The Effect of Thermal Accommodation on Unsteady Microscale Heat Transfer

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Abstract. Thermal accommodation coefficient, one of the fundamental parameters in rarefied gas dynamics, is usually introduced to account for the fraction of incident molecules interacting with solid surface in a diffusive manner. In the present study, the effects of thermal accommodation on the unsteady one-dimensional micro-flow are examined, when the oscillating flow input is applied, by employing the unsteady DSMC technique. Since the temperature jump relation has been usually accepted as the thermal boundary condition in the analysis of MEMS flow, it is also focused on in this study. To this end, the wall heat fluxes are also obtained indirectly by applying the temperature jump relation to DSMC temperature profiles. A variation in the thermal accommodation coefficient is observed to severely affect the wall properties such as heat flux and wall pressure. In addition, the difference between indirect and direct heat flux remained unchanged even if the thermal accommodation coefficient is changed.

INTRODUCTION

Recently, a great amount of effort has been exerted on the research about various microelectromechanical systems (MEMS) such as micro sensor and actuator due to their invaluable applicability and potential use for engineering problems [1]. In spite of the rapid development in the micro-fabrication technologies for MEMS devices, a fundamental understanding of fluid flow and heat transfer in micro-scale is still not satisfactory. Especially, a study of unsteady heat transfer in micro-flow is rarely found while most previous theoretical or numerical works regarding micro-systems have concentrated on the flow itself [2]. Practically, a detailed analysis of micro-flow with heat transfer would be very helpful in designing the efficient micro-space propulsion systems such as µ-arcjet and µ-resistojet [3].

Considering these points, Park et al. [4] investigated the unsteady micro-scale heat transfer by employing the unsteady DSMC technique. However, they assumed the diffuse wall therein. Different from the previous work, the present study deals with the effect of thermal accommodation on the unsteady micro-system.

Experiments about gas/surface interaction at normal temperature indicate that the reflection process can be modeled as a diffuse reflection with complete thermal accommodation. This behavior may be a consequence of such surfaces as being microscopically rough with the incident molecules suffering multiple scattering, or with the molecules being momentarily trapped or absorbed on the surface. Most analytical and numerical studies have assumed the diffuse reflection, and fortunately, this appears to be adequate for the many practical gas flows [5].

Actually, the assumption of full thermal accommodation is valid only if the characteristic time of molecular energy exchange, \( t_{\text{mol}} \), is infinitesimally small compared with other characteristic time of the system, \( t_{\text{sys}} \). However, such a simplification cannot be applied to the following problems such as the flow field around satellite [6], the ultra-fast heating of small substance by laser [7], the highly oscillating signal propagation through rarefied medium [8], etc., since in these problems, \( t_{\text{sys}} \) is comparable to \( t_{\text{mol}} \). Particularly, in the rarefied binary mixtures in which the two components have very different molecular masses, the fast sound (the frequency level is larger than \( 10^8 \) Hz) is generated [9, 10], which is one of interesting phenomena in rarefied flow.

Extended from the previous work [3], in this study the one-dimensional unsteady micro-flow caused by
oscillating flow input is investigated with emphasis on the effect of thermal accommodation. Although Park et al. [3] have pointed out that the Smoluchowski’s temperature jump relation induces some inevitable error, this study focuses on the effect of thermal accommodation on the jump relation, since it is still widely used as a thermal boundary condition for diverse governing equations [11-14]. The six different cases are considered and discussed in the below by varying system size and medium density, i.e., the Knudsen number and the acoustic Reynolds number. As a numerical tool, the DSMC method, which is validated through comparison with free molecular solutions, is adopted.

PROBLEM DEFINITION AND DSMC METHOD

As in the previous study [3], a planar system filled with monatomic argon gas is considered. A fluctuating input is continuously excited at the left end by imposing a sinusoidal mean velocity oscillation of \( u(t, x = 0) = U(t) = U_0 \sin(\omega t) \) where \( u \) is the mean velocity along x-direction, \( U_0 \) is the amplitude of excitation, \( \omega \) is excitation frequency, and \( t \) is time. Then, it is introduced into the gas medium of length \( L \) initially at rest with \( T_m = 300 \text{ K} \). A solid wall with \( T_w = 300 \text{ K} \) is located at the right end of the domain so that the impinging molecules are reflected there.

