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Maxwell boundary condition and velocity dependent accommodation coefficient

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A modification of Maxwell's boundary condition for the Boltzmann equation is developed that allows to incorporate velocity dependent accommodation coefficients into the microscopic description. As a first example, it is suggested to consider the wall-particle interaction as a thermally activated process with three parameters. A simplified averaging procedure leads to jump and slip boundary conditions for hydrodynamics. Coefficients for velocity slip, temperature jump, and thermal transpiration flow are identified and compared with those resulting from the original Maxwell model and the Cercignani-Lampis model. An extension of the model leads to temperature dependent slip and jump coefficients. © *2013 AIP Publishing LLC*. [http://dx.doi.org/10.1063/1.4829907]

I. INTRODUCTION

While the microscopic interaction between gas particles and a solid boundary (i.e., a wall) is a rather complicated affair, it is quite common in kinetic theory of gases to use simplified microscopic wall-gas interaction models which are determined by only one or two accommodation coefficients. Best known are Maxwell's boundary condition, which uses only one single accommodation coefficient,[1–3] and the Cercignani-Lampis (CL) model, which has two accommodation coefficients, one for normal momentum, and one for tangential momentum.[4,5]

Macroscopically, the interaction between gas molecules and solid walls manifests itself in temperature jump and velocity slip at the gas-wall boundary.[3,6] The strength of jump and slip can be related to the accommodation coefficients, which therefore can be measured.[7,8] According to measurements, the macroscopic accommodation coefficients that describe jump and slip are different. The simple Maxwell model, which has only a single accommodation coefficient predicts them to be equal, hence cannot fully describe experiments. The two accommodation coefficients of the CL model can be fitted to jump and slip, but the model does not allow to also fit the thermal slip coefficient.[7] Moreover, measurements reveal a temperature dependence of the macroscopic accommodation coefficients,[9,10] which is not described by the Maxwell model.

In this contribution we present a modification of Maxwell's boundary condition that includes the well-known term for isotropic scattering,[11] and *microscopic* accommodation coefficients dependent on the microscopic impact velocity. The basic model can be furnished with a wide variety of microscopic accommodation coefficients. For a first test we propose a model where the particle-wall interaction is considered as a thermally activated process. Evaluation of the model for jump and slip reveals *macroscopic* accommodation coefficients, which are compared to those for the Maxwell and CL models in the linear regime. A temperature dependence of the macroscopic accommodation coefficients arises only when an energy bonus or malus is added to the activation model. The model contains three parameters that can be used to fit the macroscopic accommodation coefficients to measurements at a given temperature, and one coefficient to describe the temperature dependence. Due to lack of data, a full fit to experiments is presently not possible.

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The paper proceeds as follows: Section II recalls the main properties of wall reflection kernels in kinetic theory. The reflection kernels for specular and diffuse reflection, thermalization, and their superposition in the Maxwell model, and the Cercignani-Lampis model are summarized in Secs. III and IV. The main contribution of this paper, i.e., the extension of the Maxwell model to velocity dependent accommodation coefficients is presented in Sec. V, and Sec. VI presents a first simple model for a velocity dependent accommodation coefficient. To obtain some insight into the influence of velocity dependence accommodation, in Sec. VII we use the Chapman-Enskog (CE) expansion to estimate macroscopic jump and slip coefficients for the model, and compare these to the classical Maxwell model as well as to the Cercignani-Lampis model. The temperature dependence of the coefficients is briefly examined in Sec. VIII. The paper closes with some final comments.

II. WALL REFLECTION KERNELS IN KINETIC THEORY

To set the stage for the subsequent discussion, we recall some basics of kinetic theory for monatomic gases and its boundary conditions: The distribution function $f(x_i, t, c_i)$ is defined such that $f(x_i, t, c_i)\, d\mathbf{c} d\mathbf{x}$ is the number of molecules with velocities in $\{\mathbf{c}, \mathbf{c}+d\mathbf{c}\}$ and positions in $\{\mathbf{x}, \mathbf{x}+d\mathbf{x}\}$ at time t. Given the distribution function, bulk properties can be computed, for instance the mass density $\rho = \int f d\mathbf{c}$, the average velocity $v_k = \frac{1}{\rho}\int c_k f d\mathbf{c}$, or the temperature $T = \frac{1}{\frac{3}{2}\rho\frac{k}{m}}\int \frac{1}{2}C^2 f d\mathbf{c}$, where $C_k = c_k - v_k$ is the peculiar velocity. In equilibrium, the distribution function is the Maxwellian,

$$f_M(\rho, T, v_k; c_k) = \rho\sqrt{\frac{m}{2\pi kT}}^3 \exp\left(-\frac{C^2}{2\frac{k}{m}T}\right). \tag{1}$$

We consider the wall interaction from the viewpoint of an observer resting with the wall, so that the wall velocity is $v_k^W = 0$, and all velocities are measured relative to the wall. When a gas particle hits the wall, it interacts with the wall particles. For non-absorbing walls, which we study exclusively, after interaction the particle will return to the gas with new direction and velocity. We write the distribution function directly in front of the wall as

$$f_W = \begin{cases} f^-, & c_n' \le 0 \\ f^+, & c_n > 0 \end{cases}, \tag{2}$$

where f^- is the distribution of incident particles (negative velocity $c_n' = c_k' n_k$ normal to the interface with normal n_k pointing into the gas), and f^+ is the distribution of reflected particles (positive normal velocity c_n). The prime at the velocity of incident particles is used to distinguish between incident and emitted particles. The relation between the incident and emitted distribution functions is expressed by means of the reflection kernel $\mathcal{R}(c_k' \to c_k)$, as[2,12,13]

$$f^+ = \frac{1}{|c_n|}\int_{c_n'<0} f^-(c_k')\,\mathcal{R}(c_k' \to c_k)\,|c_n'|\, d\mathbf{c}'. \tag{3}$$

In thermal equilibrium, wall and gas have the same temperatures, $T_W = T$, and the gas is in the corresponding Maxwellian distribution f_M, which is ensured by the microreversibility condition $f^+|_{eq} = f^-|_{eq} = f_M$.

