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SMOLUCHOWSKI'S PROBLEM FOR MOLECULAR GASES TAKING THE ACCOMMODATION COEFFICIENTS OF THE TRANSLATIONAL AND ROTATIONAL ENERGY OF THE MOLECULES INTO ACCOUNT†

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The effect of the accommodation coefficients of the energy of translational and rotational motion of molecules on the temperature jump in the classical Smoluchowski problem is investigated. Using the extension of the well-known kinetic BKW (Boltzmann–Krook–Welander) equation to the case of molecular gases, an analytical solution of this problem is obtained for diatomic and polyatomic gases taking the rotational degrees of freedom into account. A numerical analysis of the results obtained is carried out. © 2003 Elsevier Science Ltd. All rights reserved.

Despite considerable efforts, the theoretical description of the microscopic boundary conditions when gas molecules interact with a solid remains extremely incomplete even for the case of ideal surfaces and simple gases (without internal degrees of freedom of the molecules) [1]. The situation is even more complex when describing molecular gases and actual surfaces. This means that, as previously, the phenomenological microscopic boundary conditions, which use such integral characteristics of the surface as the accommodation coefficients [2], are extremely important.

For molecular gases, in addition to the accommodation coefficients of the translational energy of the molecules, used in the case of a simple gas, we need to take into account the accommodation coefficients of the internal degrees of freedom. There is experimental evidence that the accommodation coefficients of the internal degrees of freedom of gas molecules may differ considerably from unity in important practical cases, so that it is particularly important to take them into account [3, 4].

In this paper we consider relatively low temperatures for which the excitation of the oscillational degrees of freedom of the molecules can be neglected [5]. At the same time, at all temperatures, apart from extremely low ones, the rotational degrees of freedom can be considered at the classical level [5].

The effect of the accommodation coefficient of the energy was considered previously in [6] for the case of a simple gas. In the present paper we consider, for the first time, the effect of the accommodation coefficients of the energy of the translational and rotational motion of the molecules, introduced below. Here we use the kinetic equation for a molecular gas proposed in [7, 8] with a constant collision frequency of the molecules. Note that the kinetic equation for a molecular gas with a collision frequency proportional to the velocity of the molecules was introduced in [9].

It should be noted that the case of a molecular gas is essentially more complex for this problem than the case of a simple gas [6]. This is due to the fact that, for a simple gas, by taking into account the law of conservation of energy, the calculation of the energy flux transferred by molecules incident on the wall can be simplified considerably. For molecular gases it is necessary to consider fluxes of both translational and rotational energy of the molecules. Using a single law of conservation of total energy, it turns out to be impossible to simplify the calculation of both these fluxes. In this case it becomes necessary to use the exact molecule distribution function in the region of the surface.

We mean by Smoluchowski's problem (see, for example, [2, 6, 9]) the problem of finding the temperature jump in a rarefied gas in the region of the surface when the temperature gradient far from the surface is given.

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1. FORMULATION OF THE PROBLEM AND ITS SOLUTION

Suppose a constant temperature gradient K_t, orthogonal to the surface, is maintained in a half-space $x > 0$ far from the interface between a gas and a solid. We will assume that the temperature gradient is small, so that the problem can be considered in the linear approximation. The temperature profile outside the Knudsen layer has the form $T(x) = T_0 + K_t x$. We will denote the surface temperature by T_s. The quantity $\Delta T = T_0 - T_s$ is called the temperature jump. In the linear approximation $\Delta T = C_t \lambda K_t$, λ is the mean free path of the molecules, and C_t is the temperature jump coefficient. It is more convenient to introduce the relative temperature jump

$$\varepsilon_t = \Delta T / T_s = C_t \lambda k_t, \quad k_t = K_t / T_s \tag{1.1}$$

We will take the linearized kinetic equation (see [8]) for molecular gases with a constant collision frequency of the molecules ν_0, written for the case when the volume relaxation time of the energy of the translational and rotational degrees of freedom are close to one another. A similar assumption is made for the majority of molecular gases at room temperature [10]. Henceforth we will use the following dimensionless variables

$$\mathbf{c} = \sqrt{\frac{m}{2kT_s}}\mathbf{v}, \quad \nu = \sqrt{\frac{\tilde{J}}{2kT_s}}\omega, \quad x^* = \nu_0\sqrt{\frac{m}{2kT_s}}x$$

