

Application of 2DMD to gaseous microflows

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Abstract A two-dimensional molecular dynamics (2DMD) simulation is applied to gaseous microflows. Based on a velocity distribution function in equilibrium, the mean molecular speed, mean collision frequency, mean free path, and the dynamical viscosity are deduced theoretically. A Maxwell-type-like boundary condition for two-dimensional (2D) systems, which reveals a linear relationship between the slip length and the mean free path, is also derived. These expressions are consequently employed to investigate the rarefied gas flow in a submicron channel. The results show reasonable agreements with those by 3D simulations, and indicate that the 2DMD scheme can be very promising for the microflow researches because of its high efficiency in computation.

Keywords: molecular dynamics, 2D system, microscale flow, rarefaction effect.

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Due to the rapid advancement of the micro/nano-technology, known as MEMS and NEMS (micro/nano-electro-mechanical-systems) over the past decade, physics of fluid flows on the microscale has formed one of the frontiers of science and technology^[1,2]. Fluid flows are often encountered in the operating and controlling of micro- and nano-devices. Fluid flows on the microscale often show different characteristics from those on the normal scale, including boundary velocity slip, surface force effects and other unconventional effects^[3]. These effects mostly arise from the interparticle interactions of the fluid and between the fluid and its boundary, and cannot be fully explained by conventional models based on the continuum assumption.

The method of molecular dynamics (MD) simulation, which shows a significant advantage of making no routine approximations, has recently been used for probing the microfluidic mechanics. However, the scale of the simulated flow system is generally limited to nanometers because of the heavy burden of computation^[4–7]. The 2D molecular dynamics (2DMD) simulation attracted attention in probing the nature of melting/freezing transition of physisorbed gases and 2D solids in the 1980s^[8]. The phase diagram and some thermodynamic properties of a 2D system have been studied^[9]. The 2DMD simulation has also

been applied to microflow studies in recent years^[10,11]. Nevertheless, the theory and methodology of molecular kinetics in a 2D system are short of clarification yet.

The present paper focuses on the molecular kinetics of a 2D system and its application to gaseous microflows. Kinetics of gaseous molecules and the slip boundary condition (BC) for a 2D gaseous flow are studied. The outcomes are employed in a 2DMD simulation of rarefied gas flows in a microchannel.

1 Kinetic theory of gaseous molecules in a 2D system

Firstly, we introduce some necessary assumptions which are also adopted by traditional kinetic theory of gases: i) Molecular chaos: The space and velocity distribution of molecules in an equilibrium state is uniform. The molecular behaviors and their statistical characteristics in a given state are irrelevant to those before their collisions. ii) Ideal gases based on hard-sphere model: The elastic collisions between molecules take place instantaneously, and obey classical mechanics. iii) The number density of gaseous molecules cannot be too low to relate their macroscopic statistical properties with the microscopic molecular behaviors.

According to the molecular chaos and equipartition of energy theorem, the thermophysical parameters of a 2D system may be defined as

$$\bar{\varepsilon}_i = \frac{1}{N} \sum \frac{1}{2} m v_i^2 = kT, \quad (1)$$

$$P = nkT, \quad (2)$$

in which T is the temperature, P is the pressure, n is the number density, N is the molecule number, m is the molecule mass, $\bar{\varepsilon}_i$ is the mean kinetic energy of all molecules, v_i is the velocity of the molecule numbered by i , and k is the Boltzmann constant.

We now turn our attention to the velocity distribution function of molecules. On the basis of the symmetry of the velocity distribution, the distribution function can be described as

$$f(v) = A e^{-\beta(v_x^2 + v_y^2)}, \quad (3)$$

in which the integral constants A and β are determined by the conditions

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} A e^{-\beta(v_x^2 + v_y^2)} dv_x dv_y = 1, \quad (4)$$

and

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{1}{2} m (v_x^2 + v_y^2) A e^{-\beta(v_x^2 + v_y^2)} dv_x dv_y = kT. \quad (5)$$

The above equations give $A = \frac{m}{2\pi kT}$ and $\beta = \frac{m}{2kT}$.

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Thus, the distribution function for molecular velocities in a 2D system may be written as

$$f(v) = \frac{m}{2\pi kT} e^{-\frac{m(v_x^2+v_y^2)}{2kT}}. \quad (6)$$

The distribution of molecular velocities is uniform in space. It is hardly surprising that the distribution function in a 2D system is different from that in a 3D one by reason of the dimensionality reduction.

It is then easy to define the distribution function of molecular speeds as

$$f(v) = \frac{mv}{kT} e^{-\frac{mv^2}{2kT}}. \quad (7)$$

The distribution function of relative speeds is

$$f(v_r) = \frac{mv_r}{2kT} e^{-\frac{mv_r^2}{4kT}}. \quad (8)$$

On the basis of the distribution functions of molecular velocities and speeds, some parameters of a 2D molecular system are obtained as shown in table 1.

