Scattering Properties of Gas Molecules on Water Adsorbed Surfaces in High Knudsen Number Flows

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Abstract

We consider a Couette flow of a rarefied Ar gas with heat transfer between two walls and investigate the scattering behavior of gas molecules reflected either at a clean Pt surface or at a surface contaminated with adsorbates. The reflection of gas molecules on the lower wall is simulated by Molecular Dynamics (MD) method to obtain accommodation coefficients and velocity distribution functions of gas molecules. We also investigate the validity of reflection model of gas molecules on the wall by comparing with the MD results. In addition, we discuss thermal and flow properties between two walls from the obtained flow velocity and temperature distributions.

Introduction

Flows of gas between two parallel walls moving with relative velocities at different wall temperatures is an important problem. A large number of works are available on the Couette flow with heat transfer for a dilute gas [1-3]. To investigate the momentum and heat transfer between the two walls, it is essential to set appropriate boundary conditions by employing the Boltzmann equation and a model equation. The scattering behavior of gas molecules depends on the state of the wall surface. Therefore, it is interesting to investigate the velocity distribution function of reflected molecules.

In this study, we investigate the scattering behavior of the gas molecules reflected either at a clean Pt surface or at a surface contaminated with adsorbates. In general, air contains many water vapor, which easily sticks to a solid surface. Thus, we consider a wall surface on which water molecules are physically adsorbed. This study primarily aims to construct appropriate reflection models for a surface of complex structure in high Knudsen number flows.

Method of Analysis

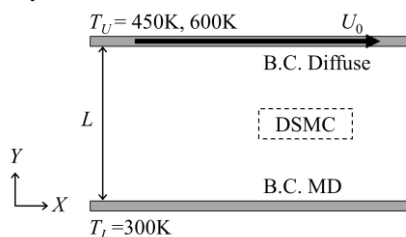The calculation system is a steady-state and it has a velocity gradient only in a normal direction between two walls. Let the distance between the two plates be L and the average number density of gas molecules be n_0. The upper wall moves with a constant velocity (U_0), while the lower wall remains stationary. The temperature of the lower wall T_L is set at 300 K, whereas that of the upper wall T_U is set at 450 or 600 K as shown in Figure 1. We apply the MD method on the lower wall to represent the gas-surface interaction. However, at the upper wall, we assume the diffuse reflection of the gas molecules. We apply the Direct Simulation Monte Carlo (DSMC) method to analyze the motions of gas molecules between the two walls. We shall mainly consider a weak rarefied gas and set the reference Knudsen number ($K_n = \lambda/L$) to be 0.2. Here, λ is the mean free path of Ar molecule in the equilibrium state with number density n_0 and temperature T_L. We divide the space between the walls into at most 80 equally divided cells. When a molecule hits the wall during the DSMC simulation, we switch to the MD method and trace the motion of every gas molecule that will interact with solid molecules at the wall.

Our MD method is nearly the same as that used in previous studies [4, 5] where we modeled a thin Pt layer. We set the surface of the layer to coincide with the (111) plane of the *fcc* lattice of Pt. One sheet of the surface layer consists of 10 Pt atoms in the X direction and another 10 atoms in the Z direction. Four molecular sheets are stacked normal to the surface in the negative Y direction. We employ the SPC/E model for water molecules. This model is characterized by three point masses, with OH distances of 0.1 nm and an HOH angle equal to the tetrahedral angle. We use the same interaction potential between the gas, solid, and adsorbed molecules used in previous studies [6]. Also, we numerically solve the Newton's equations of motion and the equations for angular momentum conservation using the leapfrog method. The time step is set at $\Delta t = 1.5 \times 10^{-15}$ s. In addition, we define the adsorption rate Θ as the ratio of the number of adsorbed water molecules to the number of Pt molecules constituting the upper surface. In this research, the adsorption rate Θ is considered to be 0 to 0.50. A simulation models of the wall surface for $\Theta = 0$ and 0.50 are shown in Figure 2.
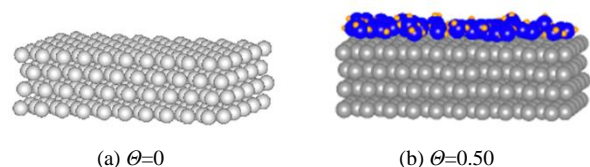

Figure 1. Couette flow with heat transfer problem.

