HEAT TRANSFER PREDICTIONS USING ACCOMMODATION COEFFICIENTS FOR
A DENSE GAS IN A MICRO/NANO-CHANNEL

S.V. Nedea*,1, A. J. Markvoort2, P. Spijker2, A. A. van Steenhoven1
1 Energy Technology, Department of Mechanical Engineering
2 BioModeling and BioInformatics, Department of Biomedical Engineering
Eindhoven University of Technology, P.O. Box 513, 5600 MB, Eindhoven, The Netherlands

ABSTRACT

The influence of gas-gas and gas-wall interactions on the heat flux predictions for a dense gas confined between two parallel walls of a micro/nano-channel is realized using combined Monte Carlo (MC) and Molecular Dynamics (MD) techniques. The accommodation coefficients are computed from explicit MD simulations. These MD coefficients are then used as effective accommodation coefficients in Maxwell-like boundary conditions in MC simulations. We find that heat flux predictions from MC based on these coefficients compare good with the results of explicit simulations except the case when there are hydrophobic gas-wall/gas-gas interactions. For this case an artificial wall was introduced in order to measure these MD accommodation coefficients at this artificial border. Good agreement is found then for both hydrophilic and hydrophobic gas-wall interactions and we show this by confronting the heat fluxes from explicit MD simulations with the the MC heat flux predictions for all the generic accommodation coefficients.

NOMENCLATURE

\begin{align*}
LJ & \text{ Lennard Jones potential} \\
tsLJ & \text{ truncated shifted Lennard Jones potential} \\
\varepsilon & \text{ interaction strength in the LJ potential} \\
L_s & \text{ distance between the parallel walls} \\
\lambda & \text{ mean free path} \\
n & \text{ number density}
\end{align*}

\begin{align*}
a & \text{ molecular diameter} \\
\eta & \text{ reduced density} \\
\alpha & \text{ accommodation coefficient} \\
q_x & \text{ heat flux} \\
T_L & \text{ temperature of incident molecules} \\
T_R & \text{ temperature of reflected molecules} \\
T_W & \text{ temperature of the wall (surface)} \\
MD & \text{ Molecular Dynamics} \\
MC & \text{ Monte Carlo}
\end{align*}

INTRODUCTION

Heat transfer at atomistic level became one of the most important issues within the microfluidics field, for instance in microchannel cooling applications. Reliable models for the gas-solid interface are essential for obtaining accurate temperature and heat flux predictions and different boundary conditions incorporating empirical accommodation coefficients have been used to study the energy transfer between the gas and the walls of a microchannel [1, 2]. A lot of studies investigating atomic or molecular scattering from solid surfaces [3–5] for understanding of fluid-wall interactions have been reported in the literature. When dealing with dilute gases, the characteristic space and time scale are much larger than molecular sizes and molecular interaction times, respectively [6]. The gas-wall interactions are modeled by assuming the solid boundary being a smooth, structureless and impenetrable surface which acts on the gas distribution function [6, 7]. The Maxwell-based models are the most widely

*Corresponding author: S.V.Nedea@tue.nl
used choice for the scattering kernel of the molecules near the solid wall. Simplified models called diffuse reflection assumes that the reflected molecules are completely accommodated with the wall surface and their velocity distribution is given by the Maxwellian distribution with the wall quantities. However, when the molecules have high energy, the diffuse reflection is not applicable, and the scattered flux shows preferred directions (e.g., specular ray direction) [8,9]. Other Maxwell-type boundary conditions are based on the assumption that a fraction $(1 - \alpha)$ of molecules is reflected specular from the surface, while $\alpha$ is re-emitted diffusely with Maxwell distribution at wall conditions. $\alpha$ is called the accommodation coefficient and can be based on the tangential momentum or on the energy of the molecules according to the flow situation [3, 4]. A more elaborated model was proposed by Cercignani and Lampis [7] and developed by Lord [10], and includes two parameters: one coefficient of the tangential momentum accommodation parallel to the surface and one of energy accommodation normal to the surface. Although the adoption of Maxwell-type boundary conditions is possible in modeling dense gases, it represents an oversimplification as their derivation is based on the assumption that the time scale of fluid-wall interactions is much shorter than the time scale of fluid-fluid interactions.

