

CALCULATION OF A HEAT FLOW FROM A SPHERICAL PARTICLE IN A DIATOMIC GAS

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The problem of heat flow from a uniformly heated spherical particle in a diatomic gas is considered. The paper reports results of numerical calculations for an analog of the Bhatnagar–Gross–Krook model of the collision integral under for purely diffuse reflection of the gas molecules from the surface.

The heat flow for an intermediate range of Knudsen number remains an urgent problem of the kinetic theory of gases. In theoretical analysis of this phenomenon, only translational degrees of freedom are taken into account, as a rule, whereas most experiments were performed with molecular gases, which requires allowance for internal degrees of freedom [1]. The contribution of each type of motion is determined by the nature of the energy spectrum. As is known (see, for example, [2]), the distance between the energy levels of rotational degrees of freedom is defined by the relation $\hbar^2/(2J)$ (\hbar is Planck's constants and J is the moment of inertia of a molecule) and is comparable to the energy of thermal motion kT (k is a Boltzmann constant) only for the lightest gases. Thus, for hydrogen molecules, $\hbar^2/(2Jk) = 85.4$ K. For heavier molecules, this value is much smaller, which allows one to ignore the discrete nature of the energy spectrum of rotational motion and consider rotational degrees of freedom in the classical approximation. Vibrational degrees of freedom are excited at temperatures of about 10^3 K, and, hence, they can be considered completely frozen.

The effect of rotational degrees of freedom on kinetic processes is studied using both direct numerical modeling [3] and various modifications of models of the collision integral [4–9]. It is common to introduce various empirical parameters are introduced, in particular, the quantity Z , which is the ratio of the energy relaxation times of translational and rotational degrees of freedom. The indicated quantity can take different values for different processes. In addition, it depends on the choice of a particular model.

Using parameters determined ambiguously by properties of gas, it is impossible to compare results obtained in different studies. Therefore, it is important to investigate the limiting case where the relaxation times of translational and rotational degrees of freedom are equal, which is valid for many gases at room temperature [1, 10].

Let us consider the problem of a heat flow from a spherical particle of radius R heated uniformly to temperature T_w and located in a diatomic gas in which constant temperature T_0 at infinity is maintained. To linearize the problem, we assume that the temperature difference $\Delta T = T_w - T_0$ is rather small.

We introduce a spherical coordinate system with origin at the center of the particle. The state of the gas surrounding the particle is described by the equation [11]

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

where φ is a correction to the equilibrium (Maxwellian) distribution function $f_0 = n_0(m/(2\pi kT_0))^{3/2} \times (J/(kT_0)) \exp(-C^2 - \gamma^2)$, $\mathbf{C} = \mathbf{V} \sqrt{m/(2kT_0)}$, $\gamma = \omega \sqrt{J/(2kT_0)}$, \mathbf{V} and ω are the natural velocities of translationally and rotationally moving molecules of the gas, respectively, I is an integral collision operator, m is the molecular weight, n_0 is the concentration of molecules at infinite distance from the particle.

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Following [12], we write

$$I[\varphi] = \nu(F - \varphi), \quad F = \sum_{i=1}^3 P_i M_i, \quad \nu = \frac{7n_0}{\alpha e} \sqrt{\frac{k^3 T_0}{8m}} = \frac{1}{\chi} \sqrt{\frac{kT_0}{2m}}.$$

Here

$$M_i = 2\pi^{-3/2} \int P_i \varphi \exp(-C^2 - \gamma^2) \gamma d\gamma d^3C, \quad (2)$$

$$P_1 = 1, \quad P_2 = \sqrt{2/5} (C^2 + \gamma^2 - 5/2), \quad P_3 = \sqrt{2} C_r,$$

and α and χ are the thermal conductivity and thermal diffusivity, respectively.

