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ANALYTICAL CALCULATION OF THE PARAMETERS OF A MOLECULAR GAS ON A SURFACE IN THE SMOLUCHOWSKI PROBLEM

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An analytical solution of the classical Smoluchowski problem on the temperature jump in molecular (monatomic, diatomic, and polyatomic) gases is presented. The gas occupies a half-space above a flat wall, with a constant temperature gradient and evaporation rate from the "gas–condensed phase" interface set far from this wall. The distribution function is explicitly constructed both in the half-space and at its boundary. Formulas for the concentration and temperature at the interface are derived; in the case of diatomic and polyatomic gases, formulas for temperatures determined by translational and rotational degrees of freedom of molecules are obtained. Numerical calculations are performed.

Introduction. The classical Smoluchowski problem of the jumps of temperature and concentration of a rarefied gas above a flat surface, with a temperature gradient perpendicular to the surface, which is set far from the latter, has been studied for a long time (see, for instance [1, 2] and the bibliography in [3]). This problem is closely associated with the problem of weak evaporation (condensation): determination of the temperature and concentration jumps, with a constant rate of evaporation (condensation) of a saturated vapor to a half-space being set.

The Bhatnagar–Gross–Krook (BGK) equation is widely used now to study heat transfer and evaporation. Thus, the problem of evaporation of a simple (monatomic) gas into vacuum from cylindrical and spherical surfaces within a wide range of Knudsen numbers was numerically solved in [4, 5] on the basis of this equation.

The Smoluchowski problem for a monatomic gas was analytically solved with the use of the BGK equation in [3, 6, 7]. Kinetic models for diatomic and polyatomic gases were proposed in [8] and [9], respectively. Exact expressions for the temperature and concentration jumps for diatomic and polyatomic gases were also obtained in [9], and numerical calculations were performed. The question of determination of translational and rotational temperatures remains open. It should be noted that these temperatures coincide far from the surface.

We assume that the relative temperature difference within the mean free path is much smaller than unity: $lK \ll 1$ (l is the mean free path of molecules and K is the logarithmic temperature gradient), and the evaporation (condensation) rate U is much smaller than the velocity of sound. If these conditions are satisfied, the kinetic equation may be linearized.

In the present work, the distribution function for monatomic, diatomic, and polyatomic gases is constructed in an explicit form. Generic formulas for temperature and concentration jumps are given for monatomic, diatomic, and polyatomic gases. Exact formulas for the relative concentration and temperature determined by translational and rotational degrees of freedom are derived analytically. Numerical calculations are performed using the exact formulas.

It should be noted that the temperature and concentration jumps were found in [10] by the variational method for the case of the Lennard-Jones and $n(r)$–6 potentials. In [11], these quantities and the parameters of the monatomic gas near the surface were calculated numerically on the basis of the Boltzmann equation for molecules

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treated as solid spheres. The gas behavior between two parallel planes, where evaporation or condensation occurs, was studied in [12]. The major attention was paid to the transitional regime in terms of the Knudsen number.

We consider a monatomic, diatomic, or polyatomic gas, which occupies a half-space $x > 0$ above a flat surface of the condensed phase. Evaporation and condensation processes may occur on the surface. There is a temperature gradient far from the surface, which is perpendicular to the latter. We introduce a Cartesian coordinate system with the origin on the surface; the region filled by the gas corresponds to the positive values of x. Then, we have $T = T_1 + Ax$ ($x \to \infty$), where $A = (dT/dx)_{x=\infty}$. We denote the surface temperature as $T_{\rm s}$, then, the temperature jump is $\Delta T = T_1 - T_{\rm s}$. In the linear approximation, the temperature jump is proportional to the temperature gradient: $\Delta T = C_{\rm t} l A$, where $C_{\rm t}$ is an unknown coefficient of proportionality, which is called the temperature-jump coefficient. Far from the surface, the gas (vapor) motion toward the surface or away from it is also possible, which corresponds to condensation or evaporation. In this case, the gas concentration and temperature can be found in the linear approximation from the following relations:

$$\varepsilon_n = \frac{n - n_{\rm s}}{n_{\rm s}} = N_1 U, \qquad \varepsilon_{\rm t} = \frac{T - T_{\rm s}}{T_{\rm s}} = N_2 U.$$

Here $n_{\rm s}$ is the concentration of the saturated vapor at a temperature $T_{\rm s}$.

