HEAT AND MASS TRANSFER PROCESSES OF A POLYATOMIC GAS IN A FLAT CHANNEL FOR ARBITRARY KNUDSEN NUMBERS

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The motion of a polyatomic gas in a flat channel under the action of pressure and temperature gradients was studied in [1]. The problem was solved numerically by using the Hansen–Morse model equation, taking account of the excitation of only one type of internal energy. The conclusion in [1] that the effect of thermal transpiration is independent of the internal degrees of freedom of the molecules is at variance with current concepts. Up till now it was assumed that such a dependence exists. Moreover, this assumption was based on an experimental determination of the rotational collision numbers [2]. In view of this, the results in [1] require further examination. In the present article we base the description of heat and mass transfer processes in a polyatomic gas in a flat channel on a model equation [3], which, in contrast with the Hansen-Morse equation used in [1], takes account of the possibility of the excitation of two types of internal energy of the molecules, for example rotational and vibrational energies. The method of solving the system of integral-moment equations gives rather accurate results over the whole range of Knudsen numbers Kn, and in addition leads to simple analytic expressions for the fluxes in the limiting cases Kn << 1 and Kn >> 1. This permits an explicit analysis of the contribution of the internal degrees of freedom of the molecules to thermal creep and to the various components of the heat fluxes resulting from pressure and temperature gradients at various Knudsen numbers.

We consider the motion of a polyatomic one-component gas between infinite parallel plates $x = \pm d/2$ as a result of longitudinal pressure and temperature gradients along the z axis. Rotational and vibrational degrees of freedom of the molecules are excited in the gas. We assume that the translational, rotational, and vibrational temperatures of the molecules in each cross section of the channel are equal to one another and equal to the temperature T. We assume that the state of the gas is weakly perturbed, and that the distribution function for molecules in the i-th rotational and the j-th vibrational states is written in the form of a small deviation from the Maxwell–Boltzmann distribution:

$$f_{ij} = P_i^{(r)} P_j^{(v)} f_0(z)\,[1 + h_{ij}(x, \mathbf{v})], \quad |h_{ij}| \ll 1,$$
$$f_0(z) = n(z)\left[\frac{m}{2\pi kT(z)}\right]^{3/2} \exp\left[-\frac{mv^2}{2kT(z)}\right], \quad P_\beta^{(\alpha)} = \tag{1}$$
$$= \frac{\exp\left[-E_\beta^{(\alpha)}/kT(z)\right]}{\sum\limits_\beta \exp\left[-E_\beta^{(\alpha)}/kT(z)\right]}, \quad \alpha = r, v, \quad \beta = i, j,$$

where n is the number density of the gas, m is the mass of a molecule, $P_\beta^{(\alpha)}$ is the probability of a state with energy $E_\beta^{(\alpha)}$, and k is the Boltzmann constant.

Since intermolecular collisions accompanied by transitions in both the rotational and vibrational spectra simultaneously are very rare [4], we neglect them.

Then, taking account of Eq. (1), the model kinetic equation [3] for the perturbation function h_{ij} is written in the following dimensionless form:

$$c_x \frac{\partial h_{ij}}{\partial y} + c_z \nu + c_z\left(c^2 - \frac{5}{2} + \varepsilon_i^{(r)} - \langle\varepsilon^{(r)}\rangle + \varepsilon_j^{(v)} - \langle\varepsilon^{(v)}\rangle\right)\tau =$$
$$= \delta\left[2uc_z + \frac{4}{5} c_z\left(c^2 - \frac{5}{2}\right)\left(\varphi_1 Q^{(t)} + \varphi_2 Q^{(r)} + \varphi_3 Q^{(v)}\right) + \right. \tag{2}$$
$$+ \frac{2k}{c_V^r} c_z\left(\varepsilon_i^{(r)} - \langle\varepsilon^{(r)}\rangle\right)\left(\varphi_4 Q^{(r)} + \varphi_5 Q^{(t)}\right) +$$

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$$+\frac{2k}{c_V^v} c_z\left(\varepsilon_j^{(v)}-\langle\varepsilon^{(v)}\rangle\right)\left(\varphi_6 Q^{(v)}+\varphi_7 Q^{(t)}\right)-h_{ij}\Big],$$

where

$$y=\frac{x}{d}, \quad \nu=\frac{d}{p}\frac{dp}{dz}, \quad \tau=\frac{d}{T}\frac{dT}{dz}, \quad \delta=\frac{1}{\tau_\eta}\left(\frac{m}{2kT_0}\right)^{1/2} d,$$

$$c_i=\left(\frac{m}{2kT_0}\right)^{1/2} v_i, \quad \varepsilon_i^{(r)}=\frac{E_i^{(r)}}{kT_0}, \quad \langle\varepsilon^{(r)}\rangle=\frac{E_0^{(r)}}{kT_0},$$