Here k is Boltzmann's constant, $\mathbf{v}$ is the velocity of translational motion of the gas molecules, $\boldsymbol{\omega}$ is the velocity of rotational motion of the gas molecules, for a diatomic molecule $\tilde{J} = J$, where J is its moment of inertia, while for a triatomic molecule $\tilde{J} = J_1\omega_1^2 + J_2\omega_2^2 + J_3\omega_3^2$ where J_i are the principal moments of inertia of a triatomic molecule. In dimensionless variables, the kinetic equation can be written as follows (the asterisk on the coordinate will be omitted):

$$c_x\frac{\partial\varphi}{\partial x} + \varphi(x, \mathbf{c}, \nu) = \int g(\mathbf{c}, \nu; \mathbf{c}', \nu')\varphi(x, \mathbf{c}', \nu')d\Omega \tag{1.2}$$

Here

$$g = 1 + 2c_x c_x' + \frac{1}{l + \frac{1}{2}}(c^2 + \nu^2 - l - \tfrac{1}{2})(c'^2 + \nu'^2 - l - \tfrac{1}{2})$$

$$d\Omega = 2^{2l-3}\pi^{\frac{1}{2}-l}\exp(-c^2 - \nu^2)\nu^{2l-3}d\nu d^3c$$

(g is the kernel of Eq. (1.2)), $l = 2$ for a diatomic gas and $l = 5/2$ for an N-atomic gas ($N \geqslant 3$).

Note that linear molecules behave as diatomic molecules when the rotational degrees of freedom are excited [5]. Hence, we will not deal with this case separately in what follows but merely include it in the general case of diatomic molecules.

We will consider the boundary condition on the wall taking into account the accommodation of the translational and rotational energy [2, 3]

$$\varphi(0, \mathbf{c}, \nu) = \varphi_0(c, \nu), \quad c_x > 0 \tag{1.3}$$

where

$$\varphi_0 = \varepsilon_n^r + \varepsilon_t^t(c^2 - 3/2) + \varepsilon_t^\omega(\nu^2 - l + 1) \tag{1.4}$$

and ε_n^r, ε_t^t, ε_t^ω are unknown quantities.

We will represent the boundary condition far from the wall in the form

$$\varphi(x, \mathbf{c}, \nu) = \varphi_{\text{as}}(x, \mathbf{c}, \nu) + o(1), \quad x \to \infty, \quad c_x < 0 \tag{1.5}$$

where

$$\varphi_{\text{as}} = k_t^*(x - c_x)(c^2 + \nu^2 - l - 3/2), \quad k_t^* = \frac{1}{\nu_0}\sqrt{\frac{2kT_s}{m}}k_t.$$

Henceforth we will omit the asterisk on k_l^*.

We will introduce the energy accommodation coefficients, defined by the translational and rotational degrees of freedom respectively

$$\alpha_t = \frac{E_i^t - E_r^t}{E_i^t - E_s^t}, \quad \alpha_\omega = \frac{E_i^\omega - E_r^\omega}{E_i^\omega - E_s^\omega} \tag{1.6}$$

Here we have introduced the energy fluxes of the translational and rotational motions of the molecules incident on the wall (the subscript *i*), reflected from the wall (the subscript *r*), and also the fluxes from the wall corresponding to the thermodynamic equilibrium of the wall and the gas

$$E_i^t = -\int_{c_x<0} c^2 c_x \varphi(0, \mathbf{c}, \nu) d\Omega, \quad E_i^\omega = -\int_{c_x<0} \nu^2 c_x \varphi(0, \mathbf{c}, \nu) d\Omega$$

$$E_r^t = \int_{c_x>0} c^2 c_x \varphi_0(\mathbf{c}, \nu) d\Omega, \quad E_r^\omega = \int_{c_x>0} \nu^2 c_x \varphi_0(\mathbf{c}, \nu) d\Omega$$

$$E_s^t = \int_{c_x>0} c^2 c_x \varphi_s(0, \mathbf{c}, \nu) d\Omega, \quad E_s^\omega = \int_{c_x>0} \nu^2 c_x \varphi_s(0, \mathbf{c}, \nu) d\Omega$$

$$\varphi_s(0, \mathbf{c}, \nu) = \varepsilon_n + \varepsilon_t(c^2 + \nu^2 - l - \tfrac{1}{2}), \quad c_x > 0 \tag{1.7}$$

where $\varphi_s(0, c, \nu)$ is the distribution function with equilibrium values of the wall parameters and ε_n is an unknown quantity.