We call both problems (on temperature and concentration jumps) in the presence of both the temperature gradient far from the wall and a constant mass flow the Smoluchowski problem, since they differ insignificantly only in boundary conditions.

1. Distribution Function in the Half-Space and at Its Boundary. For a monatomic gas, the Smoluchowski problem is to find a solution of the BGK equation

$$C_x \frac{\partial \varphi}{\partial x} + \varphi(x, \boldsymbol{C}) = \int k(\boldsymbol{C}; \boldsymbol{C}')\varphi(x, \boldsymbol{C}')\, dm \tag{1.1}$$

that satisfies the boundary conditions

$$\varphi_{x=0} = 0, \quad C_x > 0; \qquad \varphi_{x\to\infty} = \varphi_{as} + O(1), \quad C_x < 0. \tag{1.2}$$

Here $dm = \pi^{-3/2} \exp{(-C^2)} d^3C$, $k(\boldsymbol{C}, \boldsymbol{C}') = 1 + 2C_x C_x' + (2/3)(C^2 - 3/2)(C'^2 - 3/2)$, $\varphi_{as} = \varepsilon_n + 2UC_x + \varepsilon_{\rm t}(C^2 - 3/2) + K(x - C_x)(C^2 - 5/2)$, $\varepsilon_{\rm t}$ is the temperature jump, and ε_n is the concentration jump.

For diatomic and N-atomic gases ($N > 2$), the Smoluchowski problem consists in solving the equation [6]

$$C_x \frac{\partial \varphi}{\partial x} + \varphi(x, \boldsymbol{C}, \nu) = \int k(\boldsymbol{C}, \nu; \boldsymbol{C}', \nu')\varphi(x, \boldsymbol{C}', \nu')\, dm$$

with the kernel

$$k(\boldsymbol{C}, \nu; \boldsymbol{C}', \nu') = 1 + 2C_x C_x' + \frac{1}{l + 1/2}\,(C^2 + \nu^2 - l - 1/2)(C'^2 + \nu'^2 - l - 1/2)$$

($l = 2$ for a diatomic gas and $l = 5/2$ for a polyatomic gas) and the boundary conditions (1.2), in which we have

$$\varphi_{as} = \varepsilon_n + 2UC_x + \varepsilon_{\rm t}(C^2 + \nu^2 - l - 1/2) + K(x - C_x)(C^2 + \nu^2 - l - 3/2)$$

with

$$dm = 2\pi^{-3/2} \exp{(-C^2 - \nu^2)} \nu\, d\nu\, d^3C$$

for the diatomic gas and

$$dm = \pi^{-3} \exp{(-C^2 - \nu^2)}\, d^3\nu\, d^3C$$

for the polyatomic gas. Here ν is the dimensionless angular velocity of revolution of the molecule ($0 < \nu < \infty$).

The solution of problem (1.1), (1.2) is sought in the form

$$\varphi(x, \boldsymbol{C}, \nu) = h_1(x, \mu) + (C^2 - 3/2) h_2(x, \mu) \qquad (\mu = C_x)$$

in the case of a monatomic gas or

$$\varphi(x, \boldsymbol{C}, \nu) = h_1(x, \mu) + (C^2 + \nu^2 - l - 1/2) h_2(x, \mu)$$

in the case of an N-atomic gas ($N \geqslant 2$).

For all gases (monatomic, diatomic, and polyatomic), the Smoluchowski problem reduces to solving the vector equation

$$\mu \frac{\partial h}{\partial x} + h(x,\mu) = \frac{1}{\sqrt{\pi}} \int\limits_{-\infty}^{\infty} \exp(-\mu'^2) K_0(\mu,\mu') h(x,\mu')\, d\mu' \tag{1.3}$$

(relative to the vector-column with elements h_1 and h_2) with the boundary conditions

$$h(0,\mu) = \mathbf{0}, \qquad 0 < \mu < \infty, \qquad \mathbf{0} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \tag{1.4}$$

$$h(x,\mu) = h_{as}(x,\mu) + O(1), \qquad x \to \infty, \qquad \mu < 0. \tag{1.5}$$

Here

$$h_{as}(x,\mu) = \begin{bmatrix} \varepsilon_n + 2U\mu - K(x-\mu) \\ \varepsilon_{\rm t} + K(x-\mu) \end{bmatrix}, \qquad K_0(\mu,\mu') = \left[E + 2\mu\mu' \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}\right] K(\mu'),$$

E is the unit matrix, and

$$K(\mu) = \begin{bmatrix} 1 & \mu^2 - 1/2 \\ 2/(2l+1)(\mu^2 - 1/2) & 2/(2l+1)[(\mu^2 - 1/2)^2 + l] \end{bmatrix},$$

where $l = 1$ for a monatomic gas, $l = 2$ for a diatomic gas, and $l = 5/2$ for an N-atomic gas ($N \geqslant 3$).