The unsteady DSMC code used in this study is modified from the DSMC1U [5] that adopts No Time Counter (NTC) scheme and Variable Hard Sphere (VHS) Model. The oscillating molecular influx at left end is assumed in DSMC calculation by employing the Maxwellian reservoir method. Its detailed procedure is already included in previous works [3, 8] so that it is skipped here.

Throughout the computations in this study, it is always ensured that there are more than 100 particles per cell on average and each cell size is taken less than 0.1\( \lambda \) in order to obtain the satisfactory accuracy. Here, \( \lambda \) is the mean free path of the molecules in medium. According to Hadjiconstantinou and Garcia [8], the computing time step \( \Delta t \) in unsteady DSMC simulation should be taken to be significantly smaller than \( 1/c_{\text{mp}} \) in which \( c_{\text{mp}} \) is the most probable speed given by \( (2k_B T/m)^{1/2} \) where \( k_B \) is Boltzmann constant, \( T \) is temperature, and \( m \) is the mass of single molecule. Moreover, when treating the fluctuating medium like in the present situation, the time step used should also satisfy \( \Delta t << 2\pi/\omega \) to guarantee the enough resolution in the acoustic aspect. In this study, the computing time step is set to be \( \Delta t = 0.1/(c_{mp}) \). For this case, even the biggest \( \Delta t \) becomes the value of \( 2.1130 \times 10^{-10} \text{ s} \) which is much less than \( 2\pi/\omega = 6.28 \times 10^{-8} \text{ s} \). The ensemble average is obtained performing over 5000 realizations of stochastic process within a given time interval.

TEMPERATURE JUMP RELATION

In rarefied gas dynamics, one of the major problems is to model the interaction of gas molecules with a solid surface. The parameter accounting for this phenomenon is the very accommodation coefficient that represents the tendency of gas to accommodate the wall state. In terms of energy, the accommodation coefficient can be defined by [15]
\[ \sigma_T = \frac{E_i - E_r}{E_i - E_w} \]  \hspace{1cm} (1)

where \( E_i \) denotes the energy flux of the incident molecular stream, \( E_r \) denotes the energy carried away by the reflected molecules, and \( E_w \) denotes the energy that is carried away by the reflected molecules when the temperature of reflected molecular stream is assumed to be the same as the wall temperature \( T_w \). \( \sigma_T \) in Eq. (1) is usually called as “thermal accommodation coefficient” distinguished from “tangential momentum accommodation coefficient (TMAC)” \( \sigma_v \) based on momentum accommodation at surface [16]. Physically, there exist two extreme conditions for the molecular reflection at wall. The first one is the perfectly specular reflection, in which the molecules elastically collide with wall so that the molecular velocity component normal to the surface is reversed while that parallel to the surface remains unchanged. As a result, the impinging molecular stream exerts no shear stress on the surface except the normal direction to the wall. In this case, it becomes \( E_i = E_r \) so that \( \sigma_T \) becomes zero. The other condition is the perfectly diffusive reflection, in which the incident molecules have their mean energy completely adjusted or “accommodated” to the surface for which it becomes \( E_r = E_w \) so that \( \sigma_T \) is equal to unity. Rearranging Eq. (1), then we obtain:

\[ E_r = \sigma_T E_w + (1 - \sigma_T)E_i \]  \hspace{1cm} (2)

According to Eq. (2), the thermal accommodation coefficient represents a fraction of molecules that experience diffusive reflection at the solid surface. As discussed above, \( \sigma_T \) has the value ranging from 0 to 1.0.

