ABSTRACT
The replacement of the explicit wall in Molecular Dynamics (MD) simulations of nanochannels with an appropriate wall model is important to model the behavior of the gas close to the channel wall correctly. In this paper a comparison of four different wall models with explicit wall MD simulations is reported in the case of a gas confined between a warm and cold plate. Accommodation coefficients are computed from the explicit wall MD simulations using different techniques. Examples are given that for the same system different methods may produce different accommodation coefficients. The computed accommodation coefficients are subsequently used as input to some of the wall models. From comparison of simulations with explicitly modelled walls or using wall models it is shown that it is not only important to look at the distribution of outgoing velocities, but also at the correlation of incoming and outgoing velocities.

INTRODUCTION
Nanochannels are widely recognized as an important application in the cooling of microdevices, such as microprocessors. These channels allow for improved cooling with respect to conventional devices, since current techniques do not allow the latter to be miniaturized in accordance with the demands of the industry [1, 2].

Using a gas or liquid to flow through the nanochannels, the microdevices can be cooled locally in a compact and efficient way where the heat is produced. In this respect it is important to understand the transport properties, such as the heat flux, of gases at the gas-solid interface. However, in systems of micro-size flow and transport properties can no longer be described adequately by a Navier-Stokes continuum approach, since this approach requires the size of the system being not too small and the gas not very dilute [3]. For smaller length scales, it is possible to change the governing equations of the flow model from the Navier-Stokes equations to the Boltzmann equation. Nonetheless, at sufficiently small length scales the particle behavior becomes essential and, therefore, particle simulation methods are necessary, such as the direct simulation Monte Carlo (DSMC) method and molecular dynamics (MD) simulations.

MD can be used to investigate the influence of the gas-solid interface in close detail. In statistical mechanics and chemistry MD has long been used [4]. For investigation of the gas-solid interface MD is appropriate, since this technique allows the walls to be modelled explicitly, whereas the continuum approach or DSMC do not hold close to the interface [3].

Recently, several MD studies analyzing the influence of the gas-solid interface interactions on the heat flow in nanochannels have been reported, investigating the behavior of a gas confined between two plates [5–7].

Although the recent gain in computational power allows for the study of larger channels with MD, microchannels are still too large to be simulated, due to the high computational cost. Especially the explicit modelling of the solid wall in MD restrains the simulation size. Therefore, the solid wall is usually replaced
by a boundary condition. Different types of boundary conditions have been suggested over the years, ranging from simple conditions, such as the reflective or thermal wall [8, 9], to more elaborate combining the thermal and reflective wall or the Cercignani-Lampis scattering kernel [10, 11].

In this paper several boundary conditions, or wall models, are investigated to find out which one resembles MD simulations with explicitly modeled walls best. To that end velocity correlations between impinging and reflecting particles are compared, for both the explicit MD simulations and simulations with the various wall models. Furthermore, from the explicit MD simulations accommodation coefficients are computed using different techniques.

**MD SIMULATIONS**

In MD simulations the Newtonian equations of motion dictated by interacting particles are integrated, resulting in the time evolution of the system. In most MD systems these interactions are modeled by a Lennard-Jones (LJ) potential

\[
V_{LJ}(r) = 4\varepsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^{6} \right],
\]

where \(\varepsilon\) is the characteristic energy in the pair potential, \(\sigma\) the characteristic length of the pair, and \(r\) is the scalar distance between the two particles. Since the Lennard-Jones potential decays rapidly to zero for large \(r\), it is often truncated beyond a certain cut-off length and shifted in such a way that the potential energy function remains continuous.

Since the interest does not lie with specific gas-wall interactions, parameters expressed in reduced units are used in the simulations. These units have values typically around one and consequently improve the numerical stability of the simulations. Furthermore, they facilitate error estimation and when one wants to model a specific system, they can easily be converted to SI units. The reduced units in this paper have as unit for length \(\sigma^*\), as unit for mass \(m^*\), and as unit for energy \(\varepsilon^*\). All other reduced units can be derived out of these choices, such as the units for temperature \(T^*\), density \(\rho^*\), pressure \(P^*\), and time \(\tau^*\).

