Application of the Cercignani-Lampis Scattering Kernel to Channel Gas Flows

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Abstract. The Poiseuille flow, the thermal creep and the heat flux between two parallel plates are calculated applying the S model of the Boltzmann equation and the Cercignani-Lampis scattering kernel. The calculations have been carried out in wide ranges of the rarefaction parameter and of the accommodation coefficients of momentum and energy. Comparing the present results with experimental data the value of the accommodation coefficients can be calculated.

I INTRODUCTION

The gas - surface interaction law in general form is expressed via a scattering kernel $R(\mathbf{v}' \to \mathbf{v})$ as [1]

$$|v_n| f(\mathbf{v}) = \int_{v'_n < 0} |v'_n| R(\mathbf{v}' \to \mathbf{v}) f(\mathbf{v}') \, d\mathbf{v}', \tag{1}$$

where $f(\mathbf{v})$ is the distribution function, $\mathbf{v}'$ and $\mathbf{v}$ are molecular velocities of the incident and reflected particles, respectively, v_n is the normal component of the velocity. The scattering kernel must satisfy the normalization condition

$$\int_{v_n > 0} R(\mathbf{v}' \to \mathbf{v}) \, d\mathbf{v} = 1, \tag{2}$$

and the reciprocity relation

$$|v'_n| \exp\left(-\frac{mv'^2}{2kT_w}\right) R(\mathbf{v}' \to \mathbf{v}) = |v_n| \exp\left(-\frac{mv^2}{2kT_w}\right) R(-\mathbf{v} \to -\mathbf{v}'), \tag{3}$$

where m is the molecular mass of gaseous particle, k is the Boltzmann constant and T_w is the surface temperature.

In case of perfect accommodation the scattering kernel reads

$$R(\mathbf{v}' \to \mathbf{v}) = \frac{m^2 v_n}{2\pi (k T_w)^2} \exp\left(-\frac{m v^2}{2 k T_w}\right) \tag{4}$$

This kernel can be successfully used in many practical calculations. However, for some noble gases, e.g. helium, neon etc., experimental value of the mass flow rate through capillaries [2] are larger than those calculated applying the diffuse scattering kernel. To eliminate this discrepancy the diffuse - specular Maxwell kernel

$$R(\mathbf{v}' \to \mathbf{v}) = (1 - \alpha) \, \delta(\mathbf{v}' - \mathbf{v} + 2\mathbf{n}v_n) + \alpha \frac{m^2 v_n}{2\pi (k T_w)^2} \exp\left(-\frac{m v^2}{2 k T_w}\right). \tag{5}$$

is usually used. This model is simple for application and has the only parameter α called the accommodation coefficient, which can be calculated from experimental data on the Poiseuille flow (or some other type of the flow) as was made in the works [2,3]. It was very attractive to carry out experiments for various gases and various surfaces with the object to tabulate the accommodation coefficient α for every pair gas-surface. Then these tables could be used in engineering calculations like the tables of other properties (viscosity, thermal conductivity, etc.) are used nowadays. However, calculations of the parameter α from different experimental data, e.g. Poiseuille flow and the thermomolecular pressure difference (TPD), give quite different values. The values of α can be also different for the free-molecular and hydrodynamic regimes. For instance, in the work [2] (Table 5) the value $\alpha = 0.935$ is given for the pair helium-glass calculated on the basis of the free-molecular Poiseuille flow. In the same work [2] (Table 4) it is reported the value $\alpha = 0.895$, obtained from the data on the slip coefficient for the same pair gas-surface. In the paper [4] one finds the value $\alpha = 0.68$ calculated from the data on the TPD also for the helium gas and the glass surface.

One more contradiction is that, applying the Maxwell scattering kernel to a calculation of the TPD in the free-molecular regime one obtains the exponent $\gamma = 0.5$ for any value of the accommodation coefficient α, while the experimental data [5] show that a lower value of γ is possible.

So, the Maxwell model cannot correctly describe the gas-surface interaction. It became clear that one parameter for a scattering kernel is not enough, but it should have at least two parameters.