$$\varphi_1=\frac{1}{3}-\frac{5}{9}\left(\frac{c_V^r}{k}\alpha+\frac{c_V^v}{k}\alpha'\right), \quad \varphi_2=\frac{5}{6}\alpha, \quad \varphi_3=\frac{5}{6}\alpha',$$

$$\varphi_4=1-\frac{\alpha}{2}-\frac{1}{\beta}, \quad \varphi_5=\frac{1}{3}\frac{c_V^r}{k}\alpha, \quad \varphi_6=1-\frac{\alpha'}{2}-\frac{1}{\beta'}, \quad \varphi_7=\frac{1}{3}\frac{c_V^v}{k}\alpha',$$

$$\alpha=\frac{\tau_\eta}{\tau_{rr}}, \quad \alpha'=\frac{\tau_\eta}{\tau_{vv}}, \quad \beta=\frac{\tau_{Drr}}{\tau_\eta}, \quad \beta'=\frac{\tau_{Dvv}}{\tau_\eta}, \quad \tau_\eta=\frac{\eta}{p};$$

$$\begin{gathered}
u=\left(\frac{m}{2kT_0}\right)^{1/2} U=\pi^{-3/2}\sum_{ij} P_i P_j \int \exp(-c^2)\, c_z h_{ij} d\mathbf{c}, \\
Q^{(t)}=\left(\frac{m}{2kT_0}\right)^{1/2}\frac{q^{(t)}}{p_0}=\pi^{-3/2}\sum_{ij} P_i P_j \int \exp(-c^2)\, c_z\left(c^2-\frac{5}{2}\right) h_{ij} d\mathbf{c}, \\
Q^{(\alpha)}=\left(\frac{m}{2kT_0}\right)^{1/2}\frac{q^{(\alpha)}}{p_0}=\pi^{-3/2}\sum_{ij} P_i P_j \int \exp(-c^2)\, c_z\left(\varepsilon_\beta^{(\alpha)}-\langle\varepsilon^{(\alpha)}\rangle\right) h_{ij} d\mathbf{c}, \\
c_V^{(\alpha)}=k\left(\langle\varepsilon_\beta^{(\alpha)2}\rangle-\langle\varepsilon_\beta^{(\alpha)}\rangle^2\right), \quad \alpha=r, v; \quad \beta=i, j.
\end{gathered} \tag{3}$$

Here U is the macroscopic velocity of the gas, $q^{(t)}$, $q^{(r)}$, and $q^{(v)}$ are the components of the heat flux density due respectively to the translational, rotational, and vibrational degrees of freedom of the molecules, p and η are respectively the pressure and the dynamic viscosity of the gas, T_0 is the mean temperature of the gas, c_V^r and c_V^v are the contributions of the internal degrees of freedom of the molecules to the specific heat at constant volume, and the angle brackets denote the average over the internal states of the molecules. The relaxation times τ_η, τ_{rr}, τ_{vv}, τ_{Drr}, and τ_{Dvv} for a given intermolecular interaction potential can be calculated [4] or taken from experiments [5].

If the mean free path of the molecules is defined in the form [4] $l=(\pi/4)\tau_\eta(8kT_0/\pi m)^{1/2}$, the rarefaction parameter δ of the gas is related to the Knudsen number by the equation $\delta=(\sqrt{\pi}/2)\mathrm{Kn}^{-1}$.

As a boundary condition we assume completely diffuse scattering of molecules on the plates restricting the gas. Then the perturbation function is

$$h_{ij}(y=-(1/2)\operatorname{sign} c_x, \mathbf{c})=0. \tag{4}$$

By linearizing the problem, the solution of Eq. (2) can be written in the form [1]

$$h_{ij}=h_{ij}^p\nu+h_{ij}^T\tau. \tag{5}$$

By substituting Eq. (5) into Eqs. (2)-(4) and equating the terms for each of the gradients, the complete problem is separated into two: The first contains the equations describing the heat and mass transfer processes under the action of the pressure gradient, and the second under the action of the temperature gradient.

Waiting Eq. (2) in integral form, taking account of the boundary conditions (4), and substituting the expression obtained for the perturbation function into Eqs. (3), it is easy to obtain two systems of integral-moment equations for the macroscopic velocities u_p and u_T, and the translational, rotational, and vibrational components of the heat fluxes $Q_p^{(l)}$, $Q_T^{(l)}$ (l = t, r, v) due respectively to the pressure and temperature gradients:

$$u_{p,T}=\frac{\delta}{\sqrt{\pi}}\int_{-1/2}^{+1/2}\left[u_{p,T}J_{-1}+\frac{2}{5}\left(\varphi_1 Q_{p,T}^{(t)}+\varphi_2 Q_{p,T}^{(r)}+\varphi_3 Q_{p,T}^{(v)}\right)\left(J_1-\frac{1}{2}J_{-1}\right)\right]dy'+K_{p,T}^{(1)}; \tag{6}$$