The system that has been used in the MD simulations is shown in Fig. 1. It consists of gas particles trapped between two walls of different temperatures (a warm and a cold wall), which ensures a heat flow in the gas. The walls are separated in the \(x\)-direction by a distance of \(33 \sigma^*\). Each of the walls consists of 18,000 particles, which form a face centered cubic lattice, obtained from a previous crystallization simulation [5]. In both the \(y\)- and \(z\)-directions the plates extend \(47 \sigma^*\), but due to periodic boundary conditions, the plates are in fact infinitely large. Between each of the two plates 650 gas particles are present, resulting in a particle density \(n_0\) of 0.01 \(\rho^*\). The system consists of two types of particles: gas particles (G) and wall particles (S). The masses and sizes of all particles are chosen to be unity. For the wall-wall interaction, the LJ potential strength \(\varepsilon_{SS} = 6.0 \varepsilon^*\) is used, which prevents the crystal from melting. On the other hand all the other interactions (gas-wall \(\varepsilon_{GS}\) and gas-gas \(\varepsilon_{GG}\)) are either 0.1 or 0.5 \(\varepsilon^*\). The fact that the gas particles are in the gas phase and the wall particles in the solid phase is solely controlled by the Lennard-Jones parameter \(\varepsilon\).

The temperatures of both walls are controlled by coupling each of the walls separately to an external heat bath. The warm wall is kept at a temperature of \(1.0 T^*\) and the cold wall at \(0.5 T^*\). Collision of gas particles with either wall heats up or cools down the gas, thus leading to a heat flow in the gas.

Each simulation consists of two parts. In the first part the system is run until equilibrium is reached, whereas the second part is used as a production run: typically over a million time steps with step size 0.005 \(\tau^*\). During this production run macroscopic quantities, such as temperature and heat flux, are collected in the direction perpendicular to the walls. Furthermore, particles that collide with either wall have been traced. To this account for every particle moving towards the wall that crosses a virtual border, a plane located 2.5 \(\sigma^*\) from the wall, its incoming and outgoing velocities are known. The location of the virtual border is determined by two factors. First the virtual border has to be far enough away from the wall in order to prevent particles still to be influenced by the wall, which coincides with the truncation distance used for the LJ potential, and for this model equals 2.5 \(\sigma^*\). Secondly, the upper limit for the location of the virtual border is determined by the mean free path of the gas particles. The distance of the virtual border to the wall should...
be small compared to the mean free path of the gas particles to prevent collisions. The mean free path length is determined by the bulk density of the gas phase, and for a gas density of 0.01 $\rho^*$ is about 22 $\sigma^*$ [5]. In the case of free molecular flow the mean free path length is infinite and no upper limit would exist for the virtual border. Thus, locating the virtual border at 2.5 free path length is infinite and no upper limit would exist. Therefore, this model is reversed, whereas the parallel components ($v_\parallel$) remain unchanged. In terms of probability distributions both the perpendicular and parallel directions can be denoted by Dirac functions as

$$P^R_x(v_x) = \delta(v_x + v_x') \quad \text{and} \quad P^R_y(v_y) = \delta(v_y - v_y') ,$$

where the prime indicates an incoming velocity.

On the other hand the thermal wall model assumes that a particle upon collision is assigned a new velocity based on the temperature of the wall, and thus results in diffusive reflection, see Fig. 2(b). For the velocity components parallel to the wall the new velocity is drawn from a Gaussian distribution

$$P^T_x(v_x) = \sqrt{\frac{m}{2\pi kT}} e^{-\frac{m}{2kT}v_x^2} ,$$

where $m$ is the mass of the particle, $T$ the temperature of the wall, $k$ Boltzmann’s constant, $y$ can be substituted by $z$ for the other parallel direction and the superscript $T$ denotes the thermal wall. The velocity component perpendicular to the wall is randomly drawn from a Rayleigh distribution

$$P^T_y(v_y) = \frac{m}{kT} v_x e^{-\frac{m}{2kT}v_x^2} ,$$

where the sign of $v_x$ must be chosen appropriately according to the wall location [9]. Thus, a particle has no recollection whatsoever of its incoming velocity after a collision with the thermal wall.

