Slightly Rarefied Gas Flow Over
A Smooth Platinum Surface

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Abstract. The molecular dynamics method for the interaction of the gas molecule with the solid wall together with the Monte-Carlo method for the motion of gas molecules is applied to analyze the behavior of a slightly rarefied gas between two walls. The wall consists of platinum molecules and the gas is taken to be xenon or argon. The Couette flow and the thermal problem for which two walls have different temperature are considered. The slip or jump coefficient of the flow and the accommodation coefficient of the tangential momentum, normal momentum or kinetic energy are obtained at the wall of 300K temperature. The distribution function of the molecule at the wall surface is also obtained, and it is found that the Maxwell type boundary condition describes well the distribution function of the reflected molecule.

INTRODUCTION

In a slightly rarefied gas flow, we can solve the Navier-Stokes equation under the slip or jump boundary condition to obtain the flow field in most region of the flow except the Knudsen layer. The slip or jump condition is to be obtained by developing the asymptotic analysis for small Knudsen number to the Boltzmann equation. For this purpose we must specify the velocity distribution of the reflected molecule at the wall. The diffuse reflection, the Maxwell type or CL model boundary condition [1] has been assumed. However, the gas-wall interaction is not so simple and sometimes the diffuse reflection is not valid, e.g. at a very clean or high temperature wall, in an ultra vacuum, in a very high speed flow etc. As for the Maxwell type boundary condition, the accommodation coefficient should be specified. In any case, we must investigate the gas-wall interaction to get the proper distribution function of the reflected molecule.

In the present study, we shall consider a smooth and clean platinum surface and analyze the slightly rarefied gas flow between two walls by applying the molecular dynamics method for the gas-wall interaction and the Monte-Carlo method for the motion of gas molecules. We take the xenon and the argon molecules.

METHOD OF ANALYSIS

We consider a slightly rarefied gas flow between two walls and analyze the following two problems: The first one is the Couette flow. The upper wall moves with a speed $-U/2$ whereas the lower wall has the velocity $U/2$. Both walls have the same temperature of 300K. Actual calculation was made of the case that the speed ratio $S_L$ of the lower wall is taken to be 0.1 for the xenon gas and 0.25 for the argon gas, where $S_L = (U/2)/C_m$, $C_m = \sqrt{2kT_w/m}$ is the most probable speed, $m$ the mass of a molecule, $T_w$ the wall temperature taken to be 300K and $k$ the Boltzmann constant. The second one is the thermal problem. We take the temperature of the lower wall ($T_L = T_w$) to be 300K and the upper wall to be 450K. Further we assume that both walls have no motion and that the gas molecule is diffusely reflected at the upper wall. We take the Knudsen number to be 0.2 in both cases.

The same method of analysis as in previous studies [2]-[4] is applied in the present study. That is, the Monte-Carlo method [5] is applied to the analysis of the gas field between two walls. The hard sphere molecule is assumed for the interaction between gas molecules in the Monte-Carlo simulation. When a molecule hits the wall surface in the Monte-Carlo simulation, we switch to the analysis based on the molecular dynamics method...
at this point to trace the motion of the gas molecule, which is going to interact with the solid molecules of
the wall. We use the standard molecular dynamics method. For this purpose, we shall construct the wall
having the molecular structure. We assume that the wall consists of a thin platinum layer. The surface of the
layer is set on (1,1,1) plane. We take 6 Pt molecules in the X-direction and other 6 molecules in the Z-direction
on the surface. Four molecular sheets are taken normal to the surface. The periodic condition is applied to
the parallel direction to the surface as is usually assumed in the molecular dynamics. As for the interaction
potential between molecules, we take the Lennard-Jones potential for Pt—Pt, Xe—Xe or Ar—Ar interaction:
\[ \phi_{\text{L-J}}(r) = 4\epsilon \left( \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6 \right). \]

The Morse potential is used for Pt—Xe or Pt—Ar interaction:
\[ \phi_{\text{Morse}}(r) = \epsilon \left\{ \exp\left[ -2\sigma^* (r - r_0) \right] - 2 \exp\left[ -\sigma^* (r - r_0) \right] \right\}, \]
\[ \phi_{\text{Morse}}^*(r) = \epsilon \left\{ \exp\left[ -2\sigma^* (r - r_0) \right] - 1 \right\}^2. \]

Here, \( r \) is the intermolecular distance, and \( \sigma, \sigma^*, \epsilon \) and \( r_0 \) are interaction parameters. Numerical values of the
parameters involved in the potentials are taken from references [5]-[7] and shown in Table 1.

