. A large scaling factor will distribute a small number of simulated particles in the field and the computational effort will be reduced. In order to obtain sufficient accuracy of DSMC




**(a)** Velocity profile at the inlet of the channel (Transition flow with Kn = 0.12)




**(b)** Velocity profile at the middle part of the channel (Transition flow with Kn = 0.12)

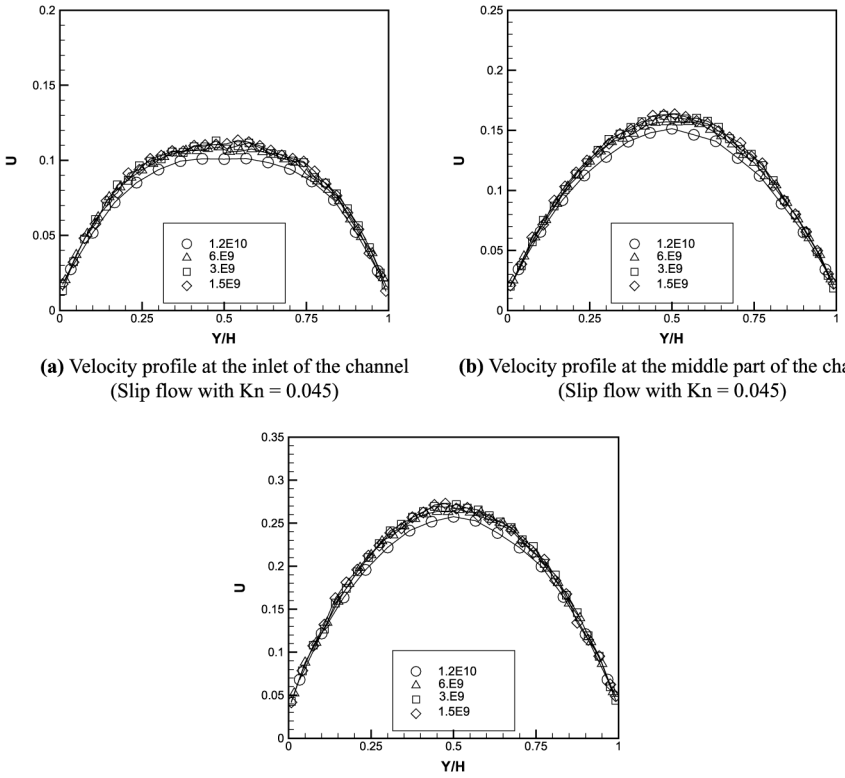



**(c)** Velocity profile at the outlet of the channel (Transition flow with Kn = 0.12)

**Figure 2.**

results, small scaling factor is preferred, but it may require a large computational effort. To save the computational effort, and in the meantime, to main the accuracy of DSMC results, it is of great interest to optimize the scaling factor in the DSMC computation. In following, we will fix the particle number per cell, and attempt to find a reasonable scaling factor in the DSMC simulation of two-dimensional micro channel flows in the "slip flow" and "transition flow" regimes.

*"Slip flow" regime*. The geometry and flow condition of this case is exactly the same as that discussed for effect of particle number per cell. It was found in the previous section that in the "slip flow" regime, 20 particles in each cell could obtain accurate DSMC results. So, in this part, we fix 20 particles in each cell. For the problem considered, the total number of real molecules in the whole flow field is fixed. So, the change of cell number is equivalent to the change of total number of particles in the flow field, and therefore the change of scaling factor. In this study, four different cell numbers of 3,000, 6,000, 12,000 and 24,000 are used so that the total number of particles in the whole field is respectively 60,000, 120,000, 240,000 and 480,000. As a consequence, the scaling factors of these four cases are $1.2 \times 10^{10}$, $6 \times 10^{9}$, $3 \times 10^{9}$ and $1.5 \times 10^{9}$. Figure 3a, b and c show the streamwise velocity distributions at the inlet, the middle part and the outlet of the channel. From the figures, it is clear that the




**(a)** Velocity profile at the inlet of the channel (Slip flow with Kn = 0.045)

**(b)** Velocity profile at the middle part of the channel (Slip flow with Kn = 0.045)

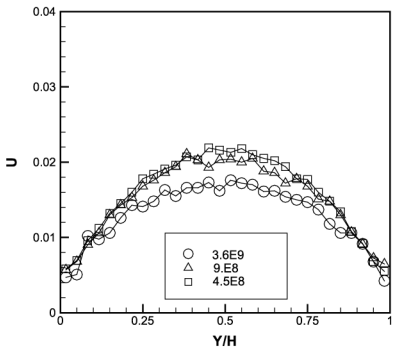
**(c)** Velocity profile at the outlet of the channel (Slip flow with Kn = 0.045)

