Molecular Dynamics Simulation of Rarefaction Effect on Shear-driven Gas Flow in Nanochannels

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Abstract. The nanoscale gas flow at normal temperature and pressure varies from the slip flow regime to the transition regime, of which the character length changes across several nanometers to several thousand nanometers. The difference in the degree of rarefaction leads to different rules of the flow in nanochannels. In order to study the influence of rare gas effect on the nanoscale gas flow, we use three-dimensional molecular dynamics method to simulate the shear flow confined by two parallel plate under different Knudsen numbers, and then obtain the distribution of flow velocity, density, normal stress and shear stress, thus calculating and analyzing the variation of the tangential momentum accommodation coefficient. Counting the gas molecules according to the velocity with positive and negative values respectively, we find that the gas flow is decomposed into two independent shear flows, which indicates strong non-equilibrium characteristics in the nanochannel.

1. Introduction

In recent years, with the rapid development of micro-nano electromechanical systems (MEMS/NEMS), nanoscale gas flow has received extensive attention and has gradually become an important research field[1-4]. Nanoscale gas flow has broad application prospects, such as biological sample extraction, integrated circuit cooling, and active flow control[5]. However, the flow characteristics at the nanoscale are quite different from the macroscopic flows. In order to understand the nanoscale flow characteristics, it is necessary to conduct an in-depth study of its mechanism.

The degree of thinness of the gas is generally expressed by the Knudsen number Kn. In the micro-nanoscale gas flow, the mean free path of the molecule is no longer a small amount compared with the flow characteristic scale, and the continuous medium assumption is no longer valid, and the gas exhibits a significant thinning effect. At the same time, the reduction of the scale will lead to an increase in the area to volume ratio, and the physical quantity associated with the wall surface will have a more pronounced effect on the flow. The difficulties of theory and experimental approach have led to the tendency to use numerical simulation methods to study the flow of thin gases. The Direct Analog Monte Carlo (DSMC) method is a widely used numerical simulation method that can effectively simulate the flow of thin gases in a transitional flow region. However, DSMC still needs to provide momentum and energy accommodation factors when dealing with the interaction of gas and wall at the boundary. For different gases and walls, the accommodation coefficients vary widely, so this method is not suitable for studying the nanoscale flow of wall dominant factors.
Molecular Dynamics (MD) method[6], as a deterministic simulation method, from the perspective of atomic motion, can not only obtain the flow details of the flow field, but also obtain the scattering regularity of gas molecules at the wall surface. Therefore, it has unique advantages in studying the micro-nano scale flow. Based on MD simulation, many scholars have conducted extensive research on micro-nano channel flow. Cao et al.[7,8] used molecular dynamics simulation method to study the gas flow in the micro-nano channel of the slip zone, and discussed the relationship between velocity slip and potential energy intensity, system temperature and wall roughness. Sun and Li[9] adopted the MD method to calculate the tangential momentum accommodation coefficient and the normal momentum accommodation coefficient in the smooth micro channel. Spijker et al.[10] used the MD method to simulate the gas flow in the nanochannel, and statistically analyzed the velocity distribution before and after the collision of the gas molecules with the wall surface, and introduced the velocity correlation cloud map when analyzing the relationship between the incident and the reflection velocity. Xie and Liu[11] simulated the Poiseuille flow of the mixed gas in the nanochannel, and found that the wall force caused the gas mixture in the channel to exhibit a special phenomenon that the chemical composition and the physical structure were no longer uniform. Barisik and Beskok[12,13] introduced an intelligent wall molecular dynamics (SWMD) method. Assuming that the wall atoms are stationary, it is found that the changes in density, velocity and pressure of the gas in the near-wall region of the channel are determined only by the wall force field. Bao et al.[14,15] used molecular dynamics to study the pressure-driven flow in finite-length nanochannels, and come to the conclusion that the pressure difference is independent of the temperature, the Knudsen number, the channel aspect ratio and wall properties. To et al.[16] studied the mean free path distribution of non-equilibrium gas in micro-nano channels by molecular dynamics simulation method, and found that the mean free path is strongly reduced near the wall surface and not sensitive to the flow type. Lim et al.[17] simulated the flow of He, Ne, Ar, Kr and Xe gases by molecular dynamics method, studied the influence of molecular mass and adsorption effect on the tangential momentum accommodation coefficient, and found that the tangential momentum accommodation coefficient with molecular mass The changes are not monotonous.