When a gas molecule hits the wall surface in the process of Monte-Carlo simulation, we put a gas molecule at a
distance of \( 8\sigma_{\text{pt}} \) above the most upper Pt molecular sheet, where \( \sigma_{\text{pt}} \) is \( \sigma \) of Pt molecule. The initial velocity of
this molecule has been calculated by the Monte-Carlo simulation. Newton’s equations of motion are integrated
with Verlet’s method. We could consider a clean surface of Pt wall without adsorbates. However, while the gas
molecule hits the clean surface successively, some of them, which have low energy, may be physically adsorbed
on the surface. We should take the platinum wall on which some Xe molecules are adsorbed, and consider the
interaction of impinging Xe molecule with the solid molecule as well as the adsorbates. Actually, we found that
ten Xe molecules are adsorbed on the surface consisting 6x6 platinum molecules when the wall temperature
is 300K. They are moving around on the surface. On the other hand, there is no physically adsorbed argon
molecule on the same platinum surface.

**RESULT**

A Distributions of flow velocity and temperature

Figure 1(a) shows the flow velocity \( q_x/(U/2) \) when \( S_L=0.1 \) for the xenon gas and \( S_L=0.25 \) for the argon gas.
The coordinate \( y \) is related with the physical coordinate \( Y \) by
\[ Y = \ell_{HS} y, \quad \ell_{HS} = (\sqrt{2\pi d^2 n_0})^{-1}, \]
where \( \ell_{HS} \) is the mean free path of the hard sphere molecule, \( d \) the diameter of the molecule and \( n_0 \) the
reference number density. We took 80 cells between two walls and about ten thousands sample numbers in one
cell. This may not be enough large to get a smooth distribution of the flow velocity. However, we can draw a
line representing the asymptotic flow velocity which is valid outside the Knudsen layer. The Knudsen layer is
the order of the mean free path, and it diminishes rapidly. We may consider that the Knudsen layer extend up
to \( y \approx 0.6 \) from the wall surface. Then, the asymptotic line, which goes through the point \( y = 2.5, q_x = 0 \), is
obtained by the least squares method using the data of \( 0.6 < y < 2.5 \), and is shown as a solid line in Fig.1(a).
Figure 1(b) shows the temperature distribution. The asymptotic temperature distribution is also obtained from

**TABLE 1. Values included in potentials.**

<table>
<thead>
<tr>
<th></th>
<th>( \sigma [\text{\AA}] )</th>
<th>( \sigma^* [1/\text{\AA}] )</th>
<th>( \epsilon/k [\text{K}] )</th>
<th>( r_0 [\text{\AA}] )</th>
<th>( m [\text{g}] )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \text{Pt—Pt} )</td>
<td>2.523</td>
<td>-</td>
<td>3771.5</td>
<td>-</td>
<td>( 3.24 \times 10^{-22} )</td>
</tr>
<tr>
<td>( \text{Xe—Xe} )</td>
<td>4.10</td>
<td>-</td>
<td>221</td>
<td>-</td>
<td>( 2.18 \times 10^{-22} )</td>
</tr>
<tr>
<td>( \text{Ar—Ar} )</td>
<td>3.405</td>
<td>-</td>
<td>119.8</td>
<td>-</td>
<td>( 6.63 \times 10^{-23} )</td>
</tr>
<tr>
<td>( \text{Pt—Xe} )</td>
<td>-</td>
<td>1.05</td>
<td>319.1</td>
<td>3.20</td>
<td>-</td>
</tr>
<tr>
<td>( \text{Pt—Ar} )</td>
<td>-</td>
<td>1.6</td>
<td>134.7</td>
<td>4.6</td>
<td>-</td>
</tr>
</tbody>
</table>
the data outside the Knudsen layer. We can obtain the so-called slip or jump coefficient at the wall surface using this asymptotic distribution. The slip and jump boundary conditions at the wall surface are written as

\[ q_x(0) = \alpha_M \ell_p \left( \frac{\partial q_x}{\partial y} \right)_0, \quad T(0) - T_w = \beta \ell_t \left( \frac{\partial T}{\partial y} \right)_0, \]  

