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Wall temperature jump in polyatomic gas flows

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Abstract. This article deals with the calculations of the temperature jump at the wall for gas flows in the slip regime. The analytical calculations are based on kinetic boundary conditions developed especially for polyatomic molecules. When compared to an expression previously obtained for unstructured molecules, the polyatomic molecule temperature jump reveals supplementary terms of bulk viscosity type due to the internal mode excitation. These terms may be important in high speed flows or in gas flows displaying significant relative density variation at the wall.

1. INTRODUCTION

In recent articles [1, 2] we proposed a model of scattering kernels, which are required to describe kinetic boundary conditions accompanying the Boltzmann equation, both for monatomic and polyatomic gases. The models involve various accommodation coefficients. We have also proposed, using the new monatomic scattering kernel, temperature jump and velocity slip expressions to be used as hydrodynamic boundary conditions in the gas slip flow regime [3]. These hydrodynamic boundary conditions concerned only unstructured atom-like molecules, and were based on a Chapman Enskog distribution function used to describe the incoming distribution function at the wall.

In this article, we extend the description of hydrodynamic boundary conditions to polyatomic gases. Thus, a temperature jump calculation is performed for polyatomic gas flows. Moreover, we have considered the polyatomic kinetic model developed by Morse [4] in describing the impinging molecule distribution function at the wall. Morse's kinetic model description is based on a multi-scale development which is suitable in polyatomic kinetic model constructions where various relaxation times arise [5].

2. BACKGROUND THEORY: SOME NEW KINETIC RESULTS

2.1. Summary of the new polyatomic scattering kernel description

A polyatomic scattering kernel was derived from an integral formulation devoted to the kinetic boundary conditions accompanying the kinetic equations. This scattering kernel displays various parameters related to the number of degrees of freedom involved in the description of gaseous particle reflections at the wall. These parameters have been shown, in a general case, to equal the accommodation coefficients corresponding to the three components of the momentum flux, and to the fluxes of the excited internal energies (rotational and vibrational energy) [2].

The construction of the model embodies a concept of specific accommodation for each external degree of freedom and for each internal energy mode; then an interplay exists between the various modes in the modeling of the reflection process. In doing so, the alternative diffuse or specular reflection is preserved for each momentum component and each internal mode (with which this alternative reduces to an elastic / inelastic alternative) . Notably, the description is suitable for taking into account possible anisotropic features of the solid wall. When the internal modes are disregarded,

the derived polyatomic scattering kernel reduces to a scattering kernel derived for a monatomic gas [1].

In the case of a single internal mode (rotational mode only), the polyatomic scattering kernel [2] may be written:

$$
B(\xi', E_{ir'}, g_{ir'}, \xi, E_{ir}, g_{ir}) = \left\{ (1 - \alpha_x)\delta(\xi'_x + \xi_x) + \alpha_x \frac{2\xi_x}{C_w^2} e^{-\frac{\xi_x^2}{C_w^2}} \right\} \times
$$

$$
\left\{ (1 - \alpha_y)\delta(\xi'_y - \xi_y) + \alpha_y \frac{1}{C_w\sqrt{\pi}} e^{-\frac{\xi_y^2}{C_w^2}} \right\} \times
$$

$$
\left\{ (1 - \alpha_y)\delta(\xi'_z - \xi_z) + \alpha_z \frac{1}{C_w\sqrt{\pi}} e^{-\frac{\xi_z^2}{C_w^2}} \right\} \times
$$

$$
\left\{ (1 - \alpha_r)\delta(E_{ir'} - E_{ir}) + \alpha_r \frac{g_{ir}}{Q_r(T_w)} e^{-\frac{E_{ir}}{kT_w}} \right\} , \tag{1}
$$

in which the dirac operator is denoted by δ. The velocity of the gaseous particles are denoted by $\xi = (\xi_x, \xi_y, \xi_z)$, where x, y and z are the three spatial coordinates with x along the normal axis to the surface, oriented toward the gas. The microscopic rotational internal energy is denoted by E_{ir}, and g_{ir} denotes the weight factor corresponding to the degeneracy of the quantum rotational states (in the case of spherical rigid rotator model $g_{ir} = 2ir + 1$). The quantities with superscript ($'$), refer to incident molecules while those without this superscript refer to reflected molecules. The three momentum accommodations of the momentum fluxes at the wall are α_x, α_y and α_z, while α_r corresponds to the accommodation coefficient of the rotational energy flux. We denote the surface temperature by T_w and $C_w^2 = 2kT_w/m$, where k is the Boltzmann constant and m the molecular mass. The particle peculiar velocities will be denoted V. The normalization partition function of the rotational mode, Q_r, is defined through

