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ACCOUNTING FOR ENERGY ACCOMMODATION IN CALCULATING THE HEAT FLUX FROM A SPHERICAL PARTICLE IN A DIATOMIC GAS

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The problem of calculation of the heat flux from a uniformly heated spherical particle in a diatomic gas is considered with account for the energy-accommodation effect. The results of numerical calculations for the analog of the BGK collision-integral model are presented.

A study of the process of heat transfer in the intermediate range of Knudsen numbers is of great theoretical and practical interest. Its results are used, in particular, to determine the character of the gas–solid surface interaction and to calculate accommodation coefficients. However, in theoretical analysis of this phenomenon, one takes into account only the translational motion of molecules, whereas the majority of experiments are conducted for molecular gases, which requires account for the internal degrees of freedom [1]. The contribution of specific types of motion is determined by the character of an energy spectrum. As is well known (see, e.g., [2]), the distance between the energy levels of the rotational degrees of freedom is determined by the relation $\hbar^2/2J$ (J is the inertia moment of a molecule) and is comparable to the thermal-motion energy kT only for lighter gases. Thus, for hydrogen molecules $\hbar^2/(2Jk)$ = 85.4 K. For heavier molecules this quantity is substantially smaller, which makes it possible to neglect the discrete character of the rotational-motion energy and to consider the rotational degrees of freedom in a classical approximation, whereas the vibrational degrees of freedom are excited at temperatures of the order of 10^3 K. Therefore, they can be considered to be completely frozen.

Let us consider a spherical particle of radius R heated uniformly to the temperature T_s and situated in a diatomic gas in which the temperature T_0, constant at infinity, is maintained. The temperature drop $\Delta T_s = T_s - T_0$ will be considered to be rather small for the problem to be linearized.

We introduce a spherical coordinate system with the origin at the center of the particle. The state of the gas surrounding the particle is described by the equation [3]

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

where φ is the correction to the equilibrium distribution function

$$f_0 = n_0 \left(\frac{m}{2\pi k T_0} \right)^{3/2} \frac{J}{kT_0} \exp(-C^2 - \gamma^2) ; \quad \mathbf{C} = \mathbf{V} \sqrt{m/2kT_0} ; \quad \gamma = \omega \sqrt{J/2kT_0} ;$$

$\mathbf{V}$ and ω are the thermal velocities of the translational and rotational motion of the gas molecules, $\mathbf{C}$ and γ are their dimensionless values, $I[\varphi]$ is the integral collision operator, and m is the molecular mass.

Taking into account the absence of reliable models for an intermolecular interaction potential, we confine ourselves to the BGK (Bhatnagar–Gross–Krook) analog [4] of the collision-integral model [5]. Assuming the relaxation times of the rotational and translational degrees of freedom to be equal, in conformity with [6] we have

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$$I[\varphi] = \nu (F - \varphi), \quad F = \sum_{i=1}^{3} P_i M_i, \quad M_i = 2\pi^{-3/2} \int P_i \, \varphi \exp(-C^2 - \gamma^2) \, \gamma d\gamma d^3 C, \quad P_1 = 1,$$

$$P_2 = \sqrt{\frac{2}{5}} \left(C^2 + \gamma^2 - \frac{5}{2} \right), \quad P_3 = \sqrt{2} \, C_r . \tag{2}$$

The parameter $\nu = \frac{7n_0}{\kappa} \sqrt{\frac{k^3 T_0}{8m}} = \frac{1}{\chi} \sqrt{\frac{kT_0}{2m}}$ characterizes the frequency of collisions between the molecules and is determined by the degree of rarefaction of the gas and κ and χ are the coefficients of thermal conductivity and thermal diffusivity.