For nanometer-scale gas flow at normal temperature and pressure, the flow varies across several nanometers to several thousand nanometers, and the flow crosses the slip flow region and the transition flow region. The degree of thinness is different, and the flow also shows different flow patterns. In order to study the effect of rare gas effect on the shear flow of nanoscale gas, the flow velocity, density, normal stress and shear stress distribution under different Knudsen conditions are investigated. The gas density of these examples remains the same, i.e. the mean free path of the gas molecules in all channels is the same, and the variation of the Knudsen number is achieved by changing the channel height.

2. The simulation method
In this paper, a three-dimensional non-equilibrium molecular dynamics method is used to simulate the shear flow of gaseous argon in micro-nano channels. The schematic diagram of the model is shown in Figure 1. The monoatomic gas is distributed in a nanochannel having a height of two infinitely long flat plates. The X and Y directions adopt periodic boundary conditions. The upper and lower walls move in opposite directions at a speed of 0.2 that drives the gas to make a shear flow. For monoatomic gases, their molecular mass $m_{\text{Ar}}=6.63\times10^{-26}$ kg, molecular diameter $\sigma_{\text{Ar}}=0.3405$ nm, and potential energy parameters $\epsilon_{\text{Ar}}=1.67\times10^{-22}$ J.

The gas-gas and gas-wall interactions are modeled using a truncated Lennard–Jones(L-J)6–12 potential energy function18, defined as:

$$U^{12}(r_{ij}) = 4\epsilon_{\sigma_{\nu}} \left\{ \left[ \left( \sigma_{\nu} / r_{ij} \right)^{12} - \left( \sigma_{\nu} / r_{\text{c}} \right)^{12} \right] - \left[ \left( \sigma_{\nu} / r_{ij} \right)^{6} - \left( \sigma_{\nu} / r_{\text{c}} \right)^{6} \right] \right\}$$

Where $r_{ij}$ is the intermolecular distance, $r_{\text{c}}$ the cutoff radius which equals $3.0\sigma_{\nu}$.
3. The simulation method

3.1. The shear gas flow in the transition regime

![Figure 1. Dimensionless velocity distribution under different Knudsen numbers.](image1)

![Figure 2. Density distribution of near-wall regions in each channel under different Knudsen numbers.](image2)

![Figure 3. Dimensionless velocity distribution under different Knudsen numbers.](image3)

![Figure 4. Normal stress distribution in the near wall area of each channel under different Knudsen numbers.](image4)

![Figure 5. Shear stress distribution in the near wall area of each channel under different Knudsen numbers.](image5)
Figure 1 shows the velocity distribution under different Knudsen conditions. It can be seen from the figure that as the height of the pipe increases, the velocity shear rate in the channel decreases. The influence of the wall force is a fixed width of 1 nm. When the height of the pipe increases, the proportion of the flow field affected by the wall force is gradually reduced. For example, when the height of the channel is 109 nm, the wall force affecting area only accounts for about 2% of the entire flow field. Figure 2 shows the velocity distribution of the near-wall region under different Knudsen conditions. We find that the flow velocity in the near-wall region increases with the decrease of the Knudsen number due to the effect of the thin gas effect.

Figure 3 and Figure 4 show the density and normal stress distribution curves in the flow field under different Knudsen conditions. It can be seen from the figure that the change of channel height does not affect the density and normal stress distribution of the gas in the channel. Figure 5 is the shear stress distribution curve in the flow field under different Knudsen conditions. The shear stress in each channel shows the same distribution law, but its value decreases with the increase of Knudsen number.

3.2. The shear gas flow in the slip regime

When the height of the channel continues to increase and the average free freeness of the gas molecules is less than 0.1 compared with the pipe height, the flow gradually transitions to the slip flow field according to the division of the thin gas flow field. For the flow in the slip flow field, the influence of the wall facing flow is limited to the Knudsen layer, and the solution can be solved according to the NS equation with the additional Maxwell slip boundary condition. The velocity dimensionless velocity distribution of the slip zone is:

$$\frac{U}{U_w} = \frac{Z}{H} + \frac{2}{1 + 2 - \frac{2}{TMAC} Kn}$$

In this section, the channel height is 272.4 nm and the gas density is 3.73 and 7.46 kg/m³ respectively. The velocity distribution in the flow field is shown in Figure 6. The solid line in the figure is the theoretical solution corresponding to the Kn. The simulation results are obtained. And the theoretical solution is in good agreement with most of the flow areas. However, in the area of the Knudsen layer close to the wall, the simulated velocity curve has a certain deviation from the theoretical solution. This is due to that the first-order slip boundary conditions of the Maxwell slip boundary condition used in the theoretical solution assume the speed linear in the Knudsen layer. In fact, with the rarefied gas effect, the velocity distribution in the Knudsen layer is a typical nonlinear distribution, which is the limitation of the slip boundary condition.