The reflection kernel $\mathcal{R}$ in (3) gives the probability that a particle which hits the wall with velocity in $\{c_k', c_k' + dc'\}$ will return to the gas with velocity in[2] $\{c_k, c_k + dc\}$. Since the probability for an incident particle to leave the reflecting interface is unity, the kernel must satisfy the normalization condition

$$\int_{c_n>0} \mathcal{R}(c_k' \to c_k)\, d\mathbf{c} = 1. \tag{4}$$

Moreover, $\mathcal{R}$ obeys the reciprocity relation,[2,12,13]

$$|c_n'|\, f_0(T_W, c')\,\mathcal{R}(c_k' \to c_k) = |c_n|\, f_0(T_W, c)\,\mathcal{R}(-c_k \to -c_k'), \tag{5}$$

where $f_0(T,c) = f_M(T,c)/\rho\sqrt{\frac{kT}{2\pi m}}$ is the reduced Maxwellian with zero velocity in the rest frame of the wall. Reciprocity guarantees microreversibility and the validity of the H-theorem at the wall.[2]

III. STANDARD REFLECTION KERNELS

Now consider the interaction between a gas particle and a wall. In case of a perfectly smooth and rigid wall, a particle coming in with velocity c'_k will be specularly reflected. That is, its tangential velocity will remain unaltered, while its normal velocity will be inversed. For this simple case the reflection kernel is a delta function,

$$\mathcal{R}_{spec}\left(c'_k \to c_k\right) = \delta\left(c'_k - c_k + 2n_j c_j n_k\right). \tag{6}$$

Real walls are not smooth, and they are not rigid. Hence, modifications of the above are in order. For a rough wall the local normal $n_{k,\,loc}$ will differ from the average wall normal n_k. A perfectly rough but rigid wall will scatter the particles into arbitrary directions, while preserving their absolute velocity c. This is described by the kernel

$$\mathcal{R}_{scat}\left(c'_k \to c_k\right) = \frac{1}{\pi}\frac{|c_n|}{c'^3}\delta\left(c' - c\right). \tag{7}$$

Moreover, the wall consists of vibrating atoms, and as a gas particle hits the wall, a molecular interaction occurs, during which the gas particle exchanges momentum and energy with the participating wall particles. In average, the collisions between gas and wall will have a tendency to bring the gas towards equilibrium with the wall. For a perfectly active wall, the gas particles leave in a Maxwellian distribution defined by wall temperature T_W and wall velocity v_k^W. One speaks of diffuse reflection, with the kernel

$$\mathcal{R}_{diff}\left(c'_k \to c_k\right) = |c_n|\, f_0\left(T_W, c_k\right). \tag{8}$$

The three kernels (6)–(8) fulfill the conditions (4) and (5).

The realistic scattering behavior lies somewhere between the extrema of specular, isotropic, and diffuse reflection. Maxwell's suggestion for a reflection kernel is a linear combination of simple kernels.[1] With constant factors Γ_0, Λ_0, Θ_0 we write

$$\mathcal{R}_M\left(c'_k \to c_k\right) = \Theta_0\mathcal{R}_{diff}\left(c'_k \to c_k\right) + \Gamma_0\mathcal{R}_{spec}\left(c'_k \to c_k\right) + \Lambda_0\mathcal{R}_{scat}\left(c'_k \to c_k\right). \tag{9}$$

Since the individual kernels fulfill reciprocity, this is also the case for the weighted sum. Normalization simply requires that the factors add up to unity,

$$\Gamma_0 = 1 - \Theta_0 - \Lambda_0\,. \tag{10}$$

In Maxwell's classical model,[1] isotropic scattering is not considered, $\Lambda_0 = 0$, so that $\Gamma_0 = 1 - \Theta_0$. Then, the coefficient Θ_0 is Maxwell's accommodation coefficient.

In his encyclopedia article,[14] Grad suggests a two accommodation factor model which is essentially the Maxwell model, but with the Maxwellian of the diffusively reflected particles, f_0, replaced by a shifted Maxwellian $\tilde{f}_0 = \frac{m^2}{2\pi(kT)^2}\exp\left(-\frac{(c-U)^2}{2\frac{k}{m}T}\right)$ where "U can be taken as a second parameter representing the wall material; e.g., in this formula, U might represent some mean value of the wall velocity and the gas velocity." Indeed, evaluation of slip with this model yields a shift of the slip velocity by U. We shall not further consider this model, but state that Grad's shift velocity U must be chosen such that it vanishes in equilibrium, where the gas Maxwellian must be centered on the wall; a reasonable choice would be to chose U proportional to the slip velocity V, that is, $U = \alpha_G V$ with a coefficient α_G.

