Study of reflection models of gas molecules on water adsorbed surfaces in high-speed flows

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Abstract
We consider a Couette flow of a rarefied Ar gas with heat transfer between two wall surfaces and investigate the scattering behavior of gas molecules reflected either at a clean Pt surface or at a surface contaminated with adsorbates. Water molecules abundantly present in the atmosphere were adopted as the adsorbates. The reflection of gas molecules on the lower wall surface was simulated by Molecular Dynamics (MD) method to obtain accommodation coefficients and velocity distribution functions of gas molecules. We applied the modified reflection model of gas molecule and investigated the velocity distribution functions of the model by comparing the MD results to verify the validity. The accommodation coefficients obtained by the MD method depend on the number of adsorbed water molecules on the lower wall surface. Specifically, tangential momentum accommodation coefficient (TMAC) tended to increase and then decrease with the increase in adsorbed water molecules, but normal momentum accommodation coefficient (NMAC) tended to decrease monotonically. The velocity distribution functions of the modified reflection model approximately show the good agreement with the MD calculation but the degree of coincidence depends on the speed difference between the upper and lower wall surfaces, and the number of adsorbed water molecules on the surface.

Keywords: Molecular dynamics, Direct simulation monte carlo, Couette flow, Rarefied gas, Reflection model

1. Introduction

In the flow around a spacecraft and the flow in MEMS/NEMS devices, the Knudsen number that is the ratio of the mean free path $\lambda$ of a gas molecule to the characteristic length $L$ of the flow becomes large. Such a flow is generally analyzed with the Boltzmann equation, a model equation, or the Direct Simulation Monte Carlo (DSMC) method, but it is necessary to specify a reflection model of gas molecules as a boundary condition on the solid wall surface. Specification of an appropriate reflection model greatly affects the validity of the analysis, so it is very important to identify the correct model to use. Currently used reflection models include the specular reflection model, diffuse reflection model, Maxwell-type model, and the CLL model. However, these models have not yet been established as systematic models and therefore, the reflection models are often selected according to fluid phenomena. For example, the diffuse reflection model is widely used in practical applications, especially in macroscale and engineering problems, in which the adsorption time is usually much longer than flows on extremely smooth surfaces. Under conditions where the adsorption time is not extremely long or short, the diffusive or specular model alone is not appropriate (Cao et al., 2009). Maxwell combined the diffuse reflection and specular reflection models, and named as Maxwell-type model (Maxwell, 1879). Although the general
Maxwell-type model describes the velocity distribution in all directions using a single parameter (i.e., \(\alpha\), called the accommodation coefficient), there are some cases where this model cannot reproduce the three-dimensional reflection of gas molecules. In other words, the general Maxwell-type model is based on the premise that there is not a large difference between accommodation coefficients for different directions, such as an isotropic flow. However, when the difference is large (i.e., the flow with macroscopic flow velocity), the differences of the accommodation coefficients in each direction is significantly different and therefore, the Maxwell-type model cannot be applied. A more informative and useful model is the CLL model, which was proposed by Cercignani and Lampis (Cercignani and Lampis, 1971) and later extended by Lord (Lord, 1991; Lord, 1995). This is guided by a function satisfying the detailed balancing condition in the thermal equilibrium state, considering the probability \(P(\mathbf{V} \rightarrow \mathbf{V}')\) of the gas molecules colliding with the solid wall surface at the incident velocity \(\mathbf{V}\) and departing from the solid wall surface at the reflection velocity \(\mathbf{V}'\). The model includes two parameters, i.e., the normal energy accommodation coefficient (NEAC) and the tangential momentum accommodation coefficient (TMAC). In order to use this model in the DSMC method, etc., it is necessary to obtain these parameters. With regard to the NEAC, there are no experimental studies, but there are some results from numerical simulations. In any case, it should be noted that the number of references for the NEAC is very limited compared with those for the TMAC (Niimi, 2011). For these reasons, further study is necessary to use the CLL model in practice.

