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Application of the Cercignani–Lampis scattering kernel to calculations of rarefied gas flows.
II. Slip and jump coefficients

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Abstract

The Cercignani–Lampis scattering kernel of the gas–surface interaction is applied to numerical calculations of the viscous slip coefficient, the thermal slip coefficient and the temperature jump coefficient. The S model of the Boltzmann equation is numerically solved by the discrete velocity method. The calculations have been carried out in the wide ranges of the accommodation coefficients of momentum and energy. Comparing the present results with experimental data on the viscous slip coefficient the values of the accommodation coefficients are calculated for some gases and glass surface.

Keywords: Gas–surface interaction; Accommodation coefficients; Viscous slip coefficient; Thermal slip coefficient; Temperature jump coefficient

1. Introduction

To calculate a rarefied gas flow applying the Boltzmann equation a boundary condition for the distribution function $f(t,\mathbf{r}',\mathbf{v})$ on a solid surface restricting the flow must be given. Here, t is the time, $\mathbf{r}'$ is the position vector and $\mathbf{v}$ is the molecular velocity. In a general form the boundary condition reads [1]

$$|v_n| f(\mathbf{v}) = \int\limits_{v_n'<0} |v_n'| R(\mathbf{v}'\to\mathbf{v}) f(\mathbf{v}')\,\mathrm{d}\mathbf{v}', \qquad v_n \geqslant 0, \tag{1}$$

where $\mathbf{v}'$ and $\mathbf{v}$ are molecular velocities of the incident and reflected particles, respectively, v_n is the normal component of the velocity $\mathbf{v}$ directed into the gas. The scattering kernel $R(\mathbf{v}'\to\mathbf{v})$ is determined by the gas–surface interaction law.

As was shown in the previous paper [2], the widely used diffuse-specular scattering kernel proposed by Maxwell does not describe correctly the gas–surface interaction. So, another model providing a more physical description of the gas–surface interaction should be applied to calculate rarefied gas flows. Among the models proposed in the papers [3–6] the scattering kernel obtained by Cercignani and Lampis [6] was chosen to apply to some classical problems of rarefied gas dynamics. This kernel reads

$$R(\mathbf{v}'\to\mathbf{v}) = \frac{m^2 v_n}{2\pi\alpha_n\alpha_t(2-\alpha_t)(kT_w)^2}\exp\left\{-\frac{m[v_n^2+(1-\alpha_n)v_n'^2]}{2kT_w\alpha_n} - \frac{m[\mathbf{v}_t-(1-\alpha_t)\mathbf{v}_t']^2}{2kT_w\alpha_t(2-\alpha_t)}\right\} I_0\left(\frac{\sqrt{1-\alpha_n}\,m v_n v_n'}{\alpha_n' k T_w}\right), \tag{2}$$

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where

$$I_0(x) = \frac{1}{2\pi}\int_0^{2\pi} \exp(x\cos\phi)\,\mathrm{d}\phi, \tag{3}$$

$\mathbf{v}_t$ is the two-dimensional vector of the tangential velocity, m is the molecular mass of the gas, k is the Boltzmann constant, T_w is the surface temperature. This kernel contains the two parameters: the first of them α_t is the accommodation coefficient of tangential momentum and the second one α_n is the accommodation coefficient of kinetic energy due to the normal velocity v_n. The accommodation coefficient α_t varies in the range from 0 to 2. Physically this means that the Cercignani–Lampis (CL) kernel (2) admits the back reflection, which may occur on a rough surface. In the limit case when $\alpha_t = 2$ and $\alpha_n = 0$ a particle changes the sign of its own velocity after a collision with a surface and then, it goes exactly in the back direction. In the case $\alpha_t = 1$ and $\alpha_n = 1$ the kernel (2) provides the diffuse reflection (perfect accommodation), while the values $\alpha_t = 0$ and $\alpha_n = 0$ give the specular reflection. A comparison of theoretical results obtained on the basis of the kernel (2) with experimental data available in the open literature will allow us to judge if this model provides an adequate description of the gas–surface interaction.

In the previous paper [2] the CL scattering kernel (2) was applied to the rarefied gas flow between two parallel plates. In the present paper we apply this kernel to other classical problems of rarefied gas dynamics, namely, a calculation of the velocity slip and temperature jump coefficients used in the boundary conditions to the hydrodynamic equations.

Some numerical results on the slip coefficients based on the CL boundary condition are given in [7] where the analytical discrete velocity method was applied. In the present work the coefficients are obtained by the numerical discrete velocity method in a wider range of the accommodation coefficient α_t.

Usually, to solve the Navier–Stokes equation the non-slip condition for the gas velocity is assumed on a solid surface. Also, to solve the Fourier equation the temperature continuity is assumed on a gas–surface boundary. It is valid when the Knudsen number is so small, say $\mathrm{Kn} < 0.01$, that the gas rarefaction can be neglected. However, for a moderately small Knudsen number, i.e., when $0.01 < \mathrm{Kn} < 0.1$, the gas rarefaction can be taken into account via the velocity slip and temperature jump boundary conditions. Such an approach allows us to take into account a gas rarefaction and, at the same time, to avoid a numerical solving of the kinetic Boltzmann equation, which requires great computational efforts. It is very important in engineering fields such as aerothermodynamics of space vehicles (see, e.g., [8]), vacuum systems (see, e.g., [9–11]), Micro-Electro-Mechanical Systems (MEMS) (see, e.g., [12–19]), and in many other fields where the Knudsen number is not so small to neglect the gas rarefaction. So, the velocity slip and temperature jump coefficients are so important in the fluid dynamics as the transport coefficients like viscosity and thermal conductivity. As Rosner and Papadopoulos wrote [20] “their engineering importance is now such that their understanding should be part of the education of all chemical engineers”.