2. Analytical Solution of the Smoluchowski Problem. According to the general Fourier method, separation of variables in Eq. (1.3) yields the expression

$$h_\eta(x,\mu) = \exp(-x/\eta)\Phi(\eta,\mu), \tag{2.1}$$

where η is the spectral parameter or the separation parameter, which is complex in the general case. Substitution of (2.1) into Eq. (1.3) yields the characteristic equation

$$(\eta - \mu)\Phi(\eta,\mu) = \eta \frac{1}{\sqrt{\pi}} \int\limits_{-\infty}^{\infty} \exp(-\mu'^2) K_0(\mu,\mu') \Phi(\eta,\mu')\, d\mu'. \tag{2.2}$$

We assume that $\Phi(\eta,\mu)$ satisfies the condition

$$\frac{1}{\sqrt{\pi}} \int\limits_{-\infty}^{\infty} \exp(-\mu'^2) K_0(\mu,\mu') \Phi(\eta,\mu')\, d\mu' = E. \tag{2.3}$$

From Eqs. (2.2) and (2.3) for $\eta \in (-\infty,\infty)$ in the half-space of generalized functions [13], we find the matrix eigenfunction

$$\Phi(\eta,\mu) = \frac{1}{\sqrt{\pi}} \eta P \frac{1}{\eta - \mu} E + \exp(\eta^2) B(\eta) \delta(\eta - \mu), \tag{2.4}$$

where Px^{-1} is the distribution (main value of the integral in integration of x^{-1}), $\delta(x)$ is the Dirac delta function, and $B(z) = K^{-1}(z)\Lambda(z)$. Here $\Lambda(z)$ is the dispersion matrix function of the problem

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

$$B(z) = \lambda_c(z) E + \frac{1}{2l} Q(z), \qquad Q(z) = \begin{bmatrix} 1/2 - z^2 & 1/2 + l - z^2 \\ 1 & 1 \end{bmatrix},$$

and $\lambda_c(z)$ is the Cercignani dispersion function

$$\lambda_c(z) = 1 - 2z\exp(-z^2) \int\limits_0^z \exp(u^2)\, du \pm i\sqrt{\pi} z \exp(-z^2), \quad \pm \mathrm{Im}\, z > 0.$$

It is shown in [8, 9] that problem (1.3)–(1.5) has a unique solution, which may be represented in the form of an expansion in eigenmatrices of the characteristic equation

TABLE 1

Gas	Smoluchowski problem		Problem of weak evaporation	
	$\delta_{\rm t}$	δ_n	$\gamma_{\rm t}$	γ_n
Monatomic	1.30272	−0.744 28	−0.22337	−0.84264
Diatomic	1.21589	−0.674 05	−0.15481	−0.89447
Polyatomic	1.19044	−0.657 06	−0.13335	−0.91042

$$h(x,\mu) = h_{as}(x,\mu) + \int\limits_0^\infty \exp\Big(-\frac{x}{\eta}\Big)\Phi(\eta,\mu)A(\eta)\,d\eta, \tag{2.5}$$

i.e.,

$$h(x,\mu) = h_{as}(x,\mu) + \frac{1}{\sqrt{\pi}}\int\limits_0^\infty \exp\Big(-\frac{x}{\eta}\Big)\Phi(\eta,\mu)A(\eta)\,d\eta + \exp\Big(\mu^2 - \frac{x}{\mu}\Big)B(\mu)A(\mu)\theta_+(\mu). \tag{2.6}$$

Here $A(\mu)$ is an unknown vector-function with elements $a_1(\mu)$ and $a_2(\mu)$, $\theta_+(\mu)$ is the Heaviside function [$\theta_+(\mu) = 1$ for $\mu > 0$ and $\theta_+(\mu) = 0$ for $\mu < 0$].