Apart from the two separate models Maxwell also proposed a linear combination of the models, considering the real reflecting surfaces as an intermediate between a perfectly elastic smooth surface (reflective wall) and a perfectly absorbing surface (thermal wall) [13]. The linear combination is governed by the accommodation coefficient $\alpha$, which represents the weight of the diffusion in the gas colliding with the wall.

Recently, Yamamoto et al. adapted the Maxwell model by allowing different accommodation coefficients for the different components of the velocity [14]. According to Yamamoto the velocity component parallel to the wall for a reflected particle is randomly drawn from the following distribution

$$P^Y_x(v_x) = \alpha T P^T_x(v_x) + (1-\alpha T) P^R_x(v_x) ,$$

where $\alpha T$ indicates the accommodation coefficient as computed from the temperature of the gas particles. For the perpendicular direction Yamamoto uses the following distribution function to draw new velocities from

$$P^Y_y(v_y) = \alpha_y P^T_y(v_y) + (1-\alpha_y) P^R_y(v_y) ,$$

where $\alpha_y$ is the accommodation coefficient computed from the perpendicular velocity components. From both perpendicular and parallel distributions it can be seen that they are a linear combination of the Rayleigh or Gaussian distribution of the thermal wall and the Dirac distribution of the reflective wall, thus each impinging particle is reflected either specularly or diffusely at the surface.

Another phenomenological model, like the above discussed Maxwell model, is the model proposed by Cercignani and Lampis [10] and later extended by Lord [11] (the CL-model). This model also uses two accommodation coefficients, albeit different ones than in the case of Yamamoto’s extension of the Maxwell model. As with all previous models, the CL-model treats the velocity components independently. The probability model.

Figure 2. Schematic representations of particle collisions with either (a) a reflective wall or (b) a thermal wall. Incoming velocities are denoted with a prime. Note that the reflective wall only reverses the $x$-component of the velocity, whereas the thermal wall is purely diffusive and new velocities are assigned to all components.

MODELS

Besides using explicitly modeled walls in MD simulations, several other models can also be employed to account for the gas-wall interaction. The simplest choices for these models are the reflective and thermal walls as introduced by Maxwell [12].

The reflective wall model simply reverses a particle when it collides with the wall, see Fig. 2(a). Thus, the perpendicular component ($v_\perp$, see figure) of a particle impinging on the wall is reversed, whereas the parallel components ($v_\parallel$, which is used to indicate both parallel components, since they are mutually interchangeable) remain unchanged. In terms of probability distributions both the perpendicular and parallel directions can be denoted by Dirac functions as

$$P^R_x(v_x) = \delta(v_x + v_x') \quad \text{and} \quad P^R_y(v_y) = \delta(v_y - v_y') ,$$

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$$P^T_x(v_x) = \sqrt{\frac{m}{2\pi kT}} e^{-\frac{m}{2kT}v_x^2} ,$$

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distribution for the parallel velocity components is given by

\[
p_{\parallel}^{CL}(v_y) = \frac{1}{kT} \frac{m}{2\pi \alpha_{v_y} (1-\alpha_{v_y})} \exp \left(-\frac{m}{2kT} \frac{v_y - (1-\alpha_{v_y})v_y'}{\alpha_{v_y} (1-\alpha_{v_y})} \right),
\]

where \( \alpha_{v_y} \) is the accommodation coefficient based on the parallel components of the velocity, and \( v_y' \) is the incoming velocity component in the y-direction. In the perpendicular direction the probability distribution equals

\[
p_{\perp}^{CL}(v_x) = \sqrt{\frac{2}{\pi}} \frac{m}{kT} \frac{\sqrt{2m}}{\alpha_{v_x} v_x} \left[ \frac{2m}{kT} \right] \right] \exp \left(-\frac{m}{2kT} \frac{v_x^2 + (1-\alpha_{v_x})v_x'^2}{\alpha_{v_x}} \right),
\]

where \( I_0 \) is the modified Bessel function of the first kind and this time the accommodation coefficient \( \alpha_{v_x} \) is computed from the temperature based on the perpendicular velocity components only, and \( v_x' \) is the incoming velocity component in the x-direction.

