Heat Transfer Predictions for Micro-/Nanochannels at the Atomistic Level Using Combined Molecular Dynamics and Monte Carlo Techniques

The thermal behavior of a gas confined between two parallel walls is investigated. Wall effects such as hydrophobic or hydrophilic wall interactions are studied, and the effect on the heat flux and other characteristic parameters such as density and temperature is shown. For a dilute gas, the dependence on gas-wall interactions of the temperature profile between the walls for the incident and reflected molecules is obtained using molecular dynamics (MD). From these profiles, the effective accommodation coefficients for different interactions and different mass fluid/wall ratio are derived. We show that Monte Carlo (MC) with Maxwell boundary conditions based on the accommodation coefficient gives good results for heat flux predictions when compared with pure molecular dynamics simulations. We use these effective coefficients to compute the heat flux predictions for a dense gas using MD and MC with Maxwell-like boundary conditions. [DOI: 10.1115/1.3056592]

Keywords: molecular dynamics, Monte Carlo simulations, heat transfer, gas-wall interactions

1 Introduction

Heat transfer at the atomistic level is one of the most important issues within many application fields. One important application is in microchannel cooling. As a lot of electronic components produce heat when operating, cooling these devices is essential for the long lifetime of these components. These devices can be cooled locally where the power is produced using a gas or fluid flow through the microchannels. As these electronic components become smaller and smaller [1] and produce relatively more power, new models for temperature and heat flux predictions are necessary.

Conventional approaches used to study heat flow range from continuum to molecular techniques. Continuum represented by the Navier–Stokes equations breaks down when the size of these devices decreases or when the flow becomes more dilute [2,3]. The governing equation of the heat flow changes from Navier–Stokes to Boltzmann equation. This equation involves molecular velocities instead of macroscopic properties. To solve this equation is very difficult since the number of independent variables contains both those of velocity and of physical space. The alternative is to use particle simulation methods to study heat transfer in micro-/nanochannels, such as direct simulation Monte Carlo (DSMC) [2] or molecular dynamics (MD) [4].

Many studies have been made for analysis of rarefied gas flows using DSMC [5–8] and different boundary conditions were used to represent the gas-solid interface [9–12]. These boundary conditions are crucial for heat predictions as the transport properties of gases at the gas-solid interface can play a very important role in the overall behavior of the channel. A lot of effort has been concentrated on studying the gas-surface interface. In most cases of these analyses, a simplified boundary condition for reflected molecules at a solid surface has been used. This boundary condition 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) [13,14].

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 is taken to be that of the tangential momentum or of the energy of the molecules according to the flow situation [15]. A more elaborated model was proposed by Cercignani and Lampis [11] 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.

An alternative is to use MD, allowing for the simulation of both wall, gas, and wall-gas interactions explicitly. The interaction of monoatomic gas molecules with solid molecules by MD method was studied by Wachman [9] and Matsui and Matsumoto [16]. They all computed the behavior of reflection or adsorption of the incident gas molecules, while Yamanishi and Matsumoto [17] constructed a gas-surface interaction model by developing a multistage collision between molecules based on the analysis of MD. Various other MD studies have been reported for specific gas-solid and fluid-solid interfaces [18,19].

In our previous work [20], we used a MD approach to study the wettability effect on heat and particle flow in nanochannels. 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. Particles were selected according to their velocities in the fluxes of particle going to the left \((V_x < 0, \text{from the cold to the warm wall})\) and to the right \((V_x > 0, \text{from the warm to the cold wall})\). In the gas-surface interface, these molecular fluxes correspond to the incident and reflected molecular fluxes.