2. Definitions

Let us introduce the Cartesian coordinates (x', y', z') with the origin at the solid surface so as the x' axis would be normal to the surface and directed into the gas. Then, the slip boundary condition at $x' = 0$, reads

$$u'_\tau = \sigma_\mathrm{P}\frac{\mu v_m}{P}\frac{\partial u'_\tau}{\partial x'} + \sigma_\mathrm{T}\frac{\mu}{\varrho}\frac{\partial \ln T}{\partial \tau}, \qquad \tau = y', z', \tag{4}$$

where μ is the stress viscosity, P is the local pressure, T is the local temperature, $\varrho = Pm/kT$ is the density, and v_m is the most probable molecular velocity at the local temperature T given by

$$v_m = \left(\frac{2kT}{m}\right)^{1/2}. \tag{5}$$

The dimensionless quantities σ_P and σ_T are the viscous and thermal slip coefficients, respectively.

The temperature jump condition on a solid surface, i.e., at $x' = 0$, reads as

$$T = T_w + \zeta_\mathrm{T}\frac{\mu v_m}{P}\frac{\partial T}{\partial x'}, \tag{6}$$

where T is the gas temperature near the surface and ζ_T is the dimensionless temperature jump coefficient.

Sometimes, the thermal slip σ_T and temperature jump ζ_T coefficients are defined via the thermal conductivity κ of the gas, which is related to the viscosity μ via the Prandtl number as

$$\mathrm{Pr} = \frac{\mu}{\kappa}c_\mathrm{P}, \tag{7}$$

where c_{P} is the specific heat of the gas at a constant pressure. Considering that $c_{\mathrm{P}} = 5k/2m$ and $\Pr \approx 2/3$ for monatomic gases we obtain the relation between κ and μ as

$$\mu = \frac{4m}{15k}\kappa. \tag{8}$$

Both Chapman–Enskog [21] and exact [22] solutions of the Boltzmann equation confirmed this relation with the accuracy 1%. Using the experimental data on the viscosity μ and conductivity κ [23] one may verify that the relation (8) is fulfilled within 1% for the noble gases. So, assuming the precision of 1% to be enough in practical calculations we may write down the expressions (4) and (6) in term of the thermal conductivity.

Note, the definitions of the slip σ_{P}, σ_{T} and jump ζ_{T} coefficients given here do not use the quantitative concept of the mean free path ℓ. Since in practical calculations one has to relate the mean free path to some transport coefficient, i.e., viscosity or thermal conductivity, it is better to exclude ℓ just in the definition.

3. Input equation

To calculate the coefficients σ_{P}, σ_{T} and ζ_{T} we consider the Knudsen layer near the surface, which has the thickness of the order of the mean free path ℓ. In this layer the velocity profile and the temperature distribution are calculated applying the stationary Boltzmann equation [1]

$$\mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{r}'} = Q, \tag{9}$$

with the boundary condition given by Eq. (1). Here, Q is the collision integral. Moreover, we have to assume an asymptotic behavior of the distribution function far from the surface, i.e., at $x' \gg \ell$. One may think that the boundary conditions (4) and (6) posed at $x' = 0$ contradict to the fact that the Boltzmann equation (9) employed to calculate the coefficients σ_{P}, σ_{T} and ζ_{T} is solved in the semi-infinite space $x' \geqslant 0$. To avoid the confuse it should be noted that on the level of the hydrodynamic equations the Knudsen layer is considered to be infinitesimal so as the conditions (4) and (6) neglect the thickness of the Knudsen layer. On the kinetic level the same layer is assumed to be very thick. Thus, the asymptotic behavior of the velocity and temperature at the infinity, i.e., at $x' \gg \ell$, from the kinetic viewpoint corresponds to the conditions (4) and (6) at the surface, i.e., at $x' = 0$, from the hydrodynamic viewpoint.

As was shown in the review [24] the S model of the Boltzmann equation (9) proposed by Shakhov [25] provides reliable numerical results for non-isothermal rarefied gas flows with modest computational efforts. In contrast to the widely used BGK equation [26], the S model provides the correct value of the Prandtl number defined by (7). So, instead of the exact collision integral Q in the right-hand side of Eq. (9) we will use its simplified form

$$Q = \frac{P}{\mu}\left\{ f^{\mathrm{M}}\left[1 + \frac{2m}{15kPT}\mathbf{q}' \cdot \mathbf{V}\left(\frac{mV^2}{2kT} - \frac{5}{2}\right)\right] - f\right\}, \tag{10}$$

where V is the magnitude of the peculiar velocity $\mathbf{V} = \mathbf{v} - \mathbf{u}'$ and f^{M} is the local Maxwellian

$$f^{\mathrm{M}} = n(\mathbf{r}')\left[\frac{m}{2\pi kT(\mathbf{r}')}\right]^{3/2} \exp\left[-\frac{mV^2}{2kT(\mathbf{r}')}\right]. \tag{11}$$

The local values of the number density n, temperature T, bulk velocity $\mathbf{u}'$ and heat flux vector $\mathbf{q}'$ are calculated via the distribution function as

$$n(\mathbf{r}') = \int f(\mathbf{r}', \mathbf{v})\,\mathrm{d}\mathbf{v}, \tag{12}$$

$$\mathbf{u}'(\mathbf{r}') = \frac{1}{n}\int \mathbf{v} f(\mathbf{r}', \mathbf{v})\,\mathrm{d}\mathbf{v}, \tag{13}$$

$$T(\mathbf{r}') = \frac{m}{3nk}\int V^2 f(\mathbf{r}', \mathbf{v})\,\mathrm{d}\mathbf{v}, \tag{14}$$

$$\mathbf{q}'(\mathbf{r}') = \frac{m}{2}\int V^2 \mathbf{V} f(\mathbf{r}', \mathbf{v})\,\mathrm{d}\mathbf{v}. \tag{15}$$

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

$$\mathbf{c}=\frac{\mathbf{v}}{v_0},\qquad \mathbf{u}=\frac{\mathbf{u}'}{v_0},\qquad \mathbf{q}=\frac{\mathbf{q}'}{P_0\,v_0},\qquad v_0=\left(\frac{2kT_0}{m}\right)^{1/2},\tag{16}$$

$$x=\frac{x'}{\ell_0},\qquad y=\frac{y'}{\ell_0},\qquad z=\frac{z'}{\ell_0},\qquad \ell_0=\frac{\mu v_0}{P_0},\tag{17}$$

where P_0 is the equilibrium pressure, T_0 is the equilibrium temperature, v_0 is the most probable velocity at the temperature T_0, and ℓ_0 is the mean free path corresponding to the pressure P_0 and temperature T_0.