Yamamoto et al. proposed a modified Maxwell-type model as a highly accurate and highly versatile reflection model (Yamamoto et al., 2006). In the modified Maxwell-type model, the distribution anisotropy is considered by assigning different accommodation coefficients to each of the \(X\), \(Y\), and \(Z\) directions at the wall surface. The authors report that this model can accurately reproduce reflections under several analytic conditions (Yamamoto et al., 2004a, 2004b; Takeuchi and Hyakutake, 2008). The validity is verified by comparing the molecular velocity distribution function of the reflected gas molecule obtained by the modified Maxwell-type model with those by the molecular dynamics (MD) method. They adopted flows of gas between two parallel wall surfaces moving with relative velocities at different wall temperatures (Takeuchi and Hyakutake, 2012). In other words, the system is a Couette flow with heat transfer. The flow system is an important problem, and many published results are available for a dilute gas (Huang and Hartley, 1968; Tij and Andres, 1995; Cao et al., 2005). The reason why many researchers investigate the Couette flow is that the phenomenon is simple and it can be applied to various fields. Moreover, 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 on the wall surface adsorbed molecules. For this reason, they investigated the influence of adsorbed molecules on the wall surface (Takeuchi et al., 2009). They selected water molecules as adsorbates because the atmosphere contains many water vapor molecules and they are easily adsorbed on a wall surface. Using this calculation system, they quantitatively investigated the influence of adsorbed water molecules on the scattering properties of gas molecules. In addition, the validity of their proposed reflection model is verified.

As mentioned above, Takeuchi et al. showed very good agreement with the MD calculation in this calculation system (Takeuchi et al., 2009). However, they only consider the case of \(S_U = 0.25, 0.50\) that is about 88 to 177 m/s and the adsorption rate \(\Theta = 0.20\). Here, \(S_U\) is defined as the ratio of the upper wall velocity and most probable speed of gas molecules, and \(\Theta\) is defined as the ratio of the number of water molecules and the number of platinum (Pt) atoms for the first layer of the wall surface. Actually, it is important whether the reflection model of gas molecules can be adapted under higher flow velocity because the flow velocity around a spacecraft reaches several hundred meters per second. It is also necessary to investigate quantitatively the influence of adsorption rate on the accommodation coefficients in a wider range. Therefore, in this study, we estimate the validity of the modified Maxwell-type model that has been validated only under limited conditions under a wider range of the speed ratio and the adsorption rate. We obtained a velocity distribution function of scattering gas molecules at higher velocity fields such as \(S_U = 2.0\) and a higher adsorption rate such as \(\Theta = 0.50\) by using this model, and verified the validity of the model at such extreme conditions by comparing it with the results of the MD method. Argon (Ar) is selected as a gas molecule. Ar scattering on a Pt surface is suitable for a model verification since it is well studied by experiments and MD simulations. We use the same system as (Yamamoto et al., 2004a) to verify a modified Maxwell-type model under extreme conditions. In this paper, the method is described in detail, and the influence of adsorbed water molecules on the accommodation coefficients and the validation of reflection model is discussed in detail. In addition, the influence of the upper wall temperature on the validation for the reflection model is newly added. In Chapters 2, 3 and 4, we explain the simulation method of this study and show the results obtained by the simulations, respectively. A summary and conclusions are finally presented in Chapter 5.
2. Simulation method