To study the impact on the heat fluxes of gas-surface interactions in realistic channels (microchannels) is computationally very expensive. The idea is to combine MD and MC to cover larger time and length scales. Hybrid methods are such techniques used to study gas-surface interface using molecular dynamics and flow region with MC. These techniques are very accurate, but to simulate the MD region taking into account explicitly the walls and the fluid in the surface region is still computationally very demanding. Previously we have introduced a hybrid simulation approach combining MD and MC simulations to study dense and dilute gases in nanochannels [21]. Yamamoto et al. [15] used another hybrid approach combining MD and DSMC for the motion of molecules between two walls and investigating the characteristics of the reflected Ni gas molecules at a Pt surface [15,22]. Based on their results on the observed trajectories of gas molecules, the gas molecules bounce on the surface (once, twice, or many times), and eventually return. In some cases, the molecules are adsorbed on the surface, and leave after a while. From the trajectories they could not deduce that the Maxwell-type distribution function consisting of the specular and diffuse reflections well describes the distribution function of the reflected molecules, but the global velocity is well described by this distribution if the accommodation coefficient involved is chosen properly. Based on this result, we investigate the gas-surface interface for a gas confined between two parallel walls [20], and we compute the accommodation coefficient for a dilute gas from a MD simulation with explicit and different wall interactions (attractive and repulsive). Also the influence of the ratio between the mass of the wall molecules and fluid molecules on the accommodation coefficient \(\alpha\) and on the heat flux \(q_s\) is shown. We then introduce these coefficients into a MC simulation based on Maxwell-type boundary conditions. The temperature and density distributions of incident and reflected molecules are shown and the effect on the heat flux is discussed.

Considering that each individual molecule is accommodated by the wall during the collision with a factor depending only on the interaction strength \(\sigma_{gas}\) between the gas molecules and wall molecule, we extend these gas-wall characteristics to study the heat flux predictions for denser gases in the channel. Thus, we transfer the accommodation coefficients computed for dilute gas to study heat flux in the microchannel for a dense gas and we accurately compute the enhanced collisions with the wall and in the wall vicinity. These accommodation coefficients are computed from the temperature profiles of the dilute gas next to the wall boundary and used in a Maxwell-type boundary condition for a MC simulation based on Enskog equation [5,23]. We compare the heat fluxes computed using the two approaches, MD and MC with Maxwell-type boundary conditions based on \(\alpha\). In the end, effective values of \(\alpha\) established confronting the MD \(q_s\) results with a map of MC \(q_s\), results for different accommodation coefficients are investigated and compared with previously computed accommodation coefficients. The differences in the heat flux predictions are shown and explained.

2 The Physical Model

Our model to study the one-dimensional heat flow in a microchannel consists of two parallel plates of length \(L\), at a distance \(L_x\) 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 \(\eta=\pi a^3/6\) [23]. 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 \(\lambda=\sqrt{2\pi a^3/\eta}\) and the molecular diameter \(a\) have the same order of magnitude. The \(\eta(V)\) factor is the pair correlation function at contact [5,23]. 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. The walls can be modeled explicitly (based on a MD model) or using boundary conditions (Maxwell or Maxwell-like boundary conditions in a MC model). Two situations were considered: (a) a dilute gas confined between the walls with the reduced density \(\eta=0.005\) and \(L_x=1.39a=32.0a\), and (b) a dense gas with \(\eta=0.2\) and \(L_x=95\lambda=46.9\mu a\).

In MD, the Lennard-Jones (LJ) potential is used to model the interactions between the gas-gas, gas-wall, and wall-wall molecules [20]. As it is a generic system we are interested in and not in one specific system, the Lennard-Jones potential serves our purpose of studying the dependency of the accommodation coefficient on the gas-wall interactions. This Lennard-Jones potentials are especially appropriate for noble gases but it captures also the essence of all systems and can thus in principle be used for metals [24,25]. Of course, more realistic potential for metals are available taking into account many-atom interactions but because LJ capture the essence of all systems and we are not directly interested in one particular metal, this potential suffices for investigating the problem we are interested in of modeling hydrophilic and hydrophobic wall interactions and study the thermal behavior in the micro-/nanochannel.