In terms of the dimensionless molecular velocity the CL kernel (2) is written as

$$R(\mathbf{c}'\to\mathbf{c})=R_x(c_x'\to c_x)R_y(c_y'\to c_y)R_z(c_z'\to c_z),\tag{18}$$

where

$$R_x(c_x'\to c_x)=\frac{2c_x}{\alpha_n}\exp\left[-\frac{c_x^2+(1-\alpha_n)c_x'^2}{\alpha_n}\right]I_0\left(\frac{2\sqrt{1-\alpha_n}\,c_xc_x'}{\alpha_n}\right),\tag{19}$$

$$R_\tau(c_\tau'\to c_\tau)=\frac{1}{[\pi\alpha_t(2-\alpha_t)]^{1/2}}\exp\left\{-\frac{[c_\tau-(1-\alpha_t)c_\tau']^2}{\alpha_t(2-\alpha_t)}\right\},\qquad \tau=y,z.\tag{20}$$

4. Viscous slip coefficient

Numerical data on the slip coefficient σ_P calculated for the diffuse scattering were reported in numerous papers. An extensive list of these papers published up to 1998 can be found in the review [24]. This list should be supplemented by the papers [27–29] published recently. All papers mentioned above reported the value

$$\sigma_\mathrm{P}=1.01619\tag{21}$$

obtained by various methods applied to the BGK model and assuming the diffuse reflection. Numerical solutions of other model equations [7,27,30–33] gave slightly different values of the slip coefficient being all of them in the range

$$0.9624\leqslant\sigma_\mathrm{P}\leqslant 1.0185.\tag{22}$$

Ohwada et al. [34] solved numerically the linearized Boltzmann equation and reported the value

$$\sigma_\mathrm{P}=\frac{1.25401}{1.270042}=0.987377\tag{23}$$

that slightly differs from that given in the review [24]. Note, to recalculate the value of σ_P given in [34] into the present notations the viscosity expression is necessary. In the review [24] an approximate expression of the viscosity μ was used, while here we use the exact expression of μ given by Pekeris and Alterman [22]. Loyalka and Hickey [35] and Siewert [29] also solved the Boltzmann equation and reported the values $\sigma_\mathrm{P}=0.9874$ and $\sigma_\mathrm{P}=0.987328$, respectively, which are very close to that given by Eq. (23).

To calculate the viscous slip coefficient σ_P we consider a monatomic rarefied gas occupying a semi-infinite space $x\geqslant 0$. The pressure P and the temperature T of the gas are assumed to be constant over the space and equal to their equilibrium values P_0 and T_0, respectively. The surface temperature T_w is equal to the equilibrium temperature T_0 too. We assume that the bulk velocity $\mathbf{u}$ has only the y component and linearly depends on the x coordinate far from the surface, i.e.,

$$u_y\to\xi_u(\sigma_\mathrm{P}+x)\quad\text{at } x\to\infty,\tag{24}$$

where ξ_u is a constant velocity gradient assumed to be small, i.e., $\xi_u\ll 1$. Such an asymptotic behavior of the bulk velocity in the Knudsen layer corresponds to the boundary condition (4) on the hydrodynamic level.

The linearization of the kinetic equation is performed representing the distribution function $f(\mathbf{r},\mathbf{c})$ as

$$f(\mathbf{r},\mathbf{c})=f_\infty^\mathrm{M}\big[1+h(x,\mathbf{c})\xi_u\big],\tag{25}$$

where f_∞^M is the local Maxwellian corresponding to the state of the gas far from the surface, i.e.,

$$f_\infty^\mathrm{M}=\frac{P_0}{kT_0}\left(\frac{m}{2\pi kT_0}\right)^{3/2}\exp\big[-c_x^2-(c_y-\xi_u x)^2-c_z^2\big].\tag{26}$$

Substituting (25) into (9) with the help of Eqs. (10)–(17) we obtain the linearized one-dimensional S model

$$c_x\frac{\partial h(x,\mathbf{c})}{\partial x}+h(x,\mathbf{c})=2\tilde{u}(x)c_y+\frac{4}{15}\tilde{q}(x)c_y\left(c^2-\frac{5}{2}\right)-2\,c_x\,c_y,\tag{27}$$

where

$$\tilde{u}(x) = \frac{u_y}{\xi_u} - x = \frac{1}{\pi^{3/2}} \int \exp(-c^2) h(x, \mathbf{c}) c_y \, \mathrm{d}\mathbf{c}, \tag{28}$$

$$\tilde{q}(x) = \frac{q_y}{\xi_u} = \frac{1}{\pi^{3/2}} \int \exp(-c^2) h(x, \mathbf{c}) c_y \left(c^2 - \frac{5}{2}\right) \mathrm{d}\mathbf{c}. \tag{29}$$

Substituting (25) into (1) with the help of Eqs. (18)–(20) we relate the perturbation function of the incident particles h^- to that of the reflected ones h^+ as

$$h^+ = \hat{A}_x \hat{A}_y \hat{A}_z h^-, \tag{30}$$

where the following scattering operators have been introduced

$$\hat{A}_x \phi = -\int_{-\infty}^{0} \frac{c'_x}{c_x} \exp\left(c_x^2 - c'^2_x\right) R_x(c'_x \to c_x) \phi(c'_x) \, \mathrm{d}c'_x, \tag{31}$$

$$\hat{A}_\tau \phi = \int_{-\infty}^{\infty} \exp\left(c_\tau^2 - c'^2_\tau\right) R_\tau(c'_\tau \to c_\tau) \phi(c'_\tau) \, \mathrm{d}c'_\tau, \quad \tau = y, z. \tag{32}$$

Here, ϕ is an arbitrary function of the molecular velocity.

