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ON ALLOWANCE FOR ENERGY ACCOMMODATION IN CALCULATING THE HEAT FLUX FROM A SPHERICAL PARTICLE AT ARBITRARY KNUDSEN NUMBERS

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The present paper considers the problem on the calculation of the heat flux from a uniformly heated spherical particle at arbitrary values of the Knudsen number with allowance for the energy accommodation effect. The results of numerical calculations of the BGK model of the collision integral are presented.

The investigation of the process of heat transfer in the intermediate range of values of the Knudsen number is of great theoretical and practical importance. This phenomenon is used, in particular, to determine the character of the gas–solid-surface interaction and calculate the accommodation coefficients. A fairly detailed review of publications on this question is given in [1, 2]. Their authors, however, restrict themselves to approximate methods, which do not give the real temperature distribution and gas molecular concentration. In [3–6], a direct numerical solution of the kinetic equation under the condition of complete energy accommodation is carried out. Moreover, the above method requires considerable resources of computer facilities, which limits its use in processing experimental results. In the present paper, the energy-accommodation effect is taken into account and a different method is proposed for solving the kinetic equation, which permits obtaining the desirable accuracy at a considerably smaller expenditure of computer time. The proposed method assumes apparent generalization to the case of more complex problems of physical kinetics and can find application in other fields of mathematical physics.

Consider a spherical particle of radius R uniformly heated to temperature T_{w} and situated in a gas in which the temperature T_0 is held constant at infinity.

We introduce a spherical system of coordinates with origin at the center of the particle. The state of the gas surrounding it is described by the equation [7]

$$C_r \frac{\partial \varphi}{\partial r} + \frac{C^2 - C_r^2}{r} \frac{\partial \varphi}{\partial C_r} = I\,[\varphi]\,, \tag{1}$$

where φ is the correction to the equilibrium distribution function

$$f_0 = n_0 \left(\frac{m}{2\pi k T_0}\right)^{3/2} \exp\,(-\,C^2)\,;$$

$\mathbf{C} = \mathbf{V}\,\sqrt{m/2kT_0}$, $\mathbf{V}$ is the thermal velocity of the gas molecules; $I[\varphi]$ is the integral collision operator.

As the boundary condition on the particle surface, we take the law of diffuse reflection of gas molecules from its surface with the Maxwell distribution function

$$\varphi\,\big|_{C_r>0,r=R} = \Phi_{\mathrm{r}} = \frac{\Delta n_{\mathrm{r}}}{n_0} + \left(C^2 - \frac{3}{2}\right)\frac{\Delta T_{\mathrm{r}}}{T_0}\,, \tag{2}$$

corresponding to the temperature T_{r} and molecular concentration n_{r} determined by the requirement on the absence of the mass gas flow

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$$\int C_r \varphi \exp(-C^2)\, d^3C = 0 \tag{3}$$

and the character of energy accommodation

$$\alpha_e = \frac{E_i - E_r}{E_i - E_w}, \tag{4}$$

where

$$E_i = -\pi^{-3/2} \int\limits_{C_r<0} C_r C^2 \varphi(R) \exp(-C^2)\, d^3C \tag{5}$$

is the dedimensionalized value of the energy brought by the incident molecules

$$E_r = \pi^{-3/2} \int\limits_{C_r>0} C_r C^2 \Phi_r \exp(-C^2)\, d^3C \tag{6}$$

and carried away by the molecules reflected from the particle;

$$E_w = \pi^{-3/2} \int\limits_{C_r>0} C_r C^2 \Phi_w \exp(-C^2)\, d^3C$$

corresponds to the energy which would be carried away by molecules if they were reflected with temperature T_w.

By virtue of the linearity of the problem the solution of Eq. (1) can be given in the form

$$\varphi = \frac{\Delta T_r}{T_0} \varphi^* .$$

Here and hereafter we agree to mark with an asterisk the quantities assigned to $\Delta T_r/T_0$ or, which is equivalent, those calculated at $\Delta T_r = T_0$.