Table 1 Comparison of parameters of 2D and 3D systems

Parameter	2D	3D
Mean speed	$\bar{v} = \sqrt{\frac{\pi kT}{2m}}$	$\bar{v} = \sqrt{\frac{8kT}{\pi m}}$
Mean relative speed	$\bar{v}_r = \sqrt{2}\bar{v}$	$\bar{v}_r = \sqrt{2}\bar{v}$
Collision frequency	$\chi = 2\sqrt{2}n\bar{v}\sigma$	$\chi = \sqrt{2}\pi n\bar{v}\sigma^2$
Mean free path	$\lambda = \frac{1}{2\sqrt{2}n\sigma}$	$\lambda = \frac{1}{\sqrt{2}\pi n\sigma^2}$
Molecular flux	$\psi = \frac{1}{\pi}n\bar{v}$	$\psi = \frac{1}{4}n\bar{v}$
Dynamical viscosity	$\mu = \frac{2}{\pi}nm\bar{v}\lambda$	$\mu = \frac{1}{2}nm\bar{v}\lambda$

2 Slip boundary condition

Because a gas-molecule cannot go through an impermeable wall, the momentum exchange across the gas-wall interface strongly depends on the frequency of collisions between the gas-molecules and the solid surface. Strictly speaking, the frequency may not be infinite generally. Therefore, discontinuity of velocity, which is often referred to as slip velocity (u_s), may appear at the gas-solid interface.

A rarefied gas flow near a solid wall in a 2D system is shown in Fig. 1. Following Maxwell, we introduce the tangential momentum accommodation coefficient ζ (TMAC), which is defined as the fraction of molecules reflected from a wall diffusively. In other words, the TMAC shows the proportion of the lost tangential mo-

mentum of incident molecules. Total momentum carried by incident molecules may be written as

$$I_{in} = \frac{1}{\pi}n\bar{v}mu_s + \frac{1}{2}\mu \frac{du}{dz}. \quad (9)$$

The molecules will give fraction ζ of their tangential momentum to the surface. Thus, momentum carried by reflected molecules is

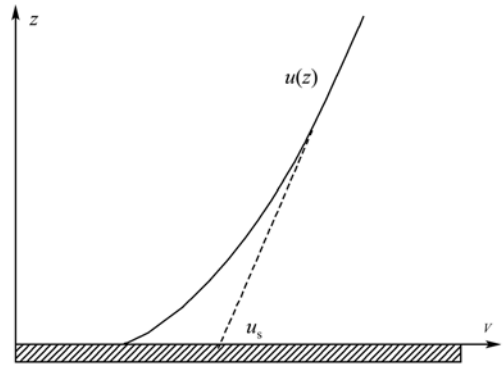


Fig. 1. Schematic of slip boundary condition.

$$I_{out} = (1-\zeta) \left(\frac{1}{\pi}n\bar{v}mu_s + \frac{1}{2}\mu \frac{du}{dz} \right). \quad (10)$$

We can write the momentum conservation equation as

$$I_{in} - I_{out} = \mu \frac{du}{dz}. \quad (11)$$

Using the physical parameters defined in a 2D system, we solve for the slip velocity as

$$u_s = \frac{2-\zeta}{\zeta} \lambda \frac{du}{dz}. \quad (12)$$

The expression is completely like the Maxwell model formally. The slip coefficient is defined as $\alpha=(2-\zeta)/\zeta$, which lies on the fraction of the reflected molecules diffusively. It is a function of the interaction between gas molecules and the surface. If all the molecules undergo diffusive reflections, the experiential value of $\alpha=1$ holds.

The slip length may be defined as

$$L_s = \alpha\lambda. \quad (13)$$

Scaled by the characteristic length of the flow system, the dimensionless slip length $l_s=L_s/H$ may be written as

$$l_s = \alpha Kn, \quad (14)$$

in which $Kn=\lambda/H$ is known as the Knudsen number characterizing the rarefaction degree of a 2D flow.

3 2DMD simulation details

(i) Simulation method. Our molecular dynamics simulation models a 2D Couette system, as shown in Fig. 2. The flows are induced by translating the walls with velocities of $U=158 \text{ m} \cdot \text{s}^{-1}$ in the positive and minus x -directions respectively. Gaseous argon undergoes shear between two platinum plates, which enclose a microchannel with a distance $H=0.1 \text{ } \mu\text{m}$. A periodic boundary condition is used in the x -direction.

To maintain a realistic gas-solid boundary condition, we build atomic structure walls based on Einstein theory that the wall atoms vibrate around the face-centered-cubic (FCC) [1,1,1] lattice sites with the Einstein frequency tethered by a harmonic spring of stiffness

$$E = \frac{16\pi^4 k^2 m^2 \theta^2}{h^2}, \quad (15)$$

where k_B and h are the Boltzmann and Planck constant, respectively, m is the mass of a wall atom, and $\theta=180 \text{ K}$ is the Einstein temperature.