Another modification of the Maxwell model was recently suggested, where distributions of normal and tangential velocities are separated, and each have their own, that is, normal and tangential accommodation coefficient.[15]

IV. THE CERCIGNANI-LAMPIS MODEL

The Cercignani-Lampis kernel introduces two accommodation coefficients, α_n and α_t, for normal and tangential momentum; the kernel reads[4]

$$\mathcal{R}_{CL}\left(c_k' \to c_k\right) = \frac{1}{2\pi}\frac{1}{\alpha_n\alpha_t\left(2-\alpha_t\right)}\frac{c_n}{\left(\frac{k}{m}T_W\right)^2}\frac{1}{2\pi}\int_0^{2\pi}\exp\left[\frac{\sqrt{1-\alpha_n}c_n c_n'\cos\phi_n}{\alpha_n\frac{k}{m}T_W}\right]d\phi_n$$
$$\times\exp\left[-\frac{c_n^2+\left(1-\alpha_n\right)c_n'^2}{2\frac{k}{m}T_W\alpha_n}-\frac{c_t^2-2\left(1-\alpha_t\right)\mathbf{c}_t\cdot\mathbf{c}_t'+\left(1-\alpha_t\right)^2c_t'^2}{2\frac{k}{m}T_W\alpha_t\left(2-\alpha_t\right)}\right]. \qquad (11)$$

Here, $\mathbf{c}_t$ is the two-dimensional vector of tangential velocity. For $\alpha_n = \alpha_t = 1$ the CL kernel reduces to diffusive reflection, for $\alpha_n = \alpha_t = 0$ it describes specular reflection, and for $\alpha_n = 0$, $\alpha_t = 2$ it describes back-wards reflection (fully inverted particle velocity). The original CL model cannot describe isotropic scattering, this requires modified kernels.[5] Thus, a wide array of reflection processes can be covered by the CL-type kernels.

While one normally speaks of the coefficients in the CL model as accommodation coefficients, their appearance in the exponentials gives them a more complicated meaning. Indeed, the exponentials are of the Boltzmann factor type, which often appears in the description of activated processes. There, typically one finds exponentials whose argument is the ratio between an (activation) energy and a thermal energy. In the CL model, the activation energy is the kinetic energy of the colliding particle weighted with the coefficients α_n and α_t, which is measured against the thermal energy kT_W of the wall.

Accordingly, the CL model predicts different outcome for the scattering of fast and slow particles, respectively. This stands in contrast to the Maxwell model, where the scattering probabilities are independent of impact. For many applications, the Maxwell model is used, due to its simplicity. Clearly, when activated processes at the surface become important, the Maxwell model might fail to give reliable results.

The differences between the Cercignani-Lampis model and Maxwell-type boundary conditions become particularly visible in thermal beam scattering. Experiments show that the beam is scattered into a plume-like structure around the line of specular reflection, and this behavior is indeed described by the Cercignani-Lampis model, with the plume shape depending strongly on the values of the accommodation coefficients α_n and α_t. All models of Maxwell-type, however, are unable to describe the plume, and instead describe the reflected beam as a single beam (produced by the specularly reflected particles), surrounded by an isotropic dome (produced by the scattered and thermalized particles).

The plume-like structure of the reflected beam will be particularly important when scattered particles move a large distance into the bulk gas, as would be the case in ultra-rarefied gases, that is, at large Knudsen numbers. For moderate Knudsen numbers, that is, for flows in the transition regime, the reflected particles travel only a short distance into the bulk before they interact with other gas particles. For these flows, it might be sufficient to use a simpler model that describes the average gas behavior, as expressed, e.g., by slip and jump coefficients, sufficiently well.

We note also that there are only few measurements of accommodation coefficients for typical technical applications. Indeed, typical experiments only measure temperature jump and velocity slip coefficients,[8,10] which describe macroscopically averaged results of collisions.

The Maxwell model with activation, that we shall develop in the following, allows for a simpler treatment than the CL model, in particular when one is interested in slip and jump boundary conditions for macroscopic transport equations, e.g., the regularized 13 moment equations.[3,16] As will be seen, it gives some additional flexibility for fitting to measurements of jump and slip coefficients.

V. MAXWELL MODEL WITH VELOCITY DEPENDENT ACCOMMODATION COEFFICIENTS

The reflection kernel describes the exchange of momentum and energy between a gas particle and the wall. In a diffusive reflection, the interaction is strong, and energy and momentum of the reflected particle are fully uncorrelated to the pre-collision state. In a specular reflection, the interaction is weak, and correlation is perfect, only the normal velocity changes its sign. Isotropic scattering stands between these two, the correlation is perfect for absolute velocity, but there is no correlation for direction. The coefficients Γ_0, Λ_0, Θ_0 provide a simple means to approximate the actual correlation by the superposition of simple kernels.

There are two factors that should influence the strength of correlation, surface activation, and particle energy. A strongly activated surface will influence the incoming particle, and thus weaken the correlation. It appears reasonable to consider the wall surface temperature T_W as a measure for surface activation. On the other hand, fast particles will loose only little of their momentum and energy to the wall, there will be a certain level of persistence of velocities, that is for fast particles, the correlation will be stronger. For an individual particle one will assume that the probability for diffuse reflection is a function of impact velocity and wall temperature. The question is now, how velocity dependent coefficients can be incorporated into a Maxwell-type reflection kernel, such that reciprocity and normalization remain valid.