An alternative to using boundary conditions is to use explicit Molecular Dynamics (MD) simulations [11], allowing thus for the simulation of wall, gas, and wall-gas interactions explicitly and to compute these accommodation coefficients on a molecular level. In our previous paper [12], we have computed these accommodation coefficients from explicit MD simulations for a dilute gas in a micro/nano-channel. We used an MD approach to study the wettability effect on heat and particle flow in nano-channels. The results on the heat flux predictions of the particles sticking to the wall (attractive wall interactions) were given, showing that the relevant parameter is the gas-wall interaction strength, whereas gas-gas is of much less importance on the resulting heat flux. Also, the higher the attraction with the wall, the higher the difference in temperature between the particles going to the left (incident) and to the right (reflected). For denser gas, the gas-gas interactions become important for the heat transfer properties and we have previously showed in [12] that for a hard-sphere gas, the accommodation coefficients imported from a dilute gas give good results for hydrophobic but not for hydrophilic wall interactions due to the overlapping effect of the clustering and attractive walls.

In this paper we compare the MC and the MD results showing the influence of both gas-gas and gas-wall interactions on the accommodation coefficients and on the heat flux predictions for a dense gas confined between two parallel walls of a micro/nano-channel. Combined Monte Carlo and Molecular Dynamics techniques [13–15] are used for these results. The deviations $\delta q_\alpha$ of the MC results from the explicit MD simulations are measured and they have the form $\delta q_\alpha = (q_{\text{MD}} - q_{\text{MC}}(\alpha))/q_{\text{MD}}$, where $q_{\text{MD}}$ is the accurate explicit MD heat flux and $q_{\text{MC}}(\alpha)$ is the MC heat flux prediction as a function of the accommodation coefficient $\alpha$ included in the Maxwell-like boundary conditions.

As these deviations of the MC heat flux predictions from the MD results show to be quite large depending on the molecular properties in the gas-surface interface, we choose to compute $\alpha$ by taking into account the interaction of a dense gas with the solid walls of the channel (attractive or repulsive gas-wall interactions). Instead of importing these coefficients from the MD gas-wall simulations of a dilute gas, we compute them exactly from the MD heat and temperature fluxes of the incident and reflected molecules of a dense gas exactly near the warm wall. These coefficients are going to be used in Maxwell-type boundary conditions in MC simulations based on the Enskog equation [6,16–18]. Comparisons of the heat fluxes derived using explicit MD simulations and MC with pure Maxwell B.C. and Maxwell-type B.C. based on these MD accommodation coefficients $\alpha$ are realised. We further investigate the case when gas-gas interactions are equal to the gas-wall interactions as the accommodation coefficients computed from the temperature profiles give very accurate heat flux predictions for attractive interaction potentials, but large deviations are registered for very hard repulsive potentials. For this case of hydrophobic gas-gas/gas-wall interactions, instead of computing $\alpha$ near the wall, we compute $\alpha$ just before the region where the clustering effect near the wall is present. This coefficient is going to be used in the B.C. for the MC simulations based on the Enskog equation [6,18] and the results for the heat flux predictions are compared to explicit MD heat flux predictions. In the end, all these accommodation coefficients computed from explicit MD simulations are compared with effective accommodation coefficients obtained by matching the MD heat flux predictions for all the interaction strengths with the map of MC heat flux dependence on the generic accommodation coefficients.