$$Q_{p,T}^{(t)}=\frac{\delta}{\sqrt{\pi}}\int_{-1/2}^{+1/2}\left[u_{p,T}\left(J_1-\frac{1}{2}J_{-1}\right)+\frac{2}{5}\left(\varphi_1 Q_{p,T}^{(t)}+\varphi_2 Q_{p,T}^{(r)}+\varphi_3 Q_{p,T}^{(v)}\right)\left(J_3-J_1+\frac{9}{4}J_{-1}\right)\right]dy'+K_{p,T}^{(2)}; \tag{7}$$

$$Q_{p,T}^{(r)} = \frac{\delta}{\sqrt{\pi}} \int_{-1/2}^{+1/2} \left(\varphi_4 Q_{p,T}^{(r)} + \varphi_5 Q_{p,T}^{(t)}\right) J_{-1} dy' + K_{p,T}^{(3)}; \tag{8}$$

$$Q_{p,T}^{(v)} = \frac{\delta}{\sqrt{\pi}} \int_{-1/2}^{+1/2} \left(\varphi_6 Q_{p,T}^{(v)} + \varphi_7 Q_{p,T}^{(t)}\right) J_{-1} dy' + K_{p,T}^{(4)}, \tag{9}$$

where

$$K_p^{(1)} = -\frac{1}{2\sqrt{\pi}} \int_{-1/2}^{+1/2} J_{-1} dy', \quad K_T^{(1)} = K_p^{(2)} = -\frac{1}{2\sqrt{\pi}} \int_{-1/2}^{+1/2} \left(J_1 - \frac{1}{2} J_{-1}\right) dy',$$

$$K_T^{(2)} = -\frac{1}{2\sqrt{\pi}} \int_{-1/2}^{+1/2} \left(J_3 - J_1 + \frac{9}{4} J_{-1}\right) dy', \quad K_p^{(3)} = K_p^{(4)} = 0,$$

$$K_T^{(3)} = \frac{c_V^r}{k} K_p^{(1)}, \quad K_T^{(4)} = \frac{c_V^v}{k} K_p^{(1)}, \quad J_n(t) = \int_0^{\infty} c^n \exp\left(-c^2 - \frac{t}{c}\right) dc.$$

The argument of the function J_n in Eqs. (6)-(9) is $(\delta|y - y'|)$. Equations (6)-(9) determine the local values of the macroscopic quantities. Of practical interest, however, are the number flux I_n and the heat flux I_q averaged over a cross section of the channel:

$$\begin{gathered} I_n = n \int_{-1/2}^{+1/2} U dy = L_{nn} X_n + L_{nq} X_q, \\ I_q = \int_{-1/2}^{+1/2} q dy = \int_{-1/2}^{+1/2} \left(q^{(t)} + q^{(r)} + q^{(v)}\right) dy = L_{qn} X_n + L_{qq} X_q, \end{gathered} \tag{10}$$

where the thermodynamic forces are chosen in the form [1]

$$X_n = -k\nu, \; X_q = -\tau/T_0. \tag{11}$$

In accordance with the fundamental assumptions of the thermodymanics of nonequilibrium processes in discontinuous systems [6], the reciprocity relation $L_{nq} = L_{qn}$ must be satisfied for the cross coefficients over the whole range of Knudsen numbers.

For numerical calculations it is convenient to use dimensionless quantities which are related to the kinetic coefficients by the following equations:

$$\begin{gathered} G_p = \left(\frac{m}{2kT_0}\right)^{1/2} \frac{k}{n_0} L_{nn}, \qquad G_T = -\left(\frac{m}{2kT_0}\right)^{1/2} \frac{k}{p_0} L_{nq}, \\ S_p^{(l)} = -\left(\frac{m}{2kT_0}\right)^{1/2} \frac{k}{p_0} L_{qn}^{(l)}, \quad S_T^{(l)} = \left(\frac{m}{2kT_0}\right)^{1/2} \frac{1}{p_0 T_0} L_{qq}^{(l)}, \; l = t, r, v, \\ L_{qn} = L_{qn}^{(t)} + L_{qn}^{(r)} + L_{qn}^{(v)}, \qquad G_T = S_p^{(t)} + S_p^{(r)} + S_p^{(v)}. \end{gathered} \tag{12}$$

The effect of thermomolecular pressure and the mechanocaloric effect are important special cases. The first is a stationary state in which the temperature gradient is kept constant and a corresponding pressure gradient is established in the system. This state is characterized by the absence of a total number flux averaged over a cross section of the channel, i.e., $I_n = 0$. Then it follows from Eqs. (10), (11), and (12) that

$$\gamma = \frac{G_T}{G_p} = \frac{\nu}{\tau} = \frac{dp/p}{dT/T}. \tag{13}$$

The mechanocaloric effect is a stationary state of second order [6], and characterizes heat transport along the channel under a constant pressure gradient with no temperature gradient $(\tau = 0)$.

It follows from Eqs. (10), (12), and (13) that

$$I_q = \frac{L_{nq}}{L_{nn}} I_n = -\gamma k T_0 I_n. \tag{14}$$

Thus, the universal indicator of thermomolecular pressure γ also determines the magnitude of the mechanocaloric effect.