(a) $\Theta=0$ (b) $\Theta=0.50$

Figure 2. Wall surface models for MD simulation.

Θ	$S_U = 1.0$						$S_U = 1.5$						$S_U = 2.0$					
	$T_U = 450K$			$T_U = 600K$			$T_U = 450K$			$T_U = 600K$			$T_U = 450K$			$T_U = 600K$		
	α_t	α_n	α_E	α_t	α_n	α_E	α_t	α_n	α_E	α_t	α_n	α_E	α_t	α_n	α_E	α_t	α_n	α_E
0.00	0.18	0.51	0.31	0.16	0.52	0.32	0.16	0.42	0.26	0.15	0.46	0.27	0.14	0.32	0.22	0.13	0.40	0.23
0.05	0.29	0.45	0.33	0.27	0.46	0.33	0.27	0.36	0.29	0.25	0.40	0.30	0.25	0.25	0.26	0.23	0.32	0.26
0.10	0.34	0.35	0.29	0.31	0.39	0.30	0.31	0.25	0.27	0.30	0.32	0.28	0.30	0.17	0.25	0.27	0.25	0.25
0.20	0.36	0.34	0.29	0.34	0.35	0.29	0.34	0.22	0.26	0.33	0.28	0.27	0.32	0.15	0.24	0.31	0.21	0.25
0.30	0.36	0.27	0.25	0.34	0.29	0.26	0.34	0.17	0.23	0.33	0.24	0.24	0.33	0.09	0.22	0.31	0.16	0.23
0.40	0.33	0.21	0.23	0.32	0.25	0.24	0.32	0.11	0.21	0.31	0.19	0.23	0.30	0.04	0.20	0.29	0.13	0.22
0.50	0.32	0.20	0.22	0.30	0.24	0.23	0.30	0.12	0.20	0.30	0.18	0.22	0.29	0.03	0.19	0.28	0.12	0.21

Table 1. Accommodation coefficients.

Results

We performed our calculations for a case where the speed ratio is $S_U = U_0/C_m = 1.0$, 1.5, or 2.0. $C_m = (2kT_L/m)^{0.5}$ is the most probable speed, k is the Boltzmann constant, and m is the mass of an Ar molecule.

Accommodation Coefficients

The tangential momentum accommodation coefficient (TMAC) α_t of gas molecules at the wall surface is defined as follows:

$$\alpha_t = \frac{\tau_i - \tau_r}{\tau_i}. \tag{1}$$

Here, τ is the X component of the momentum of molecules and subscripts i and r represent the incident and reflected molecules, respectively. The normal momentum accommodation coefficient (NMAC) α_n of gas molecules and the energy accommodation coefficient (EAC) α_E are defined as follows:

$$\alpha_n = \frac{p_i - p_r}{p_i - p_w}, \qquad \alpha_E = \frac{E_i - E_r}{E_i - E_w}, \tag{2}$$

where p is the absolute value of the Y component of the momentum of molecules, E is the total kinetic energy of molecules, and the subscripts i, r, and w represent the incident, reflected, and diffusely reflected molecules, respectively. These values of α_t, α_n, and α_E are listed in Table 1. We found that the TMAC α_t and NMAC α_n depend on the speed ratio, the upper wall temperature, and the adsorption rate.

Flow Velocity and Temperature Distributions

In Figures 3 and 4, we show the distributions of the relative flow velocity q_x/U_0 and temperature T/T_L for cases with $S_U = 1.0$ and 2.0, respectively. The ordinate Y is normalized by the distance between two plates L, and $Y = 0$ at the lower wall surface. In these figures, the plots show the distributions at each adsorption rate. The velocity slip decreases with increasing the adsorption rate. It takes the minimum value at $\Theta = 0.30$ and turns to increase with increasing the adsorption rate. This tendency is related to the dependence of TMAC on the adsorption rate. A comparison of Figures 3(a) and 4(a) shows that the effect of the adsorption rate on the distributions of flow velocity has almost the same tendency regardless of the speed ratio. In Figures 3(b) and 4(b), the temperature jump at the lower wall ($Y = 0$) increases with increasing the adsorption rate. This tendency seems to be related to the dependence of NMAC on the adsorption rate but detailed mechanism is not understood yet.