The solution of Eq. (27) can be presented as

$$h(x, \mathbf{c}) = \left[2\varphi(x, c_x) + \psi(x, c_x)\left(c_y^2 + c_z^2 - 2\right)\right] c_y. \tag{33}$$

Then Eq. (27) is split on the two equations for the functions $\varphi(x, c_x)$ and $\psi(x, c_x)$

$$c_x \frac{\partial \varphi(x, c_x)}{\partial x} + \varphi(x, c_x) = \tilde{u}(x) + \frac{2}{15} \tilde{q}(x) \left(c_x^2 - \frac{1}{2}\right) - c_x, \tag{34}$$

$$c_x \frac{\partial \psi(x, c_x)}{\partial x} + \psi(x, c_x) = \frac{4}{15} \tilde{q}(x), \tag{35}$$

which are coupled via the moments

$$\tilde{u}(x) = \frac{1}{\pi^{1/2}} \int \exp\left(-c_x^2\right) \varphi(x, c_x) \, \mathrm{d}c_x, \tag{36}$$

$$\tilde{q}(x) = \frac{1}{\pi^{1/2}} \int \exp\left(-c_x^2\right) \left[\varphi(x, c_x)\left(c_x^2 - \frac{1}{2}\right) + \psi(x, c_x)\right] \mathrm{d}c_x. \tag{37}$$

Substituting (33) into Eq. (30) we obtain the boundary conditions for the functions $\varphi(x, c_x)$ and $\psi(x, c_x)$

$$\varphi^+ = (1 - \alpha_t) \hat{A}_x \varphi^-, \qquad \psi^+ = (1 - \alpha_t)^3 \hat{A}_x \psi^-. \tag{38}$$

So, if the accommodation coefficient α_t is equal to unity the solution of Eq. (27) corresponds to that for the diffuse reflection even if the other accommodation coefficient α_n differs from unity.

Eqs. (34) and (35) with the boundary conditions (38) was solved by the discrete velocity method, which was described in the papers [36] in detail. When the velocity profile $\tilde{u}$ was known the viscous slip coefficient σ_P was calculated via the velocity value far from the surface as

$$\sigma_\mathrm{P} = \lim_{x \to \infty} \tilde{u}(x). \tag{39}$$

This relation is obtained from Eqs. (24) and (28).

The numbers of points in both physical and velocity spaces were chosen to provide the numerical error less than 0.1%. The numerical calculations were carried out in the range of the coefficient α_t from 0.25 to 2 and in the whole range of the coefficient α_n, i.e., from 0 to 1. It is difficult to expect these are the real ranges of the variation of α_t and α_n, but these data allow us to evaluate the lower and upper limits of the slip coefficient σ_P.

The numerical values of the viscous slip coefficient σ_P are given in Table 1. It should be noted that at $\alpha_t = 1$ the value of σ_P is very close to that obtained from the BGK equation, see Eq. (21). A comparison of the present results with those obtained in the work [7] by another method showed that they are in agreement to each other within the accuracy of the calculations.

As was expected the viscous slip coefficient σ_P significantly depends on the accommodation coefficient of tangential momentum α_t. In the limit case $\alpha_t = 2$ and $\alpha_n = 0$ the slip coefficient σ_P is zero. Of course, such a situation is never realized

Table 1
Viscous slip coefficient σ_P vs accommodation coefficients α_t and α_n

α_t	σ_P				
	$\alpha_n = 0$	0.25	0.5	0.75	1
0.25	6.452	6.418	6.387	6.361	6.336
0.5	2.866	2.845	2.825	2.807	2.791
0.75	1.646	1.636	1.626	1.617	1.609
1	1.018	1.018	1.018	1.018	1.018
1.25	0.6286	0.6382	0.6471	0.6556	0.6638
1.5	0.3586	0.3770	0.3943	0.4111	0.4275
1.75	0.1575	0.1840	0.2094	0.2342	0.2586
2	0.0000	0.0340	0.0669	0.0995	0.1320

Table 2
Experimental values [37] of the viscous slip coefficient σ_P and the corresponding values of the accommodation coefficient α_t assuming $\alpha_n = 1$

Gas	σ_P	α_t
He	1.255 ± 0.008	0.882 ± 0.003
Ne	1.333 ± 0.010	0.849 ± 0.004
Ar	1.180 ± 0.052	0.916 ± 0.025
Kr	1.024 ± 0.040	0.997 ± 0.022
Xe	0.993 ± 0.060	1.014 ± 0.035
H_2	1.108 ± 0.026	0.952 ± 0.013
N_2	1.192 ± 0.019	0.911 ± 0.009
CO_2	1.030 ± 0.004	0.993 ± 0.002

in practice, but this result shows that for a partially back reflection the slip coefficient σ_P can be significantly smaller than its value at the diffusion reflection. So, the slip coefficient σ_P can vary in the wide range because of its strong dependence on the momentum accommodation coefficient α_t. At the same time, the dependence of σ_P on the energy accommodation coefficient α_n is very weak.

Porodnov et al. [37] reported experimental data on the slip coefficient σ_P for some gases on a glass surface. The coefficient σ_P was measured via the mass flow rate through a packet of long capillaries. The experimental values of σ_P and the measurement error are given in the second column of Table 2. Note, the values given in Table 4 of [37] were recalculated in our notation by the factor $\sqrt{\pi}/2$. These data can be used to calculate the momentum accommodation coefficient α_t. Since the dependence of the slip coefficient σ_P on the energy accommodation coefficient α_n is weak, we assume that $\alpha_n = 1$ and then the values of α_t providing the experimental data are calculated. To simplify this task the numerical data on σ_P at $\alpha_n = 1$ were interpolated by the following simple formula

$$\sigma_\mathrm{P}(\alpha_t) = \frac{1}{\alpha_t}\big[(2-\alpha_t)\sigma_\mathrm{P}(1) - 2(1-\alpha_t)\sigma_\mathrm{P}(2)\big], \tag{40}$$

which provides the value of σ_P with the accuracy of the numerical calculations.