To determine the fluxes (10) and the indicator of the thermomolecular pressure (13) it is necessary to solve the system of integral equations (6)-(9). These equations are Fredholm equations of the second kind. Consequently, they can be solved by the Bubnov–Galerkin method [7]. In doing this the choice of the form of the trial functions for macroscopic quantities is important. It should be kept in mind that the profiles of the macroscopic quantities in an almost free-molecule regime are described exactly by the free terms of the integral equations (6)-(9). Therefore, for the solution to contain the other limiting case (Kn << 1), the choice of the form of the trial functions must be based on the behavior of the macroscopic parameters in the almost continuum limit. Taking account of the symmetry of the problem, the required functions u_{pT} and $Q_{pT}^{(l)}$ (l = t, r, v) can be written in the form of an infinite series in even basic functions $\{y^{2k}\}$ (k = 0, 1, ...). In particular, in the first approximation we can set

$$u_k(y) \approx a_k + b_k y^2, \quad Q_k^{(l)}(y) \approx c_k^{(l)}, \quad k = p, T, l = t, r, v. \tag{15}$$

The trial functions (15) have the form of solutions of the Navier–Stokes and heat-conduction equations. The solution of an analogous problem for a monatomic gas [8] showed that this approximation introduces an error of no more than 1.5% over the whole range of Knudsen numbers, i.e., the method converges very rapidly. Evidently one should expect the same accuracy for a polyatomic gas.

To determine the constants a_k, b_k, and $c_k^{(l)}$, it is necessary to substitute the trial functions (15) into Eqs. (6)-(9), and to require that the expressions obtained be orthogonal to the chosen basis functions, where the orthogonality condition for arbitrary functions f and g has the form

$$(f, g) \equiv \int_{-1/2}^{+1/2} f(y)\, g(y)\, dy = 0.$$

Thus, the quantities a_k, b_k, and $c_k^{(l)}$ are found by solving a set of five linear algebraic equations. Having determined them, expressions can be found for the fluxes I_n and I_q and the indicator of the thermomolecular pressure γ. The final expressions have a cumbersome form and are not cited here. The asymptotic expansions of these expressions for the two limiting cases are of interest:

almost free-molecule regime (δ << 1)

$$\begin{gathered} G_p = \frac{1}{2\sqrt{\pi}}(-\ln\delta + 0.6342 + 0.5908\delta),\ G_T = \frac{1}{2\sqrt{\pi}}(-0.5\ln\delta - 0.1829 + 0.5908\delta), \\ S_p^{(t)} = G_T, \quad S_p^{(r)} = S_p^{(v)} = 0, \quad S_T^{(t)} = \frac{1}{2\sqrt{\pi}}(-2.25\ln\delta + 1.4270 + 1.4770\delta), \\ S_T^{(r)} = \frac{c_V^r}{k} G_p, \quad S_T^{(v)} = \frac{c_V^v}{k} G_p; \end{gathered} \tag{16}$$

almost continuum regime ($\delta \gg 1$)

$$G_p = \frac{\delta}{12} + \frac{1}{2\sqrt{\pi}}\left(\frac{\pi}{4} + 1\right); \tag{17}$$

$$\begin{aligned} G_T = \frac{3}{20}\frac{m\lambda^t}{k\eta}\frac{1}{\delta} - \frac{3}{20\sqrt{\pi}}\frac{m\lambda^t}{k\eta}\Bigg[\frac{\pi}{2} - \frac{8}{15} + \frac{\frac{9}{5}\left(1+\frac{\alpha\beta}{2}\right)\left(1+\frac{\alpha'\beta'}{2}\right)}{\Delta_0} + \\ + \frac{\frac{\alpha\beta}{3}\left(1+\frac{\alpha'\beta'}{2}\right)\frac{m\lambda^r}{k\eta} + \frac{\alpha'\beta'}{3}\left(1+\frac{\alpha\beta}{2}\right)\frac{m\lambda^v}{k\eta}}{\Delta_1}\Bigg]\frac{1}{\delta^2} + \ldots; \end{aligned} \tag{18}$$

$$\begin{aligned} S_p^{(t)} = \frac{\frac{9}{16}\left(1+\frac{\alpha\beta}{2}\right)\left(1+\frac{\alpha'\beta'}{2}\right)}{\Delta_0}\frac{1}{\delta} - \frac{\frac{9}{16\sqrt{\pi}}\left(1+\frac{\alpha\beta}{2}\right)\left(1+\frac{\alpha'\beta'}{2}\right)}{\Delta_0}\Bigg[\frac{\pi}{2} - \frac{8}{15} + \\ + \frac{\frac{9}{5}\left(1+\frac{\alpha\beta}{2}\right)\left(1+\frac{\alpha'\beta'}{2}\right)}{\Delta_0} + \frac{\frac{5}{12}\frac{c_V^r}{k}(\alpha\beta)^2\left(1+\frac{\alpha'\beta'}{2}\right)}{\Delta_0\left(1+\frac{\alpha\beta}{2}\right)} + \frac{\frac{5}{12}\frac{c_V^v}{k}(\alpha'\beta')^2\left(1+\frac{\alpha\beta}{2}\right)}{\Delta_0\left(1+\frac{\alpha'\beta'}{2}\right)}\Bigg]\frac{1}{\delta^2} + \ldots; \end{aligned} \tag{19}$$