As a result, from (3), (5), and (6) we obtain

$$\frac{\Delta n_r}{n_0} = -\frac{1}{2} \frac{\Delta T_r}{T_0} (1 + 4I_0), \quad E_i = -\frac{I_1}{\sqrt{\pi}} \frac{\Delta T_r}{T_0}, \quad E_r = \frac{1 - 2I_0}{\sqrt{\pi}} \frac{\Delta T_r}{T_0},$$

$$I_i = \frac{1}{\pi} \int\limits_{C_r<0} C_r C^{2i} \varphi^*(R) \exp(-C^2)\, d^3C . \tag{7}$$

Analogously,

$$\frac{\Delta n_w}{n_0} = -\frac{1}{2} \frac{\Delta T_w}{T_0} - 2I_0 \frac{\Delta T_r}{T_0}, \quad E_w = \frac{1}{\sqrt{\pi}} \left(\frac{\Delta T_r}{T_0} - 2I_0 \frac{\Delta T_w}{T_0} \right).$$

Substituting the expressions obtained into condition (4), we find

$$\frac{\Delta T_r}{T_0} = \frac{\alpha_e}{1 + (1 - \alpha_e)(I_1 - 2I_0)} \frac{\Delta T_w}{T_0} . \tag{8}$$

The sought heat flux is determined by the relation

$$q = n_0 \sqrt{\frac{2k^3T_0^3}{\pi^3 m}} \int C_r C^2 \varphi \exp(-C^2)\, d^3C$$

and, by virtue of the energy conservation law, it can be given in the form

$$q = n_0 \sqrt{\frac{2k^3T_0^3}{m}} \frac{R^2}{r^2} Q .$$

The dimensionless quantity Q can be calculated at any point, in particular, on the particle surface, which yields

$$Q = E_{\mathrm{r}} - E_{\mathrm{i}} = \frac{1 - 2I_0 + I_1}{\sqrt{\pi}} \frac{\Delta T_{\mathrm{r}}}{T_0} . \tag{9}$$

The quantity

$$Q^* = \frac{1 - 2I_0 + I_1}{\sqrt{\pi}} \tag{10}$$

can be considered as the dedimensionalized value of the heat flux calculated in the case of complete accommodation of energy at $\Delta T_{\mathrm{w}} = T_0$.

Taking into account (10), relations (8) and (9) can be given in the form

$$\frac{\Delta T_{\mathrm{r}}}{T_0} = \frac{\alpha_{\mathrm{e}}}{\sqrt{\pi}\,(1 - \alpha_{\mathrm{e}})\, Q^* + \alpha_{\mathrm{e}}} \frac{\Delta T_{\mathrm{w}}}{T_0}, \quad Q = Q^* \frac{\alpha_{\mathrm{e}}}{\sqrt{\pi}\,(1 - \alpha_{\mathrm{e}})\, Q^* + \alpha_{\mathrm{e}}} \frac{\Delta T_{\mathrm{w}}}{T_0} .$$

It should be noted that this result depends neither on the form of the collision integral nor on the method of solving the problem under consideration.

It is also obvious that in the free-molecular regime the influence of the particle on the molecule distribution function in the gas volume can be neglected, and the function φ^* in the integration domain (7) and the integrals themselves can be assumed to be equal to zero. Thus, within the limit of $R \to 0$,

$$Q^* = \frac{1}{\sqrt{\pi}} .$$

In the case of a large particle, the distribution function of molecules incident on the particle is described by the Chapman–Enskog distribution, which yields

$$Q^* = \frac{\kappa}{R n_0} \sqrt{\frac{m}{2k^3 T_0}}$$

and leads to the known gas-dynamic solution

$$q = \kappa \frac{R}{r^2} \Delta T_{\mathrm{w}} .$$

To calculate Q^* in the intermediate range of values of the Knudsen number, it is necessary to solve Eq. (1). Passing to the new variable

$$\mu = \frac{(\mathbf{C}\cdot\mathbf{r})}{Cr}$$

and representing the collision operator in the form

$$I\,[\varphi] = F - \nu\varphi\,,$$

which, as is known, is possible in the case of potentials of intermolecular interaction with a limited range of action, as well as for model equations, we obtain

$$\mu\,\frac{\partial\varphi}{\partial r} + \frac{1-\mu^2}{r}\,\frac{\partial\varphi}{\partial\mu} = \frac{F-\nu\varphi}{C}\,. \tag{11}$$

