

ACCOMMODATION TWO-MOMENT BOUNDARY CONDITIONS IN PROBLEMS OF THERMAL AND ISOTHERMAL SLIP

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A new model of boundary conditions which generalizes the known Cercignani boundary condition is suggested. In this model, both the coefficient of accommodation of the tangential pulse of molecules and the coefficient of accommodation of the next moment of the distribution function are taken into account. The model is capable of approximating the mirror-diffuse boundary condition for the problems of slip with an accuracy of 1% and allows for the possibility of accommodation of different moments occurring differently on the surface. This possibility is absent in both the mirror-diffuse boundary condition and the Cercignani condition.

The problem of boundary conditions in interaction between gas molecules and the surface of a condensed phase has attracted the attention of researchers over a long period of time (see, e.g., [1]). However, despite considerable efforts, it still remains unresolved, especially for real surfaces. In this connection, mainly model boundary conditions are still used in calculations. The most popular is the Maxwell mirror-diffuse boundary condition. For the problems of slip of gases, all parameters of reflected molecules are determined by one quantity – the coefficient of accommodation of a tangential pulse.

By and large, the Maxwell model boundary conditions have shown good performance in solving specific problems [2]. At the same time, they possess a number of drawbacks. On the one hand, they are not entirely general, since it is obvious that one parameter is clearly insufficient for describing the process of scattering of molecules by the surface. On the other hand, they are not convenient enough for some of the approaches in the kinetic theory. This was the reason for the attempts at generalization of the Maxwell boundary conditions [3, 4]. The approach of Cercignani is most convenient for analytical methods of solution of kinetic equations. Conditions similar to Cercignani's boundary condition for problems of slip are also used in the problem of evaporation and temperature jump (with account for the coefficient of evaporation and accommodation of energy [2]). Unfortunately, Cercignani's boundary condition is not very adaptable to the process of scattering of gas molecules by the surface. For example, in this approach, the velocity of thermal slip of a gas does not depend at all on the coefficient of accommodation of the tangential pulse of gas molecules.

For linearized problems of slip, the distribution function can be sought in the form $f = f_0(1 + \varphi)$ [2, 3]. We introduce the Cartesian coordinate system with center on the boundary of a half-space, with the x axis being directed into the gas and the y axis directed along the gas flow. On the surface, the boundary condition must be imposed on the distribution function. Cercignani suggested it in the following form [4]:

$$\varphi(0, \mathbf{c}) = 2d_1 c_y, \quad c_x > 0.$$

It is an alternative to the mirror-diffuse one and allows for the possibility of partially retaining information by reflected molecules on the distribution function of incident molecules. The case $d_1 = 0$ corresponds to

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purely diffuse reflection of molecules from the wall. As follows from the results of [4], the parameter d_1 and the respective coefficient of accommodation q_1 lead to the same result as the coefficient of specular reflection in the Kramers problem.

The value of d_1 is determined from the requirement that the coefficient of accommodation of the tangential pulse of molecules be equal to q_1 ($0 < q_1 < 1$); q_1 can be found from the relation

$$1 - q_1 = - \left(\int_{c_x > 0} f c_x c_y d^3 c \right) / \left(\int_{c_x < 0} f c_x c_y d^3 c \right). \quad (1)$$

In this paper, we study the generalized boundary condition on the surface, which makes it possible to take into account not only the coefficient of accommodation of the tangential pulse of molecules but also the next moment of the distribution function. This boundary condition has the form

$$\varphi(0, \mathbf{c}) = 2d_1 c_y + 2d_2 c_y c_x, \quad c_x > 0. \quad (2)$$

Here the quantities d_1 and d_2 are determined from the requirement that the coefficient of accommodation of the tangential pulse of molecules and the next moment of the distribution function be equal to q_1 and q_2 ($0 < q_2 < 1$) respectively, where q_1 is determined from relation (1) and the following equality holds for q_2 :

$$1 - q_2 = \left(\int_{c_x > 0} f c_x^2 c_y d^3 c \right) / \left(\int_{c_x < 0} f c_x^2 c_y d^3 c \right). \quad (3)$$

It is reasonable to refer to relation (2) as the diffuse-moment boundary condition of second order. From this point of view, Cercignani's condition (1) is the diffuse-moment boundary condition of first order.