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

$$f_{\mathrm{ref}} = n_{\mathrm{ref}} \left(\frac{m}{2\pi k T_v} \right)^{3/2} \frac{J}{kT_\omega} \exp \left(-\frac{mV^2}{2kT_v} - \frac{J\omega^2}{2kT_\omega} \right).$$

By virtue of the linearity of the problem, we write

$$\varphi \big|_{C_r > 0, r = R} = \Phi_{\mathrm{ref}} = \frac{n_{\mathrm{ref}} - n_0}{n_0} + \left(C^2 - \frac{3}{2} \right) \tau_v + (\gamma^2 - 1) \, \tau_\omega . \tag{3}$$

The values of n_{ref}, $\tau_v = (T_v - T_0)/T_0$, and $\tau_\omega = (T_\omega - T_0)/T_0$ are determined by the requirement of the absence of the mass motion of the gas

$$2\pi^{-3/2} \int C_r \, \varphi \exp(-C^2 - \gamma^2) \, \gamma d\gamma d^3 C = 0 \tag{4}$$

and by the character of the energy accommodation [7]

$$\alpha_v = \frac{E_{\mathrm{i}}^{v} - E_{\mathrm{ref}}^{v}}{E_{\mathrm{i}}^{v} - E_{\mathrm{s}}^{v}}, \quad \alpha_\omega = \frac{E_{\mathrm{i}}^{\omega} - E_{\mathrm{ref}}^{\omega}}{E_{\mathrm{i}}^{\omega} - E_{\mathrm{s}}^{\omega}} . \tag{5}$$

Here

$$E_{\mathrm{i}}^{v} = 2\pi^{-3/2} \int_{C_r < 0} C_r C^2 \varphi(R) \exp(-C^2 - \gamma^2) \, \gamma d\gamma d^3 C \tag{6}$$

and

$$E_{\mathrm{i}}^{\omega} = 2\pi^{-3/2} \int_{C_r < 0} C_r \varphi(R) \exp(-C^2 - \gamma^2) \, \gamma^3 d\gamma d^3 C \tag{7}$$

is the dimensionless value of the energy of translational and rotational motion that is brought by the molecules incident on the particle surface;

$$E_{\mathrm{ref}}^{v} = 2\pi^{-3/2} \int_{C_r > 0} C_r C^2 \varphi(R) \exp(-C^2 - \gamma^2) \, \gamma d\gamma d^3 C \tag{8}$$

and

$$E^{\omega}_{\mathrm{ref}} = 2\pi^{-3/2} \int\limits_{C_r>0} C_r \varphi\,(R)\, \exp\,(-\,C^2 - \gamma^2)\, \gamma^3 d\gamma d^3C \tag{9}$$

the energy carried away by the molecules reflected from the particle;

$$E^{v}_{\mathrm{s}} = 2\pi^{-3/2} \int\limits_{C_r>0} C_r C^2 \Phi_{\mathrm{s}} \exp\,(-\,C^2 - \gamma^2)\, \gamma d\gamma d^3C \tag{10}$$

and

$$E^{\omega}_{\mathrm{s}} = 2\pi^{-3/2} \int\limits_{C_r>0} C_r \Phi_{\mathrm{s}} \exp\,(-\,C^2 - \gamma^2)\, \gamma^3 d\gamma d^3C \tag{11}$$

the energy that would be carried away by the molecules if they were reflected at the temperature T_{s}.

From Eqs. (4)–(11) we find

$$\frac{n_{\mathrm{ref}} - n_0}{n_0} = 2I_0 - \frac{\tau_v}{2}\,,\ \ E^{v}_{\mathrm{i}} = \frac{I_1}{\sqrt{\pi}}\,,\ \ E^{\omega}_{\mathrm{i}} = \frac{I_2}{\sqrt{\pi}}\,,\ \ E^{v}_{\mathrm{ref}} = \frac{\tau_v + 2I_0}{\sqrt{\pi}}\,,\ \ E^{\omega}_{\mathrm{ref}} = \frac{\tau_\omega + 2I_0}{\sqrt{\pi}}\,,\ \ E^{v}_{\mathrm{s}} = \frac{\tau_{\mathrm{s}} + 2I_0}{\sqrt{\pi}}\,,\ \ E^{\omega}_{\mathrm{s}} = \frac{\tau_{\mathrm{s}} + 2I_0}{\sqrt{\pi}}\,,$$

where

$$I_i = \frac{2}{\pi} \int\limits_{C_r<0} A_i C_r \exp\,(-\,C^2 - \gamma^2)\, \varphi\,(R)\, \gamma d\gamma d^3C\,; \quad \tau_{\mathrm{s}} = \Delta T_{\mathrm{s}}/T_0\,; \quad A_0 = 1\,; \quad A_1 = C^2\,; \quad A_2 = \gamma^2\,. \tag{12}$$