The simulation system is a steady state and it has a velocity gradient only in a normal direction between two wall surfaces. A schematic diagram of the simulation system is shown in Figure 1. The upper wall surface moves with a constant velocity \( U_0 \), while the lower wall surface remains stationary. The temperature of the lower wall surface \( T_L \) is set at 300 K, whereas that of the upper wall surface \( T_U \) is set at 450 or 600 K. Our simulation is performed for a case where the speed ratio is \( S_V = U_0/C_w = 1.0 \) or 2.0, where \( C_w = (2kT_c/m)^{0.5} \) is the most probable speed, \( k \) is the Boltzmann constant, and \( m \) is the mass of an argon (Ar) molecule. It covers a wide range of speed ratios compared with the previous study (Takeuchi et al., 2009), and helps to consider their influences quantitatively. We mainly considered a weak rarefied gas and set the reference Knudsen number as 0.2. Here, \( \lambda \) is the mean free path of an Ar molecule and is defined as \( \lambda = (\sqrt{2\pi d^2 n_0})^{-1} \). \( n_0 \) is the number density of the gas (Takeuchi et al., 2009). We apply the DSMC method to analyze the motions of gas molecules between the two wall surfaces. We divide the space between the wall surfaces into a maximum of 80 equal cells. Next, the gas molecules are placed randomly in the cell and given the velocity according to the Maxwellian distribution corresponding to 300 K. In the DSMC simulation, it is possible to treat molecular movement and intermolecular collision separately. Therefore, it is necessary to set the time step \( \Delta t \) to be sufficiently smaller than the average collision time \( (\tau = \lambda/C) \) of the molecule. Here, \( C \) is the average velocity of the Ar molecule and is defined as \( C = (8kT_c/\pi m)^{0.5} \). In this study, the time step \( \Delta t \) is set at about 0.2\( \tau \). Then, the dimensionless time step is set at 0.17725 by using the mean free path \( \lambda \) of gas molecules and most probable speed \( C_w \). After the system reached equilibrium in 1,000 steps, the sampling is performed in 10,000 steps. The time counter (TC) method (Bird, 1976) proposed by Bird is used to obtain the number of collisions of molecules in each cell, and we assume the Hard-Sphere model (Bird, 1994) whose molecular diameter is \( d \) for gas molecule. When a molecule collides with the upper wall surface during the DSMC simulation, we assume the diffuse reflection model. On the other hand, when a molecule collides with the lower wall surface during the DSMC simulation, we determine the velocity after collision by the MD method mentioned below.

We apply the MD method to determine the velocity of molecules after collision with the lower wall surface to represent the gas–surface interaction. Our MD method is nearly the same as that used in previous studies (Takeuchi et al., 2009; Takeuchi and Hayakutake, 2012). 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 \( 10 \times 10 = 100 \) Pt atoms arranged in the \( X \) and \( Z \) direction, respectively. Four molecular sheets are stacked normal to the surface in the negative \( Y \) direction. We apply the periodic boundary condition in the direction parallel to the surface. As for the interaction potential between molecules \( i \) and \( j \), we take the Lennard–Jones potential for Pt-Pt, given by (Yamamoto et al., 2006)

\[
\phi_{ij}(r) = 4\epsilon \left[ \left( \frac{\sigma_{Pt}}{r} \right)^{12} - \left( \frac{\sigma_{Pt}}{r} \right)^{6} \right].
\]

Here, \( r \) is the intermolecular distance, \( \epsilon \) the interaction potential well depth, and \( \sigma_{Pt} \) the core diameter. These values are listed in Table 1. In this table, \( m \) is the mass of an atom and \( k \) is the Boltzmann constant. In the present study, the SPC/E model (Berendsen et al., 1987) is used as a molecular model of water molecules. The potential function between H₂O-H₂O is given by the Lennard–Jones potential for O-O combined with the Coulomb potential between point charges \( q \) in each atom as (Berendsen et al., 1987)

\[
\phi_{H_2O-H_2O} = 4\epsilon_{O} \left[ \left( \frac{\sigma_{O}}{r_{OO}} \right)^{12} - \left( \frac{\sigma_{O}}{r_{OO}} \right)^{6} \right] + \sum_{i \neq j} \sum_{j \neq i} \frac{q_i q_j}{r_{ij}}.
\]

These interaction parameters are also listed in Table 1. We take the model developed by Spohr and Heinzinger for H₂O-Pt interactions (Spohr and Heinzinger, 1988). The potential function is described as follows:

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Fig. 1 Couette flow with heat transfer problem.

