DIFFUSION AND THERMAL SLIP OF A BINARY GAS MIXTURE

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Let us note that the phenomenon of diffusion slip at a constant gas-mixture temperature has been considered in [1], for example, and thermal slip for a single-component gas in [2]. The slip velocity of a binary gas mixture has been calculated in a field of the temperature gradient and of the partial pressure gradients. The kinetic equation is solved by an approximate method based on physical considerations. A formula has been obtained analytically for the slip velocity for arbitrary accommodation coefficients as well as for arbitrary gas concentrations and arbitrary molecule masses. The results agree to 1% accuracy with the numerical computations of other authors.

The kinetic equation in the model form proposed by Bhatnagar, Gross, and Krook [3] is utilized to describe the system. As is known, this model yields good agreement with experiment and is considerably simpler than the Boltzmann equation in mathematical respects. On the other hand, this model does not describe a number of effects since it is assumed that the time of particle collision is independent of their velocity (Maxwellian molecules). This refers primarily to the phenomenon of thermal diffusion of gases. Therefore, the subsequent reasoning is applicable to gases which possess low thermal diffusion coefficients.

Let a mixture of gases with the densities n_1 and n_2 and the molecule masses m_1 and m_2 fill the half-space $x > 0$ above the $x = 0$ plane whose temperature T_0 varies along the y coordinate. The medium is considered homogeneous in the z direction.

Let us write the system of equations for a binary gas mixture as [3]

$$v_x \frac{\partial f_i}{\partial x} + v_y \frac{\partial f_i}{\partial y} = -\frac{f_i - f_{0i}^u}{\tau_i} \qquad (i = 1,2) \tag{1}$$

$$f_{0i}^u = n_i \left(\frac{m_i}{2\pi T}\right)^{3/2} - \exp\left[\frac{v_x^2 + (v_y - u)^2 + v_z^2}{2T}\right]$$

Here u is the mass flow rate of the gas mixture along the surface (the flow is assumed one-dimensional), τ_i is the time of particle collision independent, as mentioned above, of the particle velocity, and $f_i(x, y, v)$ is the distribution function of molecules of the i-th gas in the velocities v.

The quantities n_i, u, T are functionals of f_i:

$$\rho_i = m_i n_i = m_i \int f_i(x, y, \mathrm{v})\, d\mathrm{v}$$

$$u = \frac{1}{\rho_1 + \rho_2}(\rho_1 u_1 + \rho_2 u_2) = \frac{1}{\rho_1 + \rho_2}\left(m_1 \int f_1 v_y d\mathrm{v} + m_2 \int f_2 v_y d\mathrm{v}\right)$$

$$T = \frac{1}{3(n_1 + n_2)}\left[m_1 \int (\mathrm{v} - \mathbf{u})^2 f_1 d\mathrm{v} + m_2 \int (\mathrm{v} - \mathbf{u})^2 f_2 d\mathbf{u}\right]$$

The temperature is measured in energy units. The collision terms in (1) have been chosen in simplified form; however, they conserve the number of particles of each gas and for $\tau_1 = \tau_2 = \tau$ conserve the total momentum and total energy. Therefore, τ is understood to be some mean-relaxation time of the whole gas mixture.

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The law of molecule interaction with the surface in such an approach can be arbitrary. Let us limit ourselves to the most widespread approximation in which it is assumed that part of the molecules are reflected specularly and part diffusely:

$$f_i(x=0, v_x, v_y, v_z) = (1-q) f_i(x=0, -v_x, v_y, v_z) + q_i f_{iD} \qquad (v_x > 0) \tag{2}$$

Here f_{iD} is the distribution function of the diffusely reflected molecules, and q_i is the accommodation coefficient.