**Figure 3.**

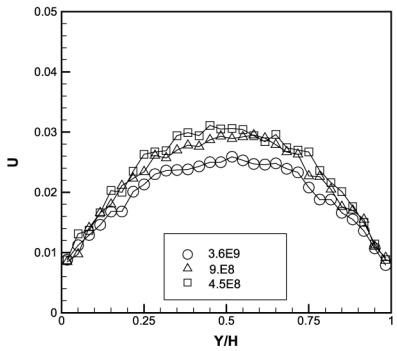
results with scaling factor of $1.2 \times 10^{10}$ are different from the others. It means that even with sufficient particles in each cell, the scaling factor has effect on the accuracy of DSMC results. The present study shows that, in order to obtain reasonable DSMC results, the maximum scaling factor should not exceed $1.0 \times 10^{10}$. This indicates that in the "slip flow" regime, a group of $1.0 \times 10^{10}$ molecules can be assumed to have the same properties and they can be grouped by one particle in the DSMC method. If the scaling factor exceeds $1.0 \times 10^{10}$, it means that too many real molecules are assumed to have the same properties, and this assumption does not reflect the real physics. An improper large scaling factor would bring physical errors in the DSMC computation.

*"Transition flow" regime*. Similarly, the geometry and flow condition of this case is exactly the same as that discussed for effect of particle number per cell. As studied in the previous section, in the "transition flow" regime, 10 particles per cell can generate reasonable DSMC results. However, for safety of this study, we still take 20 particles per cell. Like the problem in the "slip flow" regime, the total number of real molecules in the whole flow field is fixed and the particle number per cell is also fixed. So, when the number of cells is changed, the total number of particles and the scaling factors are all changed. In this study, three different cell numbers of 3,000, 12,000 and 24,000 are used

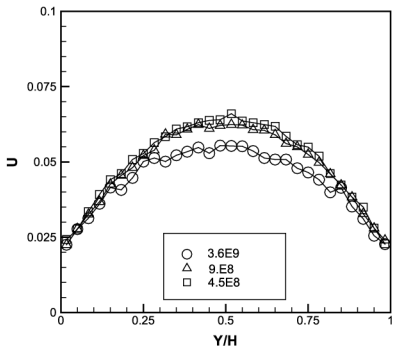
so that the total particle numbers are 60,000, 240,000 and 480,000 respectively. As a result, the scaling factors of these three cases are $3.6 \times 10^9$, $9 \times 10^8$ and $4.5 \times 10^8$. Figure 4a, b and c show the non-dimensional streamwise velocity distributions at the inlet, the middle part and the outlet of the channel. From these results, we can see that the results with scaling factors of $3.6 \times 10^9$ are quite different from the others. In order to obtain the reasonable results in the "transition flow" regime, the maximum scaling factor should not exceed $1 \times 10^9$. As compared with the results in the "slip flow" regime, the scaling factors in the "transition flow" regime are much smaller. In the "slip flow" regime, the gas is relatively denser than that in the "transition flow" regime, relatively more real molecules that have the same properties could be grouped as a particle. In "transition flow" regime, the gas is more rarefied, molecular behaviors are quite different from each other so that a small number of real molecules that have the same properties can be grouped as a particle. From the results, it can also be observed that the velocity fluctuation is quite large. This confirms that the behaviors of real molecules are different from each other in more rarefied gas, and there are more random molecular movements, and this makes the continuum assumption break down even with slip velocity boundary condition.




**(a)** Velocity profile at the inlet of the channel (Transition flow with Kn = 0.12)




**(b)** Velocity profile at the middle part of the channel (Transition flow with Kn = 0.12)



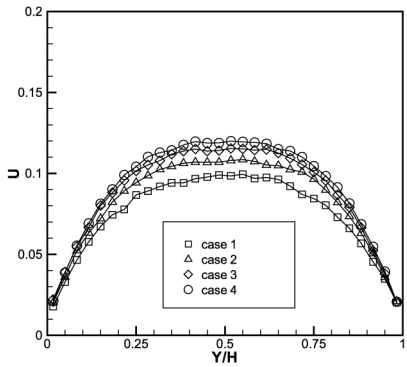

**(c)** Velocity profile at the outlet of the channel (Transition flow with Kn = 0.12)

**Figure 4.**

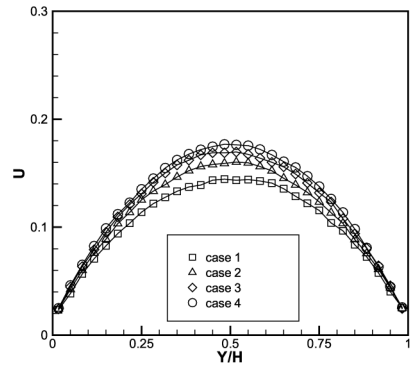
*Combined effects of particle number per cell and scaling factor per particle*