Table 1 Molecular interaction parameters.

| Atom pairs | σ [Å]  | ε/k [K]   | m [g] | r_m[Å] | A | B [Å^{12} kcal/mol] |
|------------|--------|-----------|-------|--------|---|-------------------|
| Pt-Pt      | 2.523  | 3771.5    | 3.24×10^{-22} | -      | -  | -                |
| O-O        | 3.116  | 78.2      | 2.66×10^{-23} | -      | -  | -                |
| H-H        | -      | -         | 1.67×10^{-24} | -      | -  | -                |
| Ar-Ar      | -      | -         | 6.63×10^{-23} | -      | -  | -                |
| Ar-Pt      | 0.625  | 134.7     | 4.6       | -      | -  | -                |
| Ar-O       | -      | 156.8     | 3.556     | 12.5   | -  | -                |
| Ar-H       | -      | -         | -         | -      | -  | 1.259×10^{5}     |

Table 2 Potential parameters of H_2O-Pt.

| i | a_i [J] | b_i [Å^{-1}] | c [Å^{-1}] |
|---|---------|-------------|------------|
| 1 | 1.8942×10^{-16} | 1.1004 | -          |
| 2 | 1.8863×10^{-16} | 1.0966 | -          |
| 3 | 1×10^{-13}      | 5.3568  | -          |
| 4 | 1.7142×10^{-19} | 1.2777 | -          |

\[ \phi_{\text{H}_2\text{O-Pt}} = \phi_{\text{O-Pt}} (r_{\text{O-Pt}}, \xi_{\text{O-Pt}}) + \phi_{\text{H-Pt}} (r_{\text{H-Pt}}) + \phi_{\text{H-Pt}} (r_{\text{H-Pt}}), \]
\[ \phi_{\text{O-Pt}} = [a_1 \exp(-b_1 r) - a_2 \exp(-b_2 r)]F(\xi) + a_3 \exp(-b_3 r)[1 - F(\xi)], \]
\[ \phi_{\text{H-Pt}} = a_4 \exp(-b_4 r). \]
\[ F(\xi) = \exp(-c\xi^2). \]

where \( \xi \) is the length of the projection of the distance vector onto the surface plane. The potential parameters \( a_i, b_i, \) and \( c \) are listed in Table 2. Furthermore, the potential between Ar and Pt is given by the Morse potential as (Head-gordon et al., 1991)

\[ \phi_{\text{Ar-Pt}} (r) = \varepsilon \left[ \exp\left( \frac{-2(r - r_m)}{r} \right) - 1 \right]^2. \]

We use the potential for Ar-H_2O interactions (Anderson et al., 2004) given by
Fig. 2 Wall surface model for $\Theta = 0.20$ in the MD simulation.

$$
\varphi_{\text{Ar-H}_2\text{O}} = \varphi_{\text{Ar-O}}(r_{\text{Ar-O}}) + \varphi_{\text{Ar-H}}(r_{\text{Ar-H}}) + \varphi_{\text{Ar-H}}(r_{\text{Ar-H}_2}).
$$

$$
\varphi_{\text{Ar-O}} = \frac{e}{A} \left[ 6 \exp \left( A \left( 1 - \frac{r}{r_m} \right) \right) - \left( \frac{r_m}{r} \right)^6 \right],
$$

$$
\varphi_{\text{Ar-H}} = \frac{B}{r^{12}}.
$$

These interaction parameters are also shown in Table 1. The temperature of the solid surface is set at $T_L = 300$ K. The incident position of the gas molecule to the wall surface is set at a height of $8\sigma$ away from the wall surface ($Y$ direction), enough to neglect the interaction from the surface molecules. The positions in the $X$ and $Z$ directions are randomly set. The incident velocity is set from the DSMC simulations. The MD simulation is finished when the gas molecule returns to the height of $8\sigma$ where it is not affected by the wall surface. About 10 gas molecules collide with the lower wall per one DSMC timestep, and MD simulation was performed for each of the collisions. For a single DSMC particle entrance, the MD simulation is performed using the incident molecular velocity in the DSMC simulation as the initial velocity at the height $8\sigma$ from the wall surface, and obtained reflected molecular velocities by MD simulations are handled over to DSMC simulations again. For the calculation of the Coulomb potential, the Ewald method (Ueda, 2003), which calculates the Coulomb potential with sufficient accuracy by using the Fourier series, was applied. Newton’s equations of motion and equations for angular momentum are numerically solved by the leap-frog method. To solve the rotational motion, we introduced a quaternion method (Ueda, 2003) to prevent the divergence of the calculation. The time step is taken as $\Delta t = 1.5 \times 10^{-15}$ s. In addition, we define the adsorption rate $\Theta$ in the same manner of the previous study (Takeuchi et al., 2009). In this study, the adsorption rate $\Theta$ is considered to be from 0 to 0.50. A wall surface model for $\Theta = 0.20$ is shown in Figure 2.