$$
Q_r(T_w) = \sum_{ir} g_{ir} e^{-\frac{E_{ir}}{kT_w}} . \tag{2}
$$

The reflected particle distribution function, f_i^+, is related to the incoming particle distribution function by the scattering kernel (1) through the following relation :

$$
\xi_x f_i^+ = \sum_{ir'} \int_{\Omega'} |\xi'_x| f^- B d_{\xi'} . \tag{3}
$$

2.2. A distribution function describing the incident particles

The model used here to describe the incident particle distribution function is derived from the BGKM model, which is a generalization of the well-known BGK kinetic model to polyatomic gases. This kinetic model, described in reference [4], is based on a multi-scale development which is convenient for polyatomic kinetic model constructions. However, as it is well-known in the case of monatomic gases, when starting from the basic BGK kinetic model, the description of viscosity and thermal conductivity coefficients yields an incorrect Prandtl number. This disadvantage of the BGK model can be avoided. Accordingly, we may consider an incoming distribution function given by the BGKM kinetic model [4] in which we are assuming that the viscosity and the conductivity coefficient are expressed by Chapman's description of these coefficients [6]. Thereby, the incoming distribution function reads

$$
f_i^- = F_i[1 + \varphi_t(V') - \varphi_r(E_{ir'})] , \tag{4}
$$

where $\varphi_t(V')$ and $\varphi_r(E_{ir'})$ correspond respectively to the part of the translational and the internal modes on the deviation from the Maxwell-Boltzmann distribution function, F_i, and are written,

$$
\varphi_t(V') = \frac{m}{kT_t} [\frac{\lambda_t}{nkT_t} \nabla T_t . V'(1 - \frac{2}{5C^2} V'^2) + \frac{\mu}{nkT_t} (V'_i V'_j - \frac{1}{3} V'^2 \mathbf{I}) : \frac{\partial U_i}{\partial X_j}] , \tag{5}
$$

and

$$
\varphi_r(E_{ir'}) = \frac{m\lambda_r}{nkT_t C_v^r} \frac{1}{T_t} \left(\frac{E_{ir'} - E_r(T_t)}{kT_t} \right) \nabla T_t . V' + \tag{6}
$$

$$
\frac{m\lambda_r}{nkT_t C_v} \left(\frac{mV'^2}{3kT_t} - 1 - \frac{E_{ir'} - E_r(T_t)}{C_v^r T_t} \right) \nabla . U ,
$$

in which n is the gaseous molecule number-density, μ is the viscosity coefficient, λ_t is the translational thermal conductivity, λ_r is the rotational mode thermal conductivity, C_v^r is the rotational specific heat (per molecule), C_v is the total specific heat (per molecule), **I** denotes the second order identity tensor, U is the gas macroscopic velocity, " : " denotes the double contraction of the tensorial product and, $V_i' V_j'$ and $\frac{\partial U_i}{\partial X_j}$ are the usual second order tensors. The mean rotational energy, E_r, is normally defined with the relation,

$$E_r(T_r) = \sum_{ir} \frac{g_{ir} E_{ir} e^{-\frac{E_{ir}}{kT_r}}}{Q_r(T_r)} \ . \tag{7}$$

We allow the approximation of the molecular internal structure where the molecules are considered as rigid spherical rotators and the rotational energy levels, ir, are sufficiently close to each other to be treated as a continuous variable. Thus the mean rotational energy will be given by

$$E_r(T_r) = kT_r \ . \tag{8}$$

The Maxwell-Boltzmann distribution function corresponding to only the rotational mode of excitation reads:

$$F_i(\xi, E_{ir}) = \frac{n}{(C\sqrt{\pi})^3} e^{-\frac{V^2}{C^2}} \frac{g_{ir} e^{-\frac{E_{ir}}{kT_t}}}{Q_r(T_t)} \ , \tag{9}$$

in which only one equilibrium temperature, T_t, is assumed for both the translational and rotational mode, $T_r = T_t$. This temperature represents also the gas temperature and $C^2 = 2kT_t/m$.

3. CALCULATION OF THE TEMPERATURE JUMP

3.1. Basic assumptions

The assumption used here to derive the temperature jump is that the heat flux entering the Knudsen layer is assumed equal to the heat flux in contact with the wall (i.e. at $X = 0$ in the Knudsen layer scale). This assumption is the same as the one previously used to derive a temperature jump for monatomic gases [3]; it also presumes quasi steady conditions and tangential heat flux quasi constant along the wall). Moreover, the distribution function used for the incident particles in the calculation of the heat flux in contact with the wall corresponds formally to the distribution function at the entrance of the Knudsen layer. This last assumption could be interpreted as neglecting effects from the gaseous particle collisions inside the Knudsen layer [7].