The impermeability conditions for the boundary of the half-space have the form

$$N_i = N_s, \quad N_i = N_r \tag{1.8}$$

Here

$$N_i = -\int_{c_x<0} c_x \varphi(0, \mathbf{c}, \nu) d\Omega, \quad N_r = \int_{c_x>0} c_x \varphi_0(0, \mathbf{c}, \nu) d\Omega$$

$$N_s = \int_{c_x>0} c_x \varphi_s(0, \mathbf{c}, \nu) d\Omega$$

(N_i is the flux of incident molecules, N_r is the flux of reflected molecules, and N_s is the flux of molecules corresponding to thermodynamic equilibrium).

Note that the second term in the expression for the kernel *g* makes no contribution to the right-hand side of Eq. (1.2), since the integral $\int c_x' \varphi d\Omega$ is proportional to the mass flux, which in this problem is equal to zero. The factor $c^2 + \nu^2 - l - 1/2$ in the next term of the kernel *g* can be represented in the form of the sum of two terms, equal to the factors of ε_t^t and ε_t^ω in expression (1.4). Consequently, the function φ is best sought in the form

$$\varphi = h_1(x, \mu) + (c^2 - \tfrac{3}{2}) h_2(x, \mu) + (\nu^2 - l + 1) h_3(x, \mu), \quad \mu = c_x \tag{1.9}$$

We obtain the vector equation

$$\mu \frac{\partial h}{\partial x} + h(x, \mu) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} \exp(-\mu'^2)(E + 2\mu\mu' F) K_0(\xi') h(x, \mu') d\mu' \tag{1.10}$$

Here

$$h(x, \mu) = \mathrm{col}\{h_1(x, \mu), \ h_2(x, \mu), \ h_3(x, \mu)\}, \quad \xi = \xi(\mu) = \mu^2 - \tfrac{1}{2}, \quad \xi' = \xi(\mu')$$

$$K_0(\xi) = \begin{Vmatrix} 1 & \xi & 0 \\ \xi/(l+1/2) & (\xi^2+1)/(l+1/2) & l/5 \\ \xi/(l+1/2) & (\xi^2+1)/(l+1/2) & l/5 \end{Vmatrix}, \quad F_0 = \begin{Vmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{Vmatrix}$$

where *E* is the 3×3 identity matrix.

Boundary conditions (1.3)–(1.5) can be converted into the following

$$h(0,\mu)=h_0,\quad \mu>0 \tag{1.11}$$

$$h(x,\mu)=h_{as}(x,\mu)+o(1),\quad x\to+\infty,\quad \mu<0$$

where

$$h_0=\mathrm{col}\{\varepsilon_n^r,\varepsilon_t^t,\varepsilon_t^\omega\},\quad h_{as}(x,\mu)=k_t(x-\mu)\mathrm{col}\{-1,1,1\} \tag{1.12}$$

We will introduce the new unknown function $h_4(x,\mu)=h_2(x,\mu)-h_3(x,\mu)$. Then, instead of (1.10) we obtain the following system of equations

$$\mu\frac{\partial h_1}{\partial x}+h_1(x,\mu)=\frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty}\exp(-\mu'^2)(1+2\mu\mu')[h_1(x,\mu')+\xi(\mu')h_2(x,\mu')]d\mu'$$

$$\mu\frac{\partial h_2}{\partial x}+h_2(x,\mu)=\frac{1}{\sqrt{\pi}(l+1/2)}\int_{-\infty}^{\infty}\exp(-\mu'^2)\{(\xi(\mu')h_1(x,\mu')+ \tag{1.13}$$

$$+[(\xi(\mu')^2+l]h_2(x,\mu')-h_4(x,\mu)\}d\mu'$$

$$\mu\frac{\partial h_4}{\partial x}+h_4(x,\mu)=0$$

The last equation has the obvious solution

$$h_4(x,\mu)=(\varepsilon_t^t-\varepsilon_t^\omega)\exp(-x/\mu)(1+|\mu|/\mu)/2 \tag{1.14}$$