The heat flux is determined by the relation

$$q = \int V_r \left(\frac{mV^2}{2} + \frac{J\omega^2}{2} \right) f_0\, \varphi \omega d\omega d^3V$$

and can be represented in the form

$$q = n_0 \sqrt{\frac{2k^3T_0^3}{m}}\, \frac{R^2}{r^2}\, (Q_v - Q_\omega)\,, \quad Q_v = \frac{2}{\pi^{3/2}}\, \frac{r^2}{R^2} \int C_r C^2 \varphi \exp\,(-\,C^2 - \gamma^2)\, \gamma d\gamma d^3C\,,$$

$$Q_\omega = \frac{2}{\pi^{3/2}}\, \frac{r^2}{R^2} \int C_r \varphi \exp\,(-\,C^2 - \gamma^2)\, \gamma^3 d\gamma d^3C\,.$$

The dimensionless quantities Q_v and Q_ω describe the transfer of the energy of the translational and rotational motion of the gas molecules. And, by virtue of the conservation law, the quantity $Q = Q_v + Q_\omega \equiv \mathrm{const}$ can be calculated at any point, in particular, on the particle surface where

$$Q_v \big|_{r=R} = E^{v}_{\mathrm{ref}} - E^{v}_{\mathrm{i}} = \frac{\tau_v + 2I_0 - I_1}{\sqrt{\pi}}\,, \quad Q_\omega \big|_{r=R} = E^{\omega}_{\mathrm{ref}} - E^{\omega}_{\mathrm{i}} = \frac{\tau_\omega + 2I_0 - 2I_2}{2\sqrt{\pi}}\,.$$

Substitution of the relations obtained into conditions (5) yields

$$(\sqrt{\pi}\, Q_v^v (1-\alpha_v) + \alpha_v)\, \tau_v + \sqrt{\pi}\, Q_v^\omega (1-\alpha_v)\, \tau_\omega = \alpha_v \frac{\Delta T_s}{T_0} ,$$

$$2\sqrt{\pi}\, Q_\omega^v (1-\alpha_\omega)\, \tau_v + (2\sqrt{\pi}\, Q_\omega^\omega (1-\alpha_\omega) + \alpha_\omega)\, \tau_\omega = \alpha_\omega \frac{\Delta T_s}{T_0} .$$

Whence

$$\tau_v = \frac{\Delta_v}{\Delta} \frac{\Delta T_s}{T_0} , \quad \tau_\omega = \frac{\Delta_\omega}{\Delta} \frac{\Delta T_s}{T_0} ,$$

$$\Delta_v = \alpha_v (2\sqrt{\pi}\, Q_\omega^\omega (1-\alpha_\omega) + \alpha_\omega) - \alpha_\omega \sqrt{\pi}\, Q_v^\omega (1-\alpha_v) ,$$

$$\Delta_\omega = \alpha_\omega (\sqrt{\pi}\, Q_v^v (1-\alpha_v) + \alpha_v) - \alpha_v\, 2\sqrt{\pi}\, Q_\omega^v (1-\alpha_\omega) ,$$

$$\Delta = (\sqrt{\pi}\, Q_v^v (1-\alpha_v) + \alpha_v)(2\sqrt{\pi}\, Q_\omega^\omega (1-\alpha_\omega) + \alpha_\omega) - 2\pi\, Q_v^\omega Q_\omega^v (1-\alpha_v)(1-\alpha_\omega) .$$

By Q_v^v and Q_ω^ω we mean the values of Q_v and Q_ω on the particle surface calculated at $\tau_v = 1$ and $\tau_\omega = 0$, while by Q_v^ω and Q_ω^ω we mean these values calculated at $\tau_v = 0$ and $\tau_\omega = 1$.