In previous sections, the effects of particle number per cell and scaling factor on accuracy of DSMC results are studied separately. In general, these two effects coexist in most of the DSMC computations. Their combination may have more effect on the DSMC results. In this section, we will study their combined effects in the "slip flow" regime and the "transition flow" regime respectively.

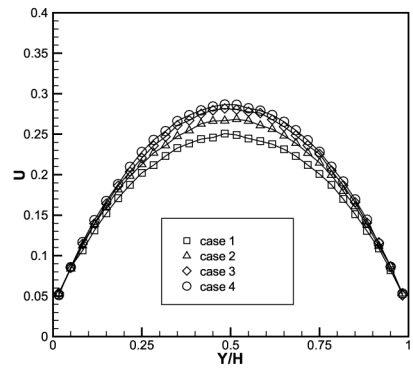
*"Slip flow" regime*. The physical geometry and pressure ratio of inlet to outlet are set to be the same as the case discussed in the previous sections. In this study, we fix the cell number in the whole flow field, which is usually adopted by many researchers. The cell number is fixed as 6,000. On the other hand, we let the particle number per cell and the total number of particles in the field be changed. In other words, both the particle number per cell and the scaling factor are changed. For the present case, the total particle numbers are taken as 60,000,120,000, 240,000 and 480,000, which are defined as case 1, case 2, case 3 and case 4. Each cell contains 10, 20, 40, 80 particles respectively for cases 1, 2, 3, 4. So, the scaling factors are $1.2 \times 10^{10}$, $6 \times 10^{9}$, $3 \times 10^{9}$ and $1.5 \times 10^{9}$ respectively for cases 1, 2, 3, 4. Figure 5a, b and c show the streamwise




**(a)** Velocity profile at the inlet of the channel (Slip flow with Kn = 0.045)




**(b)** Velocity profile at the middle part of the channel (Slip flow with Kn = 0.045)




**(c)** Velocity profile at the outlet of the channel (Slip flow with Kn = 0.045)

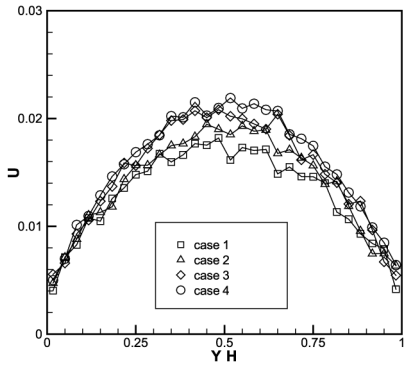
**Figure 5.**

velocity distributions at the inlet, the middle part and the outlet of the channel. From the results, it can be seen that there is no much difference between the results of cases 2, 3 and 4. But the results of case 1 have significant difference with others. This is because for case 1, the particle number per cell (10) is less than the required value and its scaling factor ($1.2 \times 10^{10}$) is larger than the required value, so the combined effects of these two aspects make the numerical results worse. This should be paid more attention. In the DSMC simulation of micro flows in the "slip flow" regime, the real molecule number is determined for a given problem. When the physical domain is divided into many cells, the choice of cell number is not arbitrary. It must meet basic requirement for the particle number per cell and the scaling factor. From present study, it can be found that with the combined effects of particle number per cell and scaling factor, the particle number in each cell should be large enough to obtain accurate DSMC results.