**ACCOMMODATION COEFFICIENT**

When discussing the more advanced Maxwell and CL-models, the accommodation coefficient has been introduced as a measure for how diffusive or reflective a collision with the wall is. However, several types of accommodation coefficients exist and each can be computed in a different way [15,16]. The general form of the equation that gives the accommodation coefficient is

\[
\alpha_k = \frac{\langle k_1 \rangle - \langle k_0 \rangle}{\langle k_1 \rangle - \langle k_T \rangle},
\]

where \( k \) can be any quantity, such as the velocity in the parallel direction \( v_y \), the total temperature \( T \), or the heat flux in perpendicular direction \( q \). The subscripts denote whether the expected value is to be computed from the incoming particles (I), the outgoing particles (O) or from the thermal wall (T). When computing accommodation coefficients involving parallel velocity components, the incoming parallel velocity component is always chosen to be positive, and the outgoing velocity is positive if it is in the same direction as the incoming and negative otherwise.

The expected values for the quantities can be obtained in several ways. The most straightforward approach is to generate histograms based on the data obtained from the macroscopic data collection during the simulations. This gives rise to a profile for a quantity across the channel, for instance the temperature gradient.

On the other hand, it is also possible to use the incoming and outgoing velocities of the impinging and reflecting particles, collected when they passed through the plane located 2.5 \( \sigma^* \) from the wall. Furthermore, the velocities of the particles going through the plane can be used to reconstruct the value of specific macroscopic quantity in the bin of the above mentioned histogram in which the plane lies. This can be done by taking into account the time a particle resided in the bin, which is indicated by the magnitude of the \( x \)-component of the velocity. Thus, the expected value can be computed in two ways from the collected velocities of the impinging and reflecting particles, either based on the plane or on the bin. With the plane averaging method each collision is weighted equally, whereas with the bin averaging method slower moving particles are weighted more than fast moving particles (by scaling the averages with respect to the \( x \)-component of the incoming velocity).

Since the thermal wall is given in closed form by Eqs. (3) and (4), it is possible to compute the expected values analytically. In Table 1 a wide range of expected values for the thermal wall are given for both averaging methods.

Using the values for the thermal wall from Table 1 and the data collected from the MD simulations different accommodation coefficients can be computed, using Eq. (9) and plugging in the desired expected values, which give the accommodation coefficient based on that quantity. In order to achieve an accurate error estimation for the accommodation coefficient, the velocities that have been collected are split into ten independent sets of velocities. For each of these groups of velocities the accommodation coefficient near the warm wall has been computed, which have been subsequently averaged to give an idea on the accuracy.

<table>
<thead>
<tr>
<th>Plane averages</th>
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<tbody>
<tr>
<td>( \langle v_x \rangle = \frac{\sqrt{2}}{\sqrt{8}} \sqrt{\frac{2kT}{m}} )</td>
</tr>
<tr>
<td>( \langle v_y \rangle = 0 )</td>
</tr>
<tr>
<td>( \langle v^2 \rangle = \frac{kT}{m} )</td>
</tr>
<tr>
<td>( \langle v_yv^2 \rangle = 0 )</td>
</tr>
<tr>
<td>( \langle v \rangle = \frac{3\sqrt{3}}{4} \sqrt{\frac{2kT}{m}} )</td>
</tr>
<tr>
<td>( \langle v^3 \rangle = \frac{15\sqrt{3}}{8} \sqrt{\frac{2kT}{m}} )</td>
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</tbody>
</table>