In proving expansion (2.5), the values of the temperature and concentration jumps are found:

$$\varepsilon_{\rm t} = \delta_{\rm t}K + \gamma_{\rm t}(2U), \qquad \varepsilon_n = \delta_n K + \gamma_n(2U). \tag{2.7}$$

Here $\delta_{\rm t} = -p_1/p_0 + \mu_0(1+\delta_1 D)$, $\gamma_{\rm t} = 2\mu_0 p_0^2 D$, $\delta_n = -\delta_{\rm t} + \mu_0 q_0^2\delta_1(2+\delta_1 D)$, $\gamma_n = q_1/q_0 - \gamma_{\rm t} + \mu_0(1+\delta_1 D)$, $D = 4(3\mu_0^2/2 - r(0)r(\mu_0) - r^2(0))/[r(\mu)(r(\mu_0)+\mu_0^2+r(0))^2]$, $r(x) = \sqrt{q(x)}$, $q(x) = (x^2-3/2)^2+4l$, and $\delta_1 = r(0)/2+3/4$; the point μ_0 is found from the equation $B_1 + R_1(\mu_0) = 0$ (special case of the problem of the Jacobi conversion for elliptical integrals);

$$B_n = -\frac{1}{2\pi}\int\limits_0^\infty \frac{b(\tau)}{r(\tau)}\,\tau^{n-1}\,d\tau; \qquad R_n(\mu_0) = -\int\limits_0^{\mu_0} \frac{\tau^{n-1}}{r(\tau)}\,d\tau;$$

$$b(\tau) = \theta_1(\tau) - \theta_2(\tau); \qquad p_1/p_0 = -A_1 - B_3 - R_3(\mu_0);$$

$$q_1/q_0 = -A_1 + B_3 + R_3(\mu_0); \qquad A_n = -\frac{1}{2\pi}\int\limits_0^\infty a(\tau)\tau^{n-1}, \qquad n = 1, 2, 3, \ldots;$$

$$a(\tau) = \theta_1(\tau) + \theta_2(\tau) - 2\pi; \qquad \theta_j(\tau) = \arg\Omega_j^+(\tau); \qquad \theta_j(0) = 0;$$

$$\Omega_j(z) = \lambda_c(z) + (3/2 - z^2)/(4l) + (-1)^{j-1}r(z)/(4l), \qquad j = 1,\ 2.$$

Relations (2.7) are the solution of the Smoluchowski problem. We present the results of numerical calculations based on these formulas, which are given in the dimensionless form (see Table 1).

It follows from the results listed in Table 1 that the temperature jump $C_{\rm t}$ for the Prandtl number $\mathrm{Pr} = 2/3$ has the following values: 2.20494 for a monatomic gas, 2.05798 for a diatomic gas, and 2.01490 for a polyatomic gas. The mean free path l was determined in accordance with [2].

In [8, 9], the unknown vector function $A(\mu)$ was also found:

$$2\sqrt{\pi}i\mu A(\mu) = [X^+(\mu) - X^-(\mu)]\Psi(\mu). \tag{2.8}$$

Here $X(z)$ is a matrix that factorizes the coefficient of the uniform Riemann–Hilbert boundary-value problem. The proof of expansion (2.5) or (2.6) reduces to solving the latter problem. The matrix $X(z)$ contains the following elements:

$$X_{11}(z) = \frac{1}{2}\Big[U_1(z)\Big(1 - \frac{z^2+1/2}{r(z)}\Big) + U_2(z)\Big(1 + \frac{z^2+1/2}{r(z)}\Big)\Big],$$

$$X_{12}(z) = -\frac{z^2-l-1/2}{r(z)}\,[U_1(z) - U_2(z)], \qquad X_{21}(z) = \frac{1}{r(z)}\,[U_1(z) - U_2(z)],$$

$$X_{22}(z) = \frac{1}{2}\Big[U_1(z)\Big(1 + \frac{z^2+1/2}{r(z)}\Big) + U_2(z)\Big(1 - \frac{z^2+1/2}{r(z)}\Big)\Big].$$

The vector column $\Psi(\mu)$ has the elements

$$\Psi_1(z) = \alpha_1 z + \alpha_0 + \frac{\alpha_{-1}}{z-\mu_0}, \qquad \Psi_2(z) = \beta_1 z + \beta_0 + \frac{\beta_{-1}}{z-\mu_0}.$$