The specific form of the function f_{iD} is essential. It follows from the condition of diffusivity of the reflection that

$$\int v_y f_{iD} d\mathbf{v} = 0$$

As usual, let us seek the solution of (1) in the form

$$f_i = f_{i0}^0 + \varphi_i \qquad (\varphi_i \ll f_{0i}^0) \tag{3}$$

Substituting (3) into (1) and linearizing [2], we obtain the system of integrodifferential equations

$$\tau v_x \frac{\partial \varphi_i}{\partial x} + \varphi_i = f_{0i}^0 \left[\frac{\delta n_i}{n_{0i}} + \frac{\delta T}{2T_0}\left(\frac{m_i v^2}{2} - 3\right) + \frac{m_i u v_y}{T_0} - \tau v_y \frac{P_{0i}'}{P_{0i}} + \tau y_y \frac{T_0'}{T_0}\left(\frac{5}{2} - \frac{m_i v^2}{2T_0}\right)\right] \tag{4}$$

$$\left(P_{0i} = T_0 n_{0i}, \quad P_{0i}' \equiv \frac{\partial P_{0i}}{\partial y}, \quad T_0' \equiv \frac{\partial T_0}{\partial y}\right)$$

Let us introduce the new variables

$$\xi = x/\tau w, \qquad c = v_x/w \tag{5}$$

$$U_i(c, \xi) = \frac{w}{n_i} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} v_y \varphi_i dv_y dv_z \tag{6}$$

$$w = \left(2T \frac{m_1 + m_2}{m_1 m_2}\right)^{1/2}$$

so that

$$u_i(\xi) = \frac{1}{n_i} \int v_y f_i d\mathbf{v} = \int_{-\infty}^{\infty} U_i(c, \xi)\, dc \tag{7}$$

Multiplying both sides of (4) by v_y and integrating over v_y and v_z, we obtain a system of equations for U_1 and U_2:

$$c \frac{\partial U_1}{\partial \xi} + U_1 = \frac{e^{-c^2/\theta_1^2}}{\theta_1 \sqrt{\pi}} \left[u - \tau \frac{T}{m_1} \frac{P_1'}{P_1} + \frac{\tau T'}{2m_1}\left(1 - 2\frac{c^2}{\theta_1^2}\right)\right] \tag{8}$$

$$c \frac{\partial U_2}{\partial \xi} + U_2 = \frac{e^{-c^2/\theta_2^2}}{\theta_2 \sqrt{\pi}} \left[u + \tau \frac{T}{m_2} \frac{P_1'}{P_2} + \frac{\tau T'}{2m_2}\left(1 - 2\frac{c^2}{\theta_2^2}\right)\right] \tag{9}$$

$$\theta_1 = \left(\frac{m_0}{m_1}\right)^{1/2}, \qquad \theta_2 = \left(\frac{m_0}{m_2}\right)^{1/2}, \qquad m_0 = \frac{m_1 m_2}{m_1 + m_2}$$

In deriving (9) it was assumed that $P = P_1 + P_2 = \text{const}$. Multiplying (8) and (9) by ρ_i/ρ and adding, we obtain

$$c \frac{\partial U}{\partial \xi} + U = u(\xi) \frac{1}{\sqrt{\pi}\rho} \left[\frac{\rho_1}{\theta_1} e^{-c^2/\theta_1^2} + \frac{\rho_2}{\theta_2} e^{-c^2/\theta_2^2}\right]$$

$$-\frac{P_1'\tau}{\sqrt{\pi}\rho} \left[\frac{1}{\theta_1} e^{-c^2/\theta_1^2} - \frac{1}{\theta_2} e^{-c^2/\theta_2^2}\right] + \frac{T'\tau}{2\sqrt{\pi}\rho} \left\{\left[\frac{n_1}{\theta_1} e^{-c_1/\theta_1^2} + \frac{n_2}{\theta_2} e^{-c^2/\theta_2^2}\right] - 2c^2 \left[\frac{n_1}{\theta_1^3} e^{-c/\theta_1^2} + \frac{n_2}{\theta_2^3} e^{-c^2/\theta_2^2}\right]\right\} \tag{10}$$

where $U = p^{-1}(U_1\rho_1 + U_2\rho_2)$.