In the third column of Table 2 the values of the accommodation coefficient α_t corresponding to the experimental values of σ_P are shown. One can see that the interaction of some gases (xenon, krypton and carbon dioxide) with the glass surface is diffuse, while for the other gases (argon, neon, helium, hydrogen, and nitrogen) the accommodation coefficient α_t slightly differs from unity. The largest deviation from unity, i.e., $\alpha_t = 0.85$, is observed for neon.

5. Thermal slip coefficient

Numerical results on the thermal slip coefficient σ_T were also reported by many authors. A critical analysis of these papers was given in the review [24]. Here, it is worth to give the results based on the linearized Boltzmann equation. Ohwada et al. [34] assuming the diffuse reflection obtained the value

$$\sigma_\mathrm{T} = \frac{3}{1.922284} \times 0.64631 = 1.0087. \tag{41}$$

Table 3
Thermal slip coefficient σ_T vs accommodation coefficients α_t and α_n

α_t	σ_T				
	$\alpha_n = 0$	0.25	0.5	0.75	1
0.25	0.8791	0.9536	1.026	1.097	1.167
0.5	0.9877	1.034	1.081	1.127	1.172
0.75	1.084	1.107	1.129	1.152	1.174
1	1.175	1.175	1.175	1.175	1.175
1.25	1.261	1.240	1.219	1.197	1.175
1.5	1.345	1.305	1.264	1.221	1.177
1.75	1.425	1.369	1.309	1.246	1.182
2	1.500	1.430	1.354	1.274	1.190

To recalculate the value given in [34] into our notations the exact expression of the heat conductivity κ given in the paper [22] was used. Loyalka [38] and Siewert [29] reported the values $\sigma_T = 3/2 \times 0.6726 = 1.0089$ and $\sigma_T = 3 \times 0.33628 = 1.00884$, respectively, which are very close to that given by Eq. (41).

To calculate the thermal slip coefficient σ_T we assume that the temperatures of the surface and of the gas have a longitudinal small gradient ξ_{Ty}. In other words, the temperature distribution of the gas occupying the semi-infinite space over the surface linearly depends on the y coordinate

$$T(y) = T_0(1 + y\,\xi_{Ty}), \quad \xi_{Ty} \ll 1. \tag{42}$$

The pressure of the gas is assumed to be constant and equal to P_0.

To linearize the kinetic equation (9) the distribution function is presented as

$$f(\mathbf{r}, \mathbf{c}) = f_\infty^{\mathrm{M}}\big[1 + h(\mathbf{r}, \mathbf{c})\xi_{Ty}\big], \tag{43}$$

where f_∞^{M} is the local Maxwellian corresponding to the gas state far from the surface

$$f^{\mathrm{M}} = \frac{P_0}{kT(y)}\left[\frac{m}{2kT(y)}\right]^{3/2} \exp\left[-\frac{c^2}{T(y)/T_0}\right]. \tag{44}$$

Substituting (43) into Eq. (9) with (10) we obtain the linearized S model

$$c_x \frac{\partial h(x, \mathbf{c})}{\partial x} + h(x, \mathbf{c}) = 2\tilde{u}(x)c_y + \left[\frac{4}{15}\tilde{q}(x) - 1\right]\left(c^2 - \frac{5}{2}\right)c_y, \tag{45}$$

where $\tilde{u}$ and $\tilde{q}$ are related to the perturbation function $h(x, \mathbf{c})$ by Eqs. (28) and (29), respectively, while the relations $\tilde{u}$ and $\tilde{q}$ to u_x and q_x are as follows

$$\tilde{u}(x) = \frac{u_x}{\xi_{Ty}}, \qquad \tilde{q}(x) = \frac{q_x}{\xi_{Ty}}. \tag{46}$$

Substituting (43) into (1) with the help of Eqs. (18)–(20) we obtain the boundary condition given by Eq. (30).

The solution of Eq. (45) can be also presented by Eq. (33) via the functions $\varphi(x, c_x)$ and $\psi(x, c_x)$ satisfying the boundary conditions (38), which mean that at $\alpha_t = 1$ the solution of Eq. (45) corresponds to that for the diffuse scattering at any value of the coefficient α_n.

Eq. (45) was solved by the discrete velocity method too. When the velocity profile was known the thermal slip coefficient σ_T was calculated via the velocity far from the surface as

$$\sigma_T = 2 \lim_{x\to\infty} \tilde{u}(x), \tag{47}$$

which follows from Eqs. (4), (16), (17) and (46).

The calculations were carried out with the numerical error less than 0.1% in the ranges $0.25 \leqslant \alpha_t \leqslant 2$ and $0 \leqslant \alpha_n \leqslant 1$. The numerical values of the coefficient σ_T are given in Table 3. A comparison of the present results with those obtained in the work [7] by another method showed that they coincide within the accuracy of the calculations. Note, the definition of σ_T in the paper [7] differs from that adopted in the present work by the factor 3.

Porodnov et al. [39] measured the thermomolecular pressure difference for a glass capillary and extracted the thermal slip coefficient σ_T from their data corresponding to the hydrodynamic regime. In Table 4 the experimental values of σ_T are given for the noble gases.

Table 4
Experimental values [39] of the thermal slip coefficient σ_T

Gas	He	Ne	Ar	Xe
σ_T	1.004 ± 0.002	0.988 ± 0.001	1.030 ± 0.003	1.116 ± 0.004

If one adopts the values of the momentum accommodation coefficient α_t given in Table 2, then one cannot find any value of the energy accommodation coefficient α_n that would provide the experimental data by Porodnov et al. [39] presented in Table 4. So, none choice of the accommodation coefficients α_t and α_n can provide the slip coefficients σ_P and σ_T that would be in agreement with the experimental data reported in [37,39].