To solve this equation, the authors of [4–6] use an iteration method analogous to that described in [3]. In so doing, they use, as the distribution function entering into the integral part of the collision operator, the values obtained at a previous iteration step. In other words, at each step the function F is assumed to be given and the problem is reduced to the numerical solution of the corresponding differential equation.

It is obvious that with such an approach Eq. (11) admits an analytical solution. Indeed, consider the system of characteristic equations

$$\frac{dr}{\mu} = \frac{r d\mu}{1-\mu^2} = \frac{C d\varphi}{F-\nu\varphi}\,.$$

The first equality

$$\frac{dr}{\mu} = \frac{r d\mu}{1-\mu^2}$$

is solved trivially and yields the equation of the characteristic

$$K_1 = r\sqrt{1-\mu^2}\,. \tag{12}$$

As the second equation, consider

$$\frac{dr}{\mu} = \frac{C d\varphi}{F-\nu\varphi}\,.$$

Substituting into this equation the value found from (12)

$$\mu = \pm\sqrt{1-K_1^2/r^2}\,,$$

we obtain

$$C\,\mathrm{sign}\,(\mu)\sqrt{1-\frac{K_1^2}{r^2}}\,\frac{d\varphi}{dr} = F - \nu\varphi\,.$$

Hence we find

$$\varphi = K_2 \exp\left(-\,\mathrm{sign}\,(\mu)\,\frac{\nu}{C}\sqrt{r^2-K_1^2}\right) + \frac{\mathrm{sign}\,(\mu)}{C}\int_R^r \exp\left(-\,\mathrm{sign}\,(\mu)\,\frac{\nu}{C}\left(\sqrt{r_1^2-K_1^2}-\sqrt{r^2-K_1^2}\right)\right)\times$$

$$\times F\left(r_1, \operatorname{sign}(\mu)\sqrt{1-K_1^2/r_1^2}\right)\frac{r_1 dr_1}{\sqrt{r_1^2-K_1^2}}. \tag{13}$$

The arguments of the function F mean that in calculating it, it is necessary to take, as r and μ, r_1 and sign (μ) $\sqrt{1-K_1^2/r_1^2}$, respectively.

To definitively determine the sought solution, it is necessary to give the boundary conditions. Obviously, relation (2) gives the value of the distribution function inside the cone of influence of the particle, i.e., for $\mu > \sqrt{1-R^2/r^2}$. Moreover, the sought solution should satisfy the finiteness condition at $r \to \infty$. And, as seen from the structure given by (13), at $\mu > 0$ this requirement is met automatically. Therefore, to determine the distribution in the region of $0 < \mu < \sqrt{1-R^2/r^2}$, one should use the continuity condition at $\mu = 0$.

The solution of Eq. (11) satisfying the above requirements is described by the function

$$\varphi = \varphi_1 H_1 + \varphi_2 H_2 + \varphi_3 H_3, \tag{14}$$

where

$$\varphi_1 = \frac{1}{C}\int_r^\infty \exp\left(-\frac{\nu}{C}\left(r\mu + \sqrt{r_1^2 - r^2(1-\mu^2)}\right)\right) F\left(r_1, -\sqrt{1-\frac{r^2}{r_1^2}(1-\mu^2)}\right)\frac{r_1 dr_1}{\sqrt{r_1^2 - r^2(1-\mu^2)}}, \tag{15}$$