Converting to the new variable $\mu = (\mathbf{C} \cdot \mathbf{r})/(Cr)$, we write (1) as

$$\mu \frac{\partial \varphi}{\partial r} + \frac{1 - \mu^2}{r} \frac{\partial \varphi}{\partial \mu} = \frac{\nu}{C} (F - \varphi). \quad (3)$$

Considering F as a specified function, we write the following system of characteristic equations:

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

The first equality $dr/\mu = r d\mu/(1 - \mu^2)$ is solved trivially. As a result, we obtain the characteristic equation

$$K_1 = r \sqrt{1 - \mu^2}. \quad (4)$$

The second equation has the form $dr/\mu = (C/\nu) d\varphi/(F - \varphi)$. Substituting the value $\mu = \pm \sqrt{1 - K_1^2/r^2}$ obtained from (4) into this equation, we obtain

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

From this, we have

$$\begin{aligned} \varphi = & K_2 \exp\left(-\text{sign}(\mu) \frac{\nu}{C} \sqrt{r^2 - K_1^2}\right) \\ & + \text{sign}(\mu) \frac{\nu}{C} \int_R^r \exp\left(\text{sign}(\mu) \frac{\nu}{C} \left(\sqrt{r_1^2 - K_1^2} - \sqrt{r^2 - K_1^2}\right)\right) F\left(r_1, \text{sign}(\mu) \sqrt{1 - \frac{K_1^2}{r_1^2}}\right) \frac{r_1 dr_1}{\sqrt{r_1^2 - K_1^2}}. \end{aligned} \quad (5)$$

The arguments of the function F imply that in the calculation of this function, r_1 and $\text{sign}(\mu) \sqrt{1 - K_1^2/r_1^2}$ should be taken as r and μ , respectively.

To obtain a unique solution, it is necessary to specify boundary conditions. Taking into account the structure of (5) and the discontinuous nature of the distribution function along the characteristic $r \sqrt{1 - \mu^2} = R$, we divide the range of the variables (r, μ) into three subregions: 1) $\mu \in [-1, 0]$; 2) $\mu \in [0, \sqrt{1 - R^2/r^2}]$; 3) $\mu \in [\sqrt{1 - R^2/r^2}, 1]$. The distribution functions in the indicated regions are denoted by corresponding subscripts.

The required solution should satisfy the finiteness condition $\varphi|_{r \rightarrow \infty} = 0$. For $\mu > 0$, this requirement is satisfied automatically, which allows one to define the distribution function to be defined only in region 1. The value of the distribution function in region 2 is given by the condition of its continuity on the boundary between regions 1 and 2, i.e., $\varphi_2(r, 0) = \varphi_1(r, 0)$ for $\mu = 0$. The boundary condition in region 3 is specified by the law of reflection of gas molecules from the particle surface $\varphi_3(R, \mu) = \Phi_w(\mu)$ at $0 < \mu < 1$ (Φ_w is the distribution function of the molecules reflected from the particle surface).

The solution of Eq. (3) satisfying the conditions listed above can be written as

$$\varphi = \varphi_1 H_1 + \varphi_2 H_2 + \varphi_3 H_3, \quad (6)$$

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

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

$$\begin{aligned} \varphi_2 = & \frac{\nu}{C} \int_{r\sqrt{1-\mu^2}}^{\infty} \exp\left(-\frac{\nu}{C}\left(r\mu + \sqrt{r_1^2 - r^2(1-\mu^2)}\right)\right) F\left(r_1, -\sqrt{1 - \frac{r^2}{r_1^2}(1-\mu^2)}\right) \frac{r_1 dr_1}{\sqrt{r_1^2 - r^2(1-\mu^2)}} \\ & + \frac{\nu}{C} \int_{r\sqrt{1-\mu^2}}^r \exp\left(\frac{\nu}{C}\left(\sqrt{r_1^2 - r^2(1-\mu^2)} - r\mu\right)\right) F\left(r_1, \sqrt{1 - \frac{r^2}{r_1^2}(1-\mu^2)}\right) \frac{r_1 dr_1}{\sqrt{r_1^2 - r^2(1-\mu^2)}}, \end{aligned} \quad (7)$$