The Lennard-Jones potential is given by the relation

\[
V_{LJ} = \epsilon \left( \frac{2R_{vdW}}{r} \right)^{12} - \frac{2R_{vdW}}{r} \left( \frac{1}{6} \right)
\]

(1)

where \(\epsilon\) is the interaction strength and \(R_{vdW}\) is the van der Waals radius, a measure of the particle size. In order to simulate hard-sphere-like interactions using MD, truncated shifted Lennard-Jones (tsLJ) potentials were used for the interactions between gas molecules. This potential is defined as

\[
V_{tsLJ} = \begin{cases} V_{LJ}(r) - V_{LJ}(r_c) & \text{if } r \leq r_c \\ 0 & \text{if } r > r_c \end{cases}
\]

(2)

where \(r_c\) is the cut-off radius. This tsLJ is used to keep only the repulsive contribution as a model for hard-sphere molecules. The walls are kept together with a relatively strong interaction strength \(\epsilon=6\) in the LJ potential. The gas-wall interactions can be hydrophilic (attractive) or hydrophobic (repulsive) wall interactions. Attractive wall interactions are modeled by LJ with \(\epsilon\) between 0.10 and 0.5, and repulsive wall interactions by tsLJ with \(\epsilon=1.0\). A figure of the potentials used in the simulations is given in Fig. 1.

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 [4,20]. The two walls consisting of 18,000 particles each forming a face centered cubic (fcc) lattice are placed in a box of size 95.0\(\times\)139.49\(\times\)139.49 in case (a) and in a box of size 1.39\(\times\)2.03\(\times\)2.03 in case (b), and are separated from each other in \(x\)-direction. For \(\eta=0.2\), the ratio \(\lambda/\sigma=0.3362\) and for \(\eta=0.005\), the ratio is \(\lambda/\sigma=23.0215\). We name one wall warm (W) and the other one cold (C). The total number of gas particles in the box in case (a) is 55.998 corresponding to a number density \(n_0=0.01\sigma^{-3}\) simulated, and 1300 corresponding to a number density \(n_0=0.01\sigma^{-3}\) simulated. The temperature of the two plates can be 033104-2 / Vol. 131, MARCH 2009 Transactions of the ASME
controlled by coupling them to a heat bath. The mass and the size of wall particles are taken as follows: \( m_2 = 1 \text{m}^3 \) and \( \sigma = 1 \text{m}^3 \). The size for both type of particles (gas and wall) is \( \sigma \) for this paper. The mass of the gas varies in our simulations as a fraction of the wall mass: \( m_1/m_2 = \frac{1}{4}, \frac{1}{2}, \frac{3}{4} \), and \( m_1/m_2 = 1 \). 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 such as density, temperature, and heat flux profiles are obtained. These simulations consist of 5,000,000 iterations and were executed on 8 CPUs of an AMD Athlon 1800+ Beowulf cluster.

3 Effective Accommodation Coefficients for a Dilute Gas

Boundary conditions have a strong effect on transport properties and heat transfer in microchannels. Wettability and hydrophilic and hydrophobic surface effects need to be studied in detail on molecular level as they have a strong impact on the heat flow in systems and devices. As explained, MD simulations for such large systems are computationally not possible. With the approach presented in this section we have the benefit that the accommodation coefficients (alpha) for the boundary conditions are computed on molecular level reflecting thus the dependency of these boundaries on molecular properties such as \( \varepsilon_{G-S} \), \( m_1/m_2 \), and T. In this section the dependency on \( \varepsilon_{G-S} \) and \( m_1/m_2 \) (gas/wall mass ratio) is shown. The Maxwell-like boundary conditions based on \( \alpha \) derived from MD simulations can be used then to reproduce the correct heat flux predictions and properties in the microchannel.

Thus, in Ref. [20], we have seen that at low densities, density peaks depending on the attractive gas-wall interaction potential are present and that this effect is reflected in increased gradients in the temperature near the wall interface. As a result of particles sticking to the wall, their velocity is adapted much more to the wall temperature, such that the higher the attraction, the higher the difference in temperature between gas particles going to the left (impinging) and particles moving to the right (reflected). We use MD with explicit wall interactions to get the temperature and density profiles averaged over time of the particles moving from the cold to the warm wall (C-W), from the warm to the cold wall (W-C), and the profiles of the total temperature and number of particles, as these properties change with the gas-wall interactions. As a result of the MD simulations, we could see that there are more particles going from the C to the W wall, than from the W to the C wall for more attractive walls, and that the numbers are almost equal for repulsive wall interactions. The reason for this is that the warm particles move faster than the cold particles. Thus, it takes longer for particles to move from the cold to the warm wall than from the warm to the cold wall and this results then in more particles moving toward the warm wall. With other words, because total flow in both directions is constant at equilibrium, this results in less warm particles and more cold particles moving toward the warm wall. The slopes of these profiles in the channel vary with the gas-surface interaction strength, \( \varepsilon_{G-S} \), and peaks are present in the temperature and density profiles when increasing \( \varepsilon_{G-S} \).