In what follows, we consider two classical problems of the kinetic theory – that of isothermal (the Kramers problem) and thermal slip. A half-space occupied by a gas is studied. Far from the wall, the gradient of mass velocity k_v , which causes isothermal slip of the gas along the plane surface, is specified. In the problem of thermal slip away from the surface, the logarithmic gradient of temperature k_T that causes thermal slip of the gas is adopted. In both problems, the velocity of slip u_0 is to be found.

Isothermal Slip. As is known [5], the function φ can be sought in the form $\varphi = c_y \psi(x, y)$ ($\mu = c_x$). Then, using the relaxation kinetic equation, we obtain that the Kramers problem boils down to finding a solution of the equation [3, 5]

$$\mu \frac{\partial}{\partial x} \psi + \psi(x, \mu) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} \exp(-\mu'^2) \psi(x, \mu') d\mu', \quad x > 0, \quad (4)$$

which satisfies conditions (1)–(3) on the wall and far from the wall goes over to the Chapman–Enskog distribution, i.e.,

$$\psi(x, \mu) = \psi_{as}(x, \mu) + o(1), \quad x \rightarrow +\infty, \quad \mu < 0, \quad (5)$$

where $\psi_{as}(x, \mu) = 2u_0 + 2k_v(x - \mu)$. From condition (2) we have

$$\psi(0, \mu) = 2d_1 + 2d_2 \mu, \quad \mu > 0, \quad (6)$$

and from relations (1) and (3) we obtain the system of moment integral equations for determining the parameters d_1 and d_2 which characterize interaction of the gas molecules with the wall:

$$(1 - q_1) \int_{-\infty}^0 \exp(-\mu^2) \mu \psi(0, \mu) d\mu = - \int_0^{\infty} \exp(-\mu^2) \mu \psi(0, \mu) d\mu, \quad (7)$$

$$(1 - q_2) \int_{-\infty}^0 \exp(-\mu^2) \mu^2 \psi(0, \mu) d\mu = \int_0^{\infty} \exp(-\mu^2) \mu^2 \psi(0, \mu) d\mu. \quad (8)$$

Using condition (3), we can transform system (7) and (8) to yield

$$(1 - q_1) \int_{-\infty}^{\infty} \exp(-\mu^2) \mu \psi(0, \mu) d\mu = -q_1 (d_1 + \sqrt{\pi} d_2/2), \quad (9)$$

$$(1 - q_2) \int_{-\infty}^{\infty} \exp(-\mu^2) \mu^2 \psi(0, \mu) d\mu = (2 - q_2) (\sqrt{\pi} d_1/2 + d_2). \quad (10)$$

We then use the laws of conservation. We obtain the following equations:

$$\int_{-\infty}^{\infty} \exp(-\mu^2) \psi(x, \mu) \mu^k d\mu = \int_{-\infty}^{\infty} \exp(-\mu^2) \psi_{as}(x, \mu) \mu^k d\mu \quad (k = 1, 2). \quad (11)$$

We note that at $k = 1$ Eq. (11) is a corollary of the law of conservation of momentum, but at $k = 2$ Eq. (11) has no obvious physical sense. Calculating the right sides of Eq. (11) and substituting them into (9) and (10), we obtain the system of equations from which we find

$$d_1 = \frac{\sqrt{\pi}}{1 - \pi/4} \left[k_v \frac{1 - q_1}{q_1} - u_0 \frac{\sqrt{\pi}}{2} \frac{1 - q_2}{2 - q_2} \right], \quad d_2 = \frac{\sqrt{\pi}}{1 - \pi/4} \left[-k_v \frac{\sqrt{\pi}}{2} \frac{1 - q_1}{q_1} + u_0 \frac{1 - q_2}{2 - q_2} \right].$$

The solution of Eq. (4) is sought in the form $\psi_{\eta}(x, \mu) = \exp(-x/\eta) f(\eta, \mu)$, where η is the spectral parameter or the separation parameter, which, generally speaking, is complex. We directly come to the characteristic equation

$$(\eta - \mu) f(\eta, \mu) = \frac{1}{\sqrt{\pi}} \eta n(\eta), \quad n(\eta) = \int_{-\infty}^{\infty} \exp(-\mu^2) f(\eta, \mu) d\mu.$$

When $\eta \in (-\infty, +\infty)$, the solution of the characteristic equation at $n(\eta) \equiv 1$ in the space of generalized functions has the form [6]

$$f(\eta, \mu) = \frac{1}{\sqrt{\pi}} \eta P \frac{1}{\eta - \mu} + \exp(\eta^2) \lambda_0(\eta) \delta(\eta - \mu),$$

where

$$\lambda_0(z) = 1 + z \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} \exp(-\tau^2) \frac{d\tau}{\tau - z}$$

is Cercignani's dispersion function [5]; the symbol Px^{-1} denotes distribution – the principal value of the integral of x^{-1} – and $\delta(x)$ is the Dirac delta-function.