Almost thirty years ago Cercignani and Lampis [6] offered the following scattering kernel

$$R(\mathbf{v}' \to \mathbf{v}) = \frac{m^2 v_n}{2\pi\alpha_n\,\alpha_t(2-\alpha_t)(kT_w)^2}$$

$$\times \exp\left\{-\frac{m[v_n^2 + (1-\alpha_n)v_n'^2]}{2kT_w\alpha_n} - \frac{m[\mathbf{v}_t - (1-\alpha_t)\mathbf{v}_t']^2}{2kT_w\alpha_t(2-\alpha_t)}\right\} J_0\left(\frac{\sqrt{1-\alpha_n}\,m\,v_n\,v_n'}{\alpha_n kT_w}\right), \qquad (6)$$

$$J_0(x) = \frac{1}{2\pi}\int_0^{2\pi} \exp(x\cos\phi)\,\mathrm{d}\phi.$$

Here, $\mathbf{v}_t$ is the two-dimensional vector of the tangential velocity. This kernel contains the two parameters α_t and α_n. The first of them α_t is the accommodation coefficient of the tangential momentum and the second one α_n is the accommodation coefficient of the kinetic energy due to the normal velocity v_n. Recently, the model has been extended to polyatomic gases [7]. In the limit case $\alpha_t = 1$ and $\alpha_n = 1$ the kernel (6) coincides with the diffuse kernel (3). In the other limit case $\alpha_t = 0$ and $\alpha_n = 0$ the kernel (6) becomes the specular one. Moreover, it admits the back scattering at $\alpha_t = 2$ and $\alpha_n = 1$, i.e. after a collision we have $\mathbf{v} = -\mathbf{v}'$. Surely, the kernel (6) satisfies the normalization condition (2) and the reciprocity relation (3).

Because of the complexity the Cercignani-Lampis kernel (6) was not applied widely yet. In the papers [8,9] this model was used to calculate the Poiseuille flow and the thermal creep through a tube in the free-molecular regime. The authors of these works assumed the coefficients α_t and α_n to be close to unity. Their theoretical result based on the Cercignani-Lampis kernel gives the exponent of the TPD lower than 0.5. This fact shows the kernel (6) provides a more physical description of the non-perfect gas-surface interaction than the Maxwell boundary condition (5). To confirm this we have to apply the kernel (6) to numerical calculations of rarefied gas flows in the wide range of the Knudsen number varying the coefficients α_t and α_n in a large interval. A comparison of these results with experimental data will allow us to calculate the accommodation coefficients α_t and α_n. Indeed, to perform a rigorous verification of the applicability of the kernel (6) or any other one a set of different experiments, e.g. Poiseuille flow, Couette flow, thermal creep, transversal heat flux between two plates etc., should be carried out with the same gas and the same surface.

The aim of the present paper is to calculate the Poiseuille flow, the thermal creep and the longitudinal heat flux between two parallel plates as a function of the accommodation coefficients α_t and α_n in the wide range of the Knudsen number.

II INPUT EQUATION

Consider a monoatomic rarefied gas confined between two infinite plates fixed at $y' = \pm a/2$. There are longitudinal gradients of the pressure P and temperature T

$$v = \frac{a}{P}\frac{dP}{dx'}, \qquad \tau = \frac{a}{T}\frac{dT}{dx'}, \tag{7}$$

which cause the gas flow along the plates. We are going to calculate the mass flow rate and the heat flux through a cross section of the channel.

For further derivations it is convenient to introduce the following dimensionless quantities

$$x = \frac{x'}{a}, \qquad y = \frac{y'}{a}, \qquad \mathbf{c} = \beta \mathbf{v}, \qquad u = \beta u'_x, \qquad q = \frac{\beta}{P} q'_x, \qquad \beta = \left(\frac{m}{2kT}\right)^{1/2}, \tag{8}$$

where u'_x is the longitudinal component of the bulk velocity, q'_x is the longitudinal component of the heat flux. We assume the bulk velocity and the heat flux vector have the only component.

Since we assume the pressure and temperature gradients to be small, the distribution function $f(\mathbf{r}, \mathbf{c})$ is linearized as

$$f(\mathbf{r}, \mathbf{c}) = f^0 \left[1 + h(y, \mathbf{c}) + vx + \left(c^2 - \frac{5}{2} \right) \tau x \right], \tag{9}$$

$$f^0 = n_0 \left(\frac{m}{2\pi k T_0} \right)^{3/2} \exp \left(-\frac{mv^2}{2kT_0} \right),$$

where n_0 and T_0 are equilibrium number density and temperature, respectively.

