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Journal of
APPLIED
MATHEMATICS
AND MECHANICS

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Journal of Applied Mathematics and Mechanics 69 (2005) 943–954

ON THE THEORY OF BULK VISCOSITY AND RELAXATION PRESSURE†

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(*Received* 16 *December* 2003)

A general theory of bulk viscosity and relaxation pressure, based on the generalized Chapman–Enskog method, is given, and also simple qualitative theories of them. Problems associated with the definition of temperature are discussed. Formulae are given for the bulk viscosity coefficient and the thermal conductivity of a gas possessing rotational degrees of freedom. The influence of bulk viscosity on the absorption and dispersion of sound and on the structure of a shock wave in nitrogen is investigated.

In aerodynamics, use has previously been made chiefly of Euler's and boundary-layer equations in which the bulk viscosity is not of the same order and is consequently omitted. In fact, the ratio of the bulk viscosity gradient to the convective part of the equation of motion will be of the order of the inverse Reynolds number, provided that the dynamic and bulk viscosity coefficients are commensurate and the velocity divergence will be of the order of the ratio of the characteristic velocity to the characteristic length. As a result, in handbooks on gas mechanics, the bulk viscosity is either generally ignored or is described insufficiently clearly [1], including, for example, in the problem of sound propagation [2]. However, at present, to calculate the laminar flows of a compressible fluid, the equations of gas dynamics in the Navier–Stokes–Fourier approximation (or, more concisely, the Navier–Stokes equations) are widely used, in which account is taken of terms of the order of the inverse Reynolds number, and therefore it is necessary to analyse the role of bulk viscosity problems of gas flows around bodies.

Different areas of the kinetic theory of bulk viscosity have been developed [3–11], but insufficient attention has been paid to its simple qualitative modest [8, 11].

The question of the definition of the temperature remains debatable [5, 6, 9]. In the case of ideal polyatomic gases, the bulk viscosity occurs in the expression for the stress tensor, provided the distribution over the internal energies of the molecules is close to local equilibriated, and the temperature T is defined from the total internal energy of the gas (as in the thermodynamics of irreversible processes). If the temperature is defined from the translational energy of the particles (the translational temperature of the gas T_t), then the stress tensor has the same form irrespective of the degree of excitation of the internal degrees of freedom of the molecules, and the bulk viscosity is not present, but similar term occurs in the expression for the internal energy of the gas. Such a definition of the temperature is more "physical", since the stress tensor is determined by transfer of the momentum of the particles [5, 6]. In non-ideal (dense) monatomic gases the bulk viscosity is governed by the potential energy of interaction of the molecules. When the temperature T_t is introduced, the expression for the bulk viscosity coefficient changes, and a similar term occurs in the formula for the internal energy of the gas [9].

A similar problem arises with the relaxation pressure – a fine effect which occurs in gas flows, provided that some of the internal degrees of freedom of the molecules are close to the locally equilibriated state while others relax [4–8, 10, 11].

A consequence of the generalized Chapman–Enskog method (Section 1) is a general system of equations of physicochemical (relaxation) gas dynamics – a system of equations with level kinetics [5, 6]. The latter describes, in particular, the regions of gas flows where the internal degrees of freedom

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†*Prikl. Mat. Mekh.* Vol. 69, No. 5, pp. 1051–1064, 2005.

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doi: 10.1016/j.jappmathmech.2005.11.016

of the molecules are frozen. The concept of the translational temperature I_t is employed. The stress tensor does not change its form as a function of the degree of excitation of the internal degrees of freedom of the molecules. Expressions for the bulk viscosity and relaxation pressure are obtained by taking the limit as $\tau/t_* \to 0$ and by redefinition of temperature T_t to T, where τ is the time of relaxation of the "rapid" process of the establishment of a quasi-equilibrium state, and t_* is the gas dynamic time. These quantities characterize the difference of T_t from the temperature T, defined taking the internal energy of molecules for rapid processes into account.

Sections 2 and 3 illustrate the positions of the general theory on the well-known [8, 12] relaxation gas dynamic models without turning to kinetic theory.

Below, we consider a gas with rotational degrees of freedom close to local equilibriated, and with the remaining internal degrees of freedom of the molecules frozen. We emphasize that, when the temperature T_t is used, the systems of equations for scalar corrections to the distribution functions are simplified (Section 4). Our main attention is devoted to a qualitative examination. Questions of the significance of bulk viscosity are illustrated by simple but representative examples (Sections 6 and 7). Similar questions for the relaxation pressure are more complex, have not been developed and are not considered here.

1. THE GENERALIZED CHAPMAN–ENSKOG METHOD

We will consider the case of ideal gases whose molecules interact only on instantaneous collisions, in the quasi-classical approximation, when the translational energy of the molecules is considered classically and the internal energy is treated quantum-mechanically [3–8]. There are no chemical reactions. The system of general equations of physiochemical gas dynamics includes equations of the balance of populations n_ω, momentum and internal energy (see the reviews [5, 6])

$$\frac{Dn_\omega}{Dt} + n_\omega \nabla \cdot \mathbf{u} + \nabla \cdot n_\omega \mathbf{V}_\omega = K_\omega, \quad K_\omega = \int J_\omega(f, f) d\boldsymbol{\xi} \tag{1.1}$$

$$\rho \frac{D\mathbf{u}}{Dt} + \nabla \cdot \mathbf{\Pi} = 0 \tag{1.2}$$

$$n \frac{D\mathscr{E}}{Dt} + \mathbf{\Pi}: \nabla \mathbf{u} + \nabla \cdot \mathbf{q} = 0 \tag{1.3}$$

Here

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla, \quad n = \sum_\omega n_\omega, \quad \rho = mn$$

n_ω is the number density of particles in quantum state ω, i.e. possessing internal energy E_ω, and $J_\omega(f, f)$ is the operator of inelastic collisions in the kinetic equation; summation is carried out for all values of the subscripts ω, $\psi = 0, 1, 2, \dots, N$, where N is the number of quantum levels, and m is the mass of a molecule.