The dispersion function has double zero at an infinite point. Corresponding to this point, as the double point of the line spectrum, there are two eigen (partial) solutions of initial equation (4): $\psi_+(x, \mu) = 1$ and $\psi_-(x, \mu) = x - \mu$. Out of the eigensolutions of the continuous spectrum, we take those decreasing when $x \rightarrow +\infty$, i.e., the set

$$\psi_\eta(x, \mu) = \exp(-x/\eta) \left[\frac{1}{\sqrt{\pi}} P \frac{1}{\eta - \mu} + \exp(\eta^2) \lambda_0(\eta) \delta(\eta - \mu) \right]$$

for $\eta > 0$.

We seek the solution of problem (4)–(6) in the form of eigenfunction expansion of the characteristic equation

$$\psi(x, \mu) = 2u_0 + 2k_v(x - \mu) + \int_0^{\infty} \exp(-x/\eta) f(\eta, \mu) a(\eta) d\eta$$

or

$$\psi(x, \mu) = 2u_0 + 2k_v(x - \mu) + \frac{1}{\sqrt{\pi}} \int_0^{\infty} \exp(-x/\eta) \frac{\eta a(\eta)}{\eta - \mu} d\eta + \exp(\mu^2 - x/\mu) \lambda_0(\mu) a(\mu) \theta_+(\mu), \quad (12)$$

where $\theta_+(\mu)$ is the Heaviside function.

Substituting (12) into (6), we obtain the singular integral equation with the Cauchy kernel

$$2d_1 + 2d_2 \mu = 2u_0 - 2k_v \mu + \frac{1}{\sqrt{\pi}} \int_0^{\infty} \frac{\eta a(\eta)}{\eta - \mu} d\eta + \exp(\mu^2) \lambda_0(\mu) a(\mu), \quad \mu > 0. \quad (13)$$

We introduce the auxiliary function

$$N(z) = \frac{1}{\sqrt{\pi}} \int_0^{\infty} \frac{\eta a(\eta)}{\eta - z} d\eta, \quad (14)$$

for which

$$N^+(\mu) - N^-(\mu) = 2\sqrt{\pi} i \mu a(\mu), \quad \mu > 0. \quad (15)$$

Using the boundary values $N(z)$ and $\lambda_0(z)$, we reduce Eq. (13) to the Riemann boundary-value problem [7], which consists of determining the analytical function $N(z)$ whose boundary values on the upper and lower edges of the cut $(0, +\infty)$ are connected by the boundary condition

$$\lambda_0^+(\mu) [N^+(\mu) + 2(u_0 - d_1) - 2(d_2 + k_v)\mu] =$$

$$= \lambda_0^-(\mu) [N^-(\mu) + 2(u_0 - d_1) - 2(d_2 + k_v)\mu], \quad \mu > 0. \quad (16)$$

We consider the corresponding homogeneous boundary-value problem

$$X^+(\mu)/X^-(\mu) = \lambda_0^+(\mu)/\lambda_0^-(\mu), \quad \mu > 0.$$

We can prove that the index of this problem is $\kappa = 1$. Consequently, it has the solution

$$X(z) = \frac{1}{z} \exp V(z), \quad V(z) = \frac{1}{\pi} \int_0^\infty \frac{\theta(\tau) - \pi}{\tau - z} d\tau,$$

where $\theta(\tau) = \arg \lambda_0^+(\tau)$.

Using the homogeneous problem, we reduce (16) to the problem of determining the analytical function from its zero jump on the cut:

$$\begin{aligned} X^+(\mu) [N^+(\mu) + 2(u_0 - d_1) - 2(d_2 + k_v)\mu] = \\ = X^-(\mu) [N^-(\mu) + 2(u_0 - d_1) - 2(d_2 + k_v)\mu], \quad \mu > 0. \end{aligned}$$

Allowing for the properties of the function $X(z)$, we find the general solution of this problem:

$$N(z) = -2(u_0 - d_1) + 2(d_2 + k_v)z + c/X(z), \quad (17)$$

where c is an arbitrary constant.