From (2) follows the boundary condition

$$U(\xi = 0, c) = U(\xi = 0, -c) - \frac{1}{\rho} [q_1 \rho_1 U_1(\xi = 0, -c) + q_2 \rho_2 U_2(\xi = 0, -c)] \tag{11}$$

$$(c > 0)$$

Equations (7), (10), (11) form a closed system to determine $U(c\xi)$. This system can be reduced to an integral equation of nondifference type. Because of the mathematical difficulties inherent in the solution of such an equation, let us try to solve the system (7), (10), (11) by the approximate method proposed in [4].

This method possesses sufficiently high accuracy in combination with simplicity. It is shown in [4] on the model of a Lorentz gas that solutions obtained by using this method differ only by several percent from the exact solutions obtained by considerably more awkward methods or by numerical machine computations. We shall be interested in solving the equations associated with sources. Since the latter decrease as $\xi \to \infty$, then the solution tends to a constant as $\xi \to \infty$:

$$u(\xi) = a \; (\xi \to \infty) \tag{12}$$

The problem is to find this quantity, which is called the slip velocity.

It follows from (10) that for $\xi \to \infty$

$$\int_{-\infty}^{\infty} cU(c, \xi)\, dc = 0$$

We therefore have

$$K = \int_{-\infty}^{\infty} cU(c, \xi)\, dc = 0 \tag{13}$$

Multiplying (10) by c and integrating, we obtain

$$L = \int_{-\infty}^{\infty} c^2 U(c, \xi)\, dc = \text{const} \tag{14}$$

The quantity a can be found by calculating L as $\xi \to \infty$ ($\underset{\xi\to\infty}{U}(c, \xi)$ is found from (10)) and equating it to the value calculated for $\xi = 0$. To do this it is necessary to know $U(c < 0, \xi = 0)$. An approximate expression can be obtained for $U(c < 0, \xi = 0)$ by putting $u = a^{(1)}$ in (10):

$$\begin{aligned} u(c<0, 0) = {} & \frac{a^{(1)}}{\sqrt{\pi}\rho}\left[\frac{\rho_1}{\theta_1} e^{-c^2/\theta_1^2} + \frac{\rho_2}{\theta_2} e^{-c^2/\theta_2^2}\right] - \frac{P_1'\tau}{\sqrt{\pi}\rho}\left[\frac{e^{-c^2/\theta_1^2}}{\theta_1} - \frac{e^{-c^2/\theta_2^2}}{\theta_2}\right] \\ & + \frac{T'\tau}{2\sqrt{\pi}\rho}\left\{\left[\frac{n_1}{\theta_1} e^{-c^2/\theta_1^2} + \frac{n_2}{\theta_2} e^{-c^2/\theta_2^2}\right] - 2v^2\left[\frac{n_1}{\theta_1^3} e^{-c^2/\theta_1^2} + \frac{n^2}{\theta_2^3} e^{-c^2/\theta_2^2}\right]\right\} \end{aligned} \tag{15}$$

$U(c > 0, 0)$ is found from the boundary condition (11) and (8), (9). To find $a^{(1)}$ we require compliance with the conservation law (13).

The reasoning confirming the sufficient accuracy of such a method of finding $U(c, 0)$ is elucidated in [4]. Performing the operation mentioned, we obtain

$$a^{(1)} = \frac{q_1\theta_1 - q_2\theta_2}{q_1\theta_1\rho_1 + q_2\theta_2\rho_2}\tau P_1' + \frac{q_1\theta_1 n_1 + q_2\theta_2 n_2}{q_1\theta_1\rho_1 + q_2\theta_2\rho_2}\frac{\tau T'}{2} \tag{16}$$

Knowing the expression for $U(c, 0)$ for $c < 0$, we can calculate the quantity a by utilizing (14), (10), (15) and taking account of the boundary condition (11):

$$a = a^{(1)} - \frac{q_1 n_1 + q_2 n_2}{2(n_1 + n_2)} a^{(1)} + \left(\frac{q_1}{m_1} - \frac{q_2}{m_2}\right)\frac{\tau P_1'}{2(n_1 + n_2)} + \left(\frac{q_1 n_1}{m_1} + \frac{q_2 n_2}{m_2}\right)\frac{\tau T'}{2(n_1 + n_2)} \tag{17}$$