The kernels for specular reflection and isotropic scattering contain delta functions, which makes it easy to modify them by multiplication with velocity dependent factors. Indeed, the kernels

$$\hat{\mathcal{R}}_{spec}\left(c_k' \to c_k\right) = \Gamma\left(c_t', \left|c_n'\right|\right)\delta\left(c_k' - c_k + 2n_j c_j n_k\right), \tag{12}$$

$$\hat{\mathcal{R}}_{scat}\left(c_k' \to c_k\right) = \Lambda\left(c'\right)\frac{1}{\pi}\frac{|c_n|}{c'^3}\delta\left(c' - c\right), \tag{13}$$

fulfill the reciprocity condition for any functions $\Gamma\left(c_t', \left|c_n'\right|\right)$ and $\Lambda(c')$. For isotropic surfaces, the scalar coefficients can only be formed with the velocity vector and the normal vector, hence Γ can only depend on the absolute value of the tangential velocity, $c_t = |\mathbf{c}_t|$.

The extension for diffusive reflection is less obvious. From the reciprocity requirement (5) follows that the modified kernel must be of the form

$$\hat{\mathcal{R}}_{diff}\left(c_k' \to c_k\right) = \chi_0 |c_n| f_0\left(T_W, c\right)\Theta\left(c_k\right)\Theta\left(c_k'\right), \tag{14}$$

with a constant χ_0 and a velocity dependent accommodation coefficient Θ that must obey $\Theta\left(c_k\right)\Theta\left(c_k'\right) = \Theta\left(-c_k\right)\Theta\left(-c_k'\right)$. The only vectors with which the scalar function $\Theta(c_k)$ can be formed are the velocity vector c_k and the normal vector n_k, hence the function must be of the form $\Theta(c_k) = \Theta(c_t, c_n)$ and be either even or odd in c_n (recall that c_t is the absolute value of tangential velocity).

Linear combination of these modified kernels yields the overall kernel

$$\begin{aligned}\hat{\mathcal{R}}_M\left(c_k' \to c_k\right) &= \chi_0 |c_n| f_0\left(T_W, c\right)\Theta\left(c_t, c_n\right)\Theta\left(c_t', c_n'\right)\\ &+ \Gamma\left(c_t', \left|c_n'\right|\right)\delta\left(c_k' - c_k + 2n_j c_j n_k\right) + \Lambda\left(c'\right)\frac{1}{\pi}\frac{|c_n|}{c'^3}\delta\left(c' - c\right),\end{aligned} \tag{15}$$

which must be further refined to ensure normalization. Integrating over c_k we have

$$1 = \int_{c_n>0}\hat{\mathcal{R}}_M\left(c_k' \to c_k\right)d\mathbf{c} = \Theta\left(c_t', c_n'\right)\chi_0\int_{c_n>0}|c_n| f_0\left(T_W, c\right)\Theta\left(c_t, c_n\right)d\mathbf{c} + \Gamma\left(c_t', \left|c_n'\right|\right) + \Lambda\left(c'\right). \tag{16}$$

It is convenient to set the constant χ_0 to

$$\frac{1}{\chi_0} = \int_{c_n>0}|c_n| f_0\left(T_W, c\right)\Theta\left(c_t, c_n\right)d\mathbf{c}, \tag{17}$$

which gives the simplified normalization condition

$$1 = \Theta\left(c_t', c_n'\right) + \Gamma\left(c_t', \left|c_n'\right|\right) + \Lambda\left(c'\right). \tag{18}$$

From the last equation follows that the coefficient Θ must be even in the normal velocity, that is

$$\Theta\left(c_t, c_n\right) = \Theta\left(c_t, |c_n|\right). \tag{19}$$

Hence, the general reflection kernel of Maxwell type with velocity dependent accommodation coefficients reads

$$\hat{\mathcal{R}}_M\left(c_k' \to c_k\right) = \frac{|c_n|\, f_0\left(T_W, c\right)\Theta\left(c_t, |c_n|\right)\Theta\left(c_t', \left|c_n'\right|\right)}{\int_{c_n>0}|c_n|\, f_0\left(T_W, c\right)\Theta\left(c_t, |c_n|\right)d\mathbf{c}} + \left(1-\Theta\left(c_t', \left|c_n'\right|\right)-\Lambda\left(c'\right)\right)\delta\left(c_k'-c_k+2n_jc_jn_k\right)+\Lambda\left(c'\right)\frac{1}{\pi}\frac{|c_n|}{c'^3}\delta\left(c'-c\right), \tag{20}$$

where $\Theta\left(c_t', \left|c_n'\right|\right)$ is the probability for a diffuse reflection, and $\Lambda(c')$ is the probability for isotropic scattering.

The accommodation coefficients $\Theta\left(c_t', \left|c_n'\right|\right)$ and $\Lambda(c')$ in the generalized Maxwell model (20) can be widely chosen, and thus offer some room for refined modelling. By meaning, Θ, Λ, and $\Gamma = 1 - \Theta - \Lambda$ are probabilities, and thus all three should assume values in [0, 1].