The function $N(z)$ determined by general solution (17) has a first-order pole at the point $z = \infty$ in contrast to the auxiliary function $N(z)$ introduced by equality (14). Eliminating this pole, we find $c = -2(d_2 + k_v)$. Now, according to (17), $N(\infty) = -2(u_0 - d_1) - cV_1$, where

$$V_k = -\frac{1}{\pi} \int_0^\infty \tau^{k-1} [\theta(\tau) - \pi] d\tau, \quad k = 1, 2, \dots, \quad V_1 = 1.0161914 \dots$$

From the condition $N(\infty) = 0$ we obtain

$$u_0 = d_1 + (d_2 + k_v) V_1. \quad (18)$$

It remains only to substitute the above-found d_1 and d_2 into formula (18); then

$$u_0 = k_v (2 - q_2) \frac{(q_1^{-1} - 1)(\sqrt{\pi} - \pi V_1/2) + (1 - \pi/4) V_1}{1 - \pi/4 + (1 - q_2)(1 + \pi/4 - \sqrt{\pi} V_1)}. \quad (19)$$

Returning to the dimensional variables, we have

$$u_0 = K_{sl} l \left(\frac{du_y}{dx} \right)_\infty,$$

where l is the mean-free path determined following Cercignani [3, 4] and K_{sl} is the coefficient of isothermal slip (see Fig. 1):

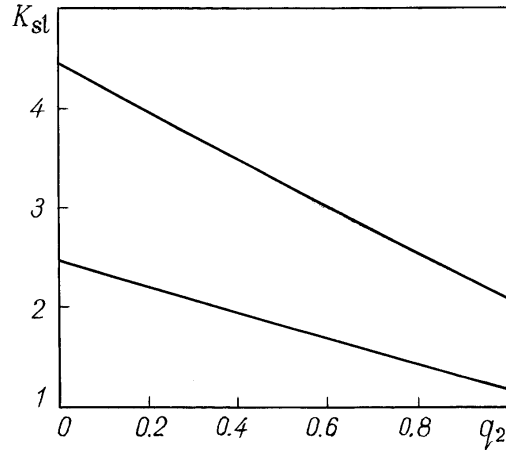


Fig. 1. Coefficient of the velocity of isothermal slip vs. q_2 at two values of q_1 : $q_1 = 0.5$ (upper curve) and $q_1 = 1$ (lower curve).

$$K_{sl} = \frac{2}{\sqrt{\pi}} (2 - q_2) \frac{(q_1^{-1} - 1) (\sqrt{\pi} - \pi V_1/2) + (1 - \pi/4) V_1}{1 - \pi/4 + (1 - q_2) (1 + \pi/4 - \sqrt{\pi} V_1)}$$

or

$$K_{sl} = (2 - q_2) \frac{0.04722 + (q_1^{-1}) \cdot 0.19885}{0.21460 - (1 - q_2) \cdot 0.01575}. \quad (20)$$

The classical Cercignani formula for the velocity of isothermal slip $u_0 = V_1 k_v$ follows from formula (19) at $q_1 = q_2 = 2$ [3, 5].

We consider the case where $q_1 \rightarrow 0$. Then, from (20) we find

$$K_{sl} = \frac{(2 - q_2) \cdot 0.19885}{0.21460 - (1 - q_2) \cdot 0.01575} q_1^{-1},$$

whence at $q_2 = 0$ we obtain the relation $K_{sl} = 2/q_1$, which coincides with the known Cercignani relation [3]. We note that with change of q_2 from 0 to 1 the coefficient of $1/q_1$ changes from 2 to 0.92661, i.e., K_{sl} decreases by 54%.

At $q_2 = 1$, it follows from formula (19) that $u_0 = k_v [0.19501 + (q_1^{-1}) \cdot 0.82118]$, and at $q_1 = 1$ we have

$$u_0 = k_v \frac{(2 - q_2) \cdot 0.21808}{0.21460 - 0.01575 (1 - q_2)}.$$

Thermal Slip. The boundary problem of thermal slip boils down to finding a solution of the inhomogeneous equation [8]

$$\mu \frac{\partial}{\partial x} \psi + \psi(x, \mu) + k_T \left(\mu^2 - \frac{1}{2} \right) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} \exp(-\mu'^2) \psi(x, \mu') d\mu', \quad (21)$$

which satisfies the boundary conditions

$$\psi(0, \mu) = 2d_1 + 2d_2\mu, \quad \mu > 0, \quad (22)$$

$$\psi(x, \mu) = 2u_0 - k_T \left(\mu^2 - \frac{1}{2} \right) + o(1), \quad x \rightarrow +\infty, \quad \mu < 0. \quad (23)$$