3. Reflection model

Based on data such as the accommodation coefficients obtained by these analyses, a modified Maxwell-type model is constructed by the following equations:

$$
f_x^+ = \alpha_x f_w + (1 - \alpha_x) f_x^- (V_y > 0),
$$

$$
f_y^+ = \alpha_x f_w + (1 - \alpha_x) f_y^- (V_y > 0),
$$

$$
f_z^+ = \alpha_E f_w + (1 - \alpha_E) f_z^- (V_y > 0).
$$

Here, the TMAC $\alpha_x$ is considered for the $X$ direction, and the NMAC $\alpha_e$ is considered for the direction normal to the
wall surface. The energy accommodation coefficient (EAC) $\alpha_E$ is used for the distribution in the Z direction. The function $f^-$ is the velocity distribution function for the incident molecules (as for $f^r$, the sign is changed), and $f_n$ is the Maxwellian distribution. In a previous study (Yamamoto et al., 2006), we used the $\alpha_i$ for the distribution in the X and Z directions, and $\alpha_r$ for the distribution in the Y direction. In this case, $\alpha_i$ is used for the X direction because the flow field that we employ has a macroscopic flow in the X direction. This assignment of accommodation coefficients is identical with that reported by Takeuchi et al. (Takeuchi et al., 2012), but it is not certain whether it can be adopted to the faster flow field and with the multitude of adsorbates. We evaluate this reflection model under these influences by comparing our model with the diffuse reflection model. The TMAC, $\alpha_t$, of gas molecules at the wall surface is defined as follows:

$$\alpha_t = \frac{\tau_i - \tau_r}{\tau_i}. \tag{9}$$

Here, $\tau$ is the $X$ component of the average momentum of molecules, and subscripts $i$ and $r$ represent the incident and reflected molecules, respectively. The NMAC, $\alpha_n$, and EAC, $\alpha_E$, of the gas molecules are defined respectively as follows:

$$\alpha_n = \frac{p_i - p_r}{p_i - p_w}, \quad \alpha_E = \frac{E_i - E_r}{E_i - E_w}, \tag{10}$$

where $p$ is the absolute value of the $Y$ component of the average momentum of the molecules, $E$ is the average total kinetic energy of the molecules, and the subscripts $i$, $r$, and $w$ represent the incident, reflected, and diffusely reflected molecules, respectively.

4. Results and discussion
4.1 Accommodation coefficients

First, we describe the accommodation coefficients necessary to construct the modified Maxwell-type model. These values of $\alpha_t$, $\alpha_n$, and $\alpha_E$ are listed in Table 3. We found that the TMAC $\alpha_t$ and NMAC $\alpha_n$ depend on the speed ratio, the upper wall temperature, and the adsorption rate. Since the authors have already investigated the influence of the speed ratio and the upper wall temperature on the accommodation coefficients (Yamamoto et al., 2004a, 2004b), we consider only the effect of adsorption rate $\Theta$ in this paper. The standard deviation of an accommodation coefficient is calculated from the 1000 data that are selected randomly from 10,000 velocity data. For example, the standard deviation of TMAC is ±0.005 when the speed ratio is 1.0 and the adsorption rate is 0.00. The results of each accommodation coefficient are shown in Figure 3. As shown in this figure, the TMAC increases with increasing the adsorption rate, peaks at $\Theta = 0.20$ to 0.30, and then decreases. On the other hand, the NMAC and EAC tend to decrease monotonically as the adsorption rate increases. This is considered to result from the roughness of the potential energy surface (PES). In the $X$ direction, the roughness of the PES has a large influence on the momentum exchange since the potential barrier is formed normal to the flow direction by water molecules. When the adsorption rate