VI. ACTIVATION MODEL FOR THE ACCOMMODATION COEFFICIENT

For a first test of the model, we proceed with the following additional simplifications:

1. The probability for diffuse reflection depends only on absolute velocity, independent of how it is distributed between normal and tangential components, thus $\Theta = \Theta(c)$.
2. Particles that are not diffusively reflected are either specularly reflected or scattered. We define the coefficient γ as the portion of these particles that are specularly reflected. Then the fraction of particles that are scattered is $\Lambda = (1-\gamma)(1-\Theta)$.
3. The coefficient γ is a measure for surface roughness, and does not depend on velocity, i.e., $\gamma = const.$

The resulting reflection kernel reads

$$\tilde{\mathcal{R}}_M\left(c_k' \to c_k\right) = \frac{|c_n|\, f_0\left(T_W, c\right)\Theta\left(c\right)\Theta\left(c'\right)}{\int\limits_{c_n>0}|c_n|\, f_0\left(T_W, c\right)\Theta\left(c\right)d\mathbf{c}} + \left(1-\Theta\left(c'\right)\right)\left[\gamma\,\delta\left(c_k'-c_k+2n_jc_jn_k\right)+\left(1-\gamma\right)\frac{1}{\pi}\frac{|c_n|}{c'^3}\delta\left(c'-c\right)\right]. \tag{21}$$

Finally, we need a model for the microscopic accommodation coefficient $\Theta(c)$. When we consider the reflection of a particle at a wall as a thermally activated process, a reasonable ansatz for the accommodation coefficient is based on Boltzmann factors. With an activation energy ϵ and an impact coefficient α we write

$$\Theta\left(c, T_W\right) = \Theta_0 \exp\left(\frac{\epsilon - \alpha\frac{m}{2}c^2}{kT_W}\right) = \Theta_T\left(T_W\right)\exp\left(\frac{-\alpha c^2}{2\frac{k}{m}T_W}\right), \tag{22}$$

where $\Theta_T\left(T_W\right) = \Theta_0 \exp\left[\frac{\epsilon}{kT_W}\right]$. This microscopic accommodation coefficient describes walls where particles coming in with high velocities are more likely to be specularly reflected or scattered with unchanged energy, while warmer walls will more effectively exchange energy with the particles, and diffuse them. For positive ϵ there is an energetic bonus, which enhances the probability of diffuse reflection. The constants $\alpha \geq 0$, ϵ , $\Theta_0 \geq 0$, must be considered as fitting parameters. The probability for elastic reflection (specular or isotropic), $1 - \Theta\left(c, T_W\right)$, is of a form very similar to the condensation coefficient proposed by Tsuruta *et al.*[17,18]

VII. JUMP AND SLIP COEFFICIENTS

The above kernels can now be used as boundary condition for the Boltzmann equation, or to find slip and jump boundary conditions for hydrodynamics.[11] We shall do the latter, in a simplified form which ignores the contributions of Knudsen layers to jump and slip.[3] While this will give an error of about 10% or so on the slip and jump coefficients, it provides a simple means to see how velocity dependent accommodation makes itself visible on the macroscopic scale.

The first order Chapman-Enskog expansion yields the bulk distribution function as a deviation from the local Maxwellian[3] $f_M(\rho, T, v_k; c_k)$

$$f_{CE} = f_M \left[1 + \frac{\sigma_{ij} C_i C_j}{2p\frac{k}{m}T} + \frac{q_k C_k}{p\frac{k}{m}T} \left(\frac{C^2}{5\frac{k}{m}T} - 1 \right) \right]. \tag{23}$$

Here, $\sigma_{ij} = \int C_{\langle i} C_{j\rangle} f d\mathbf{c}$ is the viscous stress tensor, and $q_i = \frac{1}{2} \int C^2 C_i f d\mathbf{c}$ is the non-convective heat flux. The laws of Navier-Stokes and Fourier relate these to the gradients of velocity and temperature as

$$\sigma_{ij} = -2\eta \frac{\partial v_{\langle i}}{\partial x_{j\rangle}}, \quad q_i = -\kappa \frac{\partial T}{\partial x_i}, \tag{24}$$

with viscosity η and heat conductivity κ. In the above, indices in angular brackets denote the symmetric and trace-free part of a tensor.[3]

Velocity slip and temperature jump conditions are obtained from matching of tangential momentum flux and energy flux (both in normal direction) as computed from the wall distribution, f_W, Eq. (2), and the bulk distribution (23) at the wall, that is,[3]

$$\int \mathbf{c}_t c_n (f - f_W) d\mathbf{c} = 0, \quad \int \frac{c^2}{2} c_n (f - f_W) d\mathbf{c} = 0\,. \tag{25}$$

For f_W, the distribution of the incoming particles is given by (23), $f^- = f_{CE}$, and the distribution of outgoing particles is obtained from (3) with the kernel (21), (22). For evaluation, the Chapman-Enskog distribution must be written in terms of the velocity of the observer resting with the wall, $c_i = C_i + V_i$, where V_i is the flow velocity as seen from the wall. Since the wall does not accumulate gas particles, $V_k n_k = 0$, that is V_i is the slip velocity. Moreover, we introduce the temperature jump at the wall, $\Delta T = T - T_W$. In the framework of the first order Chapman-Enskog expansion, we have to consider only the first order terms in the non-equilibrium quantities V_i, ΔT, σ_{ij}, q_i. For all kernels the continuity conditions (25) yield slip and jump conditions that can be written as

$$\begin{aligned} \frac{V_t}{\sqrt{\frac{k}{m}T_W}} &= -\frac{2-\chi}{\chi}\sqrt{\frac{\pi}{2}}\frac{\sigma_{nt}}{p} - \frac{\omega}{5}\frac{q_t}{p\sqrt{\frac{k}{m}T_W}}\,, \\ \frac{\Delta T}{T} &= -\frac{2-\lambda}{2\lambda}\sqrt{\frac{\pi}{2}}\frac{q_n}{p\sqrt{\frac{k}{m}T_W}} - \frac{\zeta}{4}\frac{\sigma_{nn}}{p}\,. \end{aligned} \tag{26}$$