Several reasons can be given to explain this failure in the comparison of the theory and experiment. First, the experimental data on the thermal slip coefficient [39] could have a larger experimental error than the author indicated, i.e., it is necessary to perform new experiments for the noble gases and a glass surface providing a better accuracy. Second, the model equation applied in the present work could give a significant error in the calculations of σ_T, i.e., another model equation with the correct Prandtl number or the Boltzmann equation itself should be solved with the CL boundary condition. Third, as was indicated in the works [33,40] the thermal slip coefficient σ_T is sensitive to the intermolecular interaction potential. So, this coefficient must be calculated on the basis of more realistic potential than the rigid sphere model, e.g., the Lennard–Jones potential.

The unfitness of the rigid sphere model to calculate the coefficient σ_T is confirmed by the significant discrepancy between its experimental value for the gas Xe (see Table 4) and its theoretical value given by Eq. (41) obtained from the Boltzmann equation for rigid spheres assuming the diffuse interaction. Note, according to Table 2 the interaction of the gas Xe with a glass surface is diffuse.

6. Temperature jump coefficient

The temperature jump coefficient ζ_T was calculated in many works on the bases of the BGK model, see, e.g., [38,41–43]. Since this model does not provide the relation (8) the numerical value of ζ_T based on the definition (6) differs from that based on the thermal conductivity. If we recalculate the numerical value reported in the papers [38,41–43] assuming the definition via the thermal conductivity we obtain

$$\zeta_T = 1.9541. \tag{48}$$

This value was obtained for the diffuse reflection.

Sone et al. [44] applying the linearized Boltzmann equation for the rigid sphere molecular model and assuming the diffuse reflection on the surface obtained the value

$$\zeta_T = 1.8723. \tag{49}$$

Loyalka [38] and Siewert [45] solving the Boltzmann equation by other methods obtained the value $\zeta_T = 1.8729$, which is very close to that given by Eq. (49). Comparing the values (48) and (49) one can see that the model equation provides a reasonable accuracy for the jump coefficient ζ_T.

To calculate the thermal jump coefficient we assume that the surface is staying at the equilibrium temperature, i.e., $T_w = T_0$, while the gas has a temperature gradient normal to the surface. This gradient is constant far from the surface

$$T(x) \to T_0\bigl[1 + (\zeta_T + x)\xi_{Tx}\bigr] \quad \text{at } x \to \infty, \tag{50}$$

where $\xi_{Tx} \ll 1$. Such an asymptotic behavior of the temperature in the Knudsen layer satisfies the boundary condition (6). The linearization is carried out as

$$f(\mathbf{r}, \mathbf{c}) = f_\infty^M\bigl[1 + h(x, \mathbf{c})\xi_{Tx}\bigr], \tag{51}$$

where f_∞^M is the local Maxwellian corresponding to the state at the infinity, i.e.,

$$f_\infty^M = \frac{P_0}{kT_\infty(x)}\left[\frac{m}{2\pi kT_\infty(x)}\right]^{3/2} \exp\left[-\frac{c^2}{T_\infty(x)/T_0}\right], \tag{52}$$

$$T_\infty(x) = T_0[1 + x\xi_{Tx}]. \tag{53}$$

Substituting (51) into Eq. (9) with Eq. (10) we obtain

$$c_x\frac{\partial h(x, \mathbf{c})}{\partial x} + h(x, \mathbf{c}) = \upsilon(x) + \left[\tau(x) - \frac{3}{2}c_x\right]\left(c^2 - \frac{5}{2}\right), \tag{54}$$

where

$$\upsilon(x)=\frac{P(x)-P_0}{P_0\,\xi_{\mathrm{T}x}}=\frac{1}{\pi^{3/2}}\int\exp\bigl(-c^2\bigr)h(x,\mathbf{c})\frac{2}{3}c^2\,\mathrm{d}\mathbf{c},\tag{55}$$

$$\tau(x)=\frac{T(x)-T_\infty(x)}{T_0\,\xi_{\mathrm{T}x}}=\frac{1}{\pi^{3/2}}\int\exp\bigl(-c^2\bigr)h(x,\mathbf{c})\left(\frac{2}{3}c^2-1\right)\mathrm{d}\mathbf{c}.\tag{56}$$

Here, the Fourier law

$$q_x'=-\kappa\frac{T_0\xi_{\mathrm{T}x}}{\ell_0},\tag{57}$$

which is valid far from the surface and the relation (8) have been used. Substituting (51) into (1) the boundary condition is obtained in the form (30).

The solution of Eq. (54) can be decomposed as

$$h(x,\mathbf{c})=\varphi(x,c_x)+\psi(x,c_x)\bigl(c_y^2+c_z^2-1\bigr).\tag{58}$$

Then Eq. (54) is split on the two equations for $\varphi(x,c_x)$ and $\psi(x,c_x)$

$$c_x\frac{\partial\varphi(x,c_x)}{\partial x}+\varphi(x,c_x)=\upsilon(x)+\left[\tau(x)-\frac{3}{2}c_x\right]\left(c_x^2-\frac{3}{2}\right),\tag{59}$$

$$c_x\frac{\partial\psi(x,c_x)}{\partial x}+\psi(x,c_x)=\tau(x)-\frac{3}{2}c_x,\tag{60}$$

which are coupled via the moments

$$\upsilon(x)=\frac{1}{\pi^{1/2}}\int\exp\bigl(-c_x^2\bigr)\varphi(x,c_x)\,\mathrm{d}c_x,\tag{61}$$

$$\upsilon(x)=\frac{2}{3\pi^{1/2}}\int\exp\bigl(-c_x^2\bigr)\bigl[\varphi(x,c_x)\bigl(c_x^2+1\bigr)+\psi(x,c_x)\bigr]\,\mathrm{d}c_x.\tag{62}$$

Substituting the presentation (58) into Eq. (30) the boundary conditions for $\varphi(x,c_x)$ and $\psi(x,c_x)$ are obtained as

$$\varphi^+=\hat{A}_x\varphi^-,\qquad\psi^+=(1-\alpha_t)^2\hat{A}_x\psi^-.\tag{63}$$

From these boundary conditions two conclusions can be made. First, in contrast to the slip coefficients σ_{P} and σ_{T}, the jump coefficient ζ_{T} depends on the energy accommodation α_n coefficients even at $\alpha_t=1$, because φ^+ is not zero at $\alpha_t=1$. Second, since φ^+ does not depend on α_t and ψ^+ depends on $(1-\alpha_t)^2$, then two values of the momentum accommodation coefficient, say α_t' and α_t'', satisfying the condition

$$1-\alpha_t'=-(1-\alpha_t'')\tag{64}$$

provide the same solution of the kinetic equation, i.e., the same value of the jump coefficient ζ_{T}. That is why the calculations can be carried out only in the range $0\leqslant\alpha_t\leqslant1$.