| $\Theta$ | $T_U = 450$ K | $T_U = 600$ K | $T_U = 450$ K | $T_U = 600$ K | $T_U = 450$ K | $T_U = 600$ K |
|---------|----------------|----------------|----------------|----------------|----------------|----------------|
| 0.00    | $\alpha_i$   | $\alpha_n$   | $\alpha_E$   | $\alpha_i$   | $\alpha_n$   | $\alpha_E$   |
| 0.18    | 0.16          | 0.15          | 0.14          | 0.16          | 0.15          | 0.14          |
| 0.05    | 0.27          | 0.25          | 0.26          | 0.27          | 0.25          | 0.26          |
| 0.10    | 0.31          | 0.30          | 0.28          | 0.31          | 0.30          | 0.27          |
| 0.20    | 0.34          | 0.32          | 0.28          | 0.34          | 0.32          | 0.27          |
| 0.30    | 0.36          | 0.34          | 0.27          | 0.36          | 0.33          | 0.26          |
| 0.40    | 0.33          | 0.32          | 0.26          | 0.33          | 0.31          | 0.23          |
| 0.50    | 0.32          | 0.30          | 0.24          | 0.32          | 0.30          | 0.22          |
is small ($\Theta = 0$ to 0.30), a rough PES is formed on the Pt surface by the small number of water molecules, as shown in Figure 4(a), and the momentum of the reflected gas molecule decreases since the gas molecules collide with the rough PES. However, as the rate of adsorbed water molecules further increases ($\Theta = 0.30$ to 0.50), the PES changes to a smoother surface by connecting these sharp peaks with each other, as shown in Figure 4(b). In other words, it is considered that potential barriers that generate a rough PES by adsorbed water molecules overlap each other, and finally, a new smooth PES is formed. The momentum of reflected gas molecules in the $X$ direction on such a smooth PES is easily reserved. As a result, in the tangential direction, the TMAC increases when the adsorption rate is small, but decreases when it is large. The NMAC and EAC tend to decrease as the adsorption rate increases, but the reason for this remains unclear; further research is needed on this aspect.

### 4.2 Distribution functions of molecular velocity

Figures 5–12 show the velocity distribution functions for gas molecules before and after reflection on the lower wall surface. Figures (a), (b), and (c) represent the distribution functions for the $X$, $Y$, and $Z$ directions, respectively. The temperature of the upper wall surface is taken to be 450 and 600 K. The molecular velocity $V$ is normalized by the most probable speed $C_m$, the open circles represent the distribution for the incident molecules, and the filled circles show the distribution of the reflected molecules obtained from the MD simulations. The distribution obtained from the diffuse reflection at the lower wall surface with temperature $T_L$ is indicated by a dashed curve for comparison. The solid curve represents the new distribution proposed in this paper based on the Maxwell-type reflection model.

Figures 5 and 6 show the results for the clean surface ($\Theta = 0$) and the water adsorbed surface ($\Theta = 0.50$) when the speed ratio is 1.0 and the temperature of the upper wall is 450 K. First, by comparing Figures 5 and 6, we consider the influence of adsorbed water molecules when the speed ratio is relatively small. In these figures, it shows that the distribution of the reflected gas molecules can be described very well for all directions by a distribution of the modified Maxwell-type reflection model. The distribution of the model showed good agreement, even in the case where the
The accommodation rate was large ($\Theta = 0.50$); therefore, we confirmed that this model can be applied regardless of the presence of the water molecules when the speed ratio is relatively small. However, the diffuse reflection model generally used shows a large difference from the MD simulation compared with the modified Maxwell-type model.

Figures 7 and 8 show the results for the clean surface ($\Theta = 0$) and the water adsorbed surface ($\Theta = 0.50$) when the speed ratio is 2.0 and the temperature of the upper wall is 450 K. We describe the influence of the speed ratio by comparing Figures 5 and 7. In the $Y$ and $Z$ directions, good agreement is shown regardless of the increase in the speed ratio. However, in the $X$ direction, it can be confirmed that a slight difference occurs when the speed ratio is 2.0. Next, by comparing Figures 6 and 8, we consider the influence of adsorbed water molecules when the speed ratio is relatively large. The difference between the modified Maxwell-type model and the MD results depends on the adsorption rate. Specifically, the difference becomes small as the adsorption rate increases, and the degree of coincidence is improved.