**THE PHYSICAL MODEL**

Our model to study the one-dimensional heat flow in a microchannel consists of two parallel plates of length $L_s$ at a distance $L_s$ apart from each other and of gas molecules confined between these two walls. Both plates have their own temperature, $T_1$ and $T_2$ respectively, where this temperature is uniform on the plate surface and constant in time, and $T_2/T_1 = 1/2$. The gas consists of spherical particles of diameter $a$ and mass $m$, at temperature $T$. The density of the gas can be expressed as $n$, being the number of particles per unit of volume, or using a reduced density $\eta$, which also takes the particle sizes into account and is related to the number density as $\eta = \pi n a^3/6$ [17]. The mean free path of the gas particles is related to this reduced density. For a relatively dense gas with $\eta = 0.1$, the mean free path $\lambda = 1/\sqrt{2\pi a^3nY(\eta)}$ and the molecular diameter $a$ have the same order of magnitude. The $Y(\eta)$ factor is the pair correlation func-
tion at contact [16, 17]. The distance \( L_x \) between the plates, in the x-direction, is always such that both plates are only a few mean free paths apart. A dense gas is considered with \( \eta = 0.2 \). The walls can be modelled explicitly (based on an MD model) or using boundary conditions (Maxwell or Maxwell-like boundary conditions in an MC model). Because we are not directly interested in one specific system, but in the dependency of the accommodation coefficient on the gas-wall interaction, the parameters used in our model are expressed in reduced units. The system consists of the following reduced units: the unit for length \( \sigma^* \), the unit for mass \( m^* \) and the unit for energy \( \epsilon^* \). Other units can be derived out of these choices [11, 19]. The two walls consisting of 18000 particles each forming a face centered cubic (fcc) lattice are placed in a box of size \( 95.0 \times 139.49 \times 139.49 \) and are separated from each other in x direction. For \( \eta = 0.2 \), the ratio \( \lambda/\sigma = 0.3362 \). We name one wall warm (w) and the other one cold (c). The total number of gas particles in the box is 55998 corresponding to a number density \( n_0 = 0.4 \sigma^{-3} \) simulated. The temperature of the two plates can be controlled by coupling them to a heat bath. The mass and the size of both particle types are taken equal \( m=1m^* \) and \( \sigma=1\sigma^* \). Every simulation, both MC and MD, consists of two parts. In the first part the system is run until equilibrium is reached, and in the second part the macroscopic quantities like density, temperature, and heat flux profiles are obtained. These simulations consists of 5000000 iterations and were executed on 8 cpu’s of an AMD Athlon 1800+ Beowulf cluster.

In MD, the Lennard Jones (LJ) potential is used to model the interactions between the gas-gas, gas-wall and wall-wall molecules [19]. Truncated shifted Lennard Jones (tsLJ) is used to keep only the repulsive contribution as a model for hard sphere molecules. The walls are kept together by a relatively strong interaction \( \epsilon_{w-w} = 6.0\epsilon^* \) in the LJ potential. The gas-wall (G-W) interactions can be hydrophilic (attractive) or hydrophobic (repulsive) wall interactions. Attractive wall interactions are modelled by LJ with \( \epsilon_{G-W} \) between 0.25\( \epsilon^* \) and 0.5\( \epsilon^* \), and repulsive wall interactions by tsLJ with \( \epsilon_{G-W}=1.0\epsilon^* \) and LJ with \( \epsilon_{G-W}=0.10\epsilon^* \). The gas-gas (G-G) interactions can be also hydrophilic or hydrophobic and are modelled exactly like the gas-wall (G-W) interactions.

**DEVIATIONS OF THE HEAT FLUX PREDICTIONS FOR A HARD-SPHERE GAS**

In [12] we showed that the relevant parameter when studying the wettability effect on heat flux for a dilute gas in micro/nano-channel is the gas-wall interaction strength, whereas gas-gas is of much less importance on the resulting heat fluxes. Considering that each individual molecule is accommodated by the wall during the collision with a factor depending only on the interaction strength \( \epsilon_{G-W} \) between the gas molecule and the wall molecule, we extended this gas-wall assumption to study the heat flux predictions for a dense gas in the channel. As for the heat transfer in a dense gas, the gas-gas interactions become important (see Table 1), we measure the deviations from the explicit MD heat flux predictions with different gas-gas/gas-wall interactions of the MC heat flux predictions when using Maxwell B.C. based on the accommodation coefficients \( \alpha \) computed in [12]. These \( \alpha \) accommodation coefficients were transferred from the gas-wall interface of a dilute gas and imported into the simulation of a dense gas. The values of the accommodation coefficients \( \alpha \) and the heat fluxes \( q_i \) from explicit MD simulations for different G-W interaction values are given in column 2 and 3 of Table 2.

The results in Table 1 show that the gas-gas interactions become important, such that the higher the \( \epsilon_{G-G} \), the lower the heat flux. When walls are very attractive, the role of gas-gas (G-G) interactions becomes less important. When we compute the deviations of the MC heat flux predictions (column 3 in Table 2) from the explicit MD heat fluxes for all the gas-gas and gas-wall interactions going from hard repulsion to hard attractive interactions in Table 1, we find that these deviations are almost always higher for hydrophilic gas-wall interactions than for hydrophobic gas-wall interactions, for all the values of the gas-gas interactions [12]. The values of these deviations are given in Table 3. For very attractive gas-gas interactions (e.g., \( \text{LJ}_{\epsilon_{G-G}}=0.50\epsilon^* \)), these deviations are very large for all the gas-wall interactions, while for moderate G-G interactions these deviations are increasing with \( \epsilon_{G-G} \). For very repulsive G-G interactions (e.g., \( \text{tsLJ}_{\epsilon_{G-G}}=1.0\epsilon^* \)), the deviations are the highest for the strongest G-W interactions and are decreasing when \( \epsilon_{G-W} \) is decreasing.