The resulting heat flux is determined by the relation

$$Q = (Q_v^v + Q_\omega^v)\, \tau_v + (Q_v^\omega + Q_\omega^\omega)\, \tau_\omega .$$

It is evident that in a free-molecular regime the influence of the particle on the molecular distribution function in the gas volume can be neglected, while the function φ in the range of integration (12) and the integrals themselves can be considered to be equal to zero. Correspondingly,

$$Q_v^v = 2Q_\omega^\omega = \frac{1}{\sqrt{\pi}} , \quad Q_v^\omega = Q_\omega^v = 0 , \quad Q = \frac{1}{\sqrt{\pi}} \left(\alpha_v + \frac{\alpha_\omega}{2} \right) \frac{\Delta T_s}{T_0} .$$

Thus, at $\alpha_\omega = 0$, i.e., in the case where only the translational degrees of freedom of the gas molecules are excited because of the reflection from the particle, the heat flux (in the limit under consideration) coincides with the value calculated for the atomic gas, and when the accommodation of energy is total it turns out to be one and a half times larger than this value.

In the case of a coarse particle, considering the distribution of the incident molecules to be coincident with the Chapman–Enskog function

$$\Phi_{\mathrm{Ch}} = \frac{4}{7} \frac{R^2}{r^2} \left(C^2 + \gamma^2 - \frac{7}{2} \right) (R\nu + C_r)\, Q ,$$

i.e., neglecting effects of the order of the Knudsen number $\mathrm{Kn} \sim (R\nu)^{-1}$, we find

$$I_0 = -I_1/2 = -I_2 = -QR\nu/7 .$$

Correspondingly,

$$Q = \frac{7}{6R\nu} \left(\tau_v + \frac{\tau_\omega}{2} \right).$$

Taking into account the fact that in the indicated approximation

$$Q_v^v = Q_\omega^\omega = -Q_v^\omega = -Q_\omega^v = \frac{1}{3\sqrt{\pi}}\,,$$

we obtain

$$\tau_v = \tau_\omega = \frac{\Delta T_\mathrm{s}}{T_0}\,, \quad Q = \frac{7}{4R\nu}\,\frac{\Delta T_\mathrm{s}}{T_0}\,,$$

which, with account for the determination, gives

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

and in this sense coincides with the solution of the problem considered for the atomic gas.

To calculate the heat flux in the intermediate range of Knudsen numbers, we must solve Eq. (1).

Following [8], the solution sought is represented in the form

$$\varphi = \varphi_1 H_1 + \varphi_2 H_2 + \varphi_3 H_3\,, \tag{13}$$

where

$$\varphi_1 = \frac{\nu}{C} \sum_{i=1}^{2} P_i \int_r^\infty \exp\left(-\frac{\nu}{C}\left(r\mu + \sqrt{r_1^2 - r^2(1-\mu^2)}\right)\right) \frac{M_i(r_1)\, r_1 dr_1}{\sqrt{r_1^2 - r^2(1-\mu^2)}}\,;$$

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

$$+ \frac{\nu}{C} \sum_{i=1}^{2} P_i \int_{r\sqrt{1-\mu^2}}^{\infty} \exp\left(-\frac{\nu}{C}\left(r\mu + \sqrt{r_1^2 - r^2(1-\mu^2)}\right)\right) \frac{M_i(r_1)\, r_1 dr_1}{\sqrt{r_1^2 - r^2(1-\mu^2)}}\,;$$

$$\varphi_3 = \frac{\nu}{C} \sum_{i=1}^{2} P_i \int_r^\infty \exp\left(\frac{\nu}{C}\left(\sqrt{r_1^2 - r^2(1-\mu^2)} - r\mu\right)\right) \frac{M_i(r_1)\, r_1 dr_1}{\sqrt{r_1^2 - r^2(1-\mu^2)}} +$$

$$+ \Phi_\mathrm{r} \exp\left(\frac{\nu}{C}\left(\sqrt{R - r^2(1-\mu^2)} - r\mu\right)\right);$$

$$H_1 = H(-\mu)\,; \quad H_3 = H\left(\mu - \sqrt{1 - R^2/r^2}\right); \quad H_2 = 1 - H_1 - H_3\,;$$

$$\mu = \frac{\mathbf{C}\cdot\mathbf{r}}{Cr}\,; \quad H(x) = \frac{|x| + x}{2x}$$

is the standard Heaviside function.