where \( \alpha_M \) and \( \beta \) are the slip and jump coefficients, \( \ell_p \) and \( \ell_t \) are the mean free paths defined by the viscosity \( \mu \) or the thermal conductivity \( \kappa \) as

\[ \ell_p = \frac{\mu}{p_0} (2RT_w)^{1/2}, \quad \ell_t = \frac{4\kappa}{\partial \rho_0} \sqrt{\frac{T_w}{2R}}, \quad p_0 = p_0 RT_w, \]  

where \( R \) is the gas constant and \( p_0 \) is the reference density. Table 2 shows the slip and jump coefficients of the flow. This table also shows the accommodation coefficients of the tangential momentum \( \sigma_M \), the normal momentum \( \sigma_N \) and the kinetic energy \( \lambda \). These are defined by

\[ \sigma_M = \frac{\tau_i - \tau_r}{\tau_i}, \quad \sigma_N = \frac{p_i - p_r}{p_i - p_w}, \quad \lambda = \frac{E_i - E_r}{E_i - E_w}, \]  

where \( \tau \) is the tangential momentum, \( p \) the normal momentum, \( E \) the energy flux, and the subscripts \( i \) and \( r \) mean the impinging and reflecting molecules, respectively, and \( w \) means the value of the molecule with the wall temperature. The slip or jump coefficient may be compared with that of the analysis based on the Maxwell type boundary condition together with the B-G-K equation \([9],[10]\). The slip coefficients \( \alpha_M \) obtained are 8.2247, 1.4876 and 1.2271 when the accommodation coefficients are 0.2, 0.8 and 0.9, respectively. The jump coefficients \( \beta \) are obtained as 3.629, 1.900 and 1.570 when the accommodation coefficients are 0.5, 0.8 and 0.9, respectively. Although the definition of the accommodation coefficient in the present study is different from that in the Maxwell model, it is interesting to see that the present slip and jump coefficients are about the same as those of the Maxwell type boundary condition. The thermal accommodation coefficient can be compared with available experimental data \([11],[12]\). Experimental values of \( \lambda \) are 0.858 and 0.55 for \( Pt - Xe \) and \( Pt - Ar \), respectively. These are also well compared with the present calculation.

**TABLE 2.** Slip, jump and accommodation coefficients.

<table>
<thead>
<tr>
<th></th>
<th>Couette flow</th>
<th>Thermal problem</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( Xe ) ( (S_L = 0.1) )</td>
<td>( Ar ) ( (S_L = 0.25) )</td>
</tr>
<tr>
<td>( \alpha_M )</td>
<td>1.4</td>
<td>9.5</td>
</tr>
<tr>
<td>( \sigma_M )</td>
<td>0.81</td>
<td>0.19</td>
</tr>
<tr>
<td>( \beta )</td>
<td>1.5</td>
<td>3.6</td>
</tr>
<tr>
<td>( \lambda )</td>
<td>0.85</td>
<td>0.43</td>
</tr>
<tr>
<td>( \sigma_N )</td>
<td>0.88</td>
<td>0.62</td>
</tr>
</tbody>
</table>

**FIGURE 1.** Distributions of (a) flow velocity and (b) temperature. \( \circ: Ar, \bullet: Xe. \)
TABLE 3. Quantities at the wall.

<table>
<thead>
<tr>
<th>Sample</th>
<th>Couette flow</th>
<th>Thermal problem</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$Xe(S_1=0.1)$</td>
<td>$Ar(S_1=0.25)$</td>
</tr>
<tr>
<td>$C_{-2}^r p/</td>
<td></td>
<td></td>
</tr><tr>
<td>ho_0$</td>
<td>0.256</td>
<td>0.256</td>
</tr>
<tr>
<td>$C_{-2}^r T/</td>
<td></td>
<td></td>
</tr><tr>
<td>ho_0$</td>
<td>-0.0185</td>
<td>-0.064</td>
</tr>
<tr>
<td>$C_{-2}^r T/</td>
<td></td>
<td></td>
</tr><tr>
<td>ho_0$</td>
<td>-0.0036</td>
<td>-0.052</td>
</tr>
<tr>
<td>$C_{-3}^r E/</td>
<td></td>
<td></td>
</tr><tr>
<td>ho_0$</td>
<td>0.292</td>
<td>0.295</td>
</tr>
<tr>
<td>$C_{-3}^r E/</td>
<td></td>
<td></td>
</tr><tr>
<td>ho_0$</td>
<td>0.291</td>
<td>0.292</td>
</tr>
</tbody>
</table>

FIGURE 2. Velocity distribution function of Ar molecule for the Couette flow. (a) parallel velocity (b) normal velocity; o: reflected, •: incident.