Regarding the gas-gas interactions we further choose to limit our comparison of the heat fluxes and deviations for two situations: when having hard repulsive gas-gas interactions and when the gas-gas interactions are equal to the gas-wall interactions \( (\epsilon_{G-W} = \epsilon_{G-G}) \). This last choice is explained by the fact that in order to understand these gas-wall accommodation coefficients, one choice is not to differentiate between the gas-gas and gas-wall interactions. Otherwise, the overlapping effects of clustering, gas-wall and gas-gas interactions will be difficult to be analysed. The choice for hard repulsive gas-gas interactions (hard-sphere) comes also natural to consider in MD as hard-sphere gas-gas interactions are considered in the MC model based on the Enskog equation [6, 16–18]. Another reason is that the deviations in these situations are quite large for all the gas-gas interactions and can be studied by varying these interaction strengths from hard repulsive to hard attractive.

From Table 2 we can also see that these deviations of the MC heat flux predictions (column 3) from the MD results (column 4 and 5) are higher for harder interactions (attractive or repulsive) and smaller for moderate interaction strengths for both situations considered (hard-sphere gas and when gas-gas equals gas-wall interactions). As already previously mentioned, in Table 2 \( \alpha T \) is computed from the explicit temperature profiles of the molecular fluxes. The temperature of the impinging and the
reflected molecules are computed from the MD simulations with explicit wall interactions by measuring the $T$ for the flux of particles moving from the cold to the warm wall and from the warm to the cold wall. To compute this $T$, individual particles are traced and according to their velocity they account for the impinging ($V_s < 0$) or for the reflected molecular fluxes ($V_s > 0$), where $V_s$ is the velocity on the $x$ direction perpendicular to the wall. From these MD simulations, we get the temperature and the density profiles. The slope of these profiles are changing with the gas-surface interaction strength, the higher the slope in $T$ next to the wall, the higher the thermal accommodation next to the wall. The effective accommodation coefficient $\alpha$ is computed then from the definition $[6, 7]$, based on the $T$ of the incident and reflected molecules in the immediate vicinity of the wall: $\alpha = (T_L - T_R)/(T_L - T_{R\text{Max}})$. Here, $T_L$ stands for the temperature of particles moving towards the wall (incident molecular flux), $T_R$ stands for the particles leaving the wall (reflected molecular flux), and $T_{R\text{Max}}$ temperature of the reflected molecular flux in case of Maxwell B.C. All these temperatures can be measured near the warm wall or next to the cold wall. In the same way, $\alpha$ can be computed based on the total energy fluxes and from the energy fluxes of impinging and reflected molecules. The values of $\alpha$ based on $T$ and on the incident and reflected molecular energy fluxes give the most accurate heat flux predictions.

As importing $\alpha$ for the Maxwell B.C. from the temperature profiles of a dilute gas into the simulation of a dense gas gives large deviations for a large set of combined gas-gas and gas-wall parameters (see Table 3), we compute the accommodation coefficient $\alpha$ based on the explicit dense gas simulations of the temperature profiles in the gas-wall interface, e.g. near the warm wall. The reason for considering the warm wall rather than the cold wall is the following. If we look at the density and temperature profiles of a dilute gas, we see that the peaks are more pronounced next to the cold wall. The origin of these peaks is explained in details in $[19]$ where we find out that for a low density gas, the temperature profile is linear in the bulk and different near the interfaces, while for a high density gas the temperature profiles are linear. These increased gradients in the $T$ near the interfaces coincides with the increased density near these interfaces $[19]$. The higher the slope in $T$ next to the wall, the higher the thermal accommodation at the wall. That’s why computing $\alpha$ from the $T$ profiles will give different values next to the cold or next to the warm wall, and it will be always higher at the cold wall. These values are taken next to the warm wall, as it is more difficult to predict accurately the local $T$ next to the cold wall due to the layering (clustering) effect for attractive wall interactions.