The higher the slope in T next to the wall, the higher the thermal accommodation at the wall and the effective accommodation coefficient \( \alpha \) based on the temperature of the incident and reflected molecules in the immediate vicinity of the wall can be computed (see Fig. 2). The high peaks correspond to the layer of particles adsorbed or sticking to the wall, and higher peaks determine increased \( \alpha \) reflected also in the T slopes.

As already stated, we define the effective accommodation coefficient based on T as

\[
\alpha = \frac{(T_{in} - T_{out})}{(T_{in} - T_3)}
\]

where \( T_{in} \) is the temperature of the particles moving toward the wall (incident), \( T_{out} \) is the temperature of particles leaving the wall (reflected), and \( T_3 \) is the temperature of the considered wall surface. We can compute all the \( \alpha \)'s from the MD temperature profiles for different G-S interactions (attractive: LJ \( \varepsilon = 0.10, 0.25, 0.5 \), and repulsive: tsLJ \( \varepsilon = 1.0 \)—see columns 1 and 2 of Table 1).

With the newly computed \( \alpha \) for each \( \varepsilon \), we can compute the heat fluxes between the walls using MC with Maxwell-like boundary conditions (BCs) based on \( \alpha [15] \). The values for \( \alpha \) are found in Table 1 (column 1) where we can also compare the heat predictions from pure MD (column 3), MC with Maxwell (last
and MC with Maxwell-like BCs based on $\alpha$ (column 4). From this table we see that the $\alpha$ accommodation coefficients computed from the temperature profiles in MD simulations give better heat flux predictions in MC simulations when used in Maxwell-like BCs based on the accommodation coefficient $\alpha$ than the pure Maxwell BCs ($\alpha=1.0$). For example, for hydrophilic wall interactions (LJ=0.25), MD predicts $q_x=0.00087[e^*/(\tau^2\sigma)]$ and $\alpha=0.25$ from the temperature profiles of the impinging and reflected molecules. MC with Maxwell-like BCs with $\alpha=0.25$ predicts the heat flux $q_x=0.00232[e^*/(\tau^2\sigma)]$, which is 2.6 times the correct MD heat flux predictions. Quantitative support for the deviations of the combined diffusive-specular boundary conditions from the pure Maxwell can also be seen in Figs. 3 and 4, where the profiles for the total temperature, and temperature of impinging and of reflected molecules can be compared using pure Maxwell boundary conditions, combined diffusive-reflective (Maxwell-like based on an accommodation coefficient $\alpha$), and explicit MD wall boundary conditions.

We analyze how the profiles of the total temperature and temperature profiles of particles moving toward and from the wall change depending on the wall properties from Maxwell to Maxwell-type based on $\alpha$, when compared with the MD profiles. In Fig. 3 we see that the total $T$ profiles have the same slope as MD when Maxwell-type BCs are used. Figure 3 shows also that MD and MC Maxwell-type based on $\alpha$ get closer to MC Maxwell predictions for higher values of $\varepsilon$, while at lower $\varepsilon$, the slopes are very much different. MD and MC (Maxwell-$\alpha$ based) are on the other side in very good agreement. To analyze the accommodation coefficient we study the behavior of the incident and reflected molecules to the wall. From the MD simulations we see that the number of molecules going from the W-C wall is smaller than the number of molecules going from the C to the W wall and they become equal for a lower $\varepsilon$. The reason for this is that warm particles move faster than the cold particles. Because total flow in both directions is constant at equilibrium, this results in less warm particles and more particles moving toward the warm wall. Also, the higher the $\varepsilon$, the better the agreement with Maxwell predictions. From the results of these temperature profiles from the C to the W and from the W to the C wall in Fig. 4, we have already computed the accommodation coefficients based on the MD results in Table 1.