B Distribution function of the molecular velocity

We next show the distribution functions of the molecular velocity at the wall surface. Figure 2 shows the distribution function of Ar molecule for the Couette flow; Fig.2(a) is for the parallel velocity to the surface, while Fig.2(b) is for normal velocity. Here, the open circle means the distribution of the reflected molecule and the filled circle is the distribution of the incident molecule obtained in the present calculation. The solid and dotted curves in Fig.2(a) are drawn from the following Maxwellian distributions $f^-_v$ for $V_y < 0$ and $f^+_v$ for $V_y > 0$, respectively:

$$f^-_v = \frac{1}{\sqrt{\pi}} e^{-(V_y - Q^-_v)^2}, \quad Q^-_v = -0.223; \quad f^+_v = \frac{1}{\sqrt{\pi}} e^{-(V_y - Q^+_v)^2}, \quad Q^+_v = -0.180,$$

where $Q^-_v$ and $Q^+_v$ are the mean velocities parallel to the wall, which are calculated using the velocities for the incoming and reflected molecules, respectively, obtained in the present calculation. Here and below, the molecular velocity and the flow velocity are normalized by the most probable speed $C_m$, and the temperature is normalized by $T_w$ (=300K). The solid and dotted curves in Fig.2(b) are also drawn from the following distributions $f^-_y$ for $V_y < 0$ and $f^+_y$ for $V_y > 0$, respectively, related to the Maxwell distribution with zero mean velocity:

$$f^-_y = -2V_y e^{-V_y^2} \quad (V_y < 0), \quad f^+_y = 2V_y e^{-V_y^2} \quad (V_y > 0).$$

It will be seen that the distribution functions obtained in the present calculation are very close to those of
The Maxwellian distributions. Figure 3 shows the distribution function of the Xe molecule for the Couette flow. The solid or dotted curve in Fig.3(a) is drawn from the same Maxwellian distribution as in Eq.(8) but with different mean parallel velocity, \( Q^- \) or \( Q^+ \), which is calculated by using the molecular velocities obtained in the present calculation and is given by

\[
Q^- = -0.0643, \quad Q^+ = -0.0125. \tag{10}
\]

The curves in Fig.3(b) are the same as those defined in Fig.2(b), i.e., these are derived from the Maxwellian distribution with zero mean velocity. We were not able to calculate the normal momentum accommodation coefficient, because the difference between the momenta of the incident and reflected molecules were very small. However, Fig.2(b) and Fig.3(b) may indicate that the normal momentum accommodation coefficient is close to unity.

We next discuss on the distribution function for the thermal problem. The velocity distribution functions of Ar molecule are shown in Fig.4 by open circles (reflected molecule) and filled circles (incident molecule). The solid and dotted curves in Fig.4(a) are drawn from the following Maxwellian distributions \( f^- \) for \( V_y < 0 \) and \( f^+ \) for \( V_y > 0 \), respectively:

\[
f^- = \frac{1}{\sqrt{\pi T_-}} e^{-V_y^2/T_-}, \quad T_- = 1.313; \quad f^+ = \frac{1}{\sqrt{\pi T_+}} e^{-V_y^2/T_+}, \quad T_+ = 1.177. \tag{11}
\]

Here, the temperature \( T_- \) and \( T_+ \) are obtained so that the heat flux to or from the wall calculated from Eq.(11) may be the same as that of the present calculation. The solid and dotted curves in Fig.4(b) are also drawn from the following distributions \( f^- \) and \( f^+ \), respectively, related to the Maxwellian distributions:

\[
f_y^- = -\frac{2}{T_-} V_y e^{-V_y^2/T_-} \quad (V_y < 0), \quad f_y^+ = \frac{2}{T_+} V_y e^{-V_y^2/T_+} \quad (V_y > 0). \tag{12}
\]

Here, \( T_- \) and \( T_+ \) are the same as in Eq.(11). From Fig.4, in this case too, we can say that the distribution function of the molecular velocity at the wall surface is very close to a Maxwellian distribution. The distribution function for Xe molecule is shown in Fig.5. The solid or dotted curves in this figure are drawn from the same Maxwellian distributions as in Eq.(11) or Eq.(12) but with different temperature \( T_- \) or \( T_+ \), which is calculated using the molecular velocities obtained in the present calculation and is given by

\[
T_- = 1.234, \quad T_+ = 1.035. \tag{13}
\]

It is interesting to see that the distribution functions obtained in the present calculation, which are shown by filled or open circles, are very close to those of the Maxwellian distributions in Fig.5.
FIGURE 4. Velocity distribution function of Ar molecule in the thermal problem. (a) parallel velocity (b) normal velocity; o: reflected, •: incident.