3.2. Schema of temperature jump derivation

As we consider only a rotational mode of excitation, disregarding the vibrational mode (that is convenient in gas flows at moderate temperatures), the total heat flux at the entrance to the Knudsen layer, Q_{Kn}, given by a Fourier law (as at the limit of the validity of the continuum model), is expressed

$$Q_{Kn} = \lambda_t \frac{\partial T_t}{\partial x} + \lambda_r \frac{\partial T_t}{\partial x} \ . \tag{10}$$

At the contact of the surface ($X = 0$), the translational and the rotational heat fluxes should be calculated using the following kinetic definitions

$$Q_{tra} = \sum_{ir'} \int_{\Omega'} \frac{1}{2} m |V_x'| V'^2 f_i^- d_{\xi'} - \sum_{ir} \int_{\Omega} \frac{1}{2} m |V_x| V^2 f_i^+ d_\xi \ , \tag{11}$$

$$Q_{rot} = \sum_{ir'} \int_{\Omega'} |V_x'| E_{ir'} f_i^- d_{\xi'} - \sum_{ir} \int_{\Omega} |V_x| E_{ir} f_i^+ d_\xi \ ,$$

and the total heat flux at the wall is given by,

$$Q_0 = Q_{tra} + Q_{rot} \ . \tag{12}$$

Then, according to our previous assumption (3.1), a temperature jump at the wall is derived through the following equality

$$Q_0 = Q_{Kn} \ . \tag{13}$$

Using scattering kernel (1) with relation (3), and incident distribution function (4), the calculation of the translational and rotational heat fluxes at the wall, defined by relation (11), yields :

$$
\begin{aligned}
Q_{tra} \ = \ & \frac{mnC}{4\sqrt{\pi}}\sigma_0(C^2 - C_w^2) - \frac{mnC}{4\sqrt{\pi}}(\alpha_y U_y^2 + \alpha_z U_z^2) + \\
& \frac{\sigma_1}{20}\frac{m\lambda_t}{kT_t}C^2\frac{\partial T_t}{\partial x} - \frac{\mu mC}{12kT_t\sqrt{\pi}}\left(\sigma_0 C_w^2 + \alpha_y U_y^2 + \alpha_z U_z^2\right)\left[3\frac{\partial U_x}{\partial x} - \nabla.U\right] + \\
& \frac{\mu mC^3}{4kT_t\sqrt{\pi}}\left[3\alpha_x\frac{\partial U_x}{\partial x} + \frac{\alpha_y - \alpha_z}{2}\frac{\partial U_y}{\partial y} + \frac{\alpha_z - \alpha_y}{2}\frac{\partial U_z}{\partial z}\right] - \\
& \frac{m^2\lambda_r}{2nkT_tC_v}\nabla.U \times \\
& \left[\frac{m}{3kT_t}\frac{3nC^5}{4\sqrt{\pi}}(\alpha_x + \alpha_y + \alpha_z) - \sigma_0\frac{nC^3}{2\sqrt{\pi}} - (\frac{m}{3kT_t}\frac{nC^3}{\sqrt{\pi}} - \frac{nC}{2\sqrt{\pi}})\left(\sigma_0 C_w^2 + \alpha_y U_y^2 + \alpha_z U_z^2\right)\right] \ ,
\end{aligned}
\tag{14}
$$

and

$$
\begin{aligned}
Q_{rot} \ = \ & \alpha_r\left[E_r(T_t) - E_r(T_w)\right] \times \left[\frac{nC}{2\sqrt{\pi}} + \frac{\mu C}{6kT_t\sqrt{\pi}}\left(3\frac{\partial U_x}{\partial x} - \nabla.U\right)\right] - \\
& \alpha_r\frac{m\lambda_r}{nkT_tC_v}\nabla.U\frac{nC}{6\sqrt{\pi}}\left[E_r(T_t) - E_r(T_w)\right] + \\
& \alpha_r\frac{\lambda_r}{2}\frac{\partial T_t}{\partial x} + \alpha_r\frac{m\lambda_r}{C_v}\frac{C}{2\sqrt{\pi}}\nabla.U \ .
\end{aligned}
\tag{15}
$$