$$
S_p^{(r)} = \frac{\frac{9}{16}\frac{c_V^r}{k}\frac{\alpha\beta}{3}\left(1+\frac{\alpha'\beta'}{2}\right)}{\Delta_0}\frac{1}{\delta} - \frac{\frac{9}{16\sqrt{\pi}}\frac{c_V^r}{k}\cdot\frac{\alpha\beta}{3}\left(1+\frac{\alpha'\beta'}{2}\right)}{\Delta_0}\left\{\frac{\pi}{2}-\frac{8}{15}+\right.
$$

$$
+\frac{\left[\frac{9}{5}\left(1+\frac{\alpha\beta}{2}\right)+\beta\left(1+\frac{5}{6}\frac{c_V^r}{k}\alpha+\frac{5}{6}\frac{c_V^v}{k}\alpha'\right)\right]\left(1+\frac{\alpha'\beta'}{}\right)}{\Delta_0}+ \tag{20}
$$

$$
\left.+\frac{\frac{5}{12}\frac{c_V^v}{k}(\alpha')^2\beta'\left[\beta'\left(1+\frac{\alpha\beta}{2}\right)-\beta\left(1+\frac{\alpha'\beta'}{2}\right)\right]}{\Delta_0\left(1+\frac{\alpha'\beta'}{2}\right)}\right\}\frac{1}{\delta^2}+\ldots;
$$

$$
S_T^{(t)} = \frac{1}{2}\frac{m\lambda^t}{k\eta}\frac{1}{\delta} - \frac{1}{2\sqrt{\pi}}\frac{m\lambda^t}{k\eta}\left[\frac{\frac{9}{5}\left(1+\frac{\alpha\beta}{2}\right)\left(1+\frac{\alpha'\beta'}{2}\right)}{\Delta_0}+\right. \tag{21}
$$

$$
\left.+\frac{\frac{\alpha\beta}{3}\left(1+\frac{\alpha'\beta'}{2}\right)\frac{m\lambda^r}{k\eta}+\frac{\alpha'\beta'}{3}\left(1+\frac{\alpha\beta}{2}\right)\frac{m\lambda^v}{k\eta}}{\Delta_1}\right]\frac{1}{\delta^2}+\ldots;
$$

$$
S_T^{(r)} = \frac{1}{2}\frac{m\lambda^r}{k\eta}\frac{1}{\delta} - \frac{1}{2\sqrt{\pi}}\frac{m\lambda^r}{k\eta}\left\{\frac{\left[\left(1+\frac{5}{6}\frac{c_V^r}{k}\alpha\right)\left(1+\frac{\alpha'\beta'}{2}\right)+\frac{5}{6}\frac{c_V^v}{k}\alpha'\right]\beta}{\Delta_0}+\right. \tag{22}
$$

$$
\left.+\frac{\alpha\left[\frac{5}{12}\alpha'\beta'\frac{m\lambda^v}{k\eta}+\frac{3}{5}\left(1+\frac{\alpha'\beta'}{2}\right)\frac{m\lambda^t}{k\eta}\right]}{\Delta_2}\right\}\frac{1}{\delta^2}+\ldots,
$$

where

$$
\Delta_0 = 1+\frac{\alpha}{2}\left(\frac{5}{3}\frac{c_V^r}{k}+\beta\right)\left(1+\frac{\alpha'\beta'}{2}\right)+\frac{\alpha'}{2}\left(\frac{5}{3}\frac{c_V^v}{k}+\beta'\right)\left(1+\frac{\alpha\beta}{2}\right)-\frac{1}{4}\alpha\alpha'\beta\beta',
$$

$$
\Delta_1 = 1+\frac{\alpha\beta}{2}\left(1+\frac{2}{3}\frac{c_V^r}{k}\right)\left(1+\frac{\alpha'\beta'}{2}\right)+\frac{\alpha'\beta'}{2}\left(1+\frac{2}{3}\frac{c_V^v}{k}\right)\left(1+\frac{\alpha\beta}{2}\right)-\frac{1}{4}\alpha\alpha'\beta\beta',
$$

$$
\Delta_2 = 1+\frac{5}{4}\alpha\left(1+\frac{2}{3}\frac{c_V^r}{k}\right)\left(1+\frac{\alpha'\beta'}{2}\right)+\frac{5}{6}\frac{c_V^v}{k}\alpha'\left(1+\frac{\alpha\beta'}{2}\right)+\frac{\alpha'\beta'}{2}.
$$

The asymptotic expansions for $S_p^{(v)}$ and $S_T^{(v)}$ are obtained from the expressions for $S_p^{(r)}$ and $S_T^{(r)}$ respectively by replacing the superscript r by v, α by α', and β by β'; λ^t, λ^r, and λ^v are the thermal conductivities due to the translational, rotational, and vibrational degrees of freedom of the molecules [4].