Figures 9 and 10 show the results for the clean surface ($\Theta = 0$) and the water adsorbed surface ($\Theta = 0.50$) when the speed ratio is 1.0 and the temperature of the upper wall is 600 K. In the case of $T_U = 600$ K, the modified Maxwell-type model showed good agreement with the MD results when the speed ratio is relatively small. This trend is similar to $T_U = 450$ K. Figures 11 and 12 show the results for the clean surface ($\Theta = 0$) and the water adsorbed surface ($\Theta = 0.50$) when the speed ratio is 2.0 and the temperature of the upper wall is 600 K. Slight differences were seen not only at low, but also at high adsorption rates in the $X$ direction. These differences were small compared with the diffuse reflection model.

From the above results, the validity of this model can be summarized. In general, it is possible to describe the distribution for all directions with only one accommodation coefficient in the case of a flow with no velocity gradient but with a temperature gradient. However, it is obvious that large differences occur when the accommodation coefficients are different in each direction, such as in the system described here. In this study, we compared our results with those obtained from the diffuse reflection model because this model is mostly used in conventional DSMC simulations, and it is important to know the difference between our model and the diffuse reflection model. In the modified Maxwell-type model suggested in this paper, the degree of agreement becomes small as the speed ratio increases, and it is somewhat dependent on the adsorption rate and the temperature of the upper wall. However, the differences between the MD results and the modified Maxwell-type reflection model are small compared with the diffuse reflection model. Therefore, this model can be applied for simulations with relatively high-speed flow and with some water molecules on the wall surfaces.
Fig. 7 Velocity distribution functions of gas molecules on the lower wall surface \((S_U = 2.0, T_U = 450 \text{ K}, \Theta = 0)\).

Fig. 8 Velocity distribution functions of gas molecules on the lower wall surface \((S_U = 2.0, T_U = 450 \text{ K}, \Theta = 0.50)\).

Fig. 9 Velocity distribution functions of gas molecules on the lower wall surface \((S_U = 1.0, T_U = 600 \text{ K}, \Theta = 0)\).

Fig. 10 Velocity distribution functions of gas molecules on the lower wall surface \((S_U = 1.0, T_U = 600 \text{ K}, \Theta = 0.50)\).
We constructed a modified Maxwell-type reflection model and verified its validity by comparing the molecular velocity distribution function at a high shear rate, a high temperature gradient, and high adsorption rates. The gas is taken to be Ar and the wall surface as made from Pt. 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 surfaces 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 $\alpha_t$ and NMAC $\alpha_e$ depend on the speed ratio, the temperature of the upper wall surface, and the adsorption rate. In this paper, the influence of adsorption rate on the accommodation coefficients is clarified. The TMAC increases with an increasing adsorption rate, and has a peak at $\Theta = 0.20$ to 0.30. On the other hand, the NMAC and EAC tend to decrease as the adsorption rate increases.

We also adapted the modified Maxwell-type reflection model for the lower wall surface and verified its validity by comparing the velocity distribution functions on the lower wall surface. It is assigned appropriate accommodation coefficients for each direction. We found that the velocity distribution of the modified Maxwell-type reflection model agreed well with the MD simulation compared with the diffuse reflection model. As the speed ratio increases, the degree of agreement becomes small and is somewhat dependent on the adsorption rate and the temperature of the upper wall. However, the differences between the MD results and the modified Maxwell-type reflection model are small compared with the diffuse reflection model. Therefore, this model can be applied for simulations with relatively high-speed flow and with some adsorption molecules on the wall surface.

5. Conclusions

Fig. 11 Velocity distribution functions of gas molecules on the lower wall surface ($S_U = 2.0$, $T_U = 600$ K, $\Theta = 0$).

Fig. 12 Velocity distribution functions of gas molecules on the lower wall surface ($S_U = 2.0$, $T_U = 600$ K, $\Theta = 0.50$).

(a) $X$ direction (along the wall surface)  (b) $Y$ direction (normal to the wall surface)  (c) $Z$ direction (across the wall surface)
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