Computing $\alpha$ from the $T$ profiles next to the wall for high $\varepsilon$’s becomes difficult due to the enhanced clustering effect next to the wall.

Table 1 Heat fluxes using MD and MC with Maxwell-like boundary conditions based on the accommodation coefficient $\alpha$. A dilute gas was considered with $\gamma=0.005$. Column 1 contains the gas-wall interaction strength for the LJ potential, column 2 contains the accommodation coefficient for each interaction, and columns 3 and 4 contain the MD and MC heat predictions.

<table>
<thead>
<tr>
<th>MD</th>
<th>$\alpha$</th>
<th>MD $q_x$</th>
<th>MC $q_x$</th>
</tr>
</thead>
<tbody>
<tr>
<td>tslJ 1.0</td>
<td>0.14</td>
<td>0.00046</td>
<td>0.00025</td>
</tr>
<tr>
<td>LJ 0.10</td>
<td>0.12</td>
<td>0.00047</td>
<td>0.00021</td>
</tr>
<tr>
<td>LJ 0.25</td>
<td>0.25</td>
<td>0.00087</td>
<td>0.00070</td>
</tr>
<tr>
<td>LJ 0.50</td>
<td>0.58</td>
<td>0.00124</td>
<td>0.00119</td>
</tr>
<tr>
<td>1.0</td>
<td></td>
<td>0.00232</td>
<td></td>
</tr>
</tbody>
</table>
cold wall and due to the shifted bulk temperature value in MC when compared with MD, caused by the fact that MC cannot predict the increased peaks near the wall.

That is why, in order to predict accurately $\alpha$, a map is given in Fig. 5. In this map, for a certain heat flux prediction in MD, we can get the effective value of the $\alpha$ coefficient from the MC heat flux predictions with Maxwell-like BC function on the accommodation coefficient $\alpha$. The $\alpha$ values measured from the temperature MD profiles, for the four values of $\epsilon$ used until now for the gas-wall interactions, are plotted also in Fig. 5 and show good agreement with the map. For lower values of $\epsilon$, the prediction is a bit lower due to higher statistical error in this case.

Table 2 shows the average number of particles, $n$, and average temperature $T$ of particles going to the left (cold-warm) and to the right (warm-cold), using MD, MC with Maxwell-like BC based on $\alpha$, and MC with fully accommodating walls ($\alpha=1$). We see also from these measurements that the density and temperature of
incident and reflected fluxes of molecules correspond very well for lower \( e \). At higher values of \( e \), the clustering next to the wall becomes important and large differences between the fluxes of particles and their \( T \) are registred when comparing MD with MC including Maxwell-like BCs based on \( \alpha \) accommodation coefficient. This \( \alpha \) is then one simple way to characterize the wall-gas interface at the immediate boundary but it is not able to predict the influence of the local effects in the wall vicinity.

We also looked at the dependency of the MD heat flux predictions on the molecular fluid/wall mass ratio. As we can see in Fig. 6, the heat flux \( q_x \) increases with decreasing mass ratio. The values of the heat fluxes on different mass ratios are shown in Table 3. The physical explanation for an increasing heat flux with decreasing mass ratio is the fact that for smaller masses of the gas, the gas particles move faster. This dependence of the mass ratio is given also by the Bird formula for the heat flux between a cold and a warm wall in case of a free molecular flow [2]. In the plots in Fig. 6, the deviations for the MD results for the total heat flux near the wall are caused because the interaction with the walls is not taken into account in the calculation of the heat flux. The values considered in the heat flux comparisons in the paper are the space averaged values for the middle of the channel.