The sum of both the expressions gives the total heat flux at the wall which may be written

$$
\begin{aligned}
Q_{tra} + Q_{rot} \ = \ & \frac{nk}{2}\sqrt{\frac{2kT_t}{\pi m}}(\sigma_0 + \alpha_r)(T_t - T_w) + \frac{\sigma_1}{10}\lambda_t\frac{\partial T_t}{\partial x} + \\
& \alpha_r\frac{\lambda_r}{2}\frac{\partial T_t}{\partial x} + \alpha_r\frac{m\lambda_r}{2C_v}\sqrt{\frac{2kT_t}{\pi m}}\nabla.U - \frac{\alpha_r}{6}\frac{m\lambda_r}{T_tC_v}\sqrt{\frac{2kT_t}{\pi m}}\nabla.U\ (T_t - T_w) - \\
& \frac{m\lambda_r}{C_v}\frac{(\alpha_y + \alpha_z)}{4}\sqrt{\frac{2kT_t}{\pi m}}\nabla.U\left[1 - \frac{2}{3(\alpha_y + \alpha_z)}\left(\sigma_0\frac{C_w^2}{C^2} + \alpha_y\frac{U_y^2}{C^2} + \alpha_z\frac{U_z^2}{C^2}\right)\right] + \\
& \frac{\mu C}{6T_t\sqrt{\pi}}\left(3\frac{\partial U_x}{\partial x} - \nabla.U\right)\left[\alpha_r\ (T_t - T_w) - \frac{m}{2k}\left(\sigma_0 C_w^2 + \alpha_y U_y^2 + \alpha_z U_z^2\right)\right] + \\
& \frac{\mu mC^3}{4kT_t\sqrt{\pi}}\left[3\alpha_x\frac{\partial U_x}{\partial x} + \frac{\alpha_y - \alpha_z}{2}\frac{\partial U_y}{\partial y} + \frac{\alpha_z - \alpha_y}{2}\frac{\partial U_z}{\partial z}\right] - \\
& \frac{mnC}{4\sqrt{\pi}}(\alpha_y U_y^2 + \alpha_z U_z^2) \ ,
\end{aligned}
\tag{16}
$$

where $\sigma_0 = \alpha_x + 1/2(\alpha_y + \alpha_z)$ and $\sigma_1 = 3\alpha_x + \alpha_y + \alpha_z$.

3.3. A temperature jump expression in polyatomic gases

Applying assumption (13) with the heat flux at the inlet of the Knudsen layer given by relation (10) and the heat flux at the wall given by relation (16), we obtain the temperature jump given by,

$$
\begin{aligned}
T_t - T_w \;=\; & \frac{1}{nk}\sqrt{\frac{\pi m}{2kT_t}}\left[\frac{(2-\frac{\sigma_1}{5})}{(\sigma_0+\alpha_r)}\lambda_t\frac{\partial T_t}{\partial x} + \frac{(2-\alpha_r)}{(\sigma_0+\alpha_r)}\lambda_r\frac{\partial T_t}{\partial x}\right] - \\[4pt]
& \frac{m\lambda_r}{2nkC_v}\left[\frac{2\alpha_r-(\alpha_y+\alpha_z)}{\sigma_0+\alpha_r}\right]\nabla.U - \\[4pt]
& \frac{1}{3nk(\sigma_0+\alpha_r)}\left(\frac{m\lambda_r}{C_v}+\mu\right)\left[(\alpha_r+\sigma_0)\frac{T_w}{T_t}-\alpha_r+\left(\alpha_y\frac{U_y^2}{C^2}+\alpha_z\frac{U_z^2}{C^2}\right)\right]\nabla.U + \\[4pt]
& \frac{\mu}{nk(\sigma_0+\alpha_r)}\left[(\alpha_r+\sigma_0)\frac{T_w}{T_t}-\alpha_r+\left(\alpha_y\frac{U_y^2}{C^2}+\alpha_z\frac{U_z^2}{C^2}\right)\right]\frac{\partial U_x}{\partial x} - \\[4pt]
& \frac{\mu}{nk(\sigma_0+\alpha_r)}\left[3\alpha_x\frac{\partial U_x}{\partial x}+\frac{\alpha_y-\alpha_z}{2}\frac{\partial U_y}{\partial y}+\frac{\alpha_z-\alpha_y}{2}\frac{\partial U_z}{\partial z}\right] + \\[4pt]
& \frac{m}{2k(\sigma_0+\alpha_r)}\left(\alpha_y U_y^2+\alpha_z U_z^2\right)\,.
\end{aligned}
\tag{17}
$$

Temperature jump (17) is globally structured in a way similar to an expression previously obtained for monatomic gases [3], i.e., it contains a pure contribution of conduction heat fluxes through the temperature gradients, and a contribution of viscous heating terms through the mean velocity gradients. Moreover, when the internal mode accommodation coefficient, α_r, vanishes and the rotational mode contribution to the heat flux entering the Knudsen layer is neglected, then temperature jump (17) reduces to the monatomic gas temperature jump expression.