We will further consider the first two equations of (1.13), using expression (1.14) in the last equation. We will represent this system in vector form

$$\mu\frac{\partial h}{\partial x}+(x,\mu)=\frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty}\exp(-\mu'^2)(E+2\mu\mu'F)K(\xi')h(x,\mu')d\mu'-$$

$$-\begin{Vmatrix}0\\ \gamma\end{Vmatrix}\frac{1}{\sqrt{\pi}}\int_0^{\infty}\exp\left(-\mu'^2-\frac{x}{\mu'}\right)d\mu',\quad h=\begin{Vmatrix}h_1\\ h_2\end{Vmatrix},\quad \gamma=\frac{l}{5}(\varepsilon_t^t-\varepsilon_t^\omega) \tag{1.15}$$

Here E is the 2×2 identify matrix

$$F=\begin{Vmatrix}1&0\\0&0\end{Vmatrix},\quad K(\xi)=\begin{Vmatrix}1&\xi\\ \xi/(l+½)&(\xi^2+1)/(l+½)\end{Vmatrix}$$

Later we will solve the boundary-value problem consisting of Eq. (1.15) and boundary conditions of the form (1.11), but now, instead of expressions (1.12), the following will occur in these conditions

$$h_0=\mathrm{col}\{\varepsilon_n^r,\varepsilon_t^t\},\quad h_{as}(x,\mu)=k_t(x-\mu)\mathrm{col}\{-1,1\}$$

We will call this Problem A.

2. ANALYTICAL SOLUTION OF PROBLEM A

Separation of the variables in the homogeneous equation corresponding to (1.15),

$$h_\eta(x,\mu)=\exp(-x/\eta)\Phi(\eta,\mu)$$

where η is a spectral parameters, leads to the following characteristic equation

$$(\eta-\mu)\Phi(\eta,\mu)=\frac{1}{\sqrt{\pi}}\eta[n^{(0)}(\eta)+2\mu En^{(1)}(\eta)-\exp(-\eta^2)\mathrm{col}\{0,\gamma\}]$$

Here

$$n^{(j)}(\eta) = \int_{-\infty}^{\infty} \exp(-\mu^2)\mu^j K(\mu)\Phi(\eta,\mu)d\mu, \quad j = 0,1 \tag{2.1}$$

The characteristic equation, after some reduction, simplifies to

$$(\eta-\mu)\Phi(\eta,\mu) = \frac{1}{\sqrt{\pi}}A(\eta), \quad A(\eta) = n^{(0)}(\eta) - \exp(-\eta^2)\operatorname{col}\{0,\gamma\} \tag{2.2}$$

From Eqs (2.1) and (2.2) when $\eta \in (0, +\infty)$ we obtain the eigenvectors [11]

$$\Phi(\eta,\mu) = \Phi^{(0)}(\eta,\mu)A(\eta) + K^{-1}(\eta)\operatorname{col}\{0,\gamma\} \tag{2.3}$$

$$\Phi^{(0)}(\eta,\mu) = \frac{1}{\sqrt{\pi}}\eta P\frac{1}{\eta-\mu}E + \exp(\eta^2)B(\eta)\delta(\eta-\mu)$$

Here

$$B(z) = K^{-1}(z)\Lambda(z) = \lambda_c(z)E + \frac{1}{2l}Q(z)$$

$$\Lambda(z) = E + z\frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty} \exp(-\mu^2)K(\mu)\frac{d\mu}{\mu-z}$$

$$\lambda_c(z) = 1 - 2z\exp(-z^2)\int_0^z \exp(u^2)du \pm i\sqrt{\pi}z\exp(-z^2), \quad \pm\operatorname{Im} z > 0$$

$$Q(z) = \begin{Vmatrix} -\xi(z) & l-\xi(z) \\ 1 & 1 \end{Vmatrix}$$

Px^{-1} denotes the principal value of the integral when integrating x^{-1}, $\delta(x)$ is the Dirac delta function and $\Lambda(z)$ is the dispersion matrix.