The values of the accommodation coefficients \( \alpha \) for different mass ratios and different wall interactions with the wall (\( e_{G,G} \)) can be derived from the temperature profile from Fig. 7. The accommodation coefficients vary with \( e \) and mass such that at low values of \( e \) (e.g., \( e_0 = 0.10 \)), the mass ratio does not influence \( \alpha \) and has values around 0.14. For higher values of \( e \) (e.g., \( e = 0.25 \)), \( \alpha \) has almost the same value for mass ratios 1.0 (\( \alpha = 0.35 \)) and 0.125 (\( \alpha = 0.32 \)), but has higher values for mass ratios 0.25 and 0.5 (\( \alpha = 0.44 \)). For very attractive walls (\( e = 0.5 \)), \( \alpha \) has the lowest value for mass ratio 0.125 (\( \alpha = 0.46 \)), followed by the case with mass ratio 1.0 (\( \alpha = 0.58 \)), and the same value for both mass ratios 0.25 and 0.5 (\( \alpha = 0.64 \)). It is interesting to see that for more attractive walls, \( \alpha \) for mass ratio 1.0 is always higher than the value for mass ratio 0.125, but lower than for 0.25 and 0.5. For repulsive walls, accommodation coefficient \( \alpha \) is higher (0.2) for mass ratio 1.0 than for the other mass ratios 0.125, 0.25, and 0.5 (\( \alpha = 0.1 \)).

4 Using the Effective Accommodation Coefficient for the Heat Flux Predictions for a Dense Gas

Assuming that the computed \( \alpha \) for different gas-wall interactions (\( e_{G,G} \)) in the MD model is a characteristic of the wall-gas interface, we use these effective values of the accommodation coefficient \( \alpha \) to compute the heat flux of a dense gas between the two walls at different temperatures.

First we determine the heat flux \( q_x \) in a channel with wall separation \( L = 95 \lambda \) and \( \eta = 0.2 \), for different wall-gas and gas-gas interactions. The results in Table 4 show that the gas-gas interactions become important, such that the higher the \( e_{G,G} \) the lower the heat flux. When walls are very attractive, the role of gas-gas interactions becomes less important.

We compute the heat flux predictions in a dense gas with \( \eta = 0.2 \) from MC simulations with Maxwell-type BCs based on the effective \( \alpha \) coefficient transferred from the gas-surface interface of a dilute gas, and we compare with MD results in the case when gas-gas interactions are considered hard-sphere (tSLJ). We see that these values are closer to MD results than MC heat predictions.

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**Table 2** Average density and temperature of the particles going from the cold to the warm wall (\( N_{C-W}, T_{C-W} \)), and from the warm to the cold wall (\( N_{W-C}, T_{W-C} \)), using MD, MC with Maxwell-like boundary conditions based on \( \alpha \), and MC with Maxwell boundary conditions (\( \alpha = 1 \)). Density is normalized with the reference density \( n_0 = 0.01 \) and temperature with \( T_0 = T_2 \) (temperature of the cold wall), and \( \eta = 0.005 \).

<table>
<thead>
<tr>
<th></th>
<th>MD</th>
<th>MC-Max (( \alpha ))</th>
<th>MC-Max (( \alpha = 1 ))</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( N_{C-W} )</td>
<td>( T_{C-W} )</td>
<td>( N_{W-C} )</td>
</tr>
<tr>
<td>tSLJ 1.0</td>
<td>0.50</td>
<td>0.71</td>
<td>0.49</td>
</tr>
<tr>
<td>LJ 0.10</td>
<td>0.51</td>
<td>0.71</td>
<td>0.48</td>
</tr>
<tr>
<td>LJ 0.25</td>
<td>0.51</td>
<td>0.68</td>
<td>0.48</td>
</tr>
<tr>
<td>LJ 0.50</td>
<td>0.52</td>
<td>0.62</td>
<td>0.47</td>
</tr>
</tbody>
</table>
with Maxwell BCs ($\alpha=1$), especially for the hydrophobic wall interactions (small $\alpha$). For attractive walls, even though better results are predicted than MC based on Maxwell BCs ($\alpha=1$), the deviations are larger due to the overlapping of attractive walls and clustering effect (see Table 5).