For our case, in Fig. 1, from the temperature profiles of a dense gas having hydrophobic gas-wall and gas-gas interactions (tsLJ: $\varepsilon_{G-G}=\varepsilon_{G-W}=1.0$) we obtain $\alpha_T$ computed near the warm wall: $\alpha_T=(T_{L(w)}-T_{R(w)})/(T_{L(w)}-T_{R\text{Max}(w)})=0.915-0.930)/(0.915-1.0)=0.18$. For computing all these coefficients $\alpha$ for different gas-gas and gas-wall interactions, results for the total heat fluxes and temperature profiles of the incident and reflected molecular fluxes for pure Maxwell B.C. and for explicit MD simulations near the warm wall are needed. Gas-gas interactions become very important for the predictions of $T_L$ and $T_R$ temperatures also for Maxwell B.C. when $\eta=0.2$. These interactions determine different properties for these incident and reflected molecular fluxes (temperature and total $q_s$), and can, thus, result in different accommodation coefficient $\alpha$. How the temperature and heat flux properties vary with the gas-gas interactions, both for explicit and pure Maxwell gas-wall B.C. is shown in Table 4 and 5. Table 4 contains the temperature near the warm wall of the incident and reflected molecules ($T_L$ and $T_R$), and also the total heat flux $q_s$ for all the G-G interactions when having pure Maxwell G-W B.C. Table 5 contains the same parameters but for the case of explicit MD with different gas-wall/gas-gas simulations. We notice that for pure Maxwell B.C., the heat flux is decreasing with $\varepsilon$ from hydrophobic to hydrophilic gas-gas interactions. For explicit MD simulations, the behavior of the heat flux $q_s$ is different: for high repulsive or high attractive gas-gas/wall interactions, $q_s$ is high and is decreasing for lower values of the interaction strengths. For instance, in Table 5, we notice that for very attractive wall interactions (LJ: $\varepsilon_{G-W}=0.5\varepsilon$) and for hardly repulsive wall (tsLJ: $\varepsilon_{G-W}=1.0\varepsilon$), the explicit MD simulations predict the same heat flux $q_s=0.015\varepsilon/((\sigma^2)^*)$, where $\tau^* = \varepsilon \sqrt{m/\sigma^3}$. From the tables 4 and 5 we see that Maxwell overestimates this thermal accommodation comparing with the explicit simulations results. Moreover, for pure Maxwell gas-wall B.C. the difference in the temperatures $T_L$ and $T_R$ of these molecular fluxes is increasing with the gas-gas interactions, while for the explicit MD gas-wall/gas-gas interactions this relation is not valid. From explicit simulations, the difference between these fluxes is the result of the complex overlapping effect of gas-gas, gas-wall and clustering effect.

We use these data for temperature and heat fluxes from tables 4 and 5, in order to compute the accommoda-

<table>
<thead>
<tr>
<th></th>
<th>G-W</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>tsLJ 1.0</td>
</tr>
<tr>
<td>G-G</td>
<td></td>
</tr>
<tr>
<td>tsLJ 1.0</td>
<td>0.015</td>
</tr>
<tr>
<td>LJ 0.10</td>
<td>0.012</td>
</tr>
<tr>
<td>LJ 0.25</td>
<td>0.012</td>
</tr>
<tr>
<td>LJ 0.50</td>
<td>0.009</td>
</tr>
</tbody>
</table>

*Table 1. Heat flux using MD with different wall-gas and gas-gas LJ interaction potential, for a dense gas with $\eta = 0.2$. The columns stand for the wall-gas interactions and the rows for the gas-gas interactions. The heat flux $q_s$ is in $[\varepsilon^*/(\sigma^2\tau^*)]$ units, where $\tau^* = \varepsilon \sqrt{m/\sigma^3}$. The values of $\alpha$ based on $T_s$ and on the incident and reflected molecular energy fluxes give the most accurate heat flux predictions.*
Table 2. Heat fluxes using MD and MC with Maxwell-like boundary conditions based on the accommodation coefficient $\alpha$ for a dilute gas and applied to a dense gas with $\eta = 0.2$ and $L_\lambda = 95.\lambda$. Column 1 contains the gas-wall interaction strength for the LJ potential, column 2 the accommodation coefficient computed from the temperature profiles of a dilute gas for each G-W interaction, column 3 the MC heat predictions using Maxwell-like B.C. based on $\alpha$, column 4 and 5 the MD heat flux predictions for the case of hydrophobic gas-gas interactions (tsLJ: $\varepsilon_{G-G} = 1.0\varepsilon^*$) and for the case of $\varepsilon_{G-G} = \varepsilon_{G-W}$ (both for LJ and tsLJ), column 6 and 7 are the deviations of the MD results from the MC ones (column 3) for these two cases. The heat flux $q_x$ is in $[\varepsilon^*/(\sigma^{2*}\tau^*)]$ units, where $\tau^* = \tau^* \sqrt{m^*/\varepsilon^*}$.