Substituting (16) into (17), we finally obtain

$$\begin{aligned} a = {} & \left\{\frac{q_1\theta_1 - q_2\theta_2}{q_1\theta_1\rho_1 + q_2\theta_2\rho_2}\left(1 - \frac{q_1 n_1 - q_2 n_2}{2n}\right) + \left(\frac{q_1}{m_1} - \frac{q_2}{m_2}\right)\frac{1}{2n}\right\}\tau P_1' \\ & + \left\{\frac{q_1\theta_1 n_1 + q_2\theta_2 n_2}{q_1\theta_1\rho_1 + q_2\theta_2\rho_2}\left(1 - \frac{q_1 n_1 + q_2 n_2}{2n}\right) + \left(\frac{q_1 n_1}{m_1} + \frac{q_2 n_2}{m_2}\right)\frac{1}{n}\right\}\frac{\tau T'}{2} \\ & (n = n_1 + n_2) \end{aligned} \tag{18}$$

The first member of (18) proportional to P_1' is called the diffusion slip velocity, while the second is the thermal slip velocity of the mixture. For $m_1 = m_2$, $q_1 = q_2 = q$ (a one-component gas), the diffusion slip velocity vanishes, as indeed it should.

Let us express the τ in (18) in terms of the transport coefficients of the gas mixture, the coefficients of diffusion and heat conduction. Since diffusion slip originates from terms of the expansion in the kinetic equation which are proportional to P', this effect is then related to the diffusion (D_{12}). Analogously, the thermal-slip effect is related to the heat conduction ($\varkappa$). The connection between τ and D_{12} can be found from the condition that the system (8), (9) correctly describes diffusion in unbounded space at great distances from the wall [5]:

$$u_1 - u_2 = -D_{12}\frac{n_1'n}{n_1n_2} \tag{19}$$

Finding the difference between u_1 and u_2 from the system (8), (9) and equating it to (19), we obtain

$$\tau = \frac{D_{12}m_1m_2n}{T\rho} \tag{20}$$

The connection between τ and $\varkappa$ is found analogously. Expressing D_{12} and $\varkappa$ in terms of τ, we finally obtain in place of (18)

$$a_i' = \left\{\frac{q_1\theta_1 - q_2\theta_2}{q_1\theta_1\rho_1 + q_2\theta_2\rho_2}\left(1 - \frac{q_1n_1 + q_2n_2}{2n}\right) + \left(\frac{q_1}{m_1} - \frac{q_2}{m_2}\right)\frac{1}{2n}\right\}\frac{m_1m_2n}{kT\rho}D_{12}P_1'$$
$$+ \left\{\frac{q_1\theta_1n_1 + q_2\theta_2n_2}{q_1\theta_1\rho_1 + q_2\theta_2\rho_2}\left(1 - \frac{q_1n_1 + q_2n_2}{2n}\right) + \left(\frac{q_1n_1}{m_1} + \frac{q_2n_2}{m_2}\right)\frac{1}{n}\right\}\frac{\varkappa}{5kT}\left[\frac{n_1}{m_1} + \frac{n_2}{m_2}\right]^{-1}T' \tag{21}$$

where k is the Boltzmann constant.

An expression for the slip velocity is obtained numerically in [6] for $T' = 0$ in the particular case

$$q_1 = q_2 = 1, \quad n_1 / n_2 \to 0, \quad m_1 / m_1 = {}^{18}/_{29} \text{ (water vapor in air)}$$

Under these conditions we obtain from (21)

$$a = -0.275 D_{12}\frac{n_1'}{n_2} \tag{22}$$

A value of the numerical coefficient, 0.277, is presented in [6] which is only 1% different from the coefficient in (22).

As has already been remarked at the beginning of the paper, the model which has been used to obtain the results can be applied to mixtures of gases having a low coefficient of thermal diffusion. However, it is later proposed to take account of thermal diffusion to calculate the thermal slip velocity of a binary mixture by applying the same approximate method of solving the kinetic equation to the linearized Boltzmamn equation.

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