### 5 Conclusions

In this paper, MD simulation including explicit walls were conducted to study the gas-surface interface, and to compute the effective accommodation coefficients to be used as boundary conditions in MC simulations. The dependence of heat flux predictions and accommodation coefficients on the wall properties (attractive and repulsive) and on the molecular fluid/wall ratio is shown and an effective map of the MC heat flux values depending on the generic accommodation coefficient is given. Confronting this map with the MD heat flux predictions, the effective accommodation coefficients that predict the same $q_x$ in MD as well as in MC were found. These effective values for accommodation coefficients are computed for a dilute gas-surface interface and are transferred then to the MC simulation of a dense gas in a nanochannel. The MC heat flux results using these coefficients were compared with the MD heat predictions. Even though better results are registered compared with other boundary conditions, still large deviations are registered due to the overlapping effect of attractive/clustering next to the wall in the case of a dense gas in the nanochannel such that $\alpha$ cannot be simply transferred.

### Table 3 Average heat flux for different molecular fluid/wall mass ratios $m_1/m_2$, for a dilute gas with $\eta=0.005$ and $\varepsilon_{G-S}=0.50$

<table>
<thead>
<tr>
<th>$m_1/m_2$</th>
<th>$1$</th>
<th>$1/2$</th>
<th>$1/4$</th>
<th>$1/8$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$q_x$</td>
<td>0.0010</td>
<td>0.0018</td>
<td>0.0022</td>
<td>0.0023</td>
</tr>
</tbody>
</table>

### Table 4 Heat flux using MD with different wall-gas and gas-gas LJ interaction potentials, for a dense gas with $\eta=0.2$. The columns stand for the wall-gas interactions and the rows for the gas-gas interactions.

<table>
<thead>
<tr>
<th>G-W</th>
<th>tsLJ 1.0</th>
<th>LJ 0.10</th>
<th>LJ 0.25</th>
<th>LJ 0.50</th>
</tr>
</thead>
<tbody>
<tr>
<td>G-G</td>
<td>$\varepsilon_{tsLJ}=1.0$</td>
<td>$\varepsilon_{LJ}=0.10$</td>
<td>$\varepsilon_{LJ}=0.25$</td>
<td>$\varepsilon_{LJ}=0.50$</td>
</tr>
<tr>
<td></td>
<td>0.015</td>
<td>0.014</td>
<td>0.016</td>
<td>0.017</td>
</tr>
<tr>
<td></td>
<td>0.012</td>
<td>0.011</td>
<td>0.014</td>
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<td></td>
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<td></td>
<td>0.009</td>
<td>0.009</td>
<td>0.012</td>
<td>0.016</td>
</tr>
</tbody>
</table>

Fig. 7 Time average of the MD temperature profiles of particles going from the C-W wall ($T_L$) and from the W-C wall ($T_R$), for different mass ratios and $\varepsilon$: (a) $m_1/m_2=1,1/2,1/4,1/8$ and $\varepsilon_{LJ}=0.10$, (b) $m_1/m_2=1,1/2,1/4,1/8$ and $\varepsilon_{LJ}=0.25$, (c) $m_1/m_2=1,1/2,1/4,1/8$ and $\varepsilon_{LJ}=0.50$, and (d) $m_1/m_2=1,1/2,1/4,1/8$ and $\varepsilon_{LJ}=1.0$. All the results are for a dilute gas with $\eta=0.005$.  

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Table 5  Heat flux using MD and MC with Maxwell-like boundary conditions based on the effective accommodation coefficient \( \alpha \). A dense gas was considered with \( \eta=0.2 \). Column 1 contains the gas-wall interaction strength for the LJ or tsLJ potential. Column 2 contains the accommodation coefficient for each interaction case as evaluated at low density from MD simulations. Columns 3 and 4 contain the MD and MC heat predictions at high gas density.

<table>
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<tr>
<th></th>
<th>MD ( \alpha )</th>
<th>MD-( q_s )</th>
<th>MC-( q_s )</th>
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<tr>
<td>tsLJ 1.0</td>
<td>0.14</td>
<td>0.015</td>
<td>0.010</td>
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<td>LJ 0.10</td>
<td>0.12</td>
<td>0.014</td>
<td>0.008</td>
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References