Eqs. (59) and (60) with the boundary conditions (63) were solved by the discrete velocity method. When the temperature deviation $\tau(x)$ was known the temperature jump coefficient ζ_{T} was calculated via the deviation value far from the surface as

$$\zeta_{\mathrm{T}}=\lim_{x\to\infty}\tau(x).\tag{65}$$

This expression is obtained from Eqs. (50) and (56).

The calculations were carries out with the numerical error less than 0.1%. The numerical values of the temperature jump coefficient ζ_{T} are given in Table 5. In the case of the diffuse reflection ($\alpha_t=1$ and $\alpha_n=1$) the value obtained here coincides within the numerical accuracy with that based on the BGK model and given by Eq. (48). Analyzing the numerical data on ζ_{T} for other values of α_t and α_n we can see that the temperature jump coefficient depends significantly on both accommodation coefficients α_t and α_n. The dependence of ζ_{T} on the energy accommodation coefficient α_n is physical, while its dependence on the momentum accommodation coefficient α_t is rather surprise.

Unfortunately, no reliable experimental data on the temperature jump coefficient are available in the open literature.

Table 5
Temperature jump coefficient ζ_T vs accommodation coefficients α_t and α_n

α_t	ζ_T				
	$\alpha_n = 0$	0.25	0.5	0.75	1
0.	–	24.82	11.45	6.965	4.722
0.25	15.03	8.684	5.763	4.087	3.009
0.5	8.653	5.828	4.170	3.088	2.335
0.75	6.855	4.833	3.549	2.670	2.040
1	6.404	4.567	3.376	2.551	1.954

7. Conclusions

The viscous slip coefficient, the thermal slip coefficient and the temperature jump coefficient used in the boundary conditions to the hydrodynamic equations for moderately rarefied gas were calculated on the basis of the Cercignani–Lampis boundary condition as a function of the tangential momentum and energy accommodation coefficients. An analysis of the numerical data showed: (i) The viscous slip coefficient significantly depends on the momentum accommodation coefficient and weakly depends on the energy accommodation coefficient. Comparing the present numerical results with experimental data for several gases it was shown that the momentum accommodation coefficient varies in the interval from 0.85 to 1 for a glass surface. (ii) The thermal slip coefficient depends on both momentum and energy accommodation coefficients. It is impossible to choose the accommodation coefficients so that to fit the theoretical data to experimental results. A further theoretical investigation of the thermal slip coefficient based on other intermolecular interaction law and other gas–surface interaction models is necessary. (iii) In spite of the fact that the temperature jump coefficient characterizes the heat transfer from the surface to gas its depends significantly on both tangential momentum and energy accommodation coefficients.

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References

[1] C. Cercignani, The Boltzmann Equation and its Application, Springer, New York, 1988.
[2] F. Sharipov, Application of the Cercignani–Lampis scattering kernel to calculations of rarefied gas flows. I. Plane flow between two parallel plates, Eur. J. Mech. B Fluids 21 (2002) 113–123.
[3] S. Nocilla, On the interaction between stream and body in free-molecular flow, in: L. Talbot (Ed.), Rarefied Gas Dynamics, Academic Press, New York, 1961, pp. 169–208.
[4] S. Nocilla, The surface re-emission law in free molecule flow, in: J.A. Laurmann (Ed.), Rarefied Gas Dynamics, Academic Press, New York, 1963, pp. 327–346.
[5] M. Epstein, A model of the wall boundary condition in kinetic theory, AIAA J. 5 (1967) 1797–1800.
[6] C. Cercignani, M. Lampis, Kinetic model for gas–surface interaction, Transport Theory Statist. Phys. 1 (1971) 101–114.
[7] C.E. Siewert, F. Sharipov, Model equations in rarefied gas dynamics: viscous-slip and thermal-slip coefficients, Phys. Fluids 14 (2002) 4123–4129.
[8] J. Fan, I.D. Boyd, C.P. Cai, K. Hennighausen, G.V. Candler, Computation of rarefied gas flows around a NACA 0012 airfoil, AIAA J. 39 (2001) 618–625.
[9] H.P. Cheng, R.Y. Jou, F.Z. Chen, Y.W. Chang, M. Iwane, T. Hanaoka, Three-dimensional flow analysis of spiral-grooved turbo booster pump in slip and continuum flow, J. Vac. Sci. Technol. A 18 (2000) 543–551.
[10] Y.-K. Hwang, J.-S. Heo, Three-dimensional rarefied flows in rotating helical channels, J. Vac. Sci. Technol. A 19 (2001) 662–672.
[11] J.-S. Heo, Y.-K. Hwang, Spiral channel flows in a disk-type drag pump, J. Vac. Sci. Technol. A 19 (2001) 656–661.
[12] J.C. Harley, Y. Huang, H.H. Bau, J.N. Zemel, Gas flow in micro-channels, J. Fluid Mech. 284 (1995) 257–274.
[13] A. Beskok, G.E. Karniadakis, W. Trimmer, Rarefaction and compressibility effects in gas microflows, Trans. ASME 118 (1996) 448–456.
[14] E.B. Arkilic, K.S. Breuer, M.A. Schmidt, Mass flow and tangential momentum accommodation in silicon micromachined channels, J. Fluid Mech. 437 (2001) 29–43.
[15] S. Colin, C. Aubert, R. Caen, Unsteady gaseous flows in rectangular microchannels: frequency response of one or two pneumatic lines connected in series, Eur. J. Mech. B Fluids 17 (1998) 79–104.
[16] H. Xue, Q. Fan, C. Shu, Prediction of micro-channel flows using direct simulation Monte Carlo, Probabilist. Eng. Mech. 15 (2000) 213–219.