The Smolochowski’s temperature jump relation can be derived by considering the kinetic approach on conductive energy balance between gas and solid surface. The net energy actually delivered to the surface can be equated to the total heat conduction across medium; Hence, the numerator of Eq. (1) can be expressed by

\[ E_i - E_w = K \left( \frac{\partial T}{\partial n} \right)_w \]  \hspace{1cm} (3)

where \( K \) is the thermal conductivity and \( n \) is the unit coordinate normal to the surface. On the other hand, in the conventional approach, the theoretical expression for the denominator of Eq. (1) is derived as follows by assuming that the state of effused molecular stream lies in equilibrium:

\[ E_i - E_w = \frac{1}{2} K \frac{\partial T}{\partial n} + \frac{1}{4} \left( \frac{\gamma + 1}{\gamma - 1} \right) \rho_g R \sqrt{\frac{2RT_g}{\pi}} (T_g - T_w) \]  \hspace{1cm} (4)

where \( T_g \) represents the gas temperature at wall, which is distinguished from the wall temperature itself. Combining and rearranging Eqs. (1), (3), and (4), the final expression for temperature jump can be obtained [17]:

\[ T_g - T_w = \frac{2 - \sigma_T}{\sigma_T} \left[ \frac{2(\gamma - 1)}{\gamma + 1} \right] \frac{1}{R_g \rho_g \sqrt{2RT_g} \sqrt{\pi}} (q_n) ; \quad q_n = K \left( \frac{\partial T}{\partial n} \right)_w \]  \hspace{1cm} (5)

or

\[ T_g - T_w = \frac{2 - \sigma_T}{\sigma_T} \left[ \frac{2\gamma}{\gamma + 1} \right] \frac{Kn}{Pr} \left( \frac{\partial T}{\partial n} \right)_w \]  \hspace{1cm} (6)

where \( T_g \) is the gas temperature at wall due to temperature jump while \( T_w \) is the actual wall temperature. \( \gamma \), \( R_g \) and \( T_\infty \) are the specific heat ratio, the gas constant, and the mean temperature at a region sufficiently far from the wall, while \( Pr \) is the Prandtl number. Physically, this represents the heat flux toward wall, \( q_n \), which can be actually calculated using the temperature difference at wall, \( T_g - T_w \). In other words, once the gas temperature profiles are obtained using the DSMC or the free molecular approximation, the indirect heat flux can be calculated using the above temperature jump relation.

However, since some fundamental inaccuracy resides in the Smolochowski’s relation, improved models satisfying a detailed balance were proposed by Cercignani and Lampis [18] and Lord [19]. Park et al. [4] also pointed out that the Smolochowski’s relation can be physically misleading in the analysis of unsteady micro-scale heat transfer.

Nevertheless, due to its simplicity and reasonable accuracy, many researchers have widely utilized the conventional temperature jump relation as a boundary condition for the rarefaction effects in the analysis of rarefied flow [11-14]. Considering these points, much part of present study focuses on the effect of thermal accommodation on the temperature jump relation.
RESULTS AND DISCUSSION

The present study examines the four cases with different system size and density for the fixed excitation condition where \( u_0 = 0.15c_0 \) and \( \omega = 1.0 \times 10^8 \) Hz. Here, \( c_0 \) is the speed of sound as defined by \((\gamma k_B T/m)^{1/2}\). The detailed computing conditions are listed in Table 1. In CASE A and B, the medium density \( \rho_0 \) is varied for a fixed system size \( L \) while CASE C and D have different domain sizes for a fixed medium density.

**TABLE 1. Computational conditions considered in the present study.**

<table>
<thead>
<tr>
<th>CASE</th>
<th>( \text{Re}_a/\gamma )</th>
<th>( \rho_0 ) [kg/m(^3)]</th>
<th>( L ) [( \mu m )]</th>
<th>( \lambda ) [( \mu m )]</th>
<th>( \tau \times 10^9 ) [sec]</th>
<th>( Kn_L )</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>0.5</td>
<td>0.1149</td>
<td>0.8067 (0.25( l ))</td>
<td>0.7840</td>
<td>2.4296</td>
<td>0.9718</td>
</tr>
<tr>
<td>B</td>
<td>1</td>
<td>0.2285</td>
<td>0.8067 (0.25( l ))</td>
<td>0.3920</td>
<td>1.2148</td>
<td>0.4859</td>
</tr>
<tr>
<td>C</td>
<td>0.5</td>
<td>0.1149</td>
<td>1.6134 (0.50( l ))</td>
<td>0.7840</td>
<td>2.4296</td>
<td>0.4859</td>
</tr>
<tr>
<td>D</td>
<td>0.5</td>
<td>0.1149</td>
<td>3.2266 (1.00( l ))</td>
<td>0.7840</td>
<td>2.4296</td>
<td>0.2430</td>
</tr>
</tbody>
</table>