Here, normal and tangential tensor components are indicated with the indices n, t, respectively. The coefficients χ, ω, λ, ζ describe different physical effects: χ is the tangential momentum accommodation coefficient (TMAC) that relates slip to shear stress (or velocity gradient). The energy accommodation coefficient (EAC) λ relates the temperature jump to the heat passing through the wall (or the normal temperature gradient). The coefficient ω describes transpiration flow that is a flow induced by a heat flux tangential to the wall.[6] Finally, the coefficient ζ describes an addition to temperature jump due to viscous normal stresses. While the coefficients χ, ω, λ, can, at least in principle, be measured in steady state experiments, this is not so for ζ, since there appear to be no steady state solutions of the Navier-Stokes-Fourier equations with $\sigma_{nn} \neq 0$. Hence, for steady flow problems, the term $\frac{\zeta}{4}\frac{\sigma_{nn}}{p}$ vanishes, and ζ cannot be measured. Indeed, the coefficient ζ is often not even mentioned.[7] Only recently, Takata and co-workers extensively studied this coefficient by considering unsteady problems in simple geometries.[19–21]

While the general form (26) results from the CE distribution, the values of the coefficients χ, ω, λ, ζ depend on the reflection kernel used. With the Maxwell kernel $\mathcal{R}_M$ with constant coefficients, (9), the coefficients are

$$\chi_M = \Theta_0 + \Lambda_0, \quad \omega_M = 1, \quad \lambda_M = \Theta_0, \quad \zeta_M = 1. \tag{27}$$

The difference between TMAC and EAC arises since isotropic scattering (described by Λ_0) changes tangential momentum of the particles, but not their energy. Accordingly, the TMAC is larger than the EAC. With $\Lambda_0 = (1-\gamma)(1-\Theta_0)$ the TMAC can also be written as $\chi_M = \gamma\Theta_0 + (1-\gamma)$.

The original Maxwell kernel, which is most often used in kinetic theory, considers only specular reflection and diffuse scattering, that is $\Lambda_0 = 0$. Then, the jump and slip coefficients reduce to $\chi_M = \lambda_M = \Theta_0$ and $\omega_M = \zeta_M = 1$. In particular, EAC and TMAC agree. Adding isotropic scattering to the original Maxwell kernel thus provides a simple means to adjust TMAC and EAC independently to experimental data, as long the measured TMAC is larger than the measured EAC.

The Cercignani-Lampis kernel $\mathcal{R}_{CL}$, which has two accommodation coefficients, $\alpha_n \in (0, 1)$ and $\alpha_t \in (0, 2)$, yields, after lengthy calculation, the macroscopic coefficients

$$\begin{aligned}
\chi_{CL} &= \alpha_t \ , \\
\omega_{CL} &= 1 \ , \\
\lambda_{CL} &= \frac{\alpha_n + \alpha_t\,(2-\alpha_t)}{2 + \frac{1}{10}\,(\alpha_t\,(2-\alpha_t) - \alpha_n)} \ , \\
\zeta_{CL} &= 2\frac{2\alpha_n - \alpha_t\,(2-\alpha_t)}{\alpha_n + \alpha_t\,(2-\alpha_t)}.
\end{aligned} \tag{28}$$

Within the simple approximation used (ignorance of Knudsen layers), the Cercignani-Lampis model can be fitted to experimental data for the slip and jump coefficients χ and λ. Depending on the values of α_n and α_t, the EAC can be smaller or larger than the TMAC; it is smaller when $\alpha_n < \alpha_t^2 \frac{12-\alpha_t}{10+\alpha_t}$. The transpiration flow coefficient ω_{CL} is independent of the accommodation coefficients. This indicates that it will be difficult, if not impossible, to fit the CL model to experimental data for transpiration flow. Indeed, numerical solutions of the linearized Boltzmann equation with the CL model show that ω cannot be fitted to experimental data.[7] The coefficients χ, ω, λ are all positive, while the normal stress coefficient ζ can be positive or negative, it changes sign at $\alpha_n = \frac{\alpha_t}{2}\,(2-\alpha_t)$.

The Maxwell accommodation model (20) with the particular velocity dependent accommodation coefficient (22) has three independent parameters (Θ_T, α, γ) that can be fitted to experimental data for χ, λ, ω. The resulting slip and jump coefficients are

$$\begin{aligned}
\chi &= \frac{\Theta_T + (1+\alpha)^3\left(\frac{1}{\gamma} - 1\right)}{\frac{1}{2}\Theta_T\left(1 - \frac{1}{\sqrt{1+\alpha}}\right) + \frac{1}{\gamma}\,(1+\alpha)^3}, \\
\omega &= 1 - \frac{6\alpha\Theta_T}{\Theta_T\,(1+\alpha) + \left(\frac{1}{\gamma} - 1\right)(1+\alpha)^4}, \\
\lambda &= \frac{\Theta_T}{\frac{1}{2}\left(1 - \frac{1}{2}\frac{2-\alpha}{\sqrt{1+\alpha}}\right)\Theta_T + (1+\alpha)^4}, \\
\zeta &= 1.
\end{aligned} \tag{29}$$