$$\varphi_2 = \frac{1}{C}\int_{r\sqrt{1-\mu^2}}^\infty \exp\left(-\frac{\nu}{C}\left(r\mu + \sqrt{r_1^2 - r^2(1-\mu^2)}\right)\right) F\left(r_1, -\sqrt{1-\frac{r^2}{r_1^2}(1-\mu^2)}\right)\frac{r_1 dr_1}{\sqrt{r_1^2 - r^2(1-\mu^2)}} +$$

$$+\frac{1}{C}\int_{r\sqrt{1-\mu^2}}^{r} \exp\left(\frac{\nu}{C}\left(\sqrt{r_1^2 - r^2(1-\mu^2)} - r\mu\right)\right) F\left(r_1, \sqrt{1-\frac{r^2}{r_1^2}(1-\mu^2)}\right)\frac{r_1 dr_1}{\sqrt{r_1^2 - r^2(1-\mu^2)}}, \tag{16}$$

$$\varphi_3 = \Phi_r \exp\left(\frac{\nu}{C}\left(\sqrt{R - r^2(1-\mu^2)} - r\mu\right)\right) + \frac{1}{C}\int_R^r \exp\left(\frac{\nu}{C}\left(\sqrt{r_1^2 - r^2(1-\mu^2)} - r\mu\right)\right)\times$$

$$\times F\left(r_1, \sqrt{1-\frac{r^2}{r_1^2}(1-\mu^2)}\right)\frac{r_1 dr_1}{\sqrt{r_1^2 - r^2(1-\mu^2)}}, \tag{17}$$

$H_1 = H(-\mu)$, $H_3 = H(\mu - \sqrt{1-R^2/r^2})$, $H_2 = 1 - H_1 - H_3$, $H(x) = \dfrac{|x| + x}{2x}$ is the standard Heaviside function.

Thus, the problem is reduced to the system of integral equations (15)–(17), for whose solution any numerical method can be used.

For a particular analysis, we restrict ourselves to the BGK model of the collision integral [8], which corresponds to

$$F = \nu \sum_{i=1}^{3} P_i(C, \mu) M_i, \quad \nu = \frac{5n_0}{\kappa}\sqrt{\frac{k^3 T_0}{8m}},$$

$$M_i = \pi^{-3/2} \int P_i \varphi \exp\,(-\,C^2)\; d^3C\,. \tag{18}$$

$$P_1 = 1\,,\quad P_2 = \sqrt{\frac{2}{3}}\left(C^2 - \frac{3}{2}\right),\quad P_3 = \sqrt{2}\;C\mu\,.$$

The choice of the above model is of particular interest, since it permits comparison with the analytical results obtained in limiting cases and makes it possible to determine the accuracy of the known approximate methods of solving the kinetic equation. Moreover, this form of the collision integral is used for solving more complex problems [4, 5].

Substitution of (14)–(17) into definition (18) leads to the system of integral equations

$$M_i\,(r) = \frac{2}{\sqrt{\pi}} \int\limits_0^{\infty} \left(\int\limits_{-1}^{0} P_i\,(C, \mu)\; \varphi_1 d\mu + \int\limits_{0}^{\sqrt{1-R^2/r^2}} P_i\,(C, \mu)\; \varphi_2 d\mu + \int\limits_{\sqrt{1-R^2/r^2}}^{1} P_i\,(C, \mu)\; \varphi_3 d\mu \right) C^2 \exp\,(-\,C^2)\; dC\,, \tag{19}$$

$$\varphi_1 = \frac{\nu}{C} \int\limits_r^{\infty} \exp\left(-\frac{\nu}{C}\left(r\mu + \sqrt{r_1^2 - r^2\,(1-\mu^2)}\right)\right) \sum_j P_j \left(C, -\sqrt{1 - \frac{r^2}{r_1^2}\,(1-\mu^2)}\right) M_j\,(r_1)\, \frac{r_1 dr_1}{\sqrt{r_1^2 - r^2\,(1-\mu^2)}}\,,$$

$$\varphi_2 = \frac{\nu}{C} \int\limits_{r\sqrt{1-\mu^2}}^{\infty} \exp\left(-\frac{\nu}{C}\left(r\mu + \sqrt{r_1^2 - r^2\,(1-\mu^2)}\right)\right) \times$$