As was shown in the review [10] the S model of the Boltzmann equation provides reliable numerical results for non-isothermal rarefied gas flows. So, in the present work the S model equations is applied, which in the linearized form reads

$$c_y \frac{\partial h}{\partial y} = \delta \left[2uc_x + \frac{4}{15} q c_x \left(c^2 - \frac{5}{2} \right) - h \right] - c_x \left[v + \tau \left(c^2 - \frac{5}{2} \right) \right], \tag{10}$$

where

$$u(y) = \frac{1}{\pi^{3/2}} \int \exp(-c^2) h(y, \mathbf{c}) \, c_x \, d\mathbf{c}, \tag{11}$$

$$q(y) = \frac{1}{\pi^{3/2}} \int \exp(-c^2) h(y, \mathbf{c}) \, c_x \left(c^2 - \frac{5}{2} \right) d\mathbf{c}. \tag{12}$$

Since Eq.(10) is linear, its solution h and the moments u and q can be decomposed into two parts as

$$h = h_P v + h_T \tau, \qquad u = u_P v + u_T \tau, \qquad q = q_P v + q_T \tau. \tag{13}$$

Then, we introduce the two mass flow rates

$$G_P = -2 \int_{-1/2}^{1/2} u_P(y) \, dy, \qquad G_T = 2 \int_{-1/2}^{1/2} u_T(y) \, dy, \tag{14}$$

and the two heat fluxes

$$Q_P = 2 \int_{-1/2}^{1/2} q_P(y) \, dy, \qquad Q_T = -2 \int_{-1/2}^{1/2} q_T(y) \, dy. \tag{15}$$

In the papers [11–13] it was proved that for any scattering kernel satisfying Eq.(3) the coefficients G_T and Q_P obey the Onsager relation

$$G_T = Q_P. \tag{16}$$

This relation can be use as an additional accuracy criterion or to reduce the computational efforts.

To eliminate the variables c_x and c_z two functions are introduced as

$$\varphi_j(y, c_y) = \frac{1}{\pi} \int \int \exp\left(-c_x^2 - c_z^2\right) h_j(y, \mathbf{c}) \, c_x \, \mathrm{d}c_x \, \mathrm{d}c_z, \qquad j = P, T \tag{17}$$

$$\psi_j(y, c_y) = \frac{1}{\pi} \int \int \exp\left(-c_x^2 - c_z^2\right) h_j(y, \mathbf{c}) \, c_x \left(c_x^2 + c_z^2 - 2\right) \mathrm{d}c_x \, \mathrm{d}c_z, \qquad j = P, T \tag{18}$$

Multiplying Eq.(10) by

$$\pi^{-1} \exp(-c_x^2 - c_z^2) c_x$$

and integrating it with respect to c_x and c_z one obtains

$$c_y \frac{\partial \varphi_j}{\partial y} = \delta\left[u_j + \frac{2}{15} q_j \left(c_y^2 - \frac{1}{2}\right) - \varphi_j\right] - S_j^\varphi, \tag{19}$$

where

$$S_P^\varphi = \frac{1}{2}, \qquad S_T^\varphi = \frac{1}{2}\left(c_y^2 - \frac{1}{2}\right).$$

Then, multiplying Eq.(10) by

$$\pi^{-1} \exp(-c_x^2 - c_z^2) c_x (c_x^2 + c_z^2 - 2)$$

the following equations for ψ_P and ψ_T are obtained

$$c_y \frac{\partial \psi_j}{\partial y} = \delta\left(\frac{4}{15} q_j - \psi_j\right) - S_j^\psi, \tag{20}$$

where

$$S_P^\psi = 0, \qquad S_T^\psi = 1.$$

The equations (19) and (20) are coupled via the moments

$$u_j(y) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} \exp(-c_y^2) \, \varphi_j(y, c_y) \, \mathrm{d}c_y, \qquad j = P, T \tag{21}$$

$$q_j(y) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} \exp(-c_y^2) \left[\varphi_j(y, c_y)\left(c_y^2 - \frac{1}{2}\right) + \psi_j(y, c_y)\right] \mathrm{d}c_y, \qquad j = P, T. \tag{22}$$

III   LINEARIZED BOUNDARY CONDITIONS

In terms of the dimensionless velocity $\mathbf{c}$ the scattering kernel $R(\mathbf{c}' \to \mathbf{c})$ can be written as

$$R(\mathbf{c}' \to \mathbf{c}) = R_n(c_n' \to c_n) \, R_x(c_x' \to c_x) \, R_z(c_z' \to c_z), \tag{23}$$

where

$$R_i = \frac{1}{[\pi \alpha_t (2 - \alpha_t)]^{1/2}} \exp\left\{-\frac{[c_i - (1 - \alpha_t)c_i']^2}{\alpha_t(2 - \alpha_t)}\right\}, \qquad i = x, z, \tag{24}$$

$$R_n(c'_n \to c_n) = \frac{2c_n}{\alpha_n} \exp\left[-\frac{c_n^2 + (1-\alpha_n)c'^2_n}{\alpha_n}\right] J_0\left(\frac{2\sqrt{1-\alpha_n}\,c_n c'_n}{\alpha_n}\right). \tag{25}$$