In an almost free-molecule regime, Eqs. (16) for the fluxes G_p, G_T, $S_p^{(t)}$, and $S_T^{(t)}$ correspond to the case of a monatomic gas. The internal components $S_p^{(r)}$ and $S_p^{(v)}$ of the heat flux produced by the pressure gradient are equal to zero in this regime, since there are no inelastic collisions between molecules — the only cause of these components.

With the exception of (17), Eqs. (17)-(22) were derived for the first time; they describe heat and mass transfer processes of a polyatomic gas in a flat channel for $\delta \gg 1$, when collisions between molecules play a significant role. If the vibrational degrees of freedom of the molecules are not excited, the first terms for G_p, G_T, and S_T agree with the expressions in [1].

However, the conclusion in [1] that the effect of thermal transpiration depends only on the Eucken translational factor is not true. It follows from (18) that the second term ($\sim\delta^{-2}$) includes also the internal components of the total Eucken factor.

Macroscopic quantities were calculated numerically with an accuracy of not less than 0.1% for any values of the rarefaction parameters δ ($0.01 \leqslant \delta \leqslant 40$). The values of the parameters α, α', β, and β' were selected from experiments. The value of α was varied from 0 (the slow exchange of energy between translational and rotational degrees of freedom of the molecules, $\tau_\eta \ll \tau_{rr}$) to 1.2 (slight exchange of energies, $\tau_\eta \sim \tau_{rr}$) [4]. Since vibrational relaxation is a very slow process on the scale of the mean free path of the molecules (vibrational collision numbers are of the order 10^3-10^7 [9]), the parameter α' was selected in the range 0-0.001. The values for $\beta = \rho D_{rr}/\eta$ and $\beta' = \rho D_{vv}/\eta$ ($\rho = mn$; D_{rr} and D_{vv} are respec-

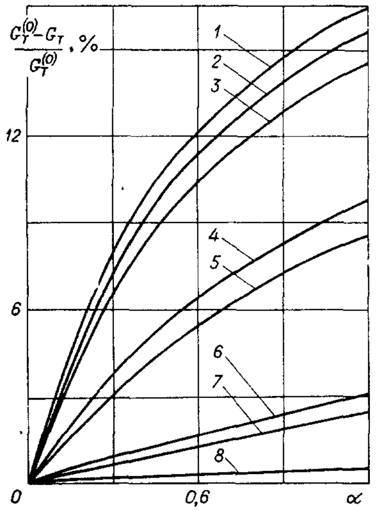

Fig. 1

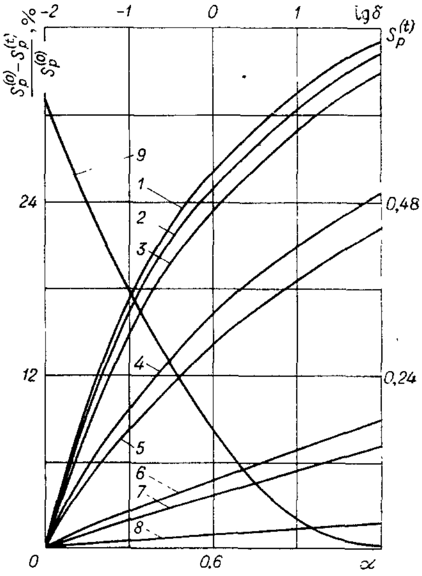

Fig. 2

tively the coefficients for the diffusion of rotationally and vibrationally excited molecules through the unexcited molecules) were chosen equal to $\beta \approx \beta' \approx 1.32$, which is valid over a wide range of temperatures for nonpolar molecules [4, 9, 10].

A comparison of our results with the numerical solution in [1] showed that if the vibrational degrees of freedom of the molecules are not excited, then for identical input parameters the maximum variance for G_p is 0.4% for $\delta = 40$, 2.8% for G_T for $\delta = 40$, and 0.4% for S_T for $\delta = 5$. Thus, as in the case of a monatomic gas [8], the Bubnov–Galerkin method converges rather rapidly. If the results obtained need to be refined, more complicated trial functions (15) must be chosen.

It is of interest to consider the mechanism and to make numerical estimates of the contribution of the internal degrees of freedom of the molecules to the fluxes. In the absence of inelastic collisions, when $\alpha = \alpha' = 0$ (the Eucken approximation), the thermal creep G_T and the translational components of the heat fluxes $S_p^{(t)}$ and $S_T^{(t)}$ are the same as the results for a monatomic gas [8], and the internal components of the heat flux caused by the pressure gradient are zero. Consequently, the internal degrees of freedom of the molecules contribute to these fluxes only when there are inelastic collisions.