<table>
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<tr>
<th>Bin averages</th>
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<tbody>
<tr>
<td>( \langle v_x \rangle = \frac{1}{\sqrt{8}} \sqrt{\frac{2kT}{m}} )</td>
</tr>
<tr>
<td>( \langle v_y \rangle = 0 )</td>
</tr>
<tr>
<td>( \langle v^2 \rangle = \frac{kT}{m} )</td>
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<tr>
<td>( \langle v_yv^2 \rangle = 0 )</td>
</tr>
<tr>
<td>( \langle v \rangle = \frac{2}{\sqrt{8}} \sqrt{\frac{2kT}{m}} )</td>
</tr>
<tr>
<td>( \langle v^3 \rangle = -\frac{1}{\sqrt{8}} \sqrt{\frac{2kT}{m}} )</td>
</tr>
</tbody>
</table>
MODEL SIMULATIONS

Using the incoming velocities from the MD simulations and the determined accommodation coefficients as input for the wall models discussed previously, new outgoing velocities can be computed for each of the wall models.

In order to compare the applicability of the model with the MD simulations, many authors look at the distributions of the outgoing velocity components in comparison to the same distributions from the MD simulations [14, 16, 18].

However, another interesting property to investigate is the correlation between incoming and outgoing velocities for each of the components. In the case of the reflective wall a strong correlation is to be expected, since particles are reflected with the same velocity, only the direction is reversed. On the other hand, the thermal wall applies diffusive reflection and no correlation is to be expected at all.

In Fig. 3 velocity correlation distributions are shown for the simulations with a low interaction with the wall. Again, only the warm wall is considered. The first column gives the correlation for the perpendicular component of the velocity, the second column for the parallel component, whereas the third column gives the correlation for the absolute velocity. It has to be mentioned that in the case of the perpendicular velocity components both the incoming and outgoing velocity are given a positive value for clarity in the figure. Finally, the last column gives the distributions of the outgoing velocities (both the parallel and perpendicular component, solid lines) in comparison with the same distributions obtained from the MD simulation (circles).

On the first row the results from the MD simulation are shown, followed by the results for the reflective and thermal walls. Thereafter the correlations and distributions from the Maxwell model (as refined by Yamamoto) and the CL-model are given.

From the MD simulation it is clear that some kind of correlation exists between incoming and outgoing velocities. Furthermore, the correlation profiles are not symmetrical along the diagonal, they lie above the diagonal, which means that the incoming gas leaves the wall with a higher temperature on average.

The velocity correlations for the reflective wall show that there is a very high correlation between incoming and outgoing velocities, which is to be expected due to the nature of the reflective wall model. On the other hand the thermal wall indeed shows

From Table 2 it can be observed that the method of computation highly influences the outcome of the accommodation coefficient, and that examining different quantities gives different accommodation coefficients. However, for low gas-solid interactions the accommodation coefficients are always lower than for high gas-solid interactions. Moreover, similar behaviors for parallel and perpendicular components can be observed.

### Table 2. Accommodation coefficients near the warm wall computed for weak (ε = 0.10 ε∗) and strong (ε = 0.50 ε∗) interactions, using two different techniques (plane and bin averages, see text). Each of the accommodation coefficients have been computed from ten independent sets of velocities.

<table>
<thead>
<tr>
<th></th>
<th>ε = 0.10 ε∗</th>
<th>ε = 0.50 ε∗</th>
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</thead>
<tbody>
<tr>
<td>α_{c_{x}}</td>
<td>0.36 ± 0.03</td>
<td>0.23 ± 0.12</td>
</tr>
<tr>
<td>α_{c_{y}}</td>
<td>0.55 ± 0.01</td>
<td>0.51 ± 0.01</td>
</tr>
<tr>
<td>α_{c_{v}}</td>
<td>0.27 ± 0.02</td>
<td>0.18 ± 0.05</td>
</tr>
<tr>
<td>α_{T_{v}}</td>
<td>0.27 ± 0.02</td>
<td>0.18 ± 0.03</td>
</tr>
<tr>
<td>α_{T_{x}}</td>
<td>0.45 ± 0.02</td>
<td>0.39 ± 0.02</td>
</tr>
<tr>
<td>α_{T_{y}}</td>
<td>0.32 ± 0.02</td>
<td>0.24 ± 0.04</td>
</tr>
</tbody>
</table>