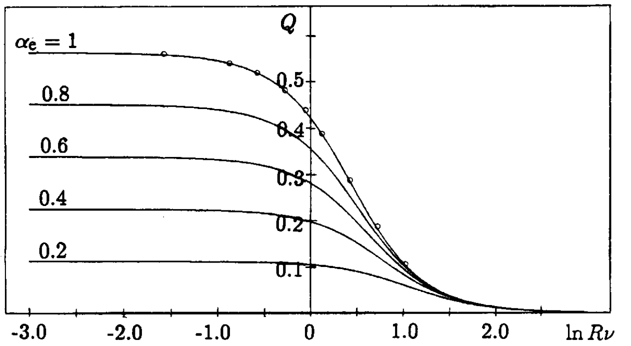
$$\times \sum_j P_j \left(C, -\sqrt{1 - \frac{r^2}{r_1^2}\,(1-\mu^2)}\right) M_j\,(r_1)\, \frac{r_1 dr_1}{\sqrt{r_1^2 - r^2\,(1-\mu^2)}} +$$

$$+\,\frac{\nu}{C} \int\limits_{r\sqrt{1-\mu^2}}^{r} \exp\left(\frac{\nu}{C}\left(\sqrt{r_1^2 - r^2\,(1-\mu^2)} - r\mu\right)\right) \sum_j P_j \left(C, \sqrt{1 - \frac{r^2}{r_1^2}\,(1-\mu^2)}\right) M_j\,(r_1)\, \frac{r_1 dr_1}{\sqrt{r_1^2 - r^2\,(1-\mu^2)}}\,,$$

$$\varphi_3 = \exp\left(\frac{\nu}{C}\left(\sqrt{R - r^2\,(1-\mu^2)} - r\mu\right)\right) \left((C^2 - 2)\, \frac{\Delta T_{\mathrm{r}}}{T_0} - \right.$$

$$\left. -\,\frac{4\nu}{C} \int\limits_0^{\infty} C^2 dC \int\limits_{-1}^{0} \mu d\mu \int\limits_R^{\infty} \exp\left(-\frac{\nu}{C}\left(R\mu + \sqrt{r_1^2 - R^2\,(1-\mu^2)}\right) - C^2\right) \times \right.$$

$$\left. \times \sum_j P_j \left(C, -\sqrt{1 - \frac{R^2}{r_1^2}\,(1-\mu^2)}\right) M_j\,(r_1)\, \frac{r_1 dr_1}{\sqrt{r_1^2 - R^2\,(1-\mu^2)}} \right) + \frac{\nu}{C} \int\limits_R^{r} \exp\left(\frac{\nu}{C}\left(\sqrt{r_1^2 - r^2\,(1-\mu^2)} - r\mu\right)\right) \times$$



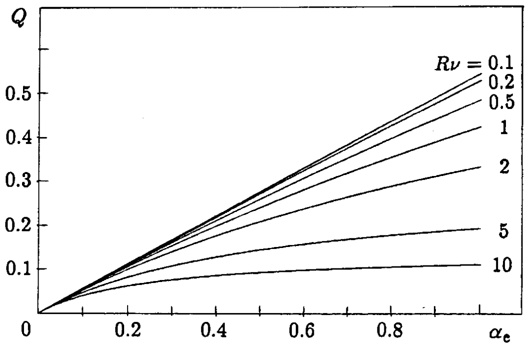


Fig. 1. Heat flux as a function of the particle size at fixed values of α_e for $\Delta T_w = T_0$. Dots show the values of Q obtained in [6] by direct integration of the kinetic equation model under consideration at complete energy accommodation.