The expression for $X_{ij}(z)$ contains the functions

$$U_j(z) = \exp\left[-A(z) + (-1)^j r(z)(B(z) + R(\mu_0, z))\right] \quad (j = 1, 2),$$

where

$$A(z) = \frac{1}{2\pi}\int\limits_0^\infty \frac{a(\tau)}{\tau - z}\,d\tau, \quad R(\mu_0, z) = \int\limits_0^{\mu_0} \frac{d\tau}{r(\tau)(\tau - z)}, \quad B(z) = \frac{1}{2\pi}\int\limits_0^\infty \frac{b(\tau)}{r(\tau)}\,\frac{d\tau}{\tau - z}.$$

From relation (2.4), we can obtain

$$\int\limits_{-\infty}^{\infty} \exp(-\mu^2)\Phi(\eta, \mu)\,d\mu = E + \frac{1}{2l}\,Q(\eta).$$

Hence, in accordance with (2.5), we have

$$\frac{1}{\sqrt{\pi}}\int\limits_{-\infty}^{\infty} \exp(-\mu^2)h(x,\mu)\,d\mu = \begin{bmatrix} \varepsilon_n - Kx \\ \varepsilon_{\rm t} + Kx \end{bmatrix} + \frac{1}{\sqrt{\pi}}\int\limits_0^\infty \exp\Big(-\frac{x}{\eta}\Big)\Big[E + \frac{1}{2l}\,Q(\eta)\Big]A(\eta)\,d\eta. \tag{2.9}$$

3. Concentration and Temperature in a Monatomic Gas. The concentration and temperature in a monatomic gas are determined by the relations

$$n(x) = \int f\,d^3v, \qquad T(x) = \frac{2}{3kn(x)}\int f\,\frac{m}{2}\,(\boldsymbol{v} - \boldsymbol{u})^2\,d^3v$$

or, with the use of the function φ,

$$\frac{n(x)}{n_0} = 1 + \pi^{-3/2}\int \exp(-C^2)\varphi(x, \boldsymbol{C})\,d^3C,$$

$$\frac{T(x)}{T_0} = 1 + \frac{2}{3}\,\pi^{-3/2}\int \exp(-C^2)\Big(C^2 - \frac{3}{2}\Big)\varphi(x, \boldsymbol{C})\,d^3C.$$

We express two latter relations via h_1 and h_2:

$$\frac{n(x)}{n_0} = 1 + \frac{1}{\sqrt{\pi}}\int\limits_{-\infty}^{\infty} \exp(-\mu^2)\Big[h_1(x,\mu) + \Big(\mu^2 - \frac{1}{2}\Big)h_2(x,\mu)\Big]\,d\mu; \tag{3.1}$$

$$\frac{T(x)}{T_0} = 1 + \frac{2}{3}\,\frac{1}{\sqrt{\pi}}\int\limits_{-\infty}^{\infty} \exp(-\mu^2)\Big\{\Big(\mu^2 - \frac{1}{2}\Big)h_1(x,\mu) + \Big[\Big(\mu^2 - \frac{1}{2}\Big)^2 + 1\Big]h_2(x,\mu)\Big\}\,d\mu. \tag{3.2}$$

We introduce the vector column $L(x) = \begin{bmatrix} n(x)/n_0 \\ T(x)/T_0 \end{bmatrix}$ and write equalities (3.1) and (3.2) in the vector form:

$$L(x) = 1 + \frac{1}{\sqrt{\pi}}\int\limits_{-\infty}^{\infty} \exp(-\mu^2)K(\mu)h(x,\mu)\,d\mu. \tag{3.3}$$

Substitution of expansion (2.5) or (2.6) into (3.3) yields the following concentration and temperature distributions in the half-space:

$$L(x) = 1 + \begin{bmatrix} \varepsilon_n - Kx \\ \varepsilon_{\rm t} + Kx \end{bmatrix} + \frac{1}{\sqrt{\pi}}\int\limits_0^\infty \exp\Big(-\frac{x}{\eta}\Big)A(\eta)\,d\eta.$$

Using analytical methods, we can find the exact values of the concentration and temperature at the boundary of the half-space, i.e., for $x = 0$. Using (2.8), we obtain

$$L(0) = 1 + \begin{bmatrix} \varepsilon_n \\ \varepsilon_{\rm t} \end{bmatrix} + \frac{1}{2\pi i} \int\limits_0^\infty [X^+(\eta) - X^-(\eta)]\Psi(\eta)\, \frac{d\eta}{\eta}.$$

Avoiding derivation (see [14]), we write the integral representation

$$X(z)\Psi(z) = h_{as}(0, z) + \frac{1}{2\pi i} \int\limits_0^\infty [X^+(\eta) - X^-(\eta)]\Psi(\eta)\, \frac{d\eta}{\eta - z}.$$

Using this representation, we obtain $L(0) = \begin{bmatrix} 1 \\ 1 \end{bmatrix} + \lim\limits_{z\to 0} X(z)\Psi(z)$.