In systems with N particles and only pair interactions, as is the case here, the heat flux vector consists of two parts (kinetic and potential), and is given by

\[
\mathbf{q} = \sum_{i} E_i \mathbf{v}_i + \frac{1}{2} \sum_{i,j} (\mathbf{F}_{ij} \cdot \mathbf{v}_i) \mathbf{r}_{ij},
\]

where \( E_i \) is the total (both kinetic and potential) energy of particle \( i \), \( \mathbf{r}_i \) the position vector of particle \( i \), \( \mathbf{v}_i \) is the velocity vector of particle \( i \), and \( \mathbf{F}_{ij} \) and \( \mathbf{r}_{ij} \) are the inter-particle separation vector and force vector between particles \( i \) and \( j \), respectively [17]. Due to the low density of our system, the resulting mean free path for the gas particles, and the corresponding location of the virtual plane almost no interactions with other gas particles will have taken place during the reflection process, and, thus, it is a safe assumption to use only the kinetic part of the heat flux vector. This allows the accommodation coefficients based on the heat flux to be computed using only \( \langle v_x v^2 \rangle \), \langle v_y v^2 \rangle and \langle v^2 \rangle. In the third column of Table 1 these values are given for the thermal wall.
Figure 3. Contour plots of the velocity correlation distribution of impinging particles versus reflecting particles (first three columns) and in the last column the corresponding velocity distributions (perpendicular blue and parallel red) for the reflecting particles (solid lines) in comparison with the same distribution obtained from the MD simulations (circles). The interaction parameter for gas-wall interactions is $\varepsilon = 0.10 \varepsilon^*$, whereas the temperature of the wall equals $1.0 T^*$. For the Yamamoto and Cercignani-Lampis models the appropriate accommodation coefficients are necessary and can be obtained from Table 2 combined with the equation describing the model.
Figure 4. Contour plots of the velocity correlation distribution of impinging particles versus reflecting particles (first three columns) and in the last column the corresponding velocity distributions (perpendicular blue and parallel red) for the reflecting particles (solid lines) in comparison with the same distribution obtained from the MD simulations (circles). The interaction parameter for gas-wall interactions is $\varepsilon = 0.50 \varepsilon^*$, whereas the temperature of the wall equals $1.0 T^*$. For the Yamamoto and Cercignani-Lampis models the appropriate accommodation coefficients are necessary and can be obtained from Table 2 combined with the equation describing the model.
no correlation (which can be best observed from the correlation distribution for the parallel direction).

The Maxwell-Yamamoto model shows a very different correlation with respect to the MD simulation. Recall from the equations for the Maxwell-Yamamoto model, Eqs. (5) and (6), that a particle is reflected either specularly or diffusively. Consequently, in the correlation profiles both the reflective and thermal wall can be easily identified.

Finally, the CL-model shows good comparison with the MD simulation. Only the shape of the correlation distribution in the parallel direction are not similar. In case of the MD simulation this is a diamond shape, whereas it is more elliptical with the CL-model.

Turning the attention to the distribution profiles (the last column in Fig. 3), different observations can be made. The reflective wall model is in good agreement with the MD simulation, as are the Maxwell-Yamamoto and the CL-model. The thermal wall model deviates only a little.

So, where the distribution profiles give the impression that three of the four models are in good agreement with the MD simulation, it is from the velocity correlation distribution that it can be observed that only the CL-model compares well with the MD simulation on both analysis methods.