Fig. 2. Heat flux as a function of the energy accommodation coefficient at fixed r.

$$\times \sum_j P_j \left(C, \sqrt{1 - \frac{r^2}{r_1^2}(1-\mu^2)} \right) M_j(r_1) \frac{r_1 dr_1}{\sqrt{r_1^2 - r^2 (1-\mu^2)}}$$

with respect to the distribution function moments depending only on the distance to the particle center. And, by virtue of (3), $M_3 = 0$. Therefore, in reality, it is necessary to solve a system of two equations, and the third equation can be used to check the accuracy of the results obtained.

It should be noted that the idea of transforming the Boltzmann equation into a system of integral equations with respect to the distribution function moments was used in considering similar problems in [9, 10]. To solve the system formed, the authors of [9, 11] used the variation method. In so doing, the trial function was chosen from the condition of accurate asymptotic behavior of macroscopic parameters in the gas-dynamic region. As a result, the heat flux was given by the relation $q = C_1/r^2$, which is really fulfilled (by virtue of the energy conservation law), whereas the temperature fields and the concentrations were determined in the form $T = C_2/r$ and $n = C_3/r$, which holds only at a large enough distance from the particle. The constants C_i were calculated from the minimum condition of the corresponding functional. In [10], the Galerkin method was used. However, the trial function was chosen from analogous considerations.

To describe the real character of the dependence $M_i(r)$, we represent it in the form of the Chebyshev polynomial series. Restricting ourselves to its first K terms, we write

$$M_i(r) = \sum_{j=0}^{K} A_j^i T_j(\xi(r)) .$$

By $\xi(r)$ is meant a monotonic function whose values range from -1 to 1. The expansion coefficients are determined by the condition

$$\sum_{l=0}^{K} T_j(\xi_l)\, T_k(\xi_l) = \frac{K+1}{2}(\delta_{0j} + 1)\,\delta_{jk}\,, \quad \xi_l = \cos\frac{(2l+1)\,\pi}{2K+2}\,.$$

Such an approach makes it possible to do without the additional integration necessary in the Galerkin method, which considerably reduces the time of calculations and, owing to this, permits increasing the number of polynomials held in the expansion but requires a more thorough selection of the expansion parameter.

As the numerical analysis shows, the most optimum from the point of view of convergence is

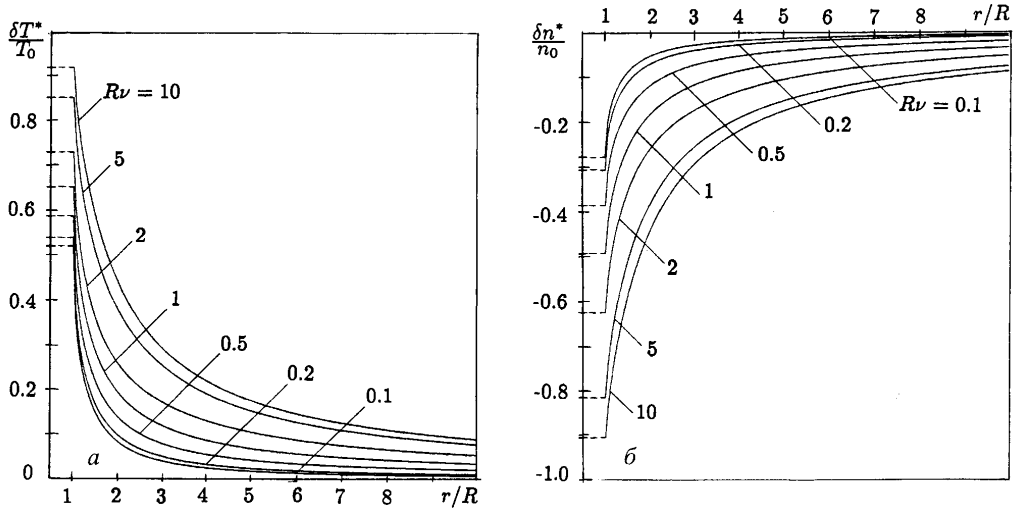


Fig. 3. Temperature (a) and concentration (b) distribution curves of gas molecules at fixed R. Horizontal dashed lines note values in the immediate vicinity of the particle surface.

$$\xi = 1 - 2\exp\left(-\beta\sqrt{r^2 - R^2}\right).$$

The quantity β was selected from the requirement that the majority of interpolation nodes lie in the region of the main change in the distribution function.