It should be noted that the expression $z^2U_2(z)$ has a finite limit in the zero, since the function $U_2(z)$ has the second-order pole in the zero. We denote $\lim\limits_{z\to 0} z^2U_2(z) = \gamma$. The dispersion function is represented in the form

$$\lambda(z) = \frac{2l}{2l+1}\, \Omega_1(z)\Omega_2(z).$$

At the same time, we can prove (see, for example, [15]) that

$$\lambda(z) = \frac{2l+3}{4(2l+1)U_1(z)U_1(-z)[U_2(z)z^2][U_2(-z)(-z)^2]},$$

whence we obtain

$$\gamma = \frac{1}{2U_1(0)} \sqrt{\frac{2l+3}{2l+1}}, \qquad l = 1, 2, 5/2.$$

The sign of the radical is chosen from the condition of continuity of the function $U_1(z)$. We denote

$$X(z)\Psi(z) = F(z) = \begin{bmatrix} f_1(z) \\ f_2(z) \end{bmatrix}.$$

We calculate the limit

$$\lim_{z\to 0} X(z)\Psi(z) = \begin{bmatrix} f_1 \\ f_2 \end{bmatrix} \equiv F.$$

It is shown that $\varphi(0) = 0$ [9], where $\varphi(z) = -\Psi_1(z) + \delta(z)\Psi_2(z)$ and $\delta(z) = [r(z) - z^2 - 1/2]/2$. Hence, we obtain $\Psi_1(0) = \delta\Psi_2(0)$, where $\delta = \delta(0) = r(0)/2 - 1/4$. As a result, we find

$$F = \Psi_2(0) \lim_{z\to 0} X(z) \begin{bmatrix} \delta \\ 1 \end{bmatrix} = \Psi_2(0) \lim_{z\to 0} \begin{bmatrix} \delta X_{11}(z) + X_{12}(z) \\ \delta X_{21}(z) + X_{22}(z) \end{bmatrix}.$$

Using the expressions for the elements of the matrix $X(z)$, we find the sought limits:

$$f_1 = \Psi_2(0)\Big[\delta U_1(0) + \gamma\, \frac{2(\delta+1)(2\delta+1)}{(4\delta+1)^2}\Big], \quad f_2 = \Psi_2(0)\Big[U_1(0) - \gamma\, \frac{4(\delta+1)}{(4\delta+1)^2}\Big].$$

Thus, we finally obtain the concentration and temperature on the wall:

$$\frac{n(0)}{n_0} = 1 + \delta U_1(0)\Psi_2(0) + \gamma\Psi_2(0)\, \frac{2(\delta+1)}{(4\delta+1)^2}; \tag{3.4}$$

$$\frac{T(0)}{T_0} = 1 + U_1(0)\Psi_2(0) - \gamma\Psi_2(0)\, \frac{4(\delta+1)}{(4\delta+1)^2}. \tag{3.5}$$

According to [14], here we have

$$\Psi_2(0) = \beta_0 - \frac{\beta_{-1}}{\mu_0} = \mu_0 q_0(1 + \delta_1 D_1)K + \mu_0 p_0 D_1(2U),$$

$$D_1 = D - \frac{1}{\alpha - \delta} = 2\, \frac{\mu_0^2 - r(0)}{r(\mu_0)[r(\mu_0) + \mu_0^2 + r(0)]}.$$

4. Concentration and Temperature of Translational and Rotational Degrees of Freedom in an N-atomic Gas ($N \geqslant 2$). The macrocharacteristics of an N-atomic gas ($N \geqslant 3$) are determined by the relations [9, 14]

$$n = \int f \, d^3\omega \, d^3v, \qquad T_v = \frac{2}{3kn} \int f \, \frac{m}{2} (\boldsymbol{v} - \boldsymbol{u})^2 \, d^3\omega \, d^3v,$$

$$\boldsymbol{u} = \frac{1}{n} \int f \boldsymbol{v} \, d^3\omega \, d^3v, \qquad T_\omega = \frac{2}{3kn} \int f \, \frac{1}{2} \sum_{i=1}^{3} J_i \omega_i^2 \, d^3\omega \, d^3v.$$

Here $\boldsymbol{\omega} = (\omega_1, \omega_2, \omega_3)$ is the vector of the dimensional angular velocity of revolution of the molecules and J_1, J_2, and J_3 are the moments of inertia of the molecule.