Here, $c_n = c_y$ at $y = -1/2$ and $c_n = -c_y$ at $y = 1/2$. Substituting (9) into (1) with the help of (2) and (3) we relate the perturbation of incident particles h^+ to the perturbation of reflected ones h^- as

$$h^+ = \hat{A}_n \hat{A}_x \hat{A}_z h^-, \tag{26}$$

where the three scattering operators have been introduced

$$\hat{A}_i\,\phi = \exp\left(c_x^2\right) \int_{-\infty}^{\infty} \exp\left(-c'^2_x\right) R_i(c'_i \to c_i)\phi(c'_i)\,\mathrm{d}c'_i, \qquad i = x, z, \tag{27}$$

$$\hat{A}_n\,\phi = \frac{1}{c_n}\exp(c_n^2) \int_{c'_n < 0} |c'_n|\exp\left(-c'^2_n\right) R_n\left(c'_n \to c_n\right)\,\phi(c'_n)\,\mathrm{d}c'_n. \tag{28}$$

Here, ϕ is an arbitrary velocity function. It can be shown that the operators $\hat{A}_x$ and $\hat{A}_z$ satisfy the relations

$$\hat{A}_x c_x = (1-\alpha_t)\,c_x, \tag{29}$$

$$\hat{A}_x c_x^2 = (1-\alpha_t)^2 c_x^2 + \frac{1}{2}\alpha_t(2-\alpha_t), \tag{30}$$

$$\hat{A}_x c_x^3 = (1-\alpha_t)^3 c_x^3 + \frac{3}{2}c_x\alpha_t(2-\alpha_t)(1-\alpha_t), \tag{31}$$

$$\hat{A}_x \hat{A}_z(c_x^2 + c_z^2 - 2) = (1-\alpha_t)^3(c_x^2 + c_z^2 - 2). \tag{32}$$

The perturbation functions h_P and h_T can be expressed via the corresponding functions $\varphi_j(c_y)$ and $\psi_j(c_y)$ as

$$h_j(\mathbf{c}) = 2\varphi_j(c_y)c_x + \psi_j(c_y)c_x(c_x^2 + c_z^2 - 2), \qquad j = P, T. \tag{33}$$

Substituting (33) into (26) and applying Eqs.(29)-(32) it is easily obtained the boundary condition for the functions $\varphi_j(c_y)$ and $\psi_j(c_y)$

$$\varphi_j^+ = (1-\alpha_t)\,\hat{A}_n\varphi_j^-, \qquad \psi_j^+ = (1-\alpha_t)^3\,\hat{A}_n\psi_j^-. \tag{34}$$

From the boundary conditions in this form we conclude that at $\alpha_t = 1$ the coefficients G_P, G_T, Q_P and Q_T do not depend on the energy accommodation coefficient α_n. The same result was obtained in the works [8,9]. Note, that it is a peculiarity of the longitudinal rarefied gas flow. If one considers a transversal heat flux between two parallel plates having different temperature one finds a dependence of the heat flux on α_n at $\alpha_t = 1$.

IV RESULTS AND DISCUSSIONS

The kinetic equations (19) and (20) with the boundary condition (34) were solved by the optimized discrete velocity method [14] with the numerical error less than 0.1%. The numerical accuracy was estimated by comparing the numerical values of the coefficients G_P, G_T, Q_P and Q_T for different grid parameters. An analysis of the numerical data showed that the Onsager relation (16) is fulfilled within the numerical accuracy. The results of the calculations are presented in Table 1.

One can see that the Poiseuille flow G_P significantly depends on the momentum accommodation coefficient α_t in the whole range of the rarefaction parameter δ considered here. It always decreases by increasing the accommodation coefficient α_t. The dependence of the Poiseuille flow G_P on the energy accommodation