The parameters d_1 and d_2 are found from the system of equations (11):

$$d_1 = -\frac{\sqrt{\pi}}{2} d_2, \quad d_2 = \frac{\sqrt{\pi}}{1 - \pi/4} \frac{1 - q_2}{2 - q_2} (u_0 - k_T/2).$$

We seek the solution of problem (21)–(23) in the form

$$\psi(x, \mu) = 2u_0 - k_T \left(\mu^2 - \frac{1}{2} \right) + \frac{1}{\sqrt{\pi}} \int_0^{\infty} \exp(-x/\eta) \frac{\eta a(\eta)}{\eta - \mu} d\eta + \exp(\mu^2 - x/\mu) \lambda_0(\mu) a(\mu) \theta_+(\mu). \quad (24)$$

Using boundary condition (5), from expansion (24) we obtain the equation on the semiaxis $\mu > 0$:

$$2(u_0 - d_1) - 2d_2 \mu - k_T \left(\mu^2 - \frac{1}{2} \right) + \frac{1}{\sqrt{\pi}} \int_0^{\infty} \frac{\eta a(\eta)}{\eta - \mu} d\eta + \exp(\mu^2) \lambda_0(\mu) a(\mu) = 0. \quad (25)$$

As before, having used the auxiliary function (17), we reduce Eq. (25) to the problem of determining the analytical function from its zero jump on the cut:

$$\begin{aligned} X^+(\mu) \left[N^+(\mu) + 2(u_0 - d_1) - 2d_2 \mu - k_T \left(\mu^2 - \frac{1}{2} \right) \right] = \\ = X^-(\mu) \left[N^-(\mu) + 2(u_0 - d_1) - 2d_2 \mu - k_T \left(\mu^2 - \frac{1}{2} \right) \right], \quad \mu > 0. \end{aligned}$$

The general solution of this problem has the form

$$N(z) = -2(u_0 - d_1) + 2d_2 z + k_T \left(z^2 - \frac{1}{2} \right) + (c_0 + c_1 z)/X(z), \quad (26)$$

where c_0 and c_1 are arbitrary constants. We note that

$$\begin{aligned} X^{-1}(z) = z \exp(-V(z)) = z - V_1 + \left(\frac{1}{2} V_1^2 - V_2 \right) \frac{1}{z} + \dots, \\ (c_0 + c_1 z)/X(z) = c_1 z^2 + (c_0 - c_1 V_1) z + \left[c_1 \left(\frac{1}{2} V_1 - V_2 \right) - c_0 V_1 \right] + \dots \end{aligned}$$

Eliminating the poles of second and first orders in solution (26) and taking into account the equality $N(\infty) = 0$, we obtain $c_1 = -k_T$, $c_0 = -2d_2 - k_T V_1$,

$$u_0 = d_1 + d_2 V_1 + \frac{1}{2} \left(\frac{1}{2} V_1^2 + V_2 - \frac{1}{2} \right) k_T. \quad (27)$$

Substituting the above-found d_1 and d_2 into (27), we have

$$u_0 = \frac{(2 - q_2)(1 - \pi/4) K_{Tsl}^1 - (1 - q_2)(\sqrt{\pi} V_1/2 - \pi/4)}{1 - \pi/4 + (1 - q_2)(1 + \pi/4 - \sqrt{\pi} V_1)} k_T, \quad (28)$$

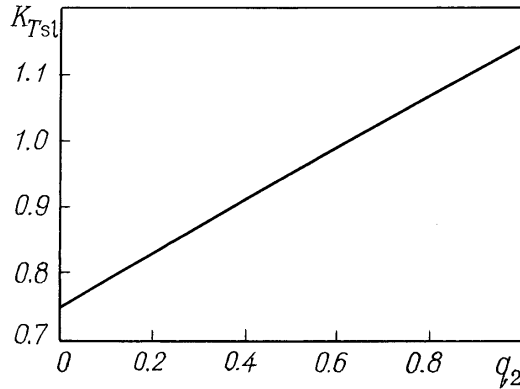


Fig. 2. Coefficient of the velocity of thermal slip K_{Tsl} vs, q_2 .

where

$$K_{Tsl}^1 = \frac{1}{2} \left(\frac{1}{2} V_1^2 + V_2 - \frac{1}{2} \right) = 0.38316 \dots \quad (29)$$