<table>
<thead>
<tr>
<th>G-W</th>
<th>$\alpha_T$</th>
<th>$q_x$ MC</th>
<th>$q_x$ tsLJ ($\varepsilon_{G-G}=1.0$)</th>
<th>$q_x$ LJ ($\varepsilon_{G-G-G-W}$)</th>
<th>$q_{dev,4}$</th>
<th>$q_{dev,5}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>tsLJ 1.0</td>
<td>0.21</td>
<td>0.0123</td>
<td>0.015</td>
<td>0.015</td>
<td>0.18</td>
<td>0.18</td>
</tr>
<tr>
<td>LJ 0.10</td>
<td>0.21</td>
<td>0.0123</td>
<td>0.014</td>
<td>0.011</td>
<td>0.12</td>
<td>0.11</td>
</tr>
<tr>
<td>LJ 0.25</td>
<td>0.40</td>
<td>0.0174</td>
<td>0.016</td>
<td>0.014</td>
<td>0.08</td>
<td>0.24</td>
</tr>
<tr>
<td>LJ 0.50</td>
<td>0.70</td>
<td>0.0203</td>
<td>0.017</td>
<td>0.016</td>
<td>0.19</td>
<td>0.26</td>
</tr>
<tr>
<td>Maxwell</td>
<td>1.0</td>
<td>0.021</td>
<td>—</td>
<td>—</td>
<td>—</td>
<td>—</td>
</tr>
</tbody>
</table>

Table 3. Deviations from the MD results of the MC heat fluxes $q_x$ with Maxwell-like boundary conditions based on the accommodation coefficient $\alpha$ for a dilute gas and applied to a dense gas with $\eta = 0.2$ and $L_\lambda = 95.\lambda$. Column 1 contains the gas-wall interaction strength for the LJ and tsLJ potential, column 2 the MC heat flux deviations from MD for tsLJ with $\varepsilon_{G-G} = 1.0\varepsilon^*$, column 3 for LJ with $\varepsilon_{G-G} = 0.1\varepsilon^*$, column 4 the deviations from MD for LJ with $\varepsilon_{G-G} = 0.5\varepsilon^*$, and column 5 the deviations from MD for LJ with $\varepsilon_{G-G} = 0.5\varepsilon^*$. All these MD and MC heat fluxes are found in Tables 1 and 2.

<table>
<thead>
<tr>
<th>G-W</th>
<th>tsLJ $dev_{q_x} (\varepsilon_{G-G} = 1.0)$</th>
<th>LJ $dev_{q_x} (\varepsilon_{G-G} = 0.10)$</th>
<th>LJ $dev_{q_x} (\varepsilon_{G-G} = 0.25)$</th>
<th>LJ $dev_{q_x} (\varepsilon_{G-G} = 0.50)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>tsLJ 1.0</td>
<td>0.18</td>
<td>0.02</td>
<td>0.02</td>
<td>0.36</td>
</tr>
<tr>
<td>LJ 0.10</td>
<td>0.12</td>
<td>0.11</td>
<td>0.11</td>
<td>0.36</td>
</tr>
<tr>
<td>LJ 0.25</td>
<td>0.08</td>
<td>0.24</td>
<td>0.24</td>
<td>0.45</td>
</tr>
<tr>
<td>LJ 0.50</td>
<td>0.19</td>
<td>0.35</td>
<td>0.26</td>
<td>0.26</td>
</tr>
</tbody>
</table>

Figure 1. Temperature profiles of the impinging and reflected molecules and total density for a dense gas with $\eta = 0.2$ using explicit MD simulations (tsLJ: $\varepsilon_{G-G} = \varepsilon_{G-W}=1.0\varepsilon^*$) and MD with Maxwell B.C.