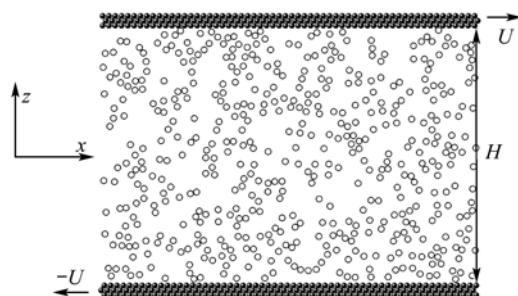


Fig. 2. Schematic snapshot of the 2D Couette system.

Particles interact with each other via a Lennard-Jones 6-12 potential of the form

$$V_{LJ} = 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right], \quad (16)$$

in which r is the intermolecular distance, ϵ and σ are the energy and molecular diameter parameters. The parameters used in this paper are listed in Table 2.

Table 2 Potential parameters used in our simulations

Parameter	Value	Parameter	Value
$\epsilon_{\text{Ar-Ar}}$	$1.67 \times 10^{-21} \text{ J}$	$\epsilon_{\text{Pt-Ar}}$	$0.894 \times 10^{-21} \text{ J}$
$\sigma_{\text{Ar-Ar}}$	$3.405 \times 10^{-10} \text{ m}$	$\sigma_{\text{Pt-Ar}}$	$3.085 \times 10^{-10} \text{ m}$

The molecules move according to Newton's second law. The equations of motion are integrated using a leap-frog-Verlet algorithm^[12] with a time step of $\Delta t = 2.14 \text{ ps}$.

To reduce the time-consuming part of the calculation of interparticle interactions, we mainly take two measures:

i) A typical potential cutoff of $r_{\text{cut}}=2.5 \sigma_{\text{Ar-Ar}}$ is used. ii) The link-cell method is adopted. The system is kept at constant temperature $T=273 \text{ K}$ for each simulation by a velocity rescaling method. Steady-state velocity profiles often require an equilibrium time about 1500000 time steps in our simulations. The averaging was then carried out for about 3000000 steps.

(ii) Analyses of computation amount. The amount of computation in the 2DMD and the 3DMD simulations can be assessed on the basis of their methodologies. At the same size of the flow system and the same Knudsen number, if the boxes of the simulated systems are assumed to be equilateral, a 3DMD has to compute more particles than a 2DMD as described by

$$N_{3D} = \frac{H}{\sigma} \frac{2}{\pi} N_{2D}, \quad (17)$$

and

$$N_{w3D} = \frac{H}{d} N_{w2D}, \quad (18)$$

in which N is the molecule number, N_w is the atom number building the walls, σ is the molecule diameter, and d is the nearest distance of neighbor wall-atoms. It is clear that the particle number in a 3D system should be much more in a larger scale system comparing with that in a 2D one. Considering the system scale the present paper simulates, we can deduce particle numbers that a 3DMD simulation need to compute (Table 3).

In molecular dynamics simulations, the calculation of the interparticle interactions is the most time-consuming part. In our simulations, an efficient Link-Cell method is used for calculation of the short ranged force between particles. Using the general cell structure in two dimensions, we need to examine N_{P2D} particle pairs of

$$N_{P2D} = \frac{1}{2} \left(9 \frac{N^2}{M^2} + 6 \frac{NM_w}{M^2} \right). \quad (19)$$

For three dimensions, we have to examine N_{P3D} pairs of

$$N_{P3D} = \frac{1}{2} \left(27 \frac{N^2}{M^3} + 18 \frac{NM_w}{M^3} \right). \quad (20)$$

Here, $M \doteq H/r_{\text{cut}}$ is the cell number of the simulated box in a certain dimension direction. Furthermore, the forces considered in a 2DMD with two dimensions is cut down about 1/3 of a 3DMD which had to calculate interactions relating to three dimensions. Taking the case of 3000 molecules in our 2DMD, the amount of a 2DMD computation is only about 1/2000 of a 3DMD.

Table 3 Particle numbers in our 2DMD and a 3DMD at the same Knudsen number (wall-atom number N_w , 2D: 2490, 3D: 1033350. Gas-molecule number N)

Kn	0.009	0.017	0.037	0.056	0.072	0.084	0.10	0.116
2D	15000	7000	3000	2000	1500	1200	1000	800
3D	3223840	1504460	644770	429850	322380	257900	214920	171940

4 Simulation results

(i) Velocity fields. Fig. 3 shows the velocity profiles of the Couette flow in the x -direction obtained by our simulations. The Knudsen numbers are from 0.009 to 0.116. The flows are in the slip regime by the traditional theory of rarefied gas dynamics, which is clearly indicated by our simulations in Fig. 3. Primarily, it shows that the profiles are linear in the middle of the channel as predicted by continuum Navier-Stokes equations, and that different velocity slips due to the rarefaction effect appear in the region adjacent to the wall with a thickness of the order of the mean free path for different Knudsen numbers. As the Knudsen numbers increase, the slip velocities become more pronounced. The results may indicate the applicability of the continuum theory accompanied by the slip condition for slip flows on the submicron scale.