We will seek a solution of Problem A in the form of an expansion in eigenvectors (2.3)

$$h(x,\mu) = h_{\text{as}}(x,\mu) + \int_0^{\infty} \exp(-x/\eta)\Phi(\eta,\mu)d\eta$$

or, in more detail,

$$h(x,\mu) = k_t(x-\mu)\begin{Vmatrix} -1 \\ 1 \end{Vmatrix} + \frac{1}{\sqrt{\pi}}\int_0^{\infty} \exp\left(-\frac{x}{\eta}\right)\frac{\eta A(\eta)}{\eta-\mu}d\eta +$$

$$+\left[\exp\left(\mu^2 - \frac{x}{\mu}\right)B(\mu)A(\mu) + \exp\left(-\frac{x}{\mu}\right)K^{-1}(\mu)\begin{Vmatrix} 0 \\ \gamma \end{Vmatrix}\right]\frac{\mu+|\mu|}{2\mu} \tag{2.4}$$

The vector function $A(\eta) = \operatorname{col}\{A_1(\eta), A_2(\eta)\}$ is the unknown in these expansions.

Substituting expression (2.4) into the first of boundary conditions (1.11) we obtain a singular integral equation with a Cauchy kernel

$$\begin{Vmatrix} k_t\mu - \varepsilon_n^r \\ -k_t\mu - \varepsilon_t^t \end{Vmatrix} + \frac{1}{\sqrt{\pi}}\int_0^{\infty} \frac{\eta A(\eta)}{\eta-\mu}d\eta + \exp(\mu^2)B(\mu)A(\mu) + K^{-1}(\mu)\begin{Vmatrix} 0 \\ \gamma \end{Vmatrix} = \begin{Vmatrix} 0 \\ 0 \end{Vmatrix}, \quad \mu > 0 \tag{2.5}$$

We substitute expansion (1.9) into the expression for N_i, (1.4) into the expression for N_r, and (1.7) into the expression for N_s. We obtain the following relations

$$N_i = \int_{c_x>0} c_x\left[h_1(0,c_x) + \left(c^2 - \frac{3}{2}\right)h_2(0,c_x)\right]d\Omega - \int c_x\varphi(0,\mathbf{c},\nu)d\Omega = N_r - \int c_x\varphi(0,\mathbf{c},\nu)d\Omega$$

$$N_r = \frac{1}{\sqrt{\pi}}\left(\frac{1}{2}\varepsilon_n^r + \frac{1}{4}\varepsilon_t^t\right), \quad N_s = \frac{1}{\sqrt{\pi}}\left(\frac{1}{2}\varepsilon_n + \frac{1}{4}\varepsilon_t\right)$$

It follows from the second condition of (1.8) that the total flux is equal to zero – this condition is automatically satisfied (this can be verified directly), while the first condition of (1.8) gives the equality

$$\varepsilon_t - \varepsilon_t^t - 2\varepsilon_n^r - 2\varepsilon_n = 0$$

We now turn to Eqs (1.6). For these equations we obtain

$$E_s^t = \frac{1}{\sqrt{\pi}}\left(\varepsilon_n + \frac{3}{2}\varepsilon_t\right), \quad E_s^\omega = \frac{l-1}{\sqrt{\pi}}\left(\frac{1}{2}\varepsilon_n + \frac{3}{4}\varepsilon_t\right)$$

$$E_r^\omega = \frac{l-1}{\sqrt{\pi}}\left(\frac{1}{2}\varepsilon_n^r + \frac{1}{4}\varepsilon_t^t + \frac{1}{2}\varepsilon_t^\omega\right)$$

The energy flux of translational motion of the molecules incident on the wall can be represented in the form

$$E_i^t = -E_0^t + E_r^t \tag{2.6}$$

$$E_0^t = \int c^2 c_x \varphi d\Omega = \int c^2 c_x [h_1(0, c_x) + \left(c^2 - \frac{3}{2}\right) h_2(0, c_x)] d\Omega =$$

$$= \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} \exp(-\mu'^2)\mu'[(\mu'^2 + 1)h_1(0, \mu') + \left(\mu'^4 + \frac{1}{2}\mu'^2 + \frac{1}{2}\right) h_2(0, \mu')] d\mu'$$