Table 4. Properties of the molecular fluxes depending on different gas-gas interactions (column 1) for pure Maxwell gas-wall B.C. Column 2 contains the temperature of the reflected molecules, column 3 of the impinging molecules and column 4 contains the total heat flux between the two walls. The heat flux $q_x$ is in $[\varepsilon^*/(\sigma^{2*}\tau^*)]$ units, where $\tau^* = \tau^* \sqrt{m^*/\varepsilon^*}$.

<table>
<thead>
<tr>
<th>G-G</th>
<th>$T_R$</th>
<th>$T_L$</th>
<th>$q_x$</th>
</tr>
</thead>
<tbody>
<tr>
<td>tsLJ 1.0</td>
<td>1.0</td>
<td>0.974</td>
<td>0.020</td>
</tr>
<tr>
<td>LJ 0.10</td>
<td>0.996</td>
<td>0.967</td>
<td>0.017</td>
</tr>
<tr>
<td>LJ 0.25</td>
<td>0.989</td>
<td>0.952</td>
<td>0.017</td>
</tr>
<tr>
<td>LJ 0.50</td>
<td>0.973</td>
<td>0.910</td>
<td>0.016</td>
</tr>
</tbody>
</table>

$\alpha_q = q_{\text{explicit}}/q_{\text{Maxwell}}$. In Table 6 we give all these accommodation coefficients for the case of explicit MD simulations when the gas-gas interactions are equal to the gas-wall interactions. Using these values of $\alpha_T$ and $\alpha_q$, we compare the $q_x$ predictions for the case of explicit MD simulations when the gas-gas interactions are equal to the gas-wall interactions.
obtained using MC with Maxwell-like B.C. based on these $\alpha$’s. We see that we get good results for the heat flux predictions $q_x$ using MC with Maxwell B.C. based on $\alpha_T$ for attractive potentials but large deviations are registered for very hard repulsive potentials (tsLJ: $\epsilon_{G-G} = \epsilon_{G-W} = 1.0 \epsilon^*$). The deviations from MD of the MC heat fluxes based on $\alpha_T$, (dev$_{\alpha_T}$) are much higher than the deviations based on $\alpha_T$ (dev$_{\alpha_T}$), while for a dilute gas these deviations were very small [12]. From these results we conclude that we can get quite accurate results for the heat fluxes by computing $\alpha_T$ from the temperature profiles, for all the values of the gas-gas/gas-wall interactions except for the high repulsive potentials. For hard repulsive gas-gas/gas-wall interactions the clustering effect becomes important and the increased collisions near the wall can not be reflected only in the accommodation coefficient computed immediately at the wall interface. Thus, for this case, we compute $\alpha_T$ for the repulsive interactions not exactly at the wall but at two molecular diameters away from the wall, that means exactly where the clustering effect and the density oscillations dissipate. This layering effect next to the wall appear both in case of a dilute gas and also of a dense gas in contact with the surface. The physical explanation is however different and it was extensively studied in [19]. The short explanation is that in case of a dilute gas, particles sticking to the wall are energetically more favorable as there are more neighbors and thus more negative energy contributions than in the gas phase. In this case, the density peak depends on the attractive part of the gas-wall interaction potential. In case of a high density gas, the density is not only the result from attractive force from the wall, but also from pushing of the molecules in the interface by the bulk gas atoms against the wall. That’s why in this case, our assumption that $\alpha$ is only a function on $\epsilon_{G-W}$ is not valid as the effect of the pushing of molecules is not included. The accommodation coefficient is computed then at two molecular diameters away from the wall, by introducing an ‘artificial wall’ and not differentiating anymore between the wall and the adsorbed molecules on the wall. From the temperature profiles of the impinging and reflected molecular fluxes, at the distance of two molecular diameters (see Fig. 1), we find that $\alpha_T=(T_{L(0)}-T_{R(2\tau)})/(T_{L(2\tau)}-T_{R(Max(2\tau))})=0.25$. The heat flux $q_x$ from MC using Maxwell-like B.C. based on this $\alpha_T=0.25$ is then $q_x = 0.014[\epsilon^*/(\sigma^* \tau^*)]$ and the deviations from the MD heat flux $q_x$ is $dev_{\alpha_T} = (q_x_{MD} - q_x(\alpha_T))/q_x_{MD}=0.05$.