[17] M. Vasudevaiah, K. Balamurugan, Heat transfer of rarefied gases in a corrugated microchannel, Int. J. Therm. Sci. 40 (2001) 454–468.

[18] H.Z. Zhao, The numerical solution of gaseous slip flows in microtubes, Int. Commun. Heat Mass 28 (2001) 585–594.

[19] J.J. Wleklinski, A calculation of gaseous slip velocity and microscale flow fields from a molecular-continuum matching analysis, Physica A 291 (2001) 197–210.

[20] D.E. Rosner, D.H. Papadopoulos, Jump, slip, and creep boundary conditions at nonequilibrium gas/solid interfaces, Ind. Eng. Chem. Res. 35 (1996) 3210–3222.

[21] J.H. Ferziger, H.G. Kaper, Mathematical Theory of Transport Processes in Gases, North-Holland, Amsterdam, 1972.

[22] C.L. Pekeris, Z. Alterman, Solution of the Boltzmann–Hilbert integral equation. II. The coefficients of viscosity and heat conduction, Proc. Nat. Acad. Sci. USA 43 (1957) 998–1007.

[23] J. Kestin, K. Knierim, E.A. Mason, B. Najafi, S.T. Ro, M. Waldman, Equilibrium and transport properties of the noble gases and their mixture at low densities, J. Phys. Chem. Ref. Data 13 (1984) 229–303.

[24] F. Sharipov, V. Seleznev, Data on internal rarefied gas flows, J. Phys. Chem. Ref. Data 27 (1998) 657–706.

[25] E.M. Shakhov, Generalization of the Krook kinetic equation, Fluid Dynamics 3 (1968) 95.

[26] P.L. Bhatnagar, E.P. Gross, M.A. Krook, A model for collision processes in gases, Phys. Rev. 94 (1954) 511–525.

[27] C.E. Siewert, Kramers' problem for a variable collision frequancy model, Eur. J. Appl. Math. 12 (2001) 179–191.

[28] L.B. Barichello, M. Camargo, P. Rodrigues, C.E. Siewert, Unified solution to classical flow problem based on the BGK model, Z. Angew. Math. Phys. 52 (2001) 517–534.

[29] C.E. Siewert, The linearized Boltzmann equation: concise and accurate solutions to basic flow problems, Z. Angew. Math. Phys. (2003).

[30] C. Cercignani, P. Foresti, F. Sernagiotto, Dependence of the slip coefficient on the form of the collision frequency, Nuovo Cimento B 57 (1968) 297–306.

[31] S.K. Loyalka, J.H. Ferziger, Model dependence of the slip coefficient, Phys. Fluids 10 (1967) 1833–1839.

[32] S.K. Loyalka, K.A. Hickey, Velocity slip and defect: hard sphere gas, Phys. Fluids A 1 (1989) 612–614.

[33] S.K. Loyalka, Slip and jump coefficients for rarefied gas flows: variational results for Lennard–Jones and $n(r) - 6$ potencial, Physica A 163 (1990) 813–821.

[34] T. Ohwada, Y. Sone, K. Aoki, Numerical analysis of the shear and thermal creep flows of a rarefied gas over a plane wall an the basis of the linearized Boltzmann equation for hard-sphere molecules, Phys. Fluids A 1 (1989) 1588–1599.

[35] S.K. Loyalka, K.A. Hickey, The Kramers problem – velocity slip and defect for a hard-sphere gas with arbitrary accommodation, Z. Angew. Math. Phys. 41 (1990) 245–253.

[36] F. Sharipov, E. Subbotin, On optimization of the discrete velocity method used in rarefied gas dynamics, Z. Angew. Math. Phys. 44 (1993) 572–577.

[37] B.T. Porodnov, P.E. Suetin, S.F. Borisov, V.D. Akinshin, Experimental investigation of rarefied gas flow in different channels, J. Fluid Mech. 64 (1974) 417–437.

[38] S.K. Loyalka, Temperature jump and thermal creep slip: rigid sphere gas, Phys. Fluids A 1 (1989) 403–408.

[39] B.T. Porodnov, A.N. Kulev, F.T. Tukhvetov, Thermal transpiration in a circular capillary with a small temperature difference, J. Fluid Mech. 88 (1978) 609–622.

[40] F. Sharipov, D. Kalempa, Slip coefficients for gaseous mixtures, in: E.P. Muntz, A. Ketsdever (Eds.), Rarfeid Gas Dynamics, Proc. 23rd Int. Symp., New York, 2002, in press.

[41] Y. Sone, Y. Onishi, Kinetic theory of evaporation and condensation, J. Phys. Soc. Japan 35 (1973) 1773–1776.

[42] L.B. Barichello, A.C.R. Bartz, M. Camargo, C.E. Siewert, The temperature-jump problem for a variable collision frequancy model, Phys. Fluids 14 (2002) 382–391.

[43] L.B. Barichello, C.E. Siewert, The temperature-jump problem in rarefied-gas dynamics, Eur. J. Appl. Math. 11 (2000) 353–364.

[44] Y. Sone, T. Ohwada, K. Aoki, Temperature jump and Knudsen layer in a rarefied gas over a plane wall: numerical analysis of the linearized Boltzmann equation for hard-sphere molecules, Phys. Fluids A 1 (1989) 363–370.

[45] C.E. Siewert, The linearized Boltzmann equation: a concise and accurate solution of the temperature-jump problem, J. Quant. Spec. Rad. Tran. 77 (2003) 417–432.