Substitution of Eq. (13) into determination (2) leads to a system of integral equations relative to M_i. Integration over γ is performed analytically. To do this, any velocity function of the gas molecules should be considered as the vector

$$f = f^1 e_1 + f^2 e_2\,, \quad e_1 = 1\,, \quad e_2 = \gamma^2 - 1\,.$$

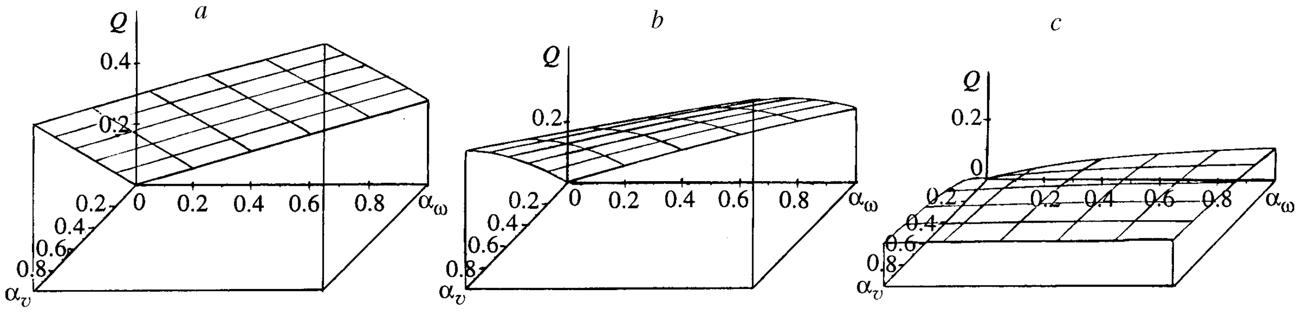

Fig. 1. Heat flux versus energy-accommodation coefficients at $R\nu = 0.1$ (a), $R\nu = 1$ (b), and $R\nu = 10$ (c).

TABLE 1. Values of the Dimensionless Flux of the Energy of Translational and Rotational Motion Calculated on the Particle Surface in the Case Where Only the Translational (Q_v^v and Q_ω^v) or Rotational (Q_v^ω and Q_ω^ω) Degrees of Freedom Are Excited in Reflection of the Gas Molecules from the Particle Surface

$R\nu$	Q_v^v	$Q_v^\omega = Q_\omega^v$	Q_ω^ω	$R\nu$	Q_v^v	$Q_v^\omega = Q_\omega^v$	Q_ω^ω
0.01	0.56318	–0.00053	0.28175	2	0.40539	–0.08156	0.23693
0.1	0.55422	–0.00525	0.27879	5	0.31230	–0.12715	0.21369
0.2	0.54357	–0.01084	0.27548	10	0.25851	–0.15262	0.20120
0.5	0.51357	–0.02654	0.26648	100	0.19378	–0.18217	0.18736
1	0.46960	–0.04917	0.25408				

Then the integration can be represented in the form of the scalar product

$$(f, g) = 2 \int_0^\infty fg\gamma \exp(-\gamma^2)\, d\gamma = f^1 g^1 + f^2 g^2 .$$