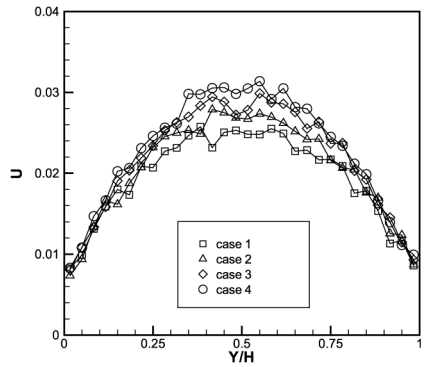
*"Transition flow" regime*. The combined effects are also studied for the micro channel flow in the "transition flow" regime. The case is the same as that discussed in the previous sections. Similar to the study of micro channel flow in the "slip flow" regime, the cell number is also fixed as 6,000, and the particle numbers in the whole field are taken as 60,000,120,000, 240,000 and 480,000, which are defined as case 1, case 2, case 3 and case 4. Each cell contains 10, 20, 40, 80 particles respectively for cases 1, 2, 3, and 4. Different from the case in the "slip flow" regime, in the present case, the scaling factors become $3.6 \times 10^9$, $1.8 \times 10^9$, $9 \times 10^8$ and $4.5 \times 10^8$ respectively for cases 1, 2, 3 and 4. Figure 6a, b and c show the streamwise velocity distributions at the inlet, the middle part and the outlet of the channel. Al the results show some fluctuations in the velocity profile. The differences among cases 2, 3 and 4 are quite small. However, case 1 shows significant discrepancies as compared with others. These results imply that in the "transition flow" regime, when the particle number in each cell exceeds 20, and each particle represents less than $1.8 \times 10^9$ real molecules, the DSMC results could be accurate. This conclusion is stricter than that given in the previous section. In the "transition flow" regime, the scaling factor is smaller than that in the "slip flow" regime, and the particle number per cell is the same. The particle number requirement will ensure the statistical accuracy. From the consideration of both two aspects, the combined effects on the DSMC results are larger than separate effect. So, stricter requirement of particle number and scaling factor are recommended in the DSMC method. From it, we know that either the particle number or the scaling factor could affect the DSMC result. The combined effect should be taken into account in DSMC computation.

## Conclusions

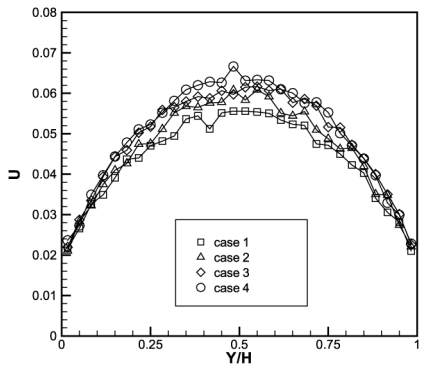
In this study, for the two-dimensional micro channel flow in the "slip flow" and "transition flow" regimes, the effects of the particle number per cell and the scaling factor of real molecules to a simulated particle on accuracy of DSMC results are studied systematically. Present investigation shows that in the DSMC method, the particle numbers in each cell should be larger than a certain critical number according to different flow regime. In the "slip flow" regime, in order to obtain sufficient intermolecular collisions, at least 20 particles should be employed to ensure the accuracy of DSMC results. In the "transition flow" regime, present results show that the required minimum particle number per cell could be smaller. This result coincides




**(a)** Velocity profile at the inlet of the channel (Transition flow with Kn = 0.12)




**(b)** Velocity profile at the middle part of the channel (Transition flow with Kn = 0.12)




**(c)** Velocity profile at the outlet of the channel (Transition flow with Kn = 0.12)

**Figure 6.**
(a) Velocity profile at the inlet of the channel (Transition flow with Kn = 0.12); (b) Velocity profile at the middle part of the channel (Transition flow with Kn = 0.12); (c) Velocity profile at the outlet of the channel (Transition flow with Kn = 0.12)

with the mechanism of molecular motion in the "transition flow" regime because in this regime, the intermolecular collision rate is less than that in the "slip flow" regime. So, even with 10 particles in each cell, by time averaging, the DSMC results are still reasonable in the "transition flow" regime. The effect of scaling factor of real molecules to a simulated particle is also studied in present paper. In the "slip flow" regime, when the scaling factor exceeds $10^{10}$, the DSMC results may have significant difference from results obtained using relatively small scaling factors. This means that if a simulated particle represents too many real molecules, it may not correctly reflect the physics of the problem and thus bring errors in DSMC simulation. In the "transition flow regime, the maximum scaling factor is reduced to $10^9$ for an accurate DSMS results. This is because in the "transition flow" regime, the individual molecular motion is enhanced, so that less number of real molecules can be grouped into a simulated particle (scaling factor), which have the same properties. It should be noted that the present study only takes the two-dimensional pressure-driven micro channel flows as an example to do investigation. For complex micro flows, the present study can serve as a guidance to

select the particle number per cell and the scaling factor. The optimal particle number per cell and the scaling factor may be different for different micro flow simulations by DSMC method.

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