A comparison of Figures 3(b) and 4(b) shows that the temperature distributions have almost the same tendency with increasing the adsorption rate. However, in the result of Figure 4(b), it can be confirmed that the temperature rises on the lower wall. This is considered to be an effect of the compressibility due to an increase in the speed ratio.

Distribution Functions of Molecular Velocity

Figures 5–8 show the velocity distribution functions for gas molecules before and after reflection on the lower wall. The temperature of the upper wall is taken to be 450 K. The molecular velocity V is normalized by the most probable speed C_m, the filled circles represent the distribution for the incident molecules, and the open circles show the distribution of the reflected molecules obtained from MD simulations. The distribution obtained from the diffuse reflection at the lower wall with temperature T_L is indicated by a solid curve for comparison. The dashed curve represents the new distribution proposed by our groups based on the Maxwell-type reflection model. It is described as follows:

$$f_x^+ = \alpha_t f_w + (1 - \alpha_t)f_x^- \qquad (V_y > 0), \tag{3}$$

$$f_y^+ = \alpha_n f_w + (1 - \alpha_n)f_y^- \qquad (V_y > 0), \tag{4}$$

$$f_z^+ = \alpha_E f_w + (1 - \alpha_E)f_z^- \qquad (V_y > 0). \tag{5}$$

Here, the TMAC α_t is considered for the X direction, and the NMAC α_n is considered for the direction normal to the wall. The EAC α_E is used for the distribution in the Z direction. The function f^- is the velocity distribution function for the incident molecules, and f_w is the Maxwellian distribution.

Figures 5 and 6 show the results for clean surface ($\Theta = 0$) and a water adsorbed surface ($\Theta = 0.50$) when the speed ratio is 1.0. In these figures, it shows that the distribution of the reflected gas molecules can be very well described by a distribution based on a Maxwell-type reflection model, regardless of the presence of the water molecules. However, the diffuse reflection model shows a large difference from the MD simulation. Figures 7 and 8 show the results for clean surface ($\Theta = 0$) and a water adsorbed surface ($\Theta = 0.50$) when the speed ratio is 2.0. In Figure 7(a), the Maxwell-type model shows a slight difference depending on the adsorption rate. Although we do not show them here, for Z directions, the velocity distribution functions obtained using a Maxwell-type reflection model also agree well with those obtained using MD simulations.
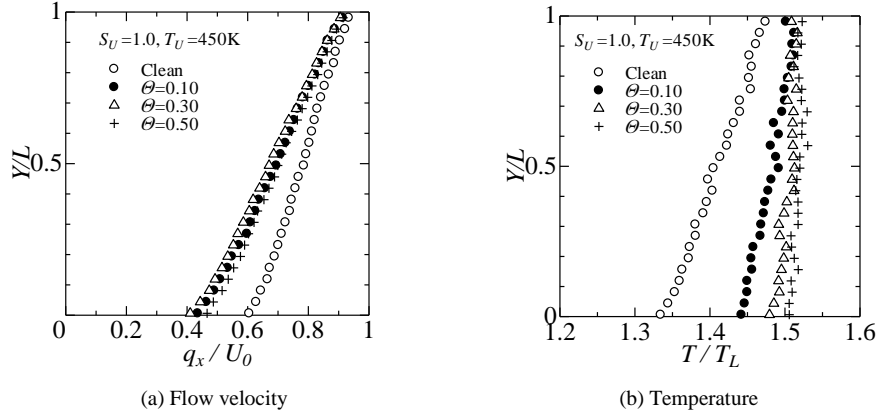
(a) Flow velocity

(b) Temperature

Figure 3.　Flow velocity and temperature distributions between two walls (S_U = 1.0, T_U= 450K).