In this case

$$P_1^1 = 1 , \quad P_1^2 = 0 , \quad P_2^1 = \sqrt{\frac{2}{5}} \left(C^2 - \frac{3}{2} \right), \quad P_2^2 = \sqrt{\frac{2}{5}} ,$$

$$\Phi_{\text{ref}}^1 = (C^2 - 2)\, \tau_v - 4\nu \sum_{i=1}^{2} \int_0^\infty P_i^1 C^2 dC \int_{-1}^{0} \mu d\mu \int_R^\infty M_i(r_1) \times$$

$$\times \exp\left(-\frac{\nu}{C} \left(R\mu + \sqrt{r_1^2 - R^2(1-\mu^2)} \right) - C^2 \right) \frac{r_1 dr}{\sqrt{r_1^2 - R^2(1-\mu^2)}} ,$$

$$\Phi_{\text{ref}}^2 = \tau_\omega .$$

As a result, the problem is reduced to the system of two integral equations

$$M_i(r) = \frac{2}{\sqrt{\pi}} \int_0^\infty \left(\int_{-1}^{0} (P_i, \varphi_1)\, d\mu + \int_0^{\sqrt{1-R^2/r^2}} (P_i, \varphi_2)\, d\mu + \int_{\sqrt{1-R^2/r^2}}^{1} (P_i, \varphi_3)\, d\mu \right) C^2 \exp(-C^2)\, dC , \quad i = 1, 2 .$$

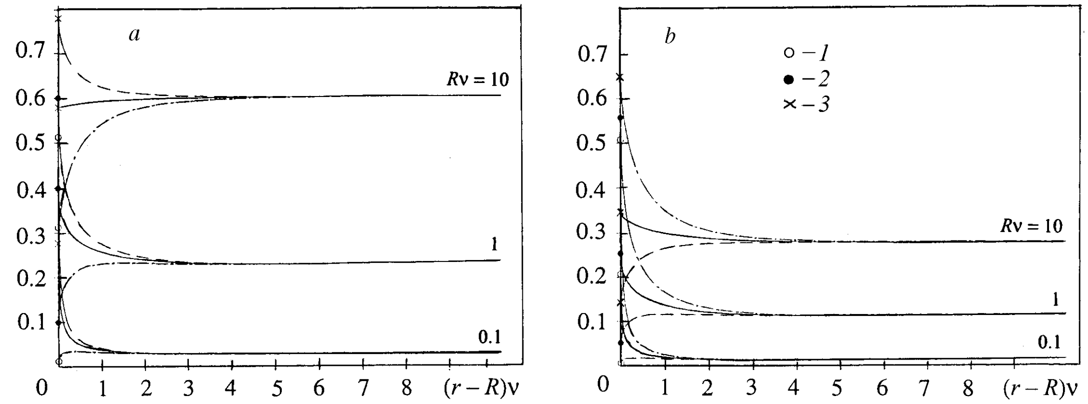

Fig. 2 Values of $\frac{\delta T}{T_0}\frac{r}{R}$ (solid line), $\frac{\delta T_v}{T_0}\frac{r}{R}$ (dashed line), and $\frac{\delta T_\omega}{T_0}\frac{r}{R}$ (dash-dot line) versus distance to the particle surface at $\tau_v = 1$, $\tau_\omega = 0$ (a) and $\tau_v = 0$, $\tau_\omega = 1$ (b): 1–3) values of the indicated quantities at $r = R$ for $R\nu = 0.1$, 1, and 10, respectively.