In Fig. 4 a similar figure, but now for the simulations with the high gas-wall interaction, is shown. This time both the reflective wall and Maxwell-Yamamoto model show poor agreement with the MD simulation based on the velocity correlation distribution. However, when looking at the probability distributions (again, the last column), it is observed that both the thermal wall and the Maxwell-Yamamoto model are in good agreement with the MD simulation, closely followed by the CL-model, whereas the reflective wall model does not agree well.

Adaption to the Maxwell-Yamamoto model

Looking again at the correlation distribution for the reflective wall, poor agreement is observed. Since the Maxwell-Yamamoto model depends on the distribution for the reflective wall, which can be clearly seen from the correlation distributions, poor agreement is also observed for this model. A closer look at the Maxwell-Yamamoto model gives an indication why this model resembles the MD simulations so poorly. From Eqs. (5) and (6) it can be seen that the new distribution is a linear combination based on the accommodation coefficient $\alpha$ of the original distribution and the distribution imposed by the thermal wall. As mentioned, this means that the particle is reflected either specularly or diffusively.

A different approach to the Maxwell-Yamamoto model is to create a linear combination of the velocities rather than of the probability distributions. Thus, when a particle collides with the wall, it keeps some part of its original incoming velocity (the reflective part) and it is given also a part of a new velocity based on the thermal wall. As with the original Maxwell-Yamamoto model the accommodation coefficient determines how much of each of the two is incorporated. For a low gas-solid interaction the reflective wall is weighted more and the thermal wall less, while the opposite is true for a high gas-solid interaction.

Using this adaption to the Maxwell-Yamamoto model for the new velocities in the parallel direction for the low gas-solid interaction results in correlations and velocities distributions as shown in Figs 5(a) and 5(c). Although the correlation profile now resembles the MD simulations much better (see first row of Fig. 3), it can be observed that the distribution is also tilted with respect to the diagonal. Furthermore, the velocity distributions show a worse agreement with the MD simulations than the original Maxwell-Yamamoto model.

However, recall that the distribution of the parallel component of the incoming velocity is a Gaussian distribution with a certain standard deviation depending on the temperature. Similarly, the distribution for the parallel component of the outgoing velocity, dictated by the thermal wall, is also a Gaussian distribution, see Eq. (3). Therefore, the adapted outgoing velocity is linear combination of two normal distributed random variables weighted by the accommodation coefficient, leading to a new Gaussian distribution, which can be written as

$$v_y[0,T_N] \sim \alpha \cdot v_y[0,T_T] + (1-\alpha) \cdot v_y[0,T_R].$$

where the first part of the right-hand side is the random variable drawn from the Gaussian distribution of the thermal wall, with temperature $T_T$, while the second part is the random variable drawn from the Gaussian distribution of the incoming velocities, with temperature $T_R$, while $T_N$ indicates the standard deviation (the new temperature) for the new Gaussian distribution. Using the additive property of random variables from Gaussian distributions, the new temperature $T_N$ equals

$$T_N = \alpha^2 T_T + (1 - \alpha)^2 T_R.$$

However, to affect the temperature correctly, the weighing accommodation factors in Eq. (12) should not be squared, since an impinging particle with the temperature of the wall, should reflect with the same temperature. Based on Eq. 12 this is not the case, and, therefore, the new temperature $T_N$ has to be simply $T_N = \alpha(T_T - T_R) + T_R$. Thus the linear combination in Eq. (11) involves $\sqrt{\alpha T}$ for the thermal part and to $\sqrt{(1-\alpha T)}$ for the reflective part.

When using this new model for the parallel directions, different velocity correlations and distribution are obtained for the low interaction strength, see Fig. 5. From this figure it can be seen that the new model removes the tilt from the velocity correlation distribution and aligns the velocity distribution with the MD simulation.
Unfortunately, a similar adaption for the perpendicular direction is not possible, since in that case two random variables are drawn from a Rayleigh distribution, see Eq. (4), and there exists no addition rule for such random variables, in contrast to the Gaussian distribution.

CONCLUSION

In this paper examples of several wall models are discussed, such as the reflective and thermal wall, as well as more elaborate methods such as the Maxwell model and the CL-model. Each of these models is analyzed to find out whether it is an appropriate model to replace the explicit solid wall.