The internal components $S_T^{(r)}$ and $S_T^{(v)}$ of the heat flux resulting from the temperature gradient behave differently. These fluxes are due both to inelastic collisions between molecules and to the diffusive transport respectively of rotationally and vibrationally excited molecules.

Let us estimate numerically the contribution of the internal degree of freedom of the molecules for various values of the rarefaction parameter δ. Calculation showed that the vibrational degrees of freedom make a very small contribution (in comparison with the rotational degrees of freedom) to all the fluxes except S_T^v.

Poiseuille flow depends very weakly on the internal degrees of freedom of the molecules: Their largest contribution is 1.2% for $\delta \simeq 1$, $\alpha = 1.2$ for a diatomic gas with rotational degrees of freedom ($c_V^r/k = 1$). In this case Poiseuille flow is decreased.

Figure 1 shows the relative contribution of the rotational degrees of freedom of diatomic molecules to the thermal creep G_T for 1) $\delta = 30$; 2) 10; 3) 5; 4) 1; 5) 0.7; 6) 0.1; 7) 0.07; 8) 0.01. The thermal creep decreases with increasing δ, and in the hydrodynamic limit is equal to zero. The relative contribution of the internal degrees of freedom increases with increasing δ. Thus, in the viscous regime with slip ($\delta = 30$) G_T becomes 16.5% smaller than $G_T^{(0)}$, the result for a monatomic gas, for an increase of α from 0 to 1.2. The decrease of the value of the thermal creep is explained by the transformation of part of the translational energy of the molecules into internal energy in inelastic collisions.

The result obtained contradicts the conclusion in [1] that the effect of thermal transpiration (13) does not depend on the internal degrees of freedom of the molecules. Although

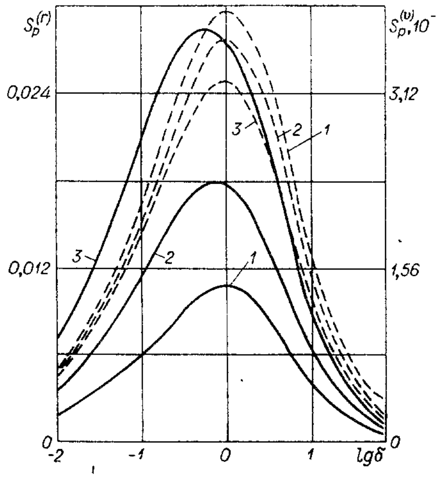

Fig. 3

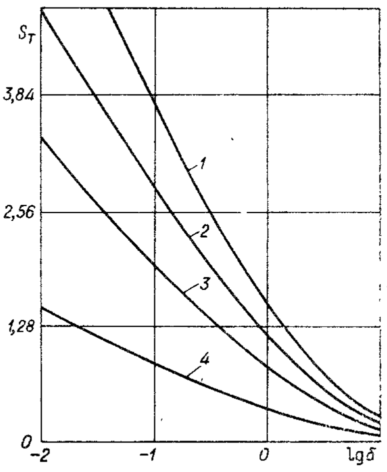

Fig. 4

all the numerical procedures were performed correctly, the conclusion in [1] is wrong because of the wrong choice of variable input parameters.

In [1] the total Eucken factor and its translational component were chosen as input parameters. However, it is known [2, 4] that each of these parameters is a function of the characteristic relaxation times, i.e., each depends on α and β.

Figures 2 and 3 show the dependence of the translational $S_p^{(t)}$ rotational $S_p^{(r)}$, and vibrational $S_p^{(v)}$ components of the heat flux which result from the pressure gradient on the rarefaction parameter δ and the value of α for a diatomic gas with $c_V^v/k = c_V^v/k = 1$, and $\alpha' = 0.001$. On Fig. 2 for curve 1) $\delta = 30$; 2) 10; 3) 5; 4) 1; 5) 0.7; 6) 0.1; 7) 0.07; 8) 0.01. Curve 9 describes the variation of $S_p^{(t)}$ with δ for $\alpha = 0.3$. On Fig. 3 the solid curves are for $S_p^{(r)}$, and the dashed curves are for $S_p^{(v)}$. For curve 1) $\alpha = 0.3$; 2) 0.6; 3) 1.2.

The contribution of the internal degrees of freedom to $S_p^{(t)}$ is rather large (Fig. 2). For $\delta = 10$ and $\alpha = 1.2$ the translational component of the heat flux is 34% smaller than $S_p^{(o)}$, the value for a monatomic gas.