TABLE 1. Coefficients G_P, G_T, Q_P and Q_T vs δ, α_t and α_n

δ	α_t	G_P $\alpha_n=0.5$	0.75	1.	$G_T = Q_P$ 0.5	0.75	1.	Q_T 0.5	0.75	1.
0.01	0.5	5.014	4.893	4.824	1.423	1.315	1.248	7.460	7.315	7.218
	0.75	3.726	3.675	3.642	1.324	1.279	1.247	6.869	6.823	6.788
	1.	3.052	3.052	3.052	1.247	1.247	1.247	6.734	6.734	6.734
0.02	0.50	4.668	4.553	4.487	1.250	1.145	1.080	6.602	6.462	6.369
	0.75	3.385	3.336	3.305	1.153	1.109	1.078	6.032	5.987	5.953
	1.00	2.714	2.714	2.714	1.078	1.078	1.078	5.900	5.900	5.900
0.1	0.5	3.952	3.865	3.812	0.8780	0.7928	0.7362	4.628	4.516	4.437
	0.75	2.693	2.655	2.630	0.7954	0.7596	0.7331	4.167	4.128	4.098
	1.0	2.039	2.039	2.039	0.7327	0.7327	0.7327	4.054	4.054	4.054
0.2	0.50	3.699	3.633	3.590	0.7306	0.6608	0.6121	3.785	3.693	3.627
	0.75	2.457	2.429	2.408	0.6604	0.6308	0.6080	3.409	3.375	3.348
	1.00	1.817	1.817	1.817	0.6075	0.6075	0.6075	3.312	3.312	3.312
1.	0.5	3.352	3.338	3.326	0.4110	0.3886	0.3698	1.934	1.897	1.866
	0.75	2.157	2.150	2.144	0.3851	0.3750	0.3660	1.797	1.782	1.767
	1.	1.554	1.554	1.554	0.3655	0.3655	0.3655	1.754	1.754	1.754
2.	0.50	3.389	3.386	3.384	0.2895	0.2828	0.2765	1.272	1.254	1.238
	0.75	2.204	2.203	2.202	0.2806	0.2774	0.2744	1.212	1.203	1.195
	1.00	1.611	1.611	1.611	0.2741	0.2741	0.2741	1.189	1.189	1.189
3.5	0.50	3.565	3.565	3.565	0.2056	0.2057	0.2058	0.8481	0.8398	0.8318
	0.75	2.383	2.383	2.383	0.2047	0.2048	0.2048	0.8224	0.8184	0.8145
	1.00	1.792	1.792	1.792	0.2047	0.2047	0.2047	0.8121	0.8121	0.8121
10.	0.5	4.564	4.557	4.551	0.09290	0.09556	0.09819	0.3458	0.3445	0.3433
	0.75	3.377	3.373	3.370	0.09554	0.09684	0.09814	0.3422	0.3416	0.3409
	1.	2.780	2.780	2.780	0.09813	0.09813	0.09813	0.3406	0.3406	0.3406
20.	0.5	6.198	6.186	6.176	0.05019	0.05200	0.05380	0.1802	0.1799	0.1796
	0.75	5.006	5.001	4.996	0.05206	0.05294	0.05383	0.1793	0.1791	0.1790
	1.	4.405	4.405	4.405	0.05383	0.05383	0.05383	0.1789	0.1789	0.1789
100.	0.5	19.49	19.47	19.46	0.01064	0.01108	0.01152	0.03721	0.03719	0.03718
	0.75	18.30	18.29	18.29	0.01110	0.01132	0.01154	0.03717	0.03716	0.03716
	1.	17.70	17.70	17.70	0.01154	0.01154	0.01154	0.03715	0.03715	0.03715

coefficient α_n is weak. It is interesting that in the interval $0.01 \le \delta \le 2.0$ this dependence decreases by increasing the rarefaction parameter and at $\delta = 3.5$ the Poiseuille flow does not depend on the energy accommodation coefficient α_n. Then, by increasing the rarefaction parameter δ this dependence appears again and begins to vanish near the hydrodynamic regime ($\delta \to \infty$).

The thermal creep G_T also depends on the momentum accommodation coefficient α_t. However, near the free molecular regime the coefficient G_T decreases, while near the hydrodynamic regime it increase, by increasing the accommodation coefficient α_t. The dependence of the thermal creep G_T on the energy accommodation coefficient α_n is similar to that on the coefficient α_t, i.e. near the free molecular regime it decreases and near the hydrodynamic regime it increases by increasing the accommodation coefficient α_n. For the rarefaction parameter $\delta = 3.5$ the thermal creep G_T is practicably constant.

Since the coefficient Q_P is equal to G_T it is not commented here.

It is rather surprising results that the heat flux Q_T weakly depends on the energy accommodation coefficient α_n. The dependence practically vanishes near the hydrodynamic regime. A significant dependence of the heat flux Q_T on the momentum accommodation coefficient α_t is observed only near free molecular regime.

V   CONCLUSIONS

So, the Poiseuille flow, thermal creep and heat flux are calculated here as function of the rarefaction parameter and of the accommodation coefficients. The calculations have been carried out on the basis of the S model kinetic equation with the Cercignani-Lampis scattering kernel. Unfortunately, because of graphic presentation of experimental data in open literature, e.g. in work [2], it is impossible to compare the present numerical

results and to calculate the accommodation coefficients. To realize this task it is necessary to perform high accuracy experiments on both isothermal and non-isothermal gas flows through a plane channel and to tabulate the experimental data.

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