The EAC is independent of the coefficient γ that describes elastic scattering. For $\alpha = 0$, the accommodation coefficient is $\Theta = \Theta_T$, and the jump and slip coefficients reduce to those of the original Maxwell model (27). For this model, TMAC χ, EAC λ, and normal stress coefficient ζ are always positive, and the TMAC is always larger than the EAC. The transpiration flow coefficient ω might become negative, when

$$\gamma > \frac{1}{1 + \Theta_T \frac{5\alpha - 1}{(1+\alpha)^4}} \ . \tag{30}$$

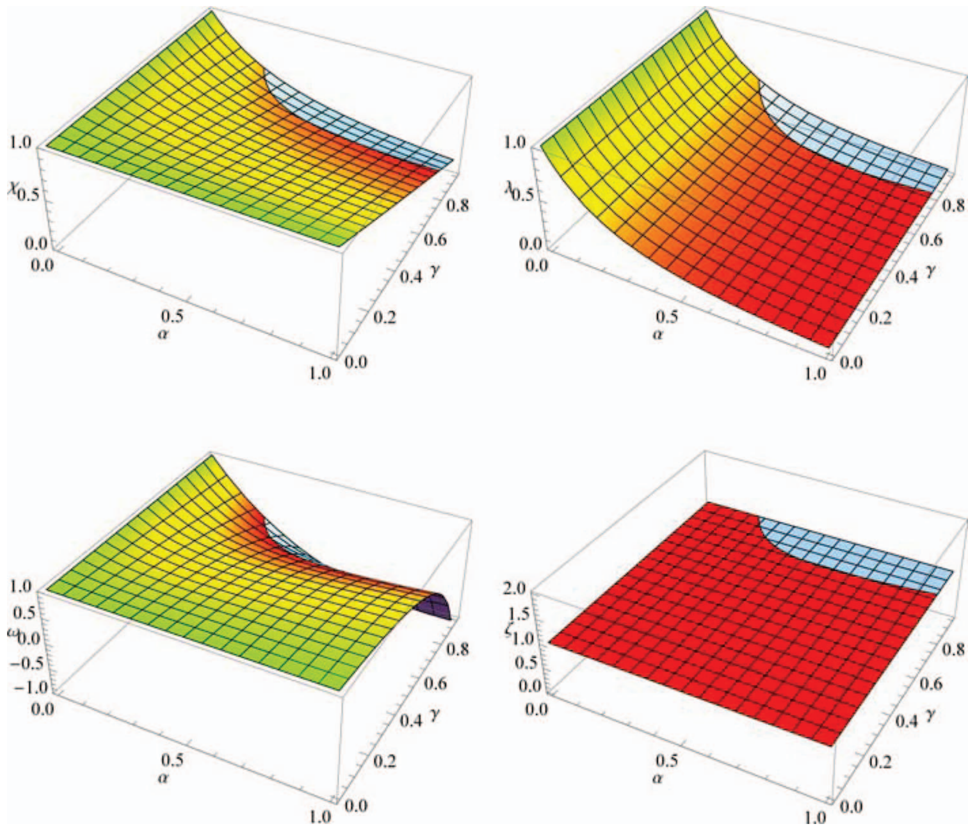

FIG. 1. Macroscopic accommodation coefficients χ, λ, ω, ζ for $\Theta_T = 1$ as function of the parameters α, γ. The region where the transpiration flow coefficient is positive is highlighted.

Transpiration flow is expected in the direction of the temperature gradient, which is the case for positive ω. Hence, one will expect values of the coefficients α and γ such that $\omega > 0$. To give an idea of the variation of the coefficients with the parameters α and γ, Fig. 1 shows, for $\Theta_T = 1$, the macroscopic coefficients χ, λ, ω, ζ as functions of $\alpha \in (0, 1)$ and $\gamma \in (0, 0.9)$. The region where $\omega > 0$ is highlighted; negative ω is only observed for larger values of γ and α, that is, for rather rough surfaces (large γ) with a relatively low percentage of diffusive reflections (large α).

Here, we shall not consider actual solutions of transport equations with slip and jump boundary conditions. Solutions of the Navier-Stokes Fourier equations with slip and jump boundary conditions can, e.g., be found in Ref. 3. A deeper test of the boundary conditions for the transition regime would be solutions for models of extended hydrodynamics, such as Grad's 13 moment equations,[14] or the regularized 13 moment equations.[3,16] While for some simple moment models the above jump and slip conditions could be used,[22] in general one will have to derive extended sets of boundary conditions from the microscopic model, e.g., following the method outlined in Ref. 16. In this context we note that larger sets of moment equations can describe explicit Knudsen layers.

VIII. TEMPERATURE DEPENDENCE

While the classical Maxwell reflection kernel has no temperature dependence, the modified kernel with velocity dependent accommodation coefficient and the Cercignani-Lampis kernel both have a dependence on the wall temperature, and on the kinetic energy of the impact. Nevertheless, the macroscopic coefficients in the jump and slip conditions (26) turn out to be independent of temperature. This can be explained by considering that in the close to equilibrium conditions of hydrodynamics, the average particle impact energy is proportional to gas temperature. Upon linearization, the temperatures T and T_W cancel out.