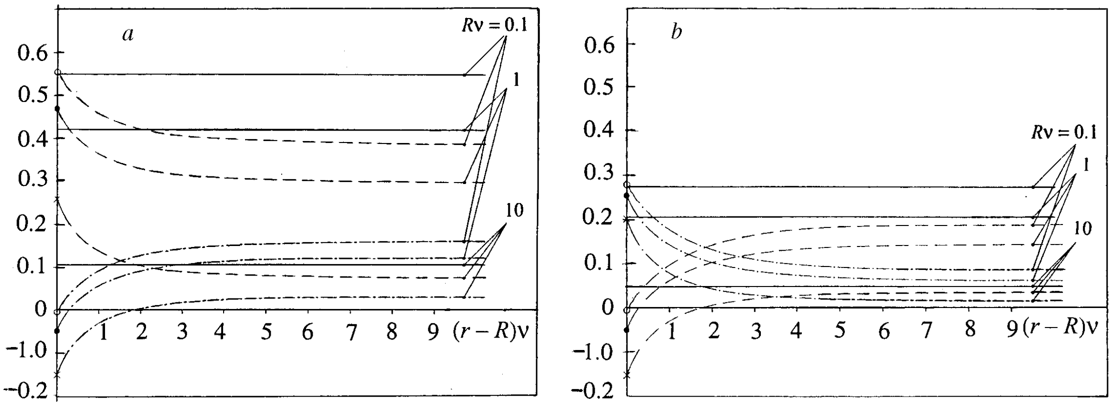

Fig. 3. Values of Q (solid line), Q_v (dashed line), and Q_ω (dash-dot line) versus distance to the particle surface at $\tau_v = 1$, $\tau_\omega = 0$ (a), and $\tau_v = 0$, $\tau_\omega = 1$ (b).

In accordance with [9], the solution of this system of equations was determined in the form of a cubic spline. To control the accuracy, we used the conservation laws and the values calculated at the intermediate (between the interpolation nodes) points.

The calculation results are given in Table 1.

Figure 1 presents the graphs of the heat flux versus the coefficients of accommodation of the energy of translational and rotational motion at $R\nu = 0.1$, 1, and 10.

Of certain interest is to analyze the energy and temperature distribution by the translational and rotational degrees of freedom of the molecules on their separate excitation, i.e., at $\tau_v = 1$ and $\tau_\omega = 0$ as well as at $\tau_v = 0$ and $\tau_\omega = 1$.

$$\frac{\delta T_v}{T_0}\frac{r}{R},\quad \frac{\delta T_\omega}{T_0}\frac{r}{R},\quad \frac{\delta T}{T_0}\frac{r}{R},$$

$$\frac{\delta T_v}{T_0} = \frac{4}{3}\pi^{-3/2}\int\left(C^2 - \frac{3}{2}\right)\varphi \exp\left(-C^2 - \gamma^2\right)\gamma d\gamma d^3C,$$

$$\frac{\delta T_\omega}{T_0} = 2\pi^{-3/2} \int (\gamma^2 - 1)\, \varphi \exp(-C^2 - \gamma^2)\, \gamma d\gamma d^3 C\,,$$

$$\frac{\delta T}{T_0} = \frac{2}{5}\left(\frac{3}{2}\frac{\delta T_v}{T_0} + \frac{\delta T_\omega}{T_0}\right),$$

Figure 2 gives the values of the relative temperature drops, normalized to r/R, that are calculated for $R\nu$ = 0.1, 1, and 10, while Fig. 3 gives the values of Q, Q_v, and Q_ω at the same parameters.

NOTATION

k, Boltzmann constant; $\hbar$, Planck constant; r, distance from the center of the particle to the point considered; T_0 and n_0, unperturbed values of the temperature and the concentration of the gas molecules at an infinite distance from the particle; T_s, temperature of the particle surface; T_v and t_ω, temperature corresponding to the energy of translational and rotational motion of the gas molecules reflected from the particle surface; τ_s, τ_v, and τ_ω, relative drops of the indicated temperatures; f_{ref} and Φ_{ref}, distribution function of the reflected molecules and correction to it; α_v and α_ω, accommodation coefficients of the energy of translational and rotational motion of the gas molecules; I_i, F, K_i, H_i, M_i, P_i, φ_i, Δ_v, Δ_ω, and μ, auxiliary quantities; δ, drop of the local values of the thermodynamic parameters: $\delta T = T(r) - T_0$; T_0, difference between the value of the corresponding parameter of the gas near the particle surface and at an infinite distance from it: $\Delta T_s = T_s - T_0$. Subscripts: i, incident; ref, reflected; s, surface; i, ith quantity; r, radial projection of the vectors **V** and **C**; v, corresponds to the velocity; ω, corresponds to the angular velocity; 0, at an infinite distance from the particle surface.

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