Two parameters of the acoustic Reynolds number \( \text{Re}_a \) and the Knudsen number \( Kn_L \) are calculated and listed to represent the acoustic feature and the rarefaction degree of the medium. The acoustic Reynolds number is defined as

\[
\text{Re}_a = \frac{c_0^2 \rho_0}{\omega \mu_0}.
\]  

(7)

where the viscosity \( \mu_0 \) is given by:

\[
\mu_0 = \frac{1}{2} \rho_0 \lambda \overline{C}_{rms}
\]  

(8)

with

\[
\overline{C}_{rms} = \sqrt{\left(\overline{\xi}^2 + \overline{\eta}^2 + \overline{\zeta}^2\right)} = \sqrt{\frac{3k_B T}{m}}
\]  

(9)

Since the excitation frequency remains constant throughout this study, the acoustic Reynolds number actually represents the effects of medium density. Different from the previous studies on rarefied sound wave propagation through infinite medium [20, 21], the present domain is finite. That is why two system parameters of \( \text{Re}_a \) and \( Kn_L \) are required to identify a system behavior. For the infinite case, since both acoustic Reynolds number and Knudsen number have the same characteristic length \( L = c_0/\omega \), there exists a following relation between \( Kn_a \) and \( \text{Re}_a \):

\[
\text{Re}_a = \sqrt{\frac{4}{3}} \times \frac{1}{Kn_a}
\]  

(10)

where the subscript ‘a’ in Knudsen and Reynolds numbers denote ‘acoustic’.

Figure 2 compares the temporal variations of normalized heat flux fluctuation at wall, \( \theta_w \), depending on thermal accommodation \( \sigma_T \) for various cases. In each graph there are two types of heat flux depending on the method used: (1) \( \theta_w(DSMC; \text{direct}) \) directly computed using the DSMC only, (2) \( \theta_w(DSMC; \Delta T) \) indirectly computed using the DSMC temperature profiles by applying temperature jump relation of Eq. (5). The classification of wall heat fluxes is summarized in Figure 3. Since both the wall temperature \( T_w \) and medium mean temperature \( T_m \) have the same value of 300 K, the fluctuation actually represents the net wall heat flux itself. \( T_0 \) and \( x^* \) in the figure denote the period \( 2\pi/\omega \) and normalized coordinate \( x/L \). Since the Park et al. [3] have already shown that the wall heat flux calculated from the higher-order modifications of the conventional Smoluchowski’s relation is not so much different from that from the original one that the conventional relation is taken into account for computation of \( \theta_w(DSMC; \Delta T) \). In the figure, the heat fluxes represented by solid and dashed lines are obtained by applying the temperature jump relation to DSMC calculations. During a specular reflection process, the molecular velocity component normal to the surface is reversed while parallel one to the surface remain unchanged. A collection of molecules with such a process macroscopically results in the thermal insulation without net energy transfer onto wall. Hence, as the thermal accommodation coefficient decreases, the magnitude of net heat flux gradually decreases because the adiabatic portion of molecules increases. The reduction of wall heat flux is purely due to the change in molecular velocities.
FIGURE 2. Temporal variations of heat fluxes at wall directly and indirectly computed depending on $\sigma_T$ for various cases: (a) CASE A; (b) CASE B; (c) CASE C; (d) CASE D.

FIGURE 3. Two kinds of wall heat fluxes

According to Park et al. [3], a deviation between direct $\theta_w$ (DSMC; direct) and indirect $\theta_w$ (DSMC; $\Delta T$), are due to the inevitable errors induced by the temperature jump relation. As indicated in previous section, in the derivation
of temperature jump relation, it is assumed that the incident molecular flux is in equilibrium. It might be true in
steady rarefied flow, however it may not be true in unsteady situation.