The presence of the heat fluxes $S_p^{(t)}$, $S_p^{(r)}$, and $S_p^{(v)}$ is a purely kinetic phenomenon, occurring only in a rarefied gas. They are not present in the continuum limit, and in Figs. 2 and 3 they clearly approach zero. Close to the free-molecule limit (16) heat transport occurs only by the translational motion of the molecules. This means that in the intermediate regime the fluxes $S_p^{(r)}$ and $S_p^{(v)}$ must have a maximum, which is seen in Fig. 3. With an increase in the parameter α the peak for the flux $S_p^{(r)}$ is displaced toward smaller δ. This is accounted for by the fact that with an increase in the fraction of inelastic collisions, the rotational degrees of freedom of the molecules are excited more quickly, and the flux $S_p^{(r)}$ reaches a maximum for a less dense medium. If the parameter α' were varied over wider limits, a similar displacement of the peak would be observed for $S_p^{(v)}$ also. It is clear that $S_p^{(v)}$ decreases with increasing α; this shows the dependence of the vibrational component of the heat flux on the fraction of translational—rotational transitions during intermolecular collisions.

Figure 4 shows the dependence on δ of the total heat fluxes S_T^{RV} for a diatomic gas with rotational and vibrational degrees of freedom (curve 1, $\alpha = 0.3$, $\alpha' = 0.001$, $c_V^r/k = c_V^v/k = 1$), S_T^R for a diatomic gas with only rotational degrees of freedom (curve 2, $\alpha = 0.3$, $c_V^r/k = 1$), and a monatomic gas (curve 3). Curves 3 and 4 describe respectively the variation of $S_T^{(t)}$ and $S_T^{(r)}$ for a gas with rotational degrees of freedom, and $S_T^{(t)}$, $S_T^{(r)}$, $S_T^{(v)}$ for a gas with rotational and vibrational degrees of freedom of the molecules. The Fourier heat-conduction law holds for each of the components of the flux $S_T^{(t)}$, $S_T^{(r)}$, and $S_T^{(v)}$ for $\delta \gg 1$. In an almost free-molecule regime the fluxes $S_T^{(r)}$ and $S_T^{(v)}$ are also different from zero (16), since rotationally and vibrationally excited molecules diffuse through the unexcited molecules.

Figure 5 shows the relative contribution of the internal degrees of freedom of the molecules to the total heat flux S_T^{RV} resulting from a temperature gradient for a gas with rotational and vibrational degrees of freedom ($\alpha' = 0.001$, $c_V^r/k = c_V^r/k = 1$, solid curves), and to S_T^R for a gas with only rotational degrees of freedom ($c_V^r/k = 1$, dashed curves) as a function of α for various values of the rarefaction parameter δ [S_{To} is the heat flux for a monatomic gas. For curve 1) $\delta = 0.1$; 2) 0.1; 3) 1; 4) 10; 5) 30]. It is clear that the total heat

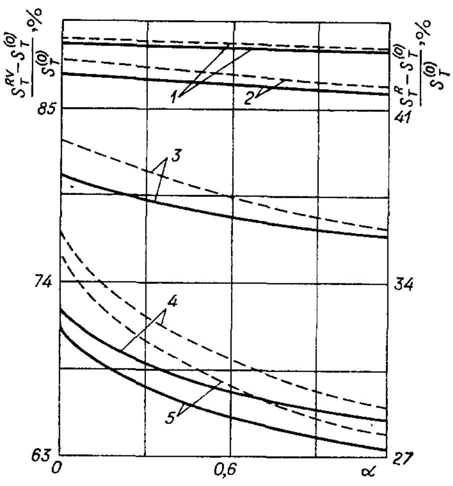

Fig. 5

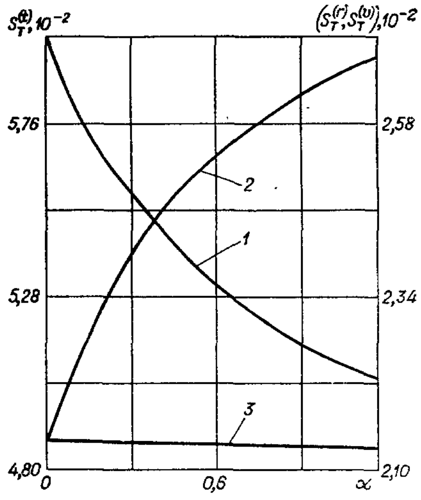

Fig. 6

flux produced by the temperature gradient depends strongly on the internal degrees of freedom of the molecules for all values of δ. For S_T^{RV} their contribution amounts to 63 to 89%, and for S_T^R from 27 to 44%. The greatest difference from the result for a monatomic gas occurs near the free-molecule limit ($\delta = 0.01$). This is accounted for by the large contribution of the diffusive transport of rotationally and vibrationally excited molecules to the heat flux in this regime. With an increase in the fraction of inelastic collisions, the total heat flux is decreased, as can be seen from Fig. 5. This occurs because with an increase in α the translational component $S_T^{(t)}$ is decreased more than the internal component of the heat flux $S_T^{(r)}$ is increased (Fig. 6, $\delta = 30$; curve 1 is for $S_T^{(t)}$, 2) $S_T^{(r)}$; 3) $S_T^{(v)}$).

In conclusion we note that our results can be used to justify and design experimental methods for determining the characteristic relaxation times in polyatomic gases.

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