Figures 1 and 2 show the values of Q calculated at $\Delta T_w = T_0$.

Of particular interest is determination of the macroscopic characteristics of gas, such as, for example, temperature distribution and molecular concentration:

$$\frac{\delta T}{T_0} = \sqrt{\frac{2}{3}}\, M_2^* \frac{\alpha_e}{\sqrt{\pi}\,(1-\alpha_e)\,Q^* + \alpha_e} \frac{\Delta T_w}{T_0}, \quad \frac{\delta n}{T_0} = M_1^* \frac{\alpha_e}{\sqrt{\pi}\,(1-\alpha_e)\,Q^* + \alpha_e} \frac{\Delta T_w}{T_0}.$$

From (19) it follows that in the case of a small particle,

$$\frac{\delta T^*}{T_0} = \sqrt{\frac{2}{3}}\, M_2^* = \frac{1}{2}\left(1 - \sqrt{1 - \frac{R^2}{r^2}}\right) + R\nu f_T, \tag{20}$$

$$\frac{\delta n^*}{n_0} = M_1^* = -\frac{1}{4}\left(1 - \sqrt{1 - \frac{R^2}{r^2}}\right) + R\nu f_n. \tag{21}$$

The first terms in (20), (21) describe the distribution of the quantities under consideration at distances comparable to the mean free path and are independent of the properties of the gas. The functions f_T and f_n are expressed in terms of integrals entering into (19) and determine the transition to the gas-dynamic solution

$$\frac{\delta T^*}{T_0} = -\frac{\delta n^*}{n_0} = \frac{R}{r}.$$

The temperature and concentration distribution in the intermediate range of $R\nu$ is given in Fig. 3.

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NOTATION

V and **C**, thermal velocity and its corresponding dedimensionalized velocity of gas molecules (subscript r denotes the radial projection); r, distance from the particle center to the point being considered; q and Q, heat flux and dedimensionalized heat flux; k, Boltzmann constant; m, mass of gas molecules; κ, heat-conductivity coefficient; R, particle radius; T_{w}, temperature of the particle surface; T_0 and n_0, unperturbed values of the temperature and concentration of gas molecules; f_0, equilibrium (Maxwellian) distribution function; φ, correction to the equilibrium distribution function; $I(\varphi)$, integral collision operator; T_{r} and Φ_{r}, temperature and distribution function of molecules reflected from the particle surface; E_{i} and E_{r}, dimensionless value of energy brought by incident molecules and carried away by molecules reflected from the particle; Φ_{w}, n_{w}, and E_{w}, distribution function, concentration, and value of energy which would be carried away by molecules reflected from the particle with the temperature of its surface; α_{e}, energy-accommodation coefficient; Δ, difference between the values of the corresponding characteristics at the particle surface and at infinity ($\Delta T = T_{\mathrm{r}} - T_0$); δ, difference between the local values of thermodynamic parameters ($\delta T = T(r) - T_0$); A_i^j, I_i, K_i, H_i, M_i, P_i, ξ_i, φ_i, F, f_T, f_n, β, μ, ν, auxiliary quantities; T_j, Chebyshev polynomial; δ_{ij}, Kronecker symbol. Subscripts: r, reflected; i, input energy; w, wall (solid surface) from which gas molecules are reflected; e, energy; 0, values of gas characteristics at an infinite distance from the particle surface.

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