The new contribution pointed out in expression (17) concerns the terms involving compressibility effects owing to the internal mode ($\lambda_r\nabla.U$). Some of these terms are due to the bulk viscosity appearing in kinetic description of polyatomic gases (this viscosity is represented by $m\lambda_r/C_v$ [6]) and they should be relevant in situations where relative variations of density become significant. Indeed, these new terms are related to relative variations of density by the continuity equation. Furthermore, significant relative variations precisely characterize the Knudsen layer and flows where temperature jump are required [8]. Moreover, following Welander assumption in the Knudsen layer, $1/n(\partial n/\partial X)\approx 1/T_t(\partial T_t/\partial X)$, these terms may be shown of the same order of magnitude as the first terms depending only on the temperature gradient. However, these new term contributions did not appear in previous studies where the macroscopic mass motion was neglected [9, 10]. They should be taken into account especially in high speed flows displaying high compressibility effect and in some low pressure heat conduction problem where sensitive density variations arise [11].

4. KNUDSEN LAYER CORRECTION TO EXPRESSION (17)

In the derivation of the temperature jump (17), the distribution function used to represent the incident gaseous particles in the calculation of the heat flux at the contact of the wall corresponds formally to the distribution function at the Knudsen layer inlet. In addition, among the flow macroscopic gradients, no distinction has been made between gradients at the inlet of the Knudsen layer and the gradients at the contact to the wall. This assumption is usually interpreted as neglecting effects from the gaseous particle collisions inside the Knudsen layer [7]. This effect may be taken into account, *a posteriori*, using the procedure described below.

Admitting that the Knudsen layer is a region of rapid variation of the gradients of the gas macroscopic parameters, then we may take into account these variations between the entrance to Knudsen layer and the contact with the wall through, for example, the following relation

$$
\frac{\partial T}{\partial x}\big|_0 = k_e\frac{\partial T}{\partial x}\big|_{KL}
\tag{18}
$$

where the quantity with subscript "$_{KL}$" refers to the entrance of the Knudsen layer and the quantity with subscript "$_0$", refers to the contact with the wall. The coefficient k_e in formula (18) represents the magnitude of the gradient variation through the Knudsen layer. Thus, in the expression of the temperature jump based on the use of relation (13)

the gradients appearing in the expression for the heat flux at the Knudsen layer inlet, i.e. in relation (10), should be distinguished from the macroscopic gradients appearing in the expression of the heat flux at the wall, i.e in relation (16). Accordingly, the expression of temperature jump deduced from the present approach, using the modification (18) may be written

$$T_t - T_w = \frac{1}{nk}\sqrt{\frac{\pi m}{2kT_t}}\left[\frac{(2-k_e\frac{\sigma_1}{5})}{(\sigma_0+\alpha_r)}\lambda_t + \frac{(2-k_e\alpha_r)}{(\sigma_0+\alpha_r)}\lambda_r\right]\frac{\partial T_t}{\partial x}|_{KL} + (...)\nabla.U \qquad (19)$$

In relation (19) the temperature gradient It could be noted that the modification (19) to the temperature jump, accounting for gradient variations through the Knudsen layer, is similar to reference corrections proposed notably by Welander [8, 10] using a BGK kinetic equation resolution in the Knudsen layer. The value of k_e given by Welander is 0.827.

5. CONCLUSION

A temperature jump, convenient as thermal boundary condition in polyatomic gas flows, has been analytically derived from a new scattering kernel developed especially for polyatomic gases. The calculation has been performed in the case of a single internal mode (only the rotational mode is excited). The temperature jump expression obtained shows that the internal mode excitation provides supplementary terms which could be important depending on the flow conditions. More investigation of these new term contributions to the temperature jump will be presented in further work.

The present thermal boundary condition could be extended to more complex flow configurations such as the inclusion of more excited internal modes (vibrational for example). However, in these cases, some relevant points should be considered. If the equilibrium temperatures involved by the different internal modes are the same, and equal to the equilibrium temperature of the translational mode, then the process remains the same as presented in this article; only a more complicate computation is required. On the contrary, if different equilibrium temperatures arise (different rotational or vibrational temperatures), as in a case of a strong non-equilibrium state between two different modes, then a different approach is required (for example a direct calculation of the temperature at the wall). Otherwise, one has to assume separately a conservation of each of the partial heat fluxes through the Knudsen layer (i.e., conservation of the translational heat flux and conservation of the heat flux of the considered internal mode).

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