FIGURE 5. Velocity distribution function of Xe molecule in the thermal problem. (a) parallel velocity (b) normal velocity; o: reflected, •: incident.

C Comparison with the Maxwell boundary condition

Finally, we discuss on the Maxwell type boundary condition. Figure 6 shows the comparison of the distribution function of the reflected molecule in the parallel direction to the surface with that of the Maxwell type boundary condition in case of the Couette flow. The Maxwell type boundary condition is taken as

\[ f^+_x = \sigma_M f_w + (1 - \sigma_M) f^-_x, \quad f_w = \exp(-V_x^2)/\sqrt{\pi}, \]

(14)

with \( \sigma_M = 0.19 \) for Ar molecule and 0.81 for Xe molecule. The function \( f^-_x \) for \( V_x < 0 \) is given by Eq.(8) with \( Q^-_x = -0.223 \) for Ar molecule and \( Q^-_x = -0.0643 \) for Xe molecule and is shown as solid curves in Fig.6. The dotted curve is drawn from Eq.(14) and the corresponding distribution function for the reflected molecule in the present calculation is shown as open circles. It will be seen that the distribution of the reflected molecule is in quite good agreement with that of the Maxwell type boundary condition in both cases. This does not mean that each molecule is reflected specularly or diffusely, but actually the global velocity distribution of the reflected molecule is quite similar to that of the Maxwell type boundary condition.
Figures 7 and 8 show the comparison of the velocity distribution functions of the reflected molecule in the thermal problem with those of the Maxwell type boundary condition. The Maxwell type boundary conditions are given by

\[ f_{\lambda}^+ = \lambda f_w + (1-\lambda) f_{\lambda}^- \, , \quad f_w = \exp(-V_x^2)/\sqrt{\pi}, \]  

\[ f_{\lambda}^- = \sigma_N f_w + (1-\sigma_N) f_{\lambda}^+ \, , \quad f_w = 2V_y \exp(-V_y^2), \]  

with \( \lambda = 0.43 \) and \( \sigma_N = 0.82 \) for \( \text{Ar} \) gas and \( \lambda = 0.85 \) and \( \sigma_N = 0.88 \) for \( \text{Xe} \) gas. The Maxwell type boundary condition is shown as dotted curves. The functions \( f_{\lambda}^+ \) and \( f_{\lambda}^- \) in these equations are the same as in Eqs.(11) and (12) and are shown as solid curves. Open circle means the distribution of the present calculation. We will see a very good agreement between the present distribution and the Maxwell type boundary condition. If we use \( \lambda \) instead of \( \sigma_N \) in Eq.(16), we will see a little bit bad agreement in case of \( \text{Ar} \) molecule but no difference in case of \( \text{Xe} \) molecule.

**CONCLUSION**

We have analyzed the flow of slightly rarefied gas of xenon or argon molecule over a smooth platinum surface of 300K temperature by applying the molecular dynamics method together with the Monte-Carlo method, and obtained the following results:

1. The accommodation coefficient of tangential momentum and the slip coefficient are 0.81 and 1.4 for xenon gas and 0.19 and 9.5 for argon gas, respectively.
2. The accommodation coefficient of kinetic energy and the jump coefficient are 0.85 and 1.5 for xenon gas and 0.43 and 3.6 for argon gas, respectively.
3. The velocity distribution function of molecules at the wall surface is approximately represented by a Maxwellian distribution function.
4. Each molecule is not reflected specularly or diffusely, but the global distribution of the reflected molecule is close to that of the Maxwell type boundary condition.

**REFERENCES**

FIGURE 7. Comparison with the Maxwell type boundary condition in the thermal problem for Ar gas. (a) parallel velocity (b) normal velocity ; o : reflected.

FIGURE 8. Comparison with the Maxwell type boundary condition in the thermal problem for Xe gas. (a) parallel velocity (b) normal velocity ; o : reflected.


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