**Figure 6.** Comparison of gas shear flow velocity distribution and theoretical solution in the slip regime.

**Figure 7.** Differences between velocity distribution and theoretical solution in the Knudsen layer.
In the Knudsen layer, it can be seen from the Figure 7. that as Kn increases, the nonlinearity of the gas velocity becomes more and more obvious, and at the same time, the deviation from the theoretical solution becomes larger. According to the velocity profile obtained by MD simulation, the velocity curve of the central region of the flow field is fitted to obtain the dimensionless velocity shear rate of the flow under different Knudsen conditions. According to the relationship between the velocity and the Knudsen number, the corresponding Tangential momentum accommodation factor. The tangential momentum accommodation coefficient under Kn 0.113 and 0.0561 is both 0.72, which is consistent with the tangential momentum accommodation coefficient of the transition flow region in the previous section, further illustrating the independence of the tangential momentum accommodation coefficient and the Knudsen number.

3.3. The analysis of the rarefaction effect

The entire flow area can be layered in the Z direction, wherein the area away from the wall surface is the wall force area, the remaining part is the main flow area, the width is , and then it is equally divided into 13 layers. Then, the velocity samples of each layer of gas molecules are subjected to classification, and the positive and negative of the velocity components of the gas molecules are classified, and the average tangential velocity of the two types of gas molecules in each layer of the flow field is obtained by statistical average. Figure 8 is a tangential velocity distribution of each layer of the flow field obtained by the above method, wherein represents the tangential average velocity of the gas molecules having a normal velocity component in each layer and represents a negative normal velocity component in each layer. The tangential average velocity of gas molecules. We found that the average tangential velocity distribution of the above two part of gas molecules is a completely antisymmetric distribution, the shear rate is exactly the same, and the two parts are added together and averaged, that is, the true velocity of each layer is obtained, which is completely consistent with the MD calculation results. Based on the above findings, it can be considered that the gas shear flow in the nanochannel is synthesized from two separate shear flows.

![Figure 8. Average tangential velocity distribution of two types of gas molecules in each layer.](image)

In order to explain the above phenomenon, it is necessary to proceed from the law of motion of a single gas molecule in a nanotube. We start tracking when the gas molecules are incident on the lower wall surface. After the collision with the lower wall surface, the tangential momentum is adjusted and the normal velocity direction is changed, and then the upper wall surface is moved. Since the channel height is relatively narrow, the gas molecules cannot be carried out in the channel. The collision of sufficient gas molecules, when it reaches the upper wall, still carries the tangential velocity information after collision with the lower wall surface; after that, the gas molecules collide with the upper wall surface to complete the adaptation of the tangential momentum with the upper wall surface. The speed direction changes again and the gas molecule moves to the lower wall surface; repeating the incomplete gas molecules in the channel and then reaching the lower wall again, thus forming a complete cycle. Each gas molecule in the channel follows the above-mentioned motion law. By ensemble averaging, we can obtain the gas tangential velocity distribution as shown in Figure 8.
4. Conclusion
In this paper, the three-dimensional non-equilibrium molecular dynamics simulation method is used to study the gas shear flow in the slip zone and the transition zone nanochannel. The distribution of the physical quantities of the gas in the channel is obtained. The flow characteristics of the near wall region are studied in depth and analyzed. The variation trend of the tangential momentum accommodation coefficient is found. The tangential momentum accommodation coefficients of the slip zone and the transition zone are consistent, and the conclusion that the tangential momentum accommodation coefficient is independent of the Knudsen number is obtained. The gas molecules in the channel are classified according to the normal velocity direction, and the velocity distribution of the two gas molecules in the flow field is obtained. It is found that the gas shear flow in the nanochannel can be decomposed into two independent flow laws. The discovery directly confirms the existence of a non-equilibrium effect of gas flow within the nanochannel.

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