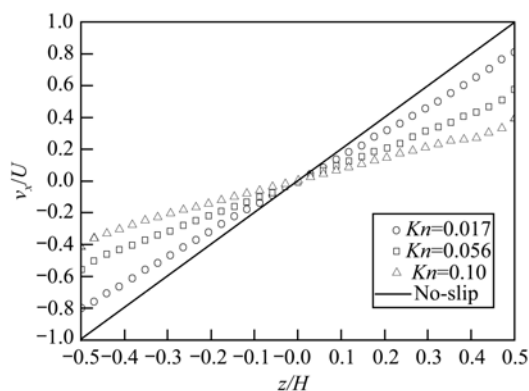


Fig. 3. Velocity profiles for various Knudsen numbers.

(ii) Slip boundary condition. In Fig. 4, we present variation of the dimensionless slip length for different Knudsen numbers obtained by our simulations. The slip lengths are derived from the linear lengthening of the velocity profiles. The dimensionless slip length appears proportional to the Knudsen number as predicted by eq. (14). The TMAC could then be extracted by fitting the slope of the l_s-Kn curve. At 273 K, the slip coefficient is about 9.14 by our simulation for flows of gaseous argon over the smooth platinum surface, which is in approximate agreement with the 3DMD result of 9.5 by Yamamoto at 300 K^[13].

(iii) Velocity distributions. In the second section of

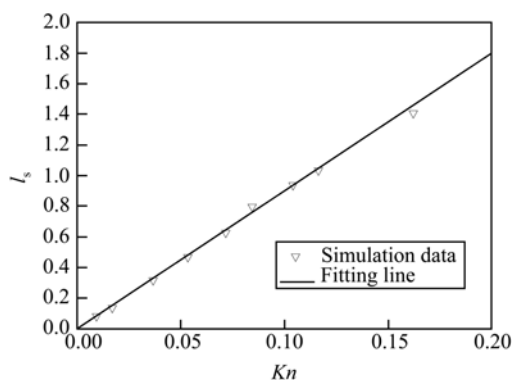


Fig. 4. Dimensionless slip length vs. Knudsen number.

this paper, the slip boundary condition has been shown to be a Maxwell-type-like model. Thus, the velocity distribution function of reflected molecules in the direction parallel to the surface may be written as

$$f_{\text{out}}(v-u_{\text{out}}) = (1-\zeta)f_{\text{in}}(v-u_{\text{in}}) + \zeta f_{\text{M}}(v-u_{\text{w}}), \quad (21)$$

in which f_{in} is the velocity distribution function of incident molecules, f_{M} is the velocity distribution function of reflected molecules diffusively (eq. 6). u_{in} , u_{out} and u_{w} are macroscopic velocities of incident molecules, reflected molecules, and wall respectively. They are generally associated by $u_{\text{w}}=(u_{\text{in}}+u_{\text{out}})/2$.

In Fig. 5, the velocity distributions are shown for incident and reflected molecules in our simulation with $Kn=0.056$. They appear in good agreement with the theoretical predictions of eq. (21).

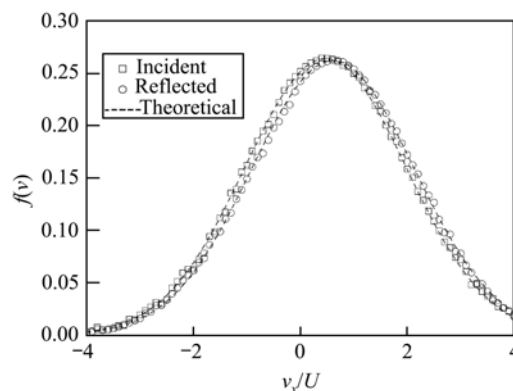


Fig. 5. Velocity distribution parallel to the wall.

5 Conclusions

1) On the basis of the velocity distribution function in equilibrium, the molecular mean speed, mean collision frequency, mean free path, and the dynamical viscosity are deduced theoretically.

2) A Maxwell-type-like boundary condition for a 2D flow system is derived. Though it has a similar appearance to the initial Maxwell model, physical parameters corresponding to a 2D system should be adopted.

3) The 2DMD simulation not only characterizes the gaseous microflow well, but is also efficient in computation.

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