(a) Flow velocity
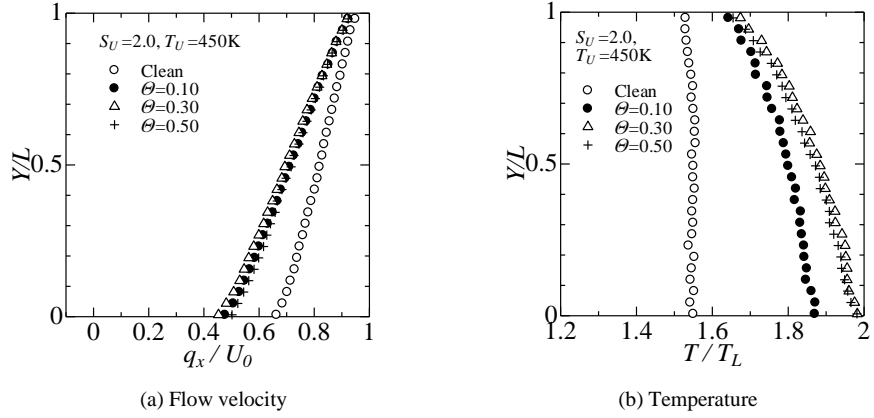
(b) Temperature

Figure 4. Flow velocity and temperature distributions between two walls (S_U = 2.0, T_U= 450K).
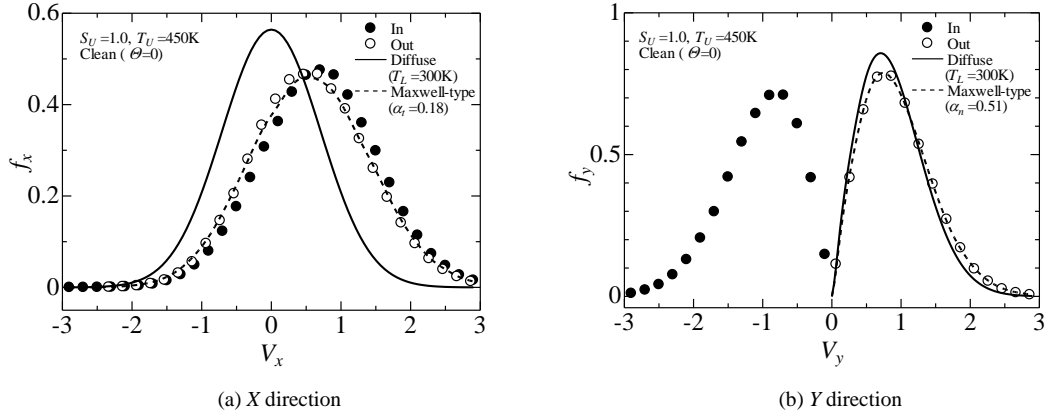

(a) X direction

(b) Y direction

Figure 5. Velocity distribution functions of gas molecules on the lower wall (S_U = 1.0, T_U= 450K, Θ= 0).

(a) X direction

(b) Y direction
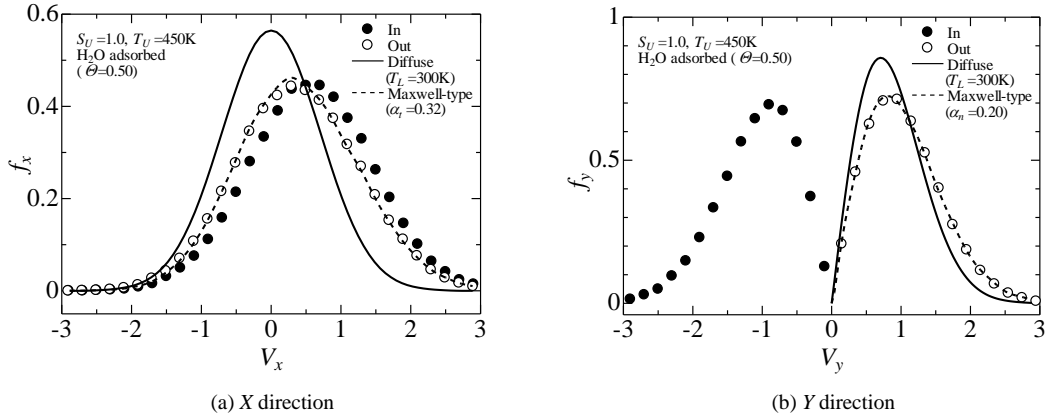
Figure 6. Velocity distribution functions of gas molecules on the lower wall (S_U =1.0, T_U=450K, Θ= 0.50).
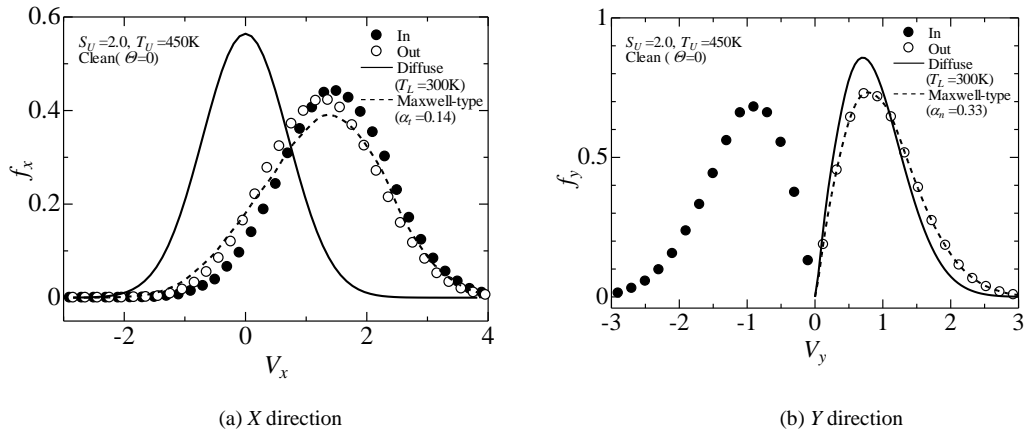
(a) *X* direction