It becomes clearer when investigating the aspect of gas kinetics. Theoretically, the translational temperature and
the heat flux toward wall are given as follows \[3, 5\]:

\[
T_r = \frac{1}{2} \frac{m}{k_B} \left( \xi^2 + \eta^2 + \zeta^2 \right)
\]

\[
q_w = \frac{N_p}{\Delta t N_{\text{amp}}} \left[ \sum_{\text{wall}} \frac{m}{2} \left( u^2 + v^2 + w^2 \right) + \sum_{\text{cell}} \frac{m}{2} \left( \xi^2 + \eta^2 + \zeta^2 \right) \right] \quad \left( \xi = \eta = \zeta = 0 \right)
\]

where the ‘cell’ indicates the summation over all the molecules in the cell interested while the ‘wall’ denotes the
statistical collection for both the incident and reflected molecules. The over-bar stands for ‘ensemble average’. \(N_p\)
is the number of molecules represented by every single simulated particle, \(\Delta t\) time step, and \(N_{\text{amp}}\) is the number
of samples. A careful examination of Eqs. (11) and (12) reveals that the wall heat flux involves one more energy term
of \(\sum_{\text{wall}} 1/2 \times m \left( u^2 + v^2 + w^2 \right)\) which is attributed to mean velocities. Some profiles in Figure 2 assume a full
thermal accommodation and furthermore, the reflected molecular stream from right wall is always in complete
equilibrium. Therefore, in that case, a degree of non-equilibrium at wall would result from a difference between
incident and reflected molecular stream. Table 2 shows that the maximum and minimum values of normalized
incident number flux when \(\sigma_T = 1.0\) for various cases. And, more incident molecules are found at positive peak of
heat flux rather than at negative peak of heat flux so that a more deviation arises between \(\theta_w(\text{direct})\) and \(\theta_w(\Delta T)\) at
positive peak of heat flux. Same discussion is also applicable to other profiles in Figure 2.

**TABLE 2.** Max. and Min. of Normalized Incident Number Flux when \(\sigma_T = 1.0\).

<table>
<thead>
<tr>
<th></th>
<th>Normalized Incident Number Flux</th>
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<tbody>
<tr>
<td></td>
<td>MAX</td>
</tr>
<tr>
<td>A, B</td>
<td>115</td>
</tr>
<tr>
<td>C</td>
<td>100</td>
</tr>
<tr>
<td>D</td>
<td>105</td>
</tr>
</tbody>
</table>

Similar to the wall heat flux, another wall property of reflected pressure is severely affected by the variation of
\(\sigma_T\) as shown in Figure 4 because the reflected molecular velocities are apparently varied depending on the degree of
thermal accommodation.

**FIGURE 4.** Temporal variations of incident and reflected wall pressure depending on \(\sigma_T\) for various cases: (a) CASE A; (b) CASE B; (c) CASE C; (d) CASE D.
Furthermore, in Figure 5, a temporal variation of difference between $\theta_w$(DSMC, direct) and $\theta_w$(DSMC, $\Delta T$) is plotted for six cases depending on $\sigma_T$. The figure shows that $\theta_w$(DSMC, direct) - $\theta_w$(DSMC, $\Delta T$) is not so influenced by the gas/surface interaction model that the degree of error induced by the Smoluchowski’s jump relation is neither reduced nor magnified depending on the surface condition. Such a feature should be always kept in mind when analyzing the problem with the temperature jump boundary condition.

**CONCLUSIONS**

A numerical study has been carried out to investigate the effect of thermal accommodation on the unsteady semi-confined one-dimensional micro-flow responding to the oscillating flow input. The unsteady DSMC technique was applied to the four cases with different system size and medium density. The thermal accommodation coefficient considered ranged from 0.7 to 1.0 with increment of 0.1. Since the temperature jump relation has been widely accepted as the thermal boundary condition in the analysis of MEMS flow, it was focused on in this study. The wall heat flux and wall pressure were strongly influenced by the variation of thermal accommodation coefficient because the degree of thermal insulation linearly increased with decreasing thermal accommodation coefficient. However, the fundamental errors induced by temperature jump relation also incurred severe discrepancies between direct and indirect results. And, the difference between indirect and direct heat flux remained unchanged in spite of the variation of thermal accommodation coefficient.

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