$$\begin{aligned} \varphi_3 = & \Phi_w \exp\left(\frac{\nu}{C}\left(\sqrt{R - r^2(1-\mu^2)} - r\mu\right)\right) \\ & + \frac{\nu}{C} \int_R^r \exp\left(\frac{\nu}{C}\left(\sqrt{r_1^2 - r^2(1-\mu^2)} - r\mu\right)\right) F\left(r_1, \sqrt{1 - \frac{r^2}{r_1^2}(1-\mu^2)}\right) \frac{r_1 dr_1}{\sqrt{r_1^2 - r^2(1-\mu^2)}}. \end{aligned}$$

Substituting (6) and (7) into the definition (2), we obtain a system of integral equations for M_i , and the integration over γ is performed analytically. For this, the distribution function should be treated as a vector:

$$\varphi = \varphi^1 e_1 + \varphi^2 e_2, \quad e_1 = 1, \quad e_2 = \gamma^2 - 1. \quad (8)$$

Then, we can write

$$2 \int_0^{\infty} P \varphi \gamma \exp(-\gamma^2) d\gamma = P \cdot \varphi = P^1 \varphi^1 + P^2 \varphi^2.$$

In addition, from the condition of absence of mass motion of the gas, we have

$$M_3 = 0. \quad (9)$$

As a result, the problem reduces to the following system of two integral equations:

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

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

$$\varphi_2 = \frac{\nu}{C} \sum_{j=1}^2 P_j \int_{r\sqrt{1-\mu^2}}^r \exp\left(\frac{\nu}{C}\left(\sqrt{r_1^2 - r^2(1-\mu^2)} - r\mu\right)\right) \frac{M_j(r_1) r_1 dr_1}{\sqrt{r_1^2 - r^2(1-\mu^2)}}$$

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

$$\varphi_3 = \frac{\nu}{C} \sum_{j=1}^2 P_j \int_R^r \exp\left(\frac{\nu}{C}\left(\sqrt{r_1^2 - r^2(1-\mu^2)} - r\mu\right)\right) \frac{M_j(r_1) r_1 dr_1}{\sqrt{r_1^2 - r^2(1-\mu^2)}} + \Phi_w \exp\left(\frac{\nu}{C}\left(\sqrt{R - r^2(1-\mu^2)} - r\mu\right)\right).$$

Here $P_1^1 = 1$, $P_1^2 = 0$, $P_2^1 = \sqrt{2/5}(C^2 - 3/2)$, and $P_2^2 = \sqrt{2/5}$.

The solution of the system obtained is sought in the form of a series in Chebyshev polynomials. Restricting ourselves to the first K terms and collecting the terms describing the asymptotic behavior of the required momenta in the gas-dynamic region, we write

$$M_i(r) = \sum_{k=0}^K A_k^i T_k(\xi(r)) + M_i^{\text{as}}, \quad \xi = 1 - 2 \exp(-\beta \sqrt{r^2 - R^2}), \quad (10)$$

$$M_1^{\text{as}} = -(4/7)(R^2 \nu / r) Q, \quad M_2^{\text{as}} = -\sqrt{5/2} M_1^{\text{as}}$$

(Q is the dimensionless heat flux). The series coefficients are given by the condition

$$\sum_{j=0}^K T_k(\xi_j) T_l(\xi_j) = \frac{K+1}{2} (\delta_{0k} + 1) \delta_{kl}, \quad \xi_j = \cos \frac{(2j+1)\pi}{2K+2}.$$

The value of β is selected such that most of the nodes of interpolation lie in the main range of the distribution function. The constant Q is linked to the sought heat flux