In the case of a diatomic gas, the molecule has one moment of inertia J, and the macrocharacteristics of the diatomic gas are determined by the following expressions [8, 9]:

$$n = \int f \omega \, d\omega \, d^3v, \qquad T_v = \frac{2}{3kn} \int f \, \frac{m}{2} \, (\boldsymbol{v} - \boldsymbol{u}) \omega \, d\omega \, d^3v,$$

$$\boldsymbol{u} = \frac{1}{n} \int f \boldsymbol{v} \omega \, d\omega \, d^3v, \qquad T_\omega = \frac{2}{3kn} \int f \, \frac{1}{2} \, J\omega^2 \omega \, d\omega \, d^3v.$$

Hereinafter, we consider the cases of diatomic and N-atomic ($N \geqslant 3$) gases together. It should be noted that the concentration distribution in the half-space (3.1) in the cases considered yields the same relation for the concentration on the wall [see (3.4)].

The temperature distributions of translational and rotational degrees of freedom with the use of h_1 and h_2 may be represented as

$$\frac{T_v(x)}{T_0} = 1 + \frac{2}{3} \frac{1}{\sqrt{\pi}} \int\limits_{-\infty}^{\infty} \exp(-\mu^2) \Big\{ \Big(\mu^2 - \frac{1}{2}\Big) h_1(x, \mu) + \Big[\Big(\mu^2 - \frac{1}{2}\Big)^2 + 1 \Big] h_2(x, \mu) \Big\} \, d\mu;$$

$$\frac{T_\omega(x)}{T_0} = 1 + \frac{1}{\sqrt{\pi}} \int\limits_{-\infty}^{\infty} \exp(-\mu^2) h_2(x, \mu) \, d\mu. \tag{4.1}$$

According to (3.3), we have

$$\frac{1}{\sqrt{\pi}} \int\limits_{-\infty}^{\infty} \exp(-\mu^2) K(\mu) h(0, \mu) \, d\mu = \begin{bmatrix} \varepsilon_n \\ \varepsilon_{\rm t} \end{bmatrix} + \frac{1}{\sqrt{\pi}} \int\limits_{0}^{\infty} A(\eta) \, d\eta = \begin{bmatrix} f_1 \\ f_2 \end{bmatrix}.$$

From this equality, using the expression for $\varepsilon_{\rm t}$, we find the translational temperature

$$\frac{T_v(0)}{T_0} = 1 + \frac{2l + 1}{3} \, f_2 - (l - 1) \, \frac{2}{3} \, \frac{1}{\sqrt{\pi}} \int\limits_{-\infty}^{\infty} \exp(-\mu^2) h_2(0, \mu) \, d\mu. \tag{4.2}$$

We have to find the rotational temperature on the wall, i.e., the value of expression (4.1) for $x = 0$. On the basis of (2.9), for $x = 0$, we obtain

$$\frac{1}{\sqrt{\pi}} \int\limits_{-\infty}^{\infty} \exp(-\mu^2) h(0, \mu) \, d\mu = \begin{bmatrix} \varepsilon_n \\ \varepsilon_{\rm t} \end{bmatrix} + \frac{1}{\sqrt{\pi}} \int\limits_{0}^{\infty} R(\eta) A(\eta) \, d\eta, \tag{4.3}$$

where $R(\eta) = E + Q(\eta)/(2l) = R_0 + R_2 \eta^2$,

$$R_0 = \begin{bmatrix} 1 + 1/(4l) & (l + 1/2)/(2l) \\ 1/(2l) & 1 + 1/(2l) \end{bmatrix}, \qquad R_2 = -\frac{1}{2l} \begin{bmatrix} 1 & 1 \\ 0 & 0 \end{bmatrix}.$$

Expanding the matrix $X(z)$ and the vector $\Psi(z)$ for $|z| \to \infty$ into asymptotic series $X(z) = X_0 + X_1/z + \ldots$ and $\Psi(z) = z\Psi_1 + \Psi_0 + \Psi_{-1}/z + \ldots$ and using the method of contour integration, we obtain the following integral representation:

$$R(z)[X(z)\Psi(z) - h_{as}(z)] - R_2(X_0\Psi_{-2} + X_1\Psi_{-1} + X_2\Psi_0)$$

$$- zR_2(X_0\Psi_{-1} + X_1\Psi_0 + X_2\Psi_1) = \frac{1}{\sqrt{\pi}} \int\limits_0^\infty R(\eta)\, \frac{\eta A(\eta)}{\eta - z}\, d\eta.$$