(b) *Y* direction

Figure 7. Velocity distribution functions of gas molecules on the lower wall (S_U = 2.0, T_U = 450K, Θ = 0).

(a) *X* direction

(b) *Y* direction
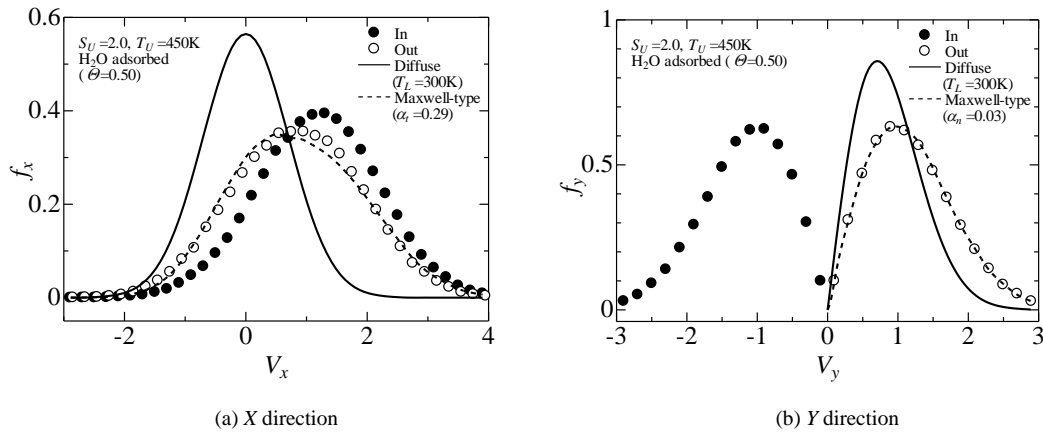
Figure 8. Velocity distribution functions of gas molecules on the lower wall (S_U = 2.0, T_U =450K, Θ = 0.50).

Conclusions

We analyzed a Couette flow with heat transfer of a rarefied gas between two parallel plates. The gas is taken to be argon and the wall is made from platinum. The analysis is based on the DSMC method for the motion of gas molecules and the MD method for the interaction between a gas molecule and the wall surface. Some types of the surface are considered; i.e., a clean surface and a surface with physically adsorbed water molecules. The reference Knudsen number is taken to be 0.2.

We first obtained the momentum and energy accommodation coefficients. We found that the TMAC α_t and NMAC α_n depend on the speed ratio, temperature of the upper wall, and adsorption rate. The influence of these parameters is quantitatively clarified by the accommodation coefficients.

Secondly, we investigated the flow velocity and temperature distributions between two walls and clarified the influence of the adsorption rate on the velocity slip and temperature jump on the lower wall.

Finally, we investigated the velocity distribution functions on the lower wall. A proposed reflection model based on the Maxwell-type reflection model is constructed with appropriate accommodation coefficients in each direction. We found that the velocity distribution based on a Maxwell-type reflection model agreed well with the MD simulation compared with the diffuse reflection. However, it was found that the degree of coincidence depends on adsorption rate and speed ratio.

References

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