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

by the relation

$$q = n_0 \sqrt{2k^3 T_0^3 / m} (R^2 / r^2) Q,$$

and, according to the energy conservation law, the quantity Q can be evaluated at any point, in particular on the particle surface. From this, we have

$$\begin{aligned} Q = 2\pi^{-3/2} \int \mu C (C^2 + \gamma^2) \varphi \exp(-C^2 - \gamma^2) \gamma d\gamma d\mathbf{C} &= \frac{4}{\sqrt{\pi}} \int_0^\infty dC \int_0^\infty d\gamma \int_0^1 \Phi_w \mu C^3 (C^2 + \gamma^2) \exp(-C^2 - \gamma^2) d\mu \\ &+ \frac{2\nu}{\sqrt{\pi}} \sum_{j=1}^2 \int_0^\infty (P_j^1 (C^2 + 1) + P_j^2) C^2 dC \int_{-1}^0 \mu d\mu \int_R^\infty M_j(r_1) \\ &\times \exp\left(-\frac{\nu}{C} \left(R\mu + \sqrt{r_1^2 - R^2(1 - \mu^2)}\right) - C^2\right) \frac{r_1 dr_1}{\sqrt{r_1^2 - R^2(1 - \mu^2)}}. \end{aligned} \quad (11)$$

We consider the case of purely diffuse reflection of gas molecules from the particle surface

$$\Phi_w = \Delta n / n_0 + (C^2 + \gamma^2 - 5/2) \Delta T / T_0.$$

The difference in gas molecule concentration Δn is given by condition (9), which is equivalent to the relation

$$\frac{\Delta n}{n_0} = -\frac{1}{2} \frac{\Delta T}{T_0} - 8 \int_0^\infty dC \int_0^\infty d\gamma \int_{-1}^0 \varphi(R) \gamma \mu C^3 \exp(-C^2 - \gamma^2) d\mu.$$

Taking into account the definition (8), we have

$$\Phi_w = \Phi_w^1 e_1 + \Phi_w^2 e_2,$$

where

$$\Phi_w^1 = (C^2 - 2) \frac{\Delta T}{T_0} - 4\nu \sum_{j=1}^2 \int_0^\infty P_j^1 C^2 dC \int_{-1}^0 \mu d\mu \int_R^\infty M_j(r_1) \exp\left(-\frac{\nu}{C} \left(R\mu + \sqrt{r_1^2 - R^2(1 - \mu^2)}\right) - C^2\right) \frac{r_1 dr_1}{\sqrt{r_1^2 - R^2(1 - \mu^2)}},$$

$$\Phi_w^2 = \Delta T / T_0.$$

As a result, relation (11) leads to

$$\begin{aligned} Q = \frac{3}{2\sqrt{\pi}} \frac{\Delta T}{T_0} + \frac{2\nu}{\sqrt{\pi}} \sum_{j=1}^2 \int_0^\infty (P_j^1 (C^2 - 2) + P_j^2) C^2 dC \int_{-1}^0 \mu d\mu \int_R^\infty M_j(r_1) \\ \times \exp\left(-\frac{\nu}{C} \left(R\mu + \sqrt{r_1^2 - R^2(1 - \mu^2)}\right) - C^2\right) \frac{r_1 dr_1}{\sqrt{r_1^2 - R^2(1 - \mu^2)}}. \end{aligned} \quad (12)$$