Hence, for $z = 0$, we have

$$\frac{1}{\sqrt{\pi}} \int\limits_0^\infty R(\eta)A(\eta)\, d\eta = R_0 \begin{bmatrix} f_1 - \varepsilon_n \\ f_2 - \varepsilon_{\rm t} \end{bmatrix} - R_2(X_0\Psi_{-2} + X_1\Psi_{-1} + X_2\Psi_0). \tag{4.4}$$

Substituting (4.4) into (4.3) and using the expression for $f_2 - \varepsilon_{\rm t}$ from (4.4), we obtain

$$\frac{1}{\sqrt{\pi}} \int\limits_{-\infty}^\infty \exp(-\mu^2) h_2(0, \mu)\, d\mu = -\frac{1}{2l}\, (\varepsilon_n + \varepsilon_{\rm t}) + \frac{1}{2l}\, f_1 + \frac{2l + 1}{2l}\, f_2. \tag{4.5}$$

To find the translational and rotational temperatures, we substitute (4.5) into (4.2) and (4.1) for $x = 0$:

$$\frac{T_v(0)}{T_0} = 1 + \frac{l - 1}{3l}\, (\varepsilon_n + \varepsilon_{\rm t}) - \frac{l - 1}{3l}\, f_1 + \frac{2l + 1}{3l}\, f_2; \tag{4.6}$$

$$\frac{T_\omega(0)}{T_0} = 1 - \frac{1}{2l}\, (\varepsilon_n + \varepsilon_{\rm t}) + \frac{1}{2l}\, f_1 + \frac{2l + 1}{2l}\, f_2. \tag{4.7}$$

Remark 1. For $l = 1$, formula (4.6) has no second and third terms and coincides with formula (3.5) for a monatomic gas.

We present some results of numerical calculations. For a monatomic gas, from formulas (3.5) and (3.4), we have $T(0)/T_0 = 1 + 0.85351K - 0.40958U$ and $n(0)/n_0 = 1 - 0.39657K - 1.32226U$.

For a diatomic gas, formulas (4.6), (4.7), and (3.4) yield the following results: $T_v(0)/T_0 = 1 + 0.82149K - 0.33938U$, $T_\omega(0)/T_0 = 1 + 0.77028K - 0.13676U$, and $n(0)/n_0 = 1 - 0.38207K - 1.35394U$.

Finally, for an N-atomic gas ($N \geqslant 3$), from formulas (4.6), (4.7), and (3.4), we obtain $T_v(0)/T_0 = 1 + 0.81174K - 0.31975U$, $T_\omega(0)/T_0 = 1 + 0.76172K - 0.11719U$, and $n(0)/n_0 = 1 - 0.37840K - 1.36265U$.

Conclusions. The parameters of a monatomic gas near the surface were calculated in several papers (see [11, 12]). Aoki and Mazukawa [12] determined the gas parameters between two planes in the case of evaporation or condensation. However, the results of [12] are presented in such a form that does not allow a direct comparison with the results of the present work. We cite the results of Loyalka [11], which were obtained for a monatomic gas on the basis of the numerical solution of the Boltzmann equation for molecules treated as solid spheres (recalculated in the notation of the present work): $T(0)/T_0 = 1 + 0.8650K - 0.4036U$, $n(0)/n_0 = 1 - 0.4141K - 1.3074U$, $\varepsilon_{\rm t} = 1.2487K - 0.4556U$, and $\varepsilon_n = -0.6789K - 1.6856U$. A comparison of the results of [11] with the data of the present work shows that the difference is 4% for the temperature jump and 8% for the concentration jump in the Smoluchowski problem; the difference is 2% for the temperature jump and 0.02% for the concentration jump in the problem of weak evaporation. It should be noted that the temperature jump for a monatomic gas $\varepsilon_{\rm t} = 1.3027$ was found by numerical methods in [16], which coincides with the above value.

The formulas for the temperature jump of a molecular gas, which were obtained in the present work, may be used for analysis of the dynamics of moderately large aerosol particles, for analysis of measurements of the thermal conductivity of molecular gases, and in other problems of heat transfer between the molecular gas and the condensed phase.

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