In exactly the same way, the energy flux of the rotational motion of the molecules incident on the wall can be expressed in the form

$$E_i^\omega = -E_0^\omega + E_r^\omega \tag{2.7}$$

$$E_0^\omega = \int \nu^2 c_x \varphi d\Omega = \frac{l-1}{\sqrt{\pi}} \int_{-\infty}^{\infty} \exp(-\mu'^2)\mu'[h_1(0, \mu') + \left(\mu'^2 + \frac{1}{2}\right) h_2(0, \mu')] d\mu'$$

To calculate E_0^t and E_0^ω we use the following representations

$$h_j(0, \mu) = (-1)^{j+1} k_t \mu + \int_0^\infty [\Phi_{j1}^{(0)}(\eta, \mu) A_1(\eta) + \Phi_{j2}^{(0)}(\eta, \mu) A_2(\eta)] d\eta, \quad j = 1, 2$$

We put

$$n_{mj}^{(2g+1)}(\eta) = \int_{-\infty}^{\infty} \exp(-\mu^2)\mu^{2g+1}\Phi_{mj}^{(0)}(\eta, \mu) d\mu, \quad g = 0, 1, 2; \quad m, j = 1, 2$$

Then, the expression for the flux of translational energy takes the form

$$E_0^t = -\frac{5}{4}k_t + \frac{1}{\sqrt{\pi}} \int_0^\infty \sum_{j=1}^{3} A_j(\eta)\left[n_{1j}^{(1)}(\eta) + \frac{1}{2}n_{2j}^{(1)}(\eta) + n_{1j}^{(3)}(\eta) + \frac{1}{2}n_{2j}^{(3)}(\eta) + n_{2j}^{(5)}(\eta)\right] d\eta$$

Direct calculations show that

$$n^{(1)}(\eta) = \frac{1}{2l}Q(\eta), \quad n^{(3)}(\eta) = -\frac{1}{2}\eta E + \frac{1}{2l}\eta^3 Q(\eta)$$

$$n^{(5)}(\eta) = \left(-\frac{3}{4}\eta - \frac{1}{2}\eta^3\right)E + \frac{1}{2l}\eta^5 Q(\eta)$$

Using these equations we obtain that

$$E_0^t = -\frac{5}{4}k_t - I, \quad E_0^\omega = -\frac{l-1}{2}k_t + I, \quad I = \frac{1 - l^{-1}}{2\sqrt{\pi}} \int_0^\infty \eta[A_1(\eta) + A_2(\eta)] d\eta$$

Now, from Eqs (1.6), using expressions (2.6) and (2.7), we obtain

$$(\alpha_\varsigma^{-1}-1)E_0^\varsigma+E_r^\varsigma-E_s^\varsigma=0,\quad \varsigma=t,\omega$$

Further, we obtain (see [6–8]) an analytical solution of Eq. (2.5) and, calculating it using integral I, we obtain the following missing equations for determining all the unknown parameters

$$\begin{aligned}
&\alpha_2=(1-l^{-1})(-\varepsilon_t^t+\varepsilon_t^\omega)p_0,\quad q_0\alpha_1+q_1\alpha_2=k_t q_0^2\\
&l^{-1}\varepsilon_t^t+(1-l^{-1})\varepsilon_t^\omega+(p_0-q_0)\alpha_2+p_0\beta_0=p_1p_0^{-1}k_t\\
&-2^{-1}(1-l^{-1})\varepsilon_t^t+2^{-1}(1-l^{-1})\varepsilon_t^\omega+\varepsilon_n^r+(q_2+q_0-p_0)\alpha_2+q_1\alpha_1+q_0\alpha_0-(p_0-q_0)\beta_0=\\
&=-k_tq_0(p_1-q_1)\\
&\mu_0\alpha_1-\alpha_0+\delta\beta_0=-k_t\mu_0\delta q_0\quad(\alpha-\delta)\beta_{-1}=\mu_0^2(\delta q_0k_t-\alpha_1)\\
&\mu_0^2\alpha_2+\mu_0\alpha_1+\alpha_0-\alpha\beta_0-\alpha'\beta_{-1}=-\alpha\mu_0q_0k_t\\
&(\alpha_t^{-1}-1)[q_3\alpha_2+q_2\alpha_1+q_1(\alpha_0+\beta_0)+q_0(1+\alpha)\beta_{-1}]+\\
&+\frac{1}{\sqrt{\pi}(1-l^{-1})}[2\varepsilon_n^r+3\varepsilon_t^t-2\varepsilon_n-3\varepsilon_t]=(\alpha_t^{-1}-1)k_t\left[\frac{5}{2(1-l^{-1})}+q_0q_2\right]\\
&(\alpha_w^{-1}-1)[q_3\alpha_2+q_2\alpha_1+q_1(\alpha_0+\beta_0)+q_0(1+\alpha)\beta_{-1}]-\\
&-\frac{l}{2\sqrt{\pi}}[2\varepsilon_n^r+\varepsilon_t^t+2\varepsilon_t^\omega-2\varepsilon_n-3\varepsilon_t]=(\alpha_\omega^{-1}-1)k_t(-l+q_0q_2)
\end{aligned}\tag{2.8}$$