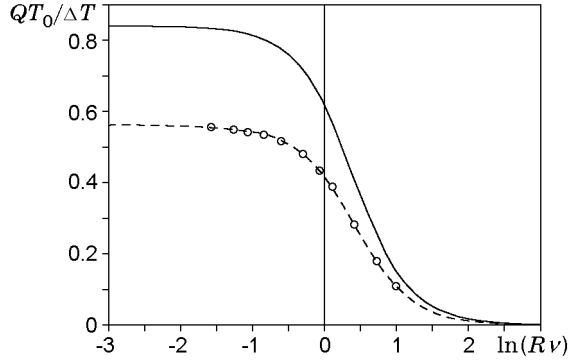


Fig. 1

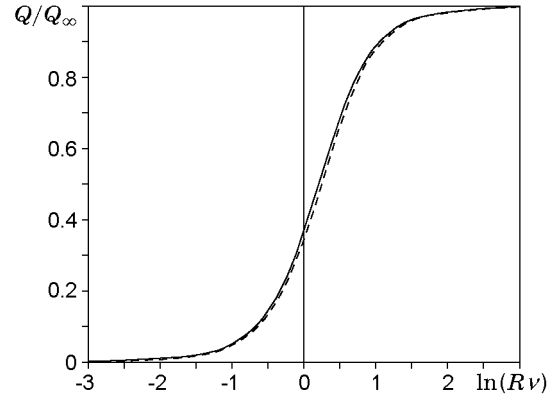


Fig. 2

TABLE 1

$R\nu$	Diatomic gas					Atomic gas ($K = 20$)
	$K = 3$	$K = 5$	$K = 10$	$K = 15$	$K = 20$	
0.01	0.8456	0.8454	0.8448	0.8441	0.8437	0.5622
0.1	0.8326	0.8248	0.8174	0.8201	0.8209	0.5466
0.2	0.8113	0.7935	0.7938	0.7964	0.7966	0.5304
0.5	0.7303	0.7125	0.7278	0.7280	0.7286	0.4864
1	0.6072	0.6215	0.6297	0.6307	0.6313	0.4244
2	0.4568	0.4906	0.4911	0.4906	0.4947	0.3341
5	0.2725	0.2785	0.2786	0.2786	0.2786	0.1945
10	0.1587	0.1575	0.1577	0.1577	0.1577	0.1113
100	0.01731	0.01732	0.01732	0.01732	0.01732	0.01258

In the case of a small particle, the second term in (12) can be ignored. Consequently, in the free-molecular regime, the heat flux is

$$Q = (3/(2\sqrt{\pi}))\Delta T/T_0,$$

i.e., it is a factor of 1.5 greater than that in an atomic gas. This difference does not depend on the form of the collision integral and is determined exclusively by the presence of additional degrees of freedom (see, e.g., [11]).

In the gas-dynamic limit ($R\nu \gg 1$), the distribution function is defined by the Chapman–Enskog distribution. As a result,

$$Q = Q_\infty = (7/(4R\nu))\Delta T/T_0,$$

and, taking into account the definition of ν , we have $q = \alpha R\Delta T/r^2$. This expression coincides with the solution of the problem considered for the case of an atomic gas.

A curve of Q versus particle size is given in Fig. 1 (solid curve). The figure also shows the results of solution of the kinetic equation for an atomic gas using the Bhatnagar–Gross–Krook model (dashed curve is the data of the present study and the points are the results of numerical integration of the kinetic equation of [13]).

It should be noted that in most papers, results are presented in the form of the ratio Q/Q_∞ . In Fig. 2 (notation same as in Fig. 1) it is evident that such representation of the results does not fit the real dependence of the heat flux on particle size and leads to the wrong conclusion [14] that the dependences for one-atomic and polyatomic gases are identical. In this case, the dependence $Q/Q_\infty(\ln(R\nu))$ agrees with the results of [14] obtained in later experiments on measuring the heat flux between coaxial cylinders [15].

We also note that the idea of converting the Boltzmann equation to a system of integral equations for the moments of the distribution function was used to solve similar problems in [16–18]. In [16, 17], the system formulated was solved by the variational method. In this case, the trial function was chosen such that it provided an exact asymptotic description of the macroscopic parameters in the gas-dynamic region. As a result, the heat flux was specified by the relation $q = C_1/r^2$, which represents the facts adequately by virtue of the energy conservation law, whereas the temperature and concentration distributions were defined as $T = C_2/r$ and $n = C_3/r$, which is

valid only at large distance from the particle. The constants C_i were calculated from the condition of minimum of the corresponding functional. In [18], the Galerkin method was used but the trial function was selected similarly to [16, 17].

Use of Chebyshev polynomials eliminates additional integration, required when using the Galerkin method. This reduces the computation time considerably and makes it possible to calculate a larger number of polynomials in the series (10). Values of the parameter $QT_0/\Delta T$ versus the number of polynomials retained are listed in Table 1. For comparison, the table lists values of this parameter obtained by the same method for atomic gases.

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