In the end, we compare these accommodation coefficients found until now from the $T$ of the molecular fluxes with the effective accommodation coefficients. We match then the explicit MD heat fluxes $q_x$, with the map of MC $q_x$ dependence on the generic accommodation coefficient $\alpha$ when considering Maxwell-like B.C. based on a accommodation coefficient $\alpha$. These effective values are derived then from Fig. 2, where we can just estimate the effective $\alpha$ having the exact MD heat flux values for all the gas-gas/gas-wall interactions. In Table 7 we consider again the case when gas-gas interactions equal gas-wall interactions (in LJ: $\epsilon_{G-G} = \epsilon_{G-W} = 0.10 \epsilon^*$, 0.25$\epsilon^*$, 0.50$\epsilon^*$, and for tsLJ: $\epsilon_{G-G} = \epsilon_{G-W} = 1.0 \epsilon^*$)

<table>
<thead>
<tr>
<th>$\epsilon_{G-G} = \epsilon_{G-W}$</th>
<th>$T_R$</th>
<th>$T_L$</th>
<th>$q_x$</th>
</tr>
</thead>
<tbody>
<tr>
<td>tsLJ 1.0</td>
<td>0.930</td>
<td>0.915</td>
<td>0.015</td>
</tr>
<tr>
<td>LJ 0.10</td>
<td>0.903</td>
<td>0.886</td>
<td>0.010</td>
</tr>
<tr>
<td>LJ 0.25</td>
<td>0.925</td>
<td>0.910</td>
<td>0.013</td>
</tr>
<tr>
<td>LJ 0.50</td>
<td>0.944</td>
<td>0.927</td>
<td>0.015</td>
</tr>
</tbody>
</table>

Table 5. Properties of the molecular fluxes for different gas-gas interactions and explicit wall interactions with $\epsilon_{G-G} = \epsilon_{G-W}$ (column 1). Column 2 contains the MD temperature of the reflected molecules, column 3 of the impinging molecules and column 4 contains the total MD heat flux between the two walls. The heat flux $q_x$ is in $[\epsilon^*/(\sigma^* \tau^*)]$ units, where $\tau^* = \sigma^*/\sqrt{m \epsilon^*}$.

**REFERENCES**

1. In the previous paper [12] we computed the accommodation coefficients for different gas-wall interaction strengths of a dilute gas and we showed that these coefficients used in Maxwell-like B.C. give good heat flux predictions compared to MD results. In this paper we show that for a dense gas, the thermal accommodation of the gas molecules colliding with the wall is not only dependent on the interaction strength between the gas-wall molecules, but also on the gas-gas interaction strength and on
Table 6. Accommodation coefficients for a dense gas ($\eta = 0.2$) for all the gas-gas/gas-wall interactions (column 1) computed from the temperature profiles ($\alpha_T$) and heat fluxes ($q_{\alpha_q}$) (column 2 and 3). Based on these coefficients, the heat fluxes $q_{\alpha_q}(\alpha_T)$ (column 4) and $q_{\alpha}(\alpha_T)$ (column 5) are computed using MC with Maxwell-like B.C. based on $\alpha_T$ and $\alpha_q$. Column 6 contains the explicit MD heat flux $q_{\alpha_M}$ for all the gas-gas/gas-wall interactions. Column 7 and 8 contain the deviations of the MC heat flux from the MD results. The heat flux $q_x$ is in $[\epsilon^*/(\alpha^2\tau^* )]$ units, where $\tau^* = \sqrt{\sigma^*/\epsilon^*}$.

Table 7. Accommodation coefficients $\alpha_T$ computed from the temperature of the impinging and reflected molecules for a dense gas with $\eta = 0.2$ (column 2) and the effective accommodation coefficients derived from the MC heat flux dependency on a generic $\alpha$ (column 3), for all the hydrophilic (LJ $E_{G-G} = E_{G-W} = 0.25\epsilon^* \text{ and } 0.50\epsilon^*$) and hydrophobic interaction strengths (tsLJ $E_{G-G} = E_{G-W} = 1.0\epsilon^*$ and LJ $E_{G-G} = E_{G-W} = 0.10\epsilon^*$).

REFERENCES


[12] Nedea, S., Markvoort, A., van Steenhoven, A., and...
P.A.J. Hilbers, June, 2007. “Heat transfer predictions for micro/nano-channels at atomistic level using combined molecular dynamics and monte carlo techniques”. Fifth International Conference on Nanochannels, Microchannels and Minichannels, Puebla, Mexico, ICNMM2007-30039, CD.