In these equations

$$\begin{aligned}
&p_0=\exp(-S_2),\quad q_0=1/p_0,\quad p_1=p_0(-R_1-S_3),\quad q_1=q_0(-R_1+S_3)\\
&q_2=q_0\left(-R_2+S_4-\frac{3}{2}S_2\right)+\frac{1}{2}q_1(-R_1+S_3),\quad q_3=q_0\left(-R_3+S_5-\frac{3}{2}S_3\right)+\\
&+\frac{2}{3}q_1\left(-R_2+S_4-\frac{3}{2}S_2\right)+\frac{1}{3}q_2(-R_1+S_3),\quad \delta=\frac{1}{2}\left(r(0)-\frac{1}{2}\right)\\
&\alpha=-\frac{1}{2}\left(r(\mu_0)+\mu_0^2+\frac{1}{2}\right),\quad \alpha'=-\frac{\mu_0}{r(\mu_0)}\left[r(\mu_0)+\mu_0^2-\frac{3}{2}\right]
\end{aligned}$$

The point μ_0 is found from the equation $S_1=0$ (a special case of the problem of Jacobi inversion for elliptic integrals), where

$$\begin{aligned}
&S_n=-\frac{1}{2\pi}\int_0^\infty\frac{\theta_1(u)-\theta_2(u)}{r(u)}u^{n-1}du-\int_0^{\mu_0}\frac{u^{n-1}}{r(u)}du\\
&R_n=-\frac{1}{2\pi}\int_0^\infty(\theta_1(u)+\theta_2(u))u^{n-1}du,\quad n=1,2,3\ldots\\
&\theta_j(u)=-\frac{\pi}{2}-\operatorname{arctg}\frac{\Omega_j(u)}{\sqrt{\pi}u\exp(-u^2)},\quad r(z)=\sqrt{\left(z^2-\frac{3}{2}\right)^2+4l}\\
&\Omega_j(z)=\lambda_c(z)+\frac{1}{4l}\left(\frac{3}{2}-z^2+(-1)^jr(z)\right),\quad j=1,2,\quad l=2,\frac{5}{2}
\end{aligned}$$

The solution of system of linear equations (2.8) leads to the following expression for the temperature jump

$$\varepsilon_t=D(\alpha_t,\alpha_\omega)k_t$$

where

$$D = 1.13019\frac{1 - 0.44595\alpha_t - 0.04272\alpha_\omega + 0.00755\alpha_t\alpha_\omega}{0.36436\alpha_t + 0.18219\alpha_\omega - 0.02768\alpha_t\alpha_\omega}$$

for a diatomic gas and

$$D = 1.19044\frac{1 - 0.43332\alpha_t - 0.17771\alpha_\omega + 0.07572\alpha_t\alpha_\omega}{0.33582\alpha_t + 0.25186\alpha_\omega - 0.12298\alpha_t\alpha_\omega}$$

for a polyatomic gas.