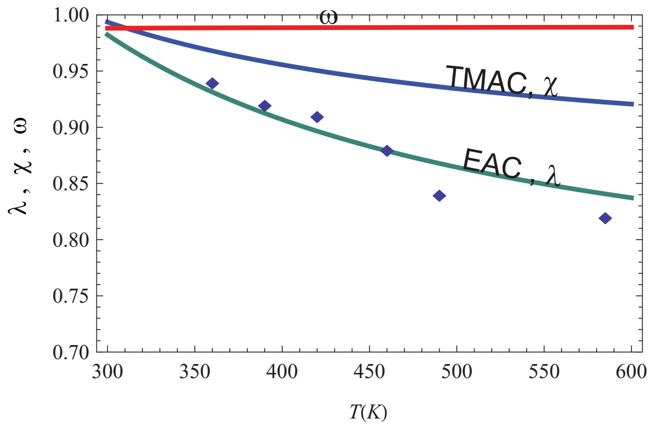

FIG. 2. TMAC, EAC, and transpiration flow coefficient ω for the modified Maxwell model with $\alpha = 0.004$, $\gamma = 0.5$, $\Theta_T = \Theta_0 \exp\left[\hat{\epsilon}\frac{T_0}{T}\right]$ with $\Theta_0 = \exp\left[-\hat{\epsilon}\right]$ and $\hat{\epsilon} = 0.32$, $T_0 = 300\ K$. Symbols indicate measurements of the EAC of argon from Ref. 8.

To allow a more detailed temperature dependence of the coefficients, we introduced in (22) the activation energy ϵ for the wall-particle interaction, which is hidden in the coefficient $\Theta_T = \Theta_0 \exp\left[\frac{\epsilon}{kT_W}\right]$. The energy ϵ provides an easy means to bring the temperature dependence into the model. Experimental data suggest that the accommodation coefficients decrease with increasing temperature,[8–10] which indicates positive ϵ. The absolute value of ϵ will depend on wall material and gas-type, and must be determined from experiments.

Figure 2 shows, as an example, the temperature dependent curves for TMAC χ, EAC λ, and transpiration flow coefficient ω. Coefficients were chosen in an attempt to fit the EAC to measurements presented in Ref. 8. Figure 9 in Ref. 8 shows data for their coefficient $\alpha_{[8]}$, which is related to our EAC by $\lambda = \frac{2\alpha_{[8]}}{1+\alpha_{[8]}}$, for temperatures between 360K and 585K. The values used for fitting are $\alpha = 0.004$, $\gamma = 0.5$, $\Theta_T = \Theta_0 \exp\left[\hat{\epsilon}\frac{T_0}{T}\right]$ with $\Theta_0 = \exp\left[-\hat{\epsilon}\right]$ and $\hat{\epsilon} = 0.32$, and $T_0 = 300\ K$. Note that the EAC is independent of the coefficient γ that only affects TMAC χ and the transpiration flow coefficient ω; the value used is arbitrary, since no corresponding values for TMAC are available. We see that TMAC and EAC decrease with temperature, while the transpiration flow coefficient is close to unity with a small increase; this behavior is similar for other values of γ, where larger values give smaller TMAC and ω.

Due to lack of experimental data that cover all three coefficients for a wider temperature range for the same gas-surface pairing, we cannot, at this time, perform a better fitting procedure to experimental data. We also remind the reader that the velocity dependent accommodation coefficient (22) is simply an example, while the generalized Maxwell reflection kernel (20) can be used with a wide variety of possible velocity dependent accommodation coefficients $\Theta(c_t, |c_n|)$ and $\Lambda(c)$.

IX. CONCLUSIONS

We have proposed an extension of Maxwell's classical boundary condition for the Boltzmann equation that incorporates a velocity dependent accommodation coefficient as well as isotropic scattering. The model was furnished with a particular accommodation coefficient that describes the gas wall interaction as thermally activated process. For evaluation we approximated macroscopic jump and slip coefficients from the first order Chapman-Enskog expansion (Knudsen layers ignored). We summarize our findings as follows:

- The classical Maxwell model has just a single accommodation coefficient, and predicts the same values for momentum (TMAC) and energy (EAC) accommodation coefficients. Thus it has a limited capability to be fitted to realistic experiments.

- The addition of isotropic scattering to the Maxwell model gives the simplest model in which TMAC and EAC can be separately fitted to experimental data.
- The Cercignani-Lampis model offers two coefficients to adjust for experimental values of TMAC and EAC, just as the Maxwell model with isotropic scattering. Both models give the same transpiration flow coefficient.
- The Maxwell model with velocity dependent accommodation coefficient provides large modelling flexibility. Its predictions depend on the particular form of the velocity dependent accommodation coefficient.
- Considering the diffuse reflection of particles as thermally activated process gives a simple model for the velocity dependent accommodation coefficient with three parameters, and thus greater flexibility for fitting.
- The activation model provides a simple means to include temperature dependence of macroscopic accommodation coefficients.
- All Maxwell models examined predict TMAC $\geq$ EAC, while the CL model allows a larger EAC as well.
- Compared to the CL model, the Maxwell models are easier to treat mathematically, which gives them some advantage for determination of boundary conditions for extended moment equations as, e.g., in Ref. 16.

We close with a call for more experimental data. We could not find any systematic measurements of TMAC, EAC, and transpiration flow coefficients for the same gas-wall pairs over a wider range of temperatures. This makes it almost impossible to fit any of the models to data. As long as no complete data sets are available, the standard Maxwell model appears to be as good for modelling of rarefied gas flows as any other model.

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