To be able to compute the Maxwell and CL-model it is necessary to have knowledge on the accommodation coefficient for the gas. From the MD simulations the velocities of particles impinging and reflecting on the wall have been collected. Using this data the accommodation coefficient is computed using two different methods: plane or bin averaging. The first method computes the standard averages, whereas the second method takes the perpendicular velocity component into account to reproduce accurate profiles for the desired quantity, such as velocity, temperature or heat flux. However, since there is no agreement in literature based on which quantity the accommodation coefficient should be computed, different accommodation coefficients are determined, see Table 2. From this table it is clear that the method used to compute the accommodation coefficient, as well as based on which quantity the accommodation coefficient is computed, highly affects the value for the accommodation coefficient.

Accommodation coefficients computed using the bin averaging method are always lower than when computed using the plane averaging method. Moreover, the standard deviation on the computed accommodation coefficient is much larger for the bin averaging methods, especially for the accommodation coefficients computed directly from the velocities. Especially the standard deviation for the bin averaging method for the perpendicular velocity is large compared to the computed accommodation coefficient. However, this large standard deviation can be explained by the used averaging method (scaling with respect to perpendicular velocity component) and probably not enough data to arrive at more accurate statistics.

Some of the accommodation coefficients served as input for the Maxwell and CL-model. Both of the models required accommodation coefficients computed from the plane averaging method. Therefore it seems to be more appropriate to use the plane averaging method for the computation of the accommodation coefficients.

Subsequently the previously mentioned wall models have been used to generate velocities for reflected particles, with the velocities of the impinging particles taken from the MD simulations. For these wall models not only the outgoing velocity distribution is compared with the same distribution from the MD simulations, but also the correlation distributions between incoming and outgoing velocities is investigated.

Based on these correlation distributions (see Figs. 3 and 4) it is observed that neither the reflective nor the thermal wall model the behavior of the explicit wall correctly. Furthermore, the Maxwell-Yamamoto model shows poor agreement with the MD simulations, whereas the CL-model performs well. However, in the case of the CL-model, still differences with the MD simulations are observed, especially when considering low gas-wall interactions. The MD simulations show a diamond shaped correlation distribution for the parallel velocity component, which is not reproduced by the CL-model, nor by any other model.

From examining the comparison of the probability distributions of the outgoing velocities of the models with the MD simulations, it can be wrongly concluded that the reflective wall model (in the case of the low interaction strength), or the thermal wall model (in the case of the high interaction strength) or
the Maxwell-Yamamoto model (in both cases) resemble the MD simulations well. However, from the correlation distributions it is clear that no resemblance exists. Again, the CL-model is in best agreement with the MD simulations.

The correlation distributions of the Maxwell-Yamamoto model show clearly that a particle is either reflected specularly or diffusively. Based on the argument of additivity of Gaussian distributions a new model has been constructed for the parallel direction only. Implementation of this adapted model showed far better agreement with the MD simulations, see Fig. 5.

Although none of the discussed wall models truly resemble the MD simulations, the CL-model agrees best. However, in all models it is assumed that every velocity component can be treated independently. The correlation distributions show that this assumption is not valid.

When discussing the computed accommodation coefficients, as listed in Table 2, it has been noted that depending on the method used to compute the accommodation coefficient (either using the plane or bin averaging method), large differences can occur. However, if every collision would result into the same accommodation coefficient, the method of averaging should not matter. From the table of accommodation factors it is clear that this is not the case, which stresses the observation from the velocity correlation distributions, that neither wall model reproduces the correlations observed from the MD simulations, indicating that models should incorporate an accommodation factor that depends on the incoming velocity.

It is important to choose the best wall model to replace the explicit solid wall, in order to obtain the correct gas-wall behavior, which is of great importance to understand the heat capacity of nanochannels. In the case of a gas or liquid flow this is even more important. Currently a wall model is being developed that takes the correlation between velocity components into account.

REFERENCES