Note that when $\alpha_t = \alpha_\omega = 1$ the last formulae give respectively: $\varepsilon_t = 1.13019\ k_t$ for a diatomic gas and $\varepsilon_t = 1.19044\ k_t$ for a polyatomic gas, which agrees exactly with known results [8]. We will use the definition of the mean free path [12] $\lambda = \eta\rho^{-1}\ (\pi m/(2kT_s))^{1/2}$, where η is the dynamic viscosity and ρ is the density of the gas. This expression can be rewritten in the equivalent form $\lambda = \chi\mathrm{Pr}(\pi m/(2kT_s))^{1/2}$, where χ is the thermal diffusivity and Pr is the Prandtl number. The expression for the coefficient C_t, introduced by equality (1), can then be represented in the form $C_t = ({}^2\!/_3\mathrm{Pr})C_t^*$, where $C_t^* = 2.01497D(\alpha_t, \alpha_\omega)$ for a diatomic gas and $C_t^* = 2.11571D(\alpha_t, \alpha_\omega)$ for a polyatomic gas.

Note that when one of the quantities α_t or α_ω approaches zero the temperature jumps of the molecular gas remain finite. Only when α_t and α_ω simultaneously approach zero do the expressions for the temperature jump diverge. This is due to the fact that, in the latter case, thermal contact between the gas and the solid breaks down.

The figure shows the temperature jump coefficient of a diatomic gas (a) and a polyatomic gas (b) as a function of the accommodation coefficient α_t for different values of α_ω. It can be seen from an analysis of the graphs that the difference in the behaviour of diatomic and polyatomic gases increases as the accommodation coefficient of the rotational energy of the molecules decreases. This is due to the fact that a reduction in the value of the accommodation coefficient of the rotational energy of the molecules manifests itself in a different way in the case of diatomic and polyatomic gases. A reduction in the value of α_ω reduces the heat exchange of a solid with two-degree-of-freedom diatomic gas and with three-degree-of-freedom polyatomic gas.

The value of the temperature jump in a diatomic gas when $\alpha_\omega = 0$ and $\alpha_t = 1$ is equal to $\varepsilon_t = 1.71854\ k_t$, which is 52% greater than the value of the temperature jump for complete accommodation. For a polyatomic gas, for the similar case, we have $\varepsilon_t = 2.00883\ k_t$, which is 69% greater than the value of the temperature jump for complete accommodation. It follows from a comparison of these quantities

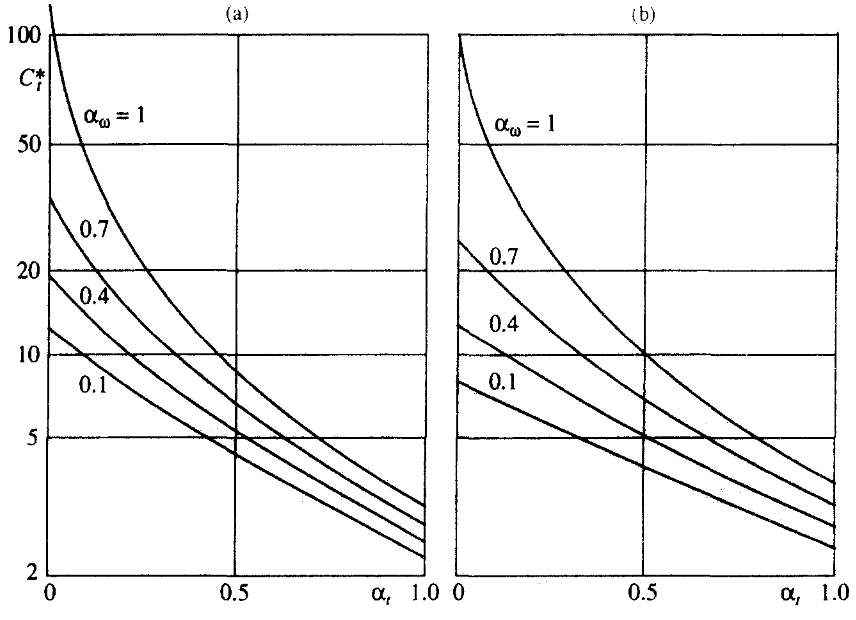

Fig. 1

that the value of the accommodation coefficient of the rotational energy of the molecules in fact has a more pronounced effect on the temperature jumps in a polyatomic gas than in a diatomic gas.

The formulae derived for the temperature jump of a molecular gas can be used when analysing the dynamics of moderately large aerosol particles, when analysing an experiment to determine the thermal conductivity of molecular gases and in other problems related to heat exchange between a molecular gas and a solid.

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