Returning to the dimensional variables, we obtain that the velocity of thermal slip of the gas is determined by the formula

$$u_0 = \nu K_{Tsl} \left(\frac{d \ln T}{dy} \right)_{\infty},$$

where ν is the kinematic viscosity and K_{Tsl} is the coefficient of the velocity of thermal slip (see Fig. 2),

$$K_{Tsl} = 3 \frac{(2 - q_2) (1 - \pi/4) K_{Tsl}^1 - (1 - q_2) (\sqrt{\pi} V_1/2 - \pi/4)}{1 - \pi/4 + (1 - q_2) (1 + \pi/4 - \sqrt{\pi} V_1)},$$

or

$$K_{Tsl} = \frac{(2 - q_2) \cdot 0.24668 - (1 - q_2) \cdot 0.34553}{0.21460 - (1 - q_2) \cdot 0.01575}.$$

From this, at $q_2 = 0$ we obtain $K_{Tsl}^0 = 0.74342$. As is seen from (28), the coefficient K_{Tsl} does not depend on the value of the coefficient of the tangential pulse of molecules q_1 . At $q_2 = 1$, the boundary conditions correspond to purely diffuse reflection of molecules from the surface, with the coefficient K_{Tsl} passing into the well-known expression (29) (see, e.g., [8, 9]).

For purely specular reflection of molecules from the surface, the coefficient of the velocity of thermal slip is $K_{Tsl}^* = 0.75$. We note that the difference between the coefficient of thermal slip $K_{Tsl}^* = 0.75$ and the coefficient K_{Tsl}^0 calculated at $q_2 = 0$ is 0.9%.

It is seen from the graphs of Figs. 1 and 2 that K_{sl} decreases monotonically with increase in q_2 , whereas K_{Tsl} increases monotonically. As the coefficient q_1 decreases, the range of K_{sl} values increases (broadens) and shifts upward.

The available analysis of the experimental data on the coefficient of accommodation of the tangential pulse q_1 [1] shows in most cases that the values of q_1 are close to unity. As a rule, they lie within the range 0.95–1.00. At the same time, direct experimental data on the coefficient of accommodation q_2 are absent. However, the value of K_{Tsl} can be evaluated from the data on the rate of thermophoresis aerosol particles. For

large spherical particles, when $\text{Kn} = l/R \ll 1$ (l is the free path and R is the particle radius), the following relation holds for the rate of thermophoresis [10]:

$$\mathbf{u}_T = -2\nu K_{Tsl} \frac{\kappa_e}{\kappa_i + 2\kappa_e} \text{grad}(\ln T)$$

It follows from the analysis of experimental data [10] that the values of the coefficient K_{Tsl} lie within the range 1.1–1.2. Hence, we can make inference that the values of q_2 are close to unity. Thus, Cercignani's kinetic model, where $q_2 = 0$, is in contradiction with the experimental data.

The foregoing analysis of the dependence of the coefficients of isothermal and thermal slip on the parameters q_1 and q_2 shows that the use of these coefficients allows one to approximate (simulate) mirror-diffuse boundary conditions with an accuracy higher than 1% for problems of gas slip. At the same time, the boundary conditions considered are more adaptable than the mirror-diffuse ones, since they make it possible to take into account different degrees of accommodation of any moment of the distribution function over the velocities of gas molecules.

The boundary conditions suggested can be used for describing other types of slip (Barnett, diffuse, etc.) of both simple gas and gas mixtures.

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NOTATION

f_0 , absolute Maxwellian; \mathbf{c} , dimensionless velocity of molecules, $\mathbf{c} = \sqrt{m/2kT}\mathbf{v}$; \mathbf{v} , dimensional velocity of molecules; k , Boltzmann constant; m , mass of a molecule; q_1 , coefficient of accommodation of the tangential pulse of molecules (first moment of the distribution function); q_2 , coefficient of accommodation of second moment of the distribution function; K_{sl} , coefficient of isothermal slip; K_{Tsl} , coefficient of thermal slip; k_v and k_T , gradients of mass velocity and temperature; l , mean free path determined according to Cercignani [3, 4]; ν , kinematic viscosity of the gas; κ_e , thermal conductivity of the gas; κ_i , thermal conductivity of the particle; Kn , Knudsen number; R , particle radius. Subscripts: as, asymptotics; sl, slip; Tsl, thermal slip; T , temperature; e, external; i, internal.

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