Summing Eq. (1.1) over ω, we obtain the continuity equation

$$\frac{Dn}{Dt} + n \nabla \cdot \mathbf{u} = 0 \tag{1.4}$$

The generalized Chapman–Enskog method gives the series for the distribution functions $f_\omega = f_\omega^{(0)} + f_\omega^{(1)} \dots$ according to the Knudsen number $\mathrm{Kn} \ll 1$ relative to the locally Maxwell function

$$f_\omega^{(0)} = n_\omega \left(\frac{h}{\pi}\right)^{3/2} \exp(-hc^2), \quad \mathbf{c} = \boldsymbol{\xi} - \mathbf{u}, \quad h = \frac{m}{2kT_t} \tag{1.5}$$

where m is the mass and ξ is the velocity of the particle. The perturbation

$$f_\omega^{(1)} = f_\omega^{(0)} \left\{ -A_\omega \mathbf{c} \cdot \nabla \ln T_t - B_\omega \left(\mathbf{cc} - \frac{1}{3} \mathbf{I} c^2 \right): \nabla \mathbf{u} - \sum_\psi D_{\omega\psi} \mathbf{c} \cdot \nabla \frac{n_\psi}{n} - G_\omega \right\}$$
$$\frac{f_\omega^{(1)}}{f_\omega^{(0)}} = O(\mathrm{Kn}) \tag{1.6}$$

Here **I** is the unit tensor, and A, B, D and G are scalar coefficients of the order of the Knudsen number Kn; they depend on hc^2 and the independent of the gradients of the macroparameters and explicitly of **u**.

We will consider the version of the method when the following quantities are defined in terms of $f_\omega^{(0)}$

$$n_\omega = \int f_\omega^{(0)} d\boldsymbol{\xi}, \quad \mathbf{u} = \frac{1}{n}\sum_\omega \int f_\omega^{(0)} \boldsymbol{\xi} d\boldsymbol{\xi}, \quad T_t = \left(\frac{3}{2}nk\right)^{-1} \sum_\omega \int f_\omega^{(0)} \frac{m}{2} c^2 d\mathbf{c}$$
$$\mathscr{E} = \frac{3}{2}kT_t + \mathscr{E}^{\text{in}}, \quad \mathscr{E}^{\text{in}} = \sum_\omega \frac{n_\omega}{n} E_\omega \tag{1.7}$$

where $\mathscr{E}$ is the specific internal energy of the gas, k is Boltzmann's constant and the quantity $\mathscr{E}^{\text{in}}$ is governed by the internal energy of the molecules.

Formulae (1.7) yield the conditions for the solution of the integral equations for the coefficients A, B, D and G to be unique. The vector terms (in terms of **c**) of expression (1.6) define the diffusion rates $\mathbf{V}_\omega$ and the heat flux vector **q**. The stress tensor

$$\mathbf{\Pi} = \sum_\omega m \int (f_\omega^{(0)} + f_\omega^{(1)}) \mathbf{cc} d\mathbf{c} = P\mathbf{I} + \boldsymbol{\pi}, \quad P = nkT_t \tag{1.8}$$

where P is the trace of the stress tensor, π is the divergentless tensor (with zero trace)

$$\boldsymbol{\pi} = -\sum_\omega m \int f_\omega^{(0)} B_\omega \left(\mathbf{cc} - \frac{1}{3}\mathbf{I}c^2\right) : \nabla \mathbf{u} \mathbf{cc} d\mathbf{c} = -2\eta \mathbf{S} \tag{1.9}$$

η is the dynamic viscosity coefficient and **S** is the shear rate tensor with the Cartesian components

$$S_{ij} = \frac{1}{2}\left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j}\right) - \frac{1}{3}\nabla \cdot \mathbf{u} I_{ij}, \quad i, j = 1, 2, 3$$

Finally, the right-hand side of Eq. (1.1)

$$K_\omega = K_\omega^{(0)} + K_\omega^{(1)}(G); \quad K_\omega^{(0)} = \int J(f^{(0)}, f^{(0)}) d\mathbf{c}, \quad K_\omega^{(1)} = \int L(f^{(0)}, f^{(0)} G) d\mathbf{c} \tag{1.10}$$

i.e. $K_\omega^{(0)}$ is calculated from $f = f^{(0)}$, and L is the linearized (with respect to $f^{(0)}$) and symmetrized [5, 6] operator of inelastic collisions. Only the scalar term G_ω (in terms of **c**) of expression (1.6) contributes to $K_\omega^{(1)}$. The fact that, in near-equilibrium situations, the terms of formula (1.10) are quantities of identical order [5, 6] is fundamental.

If rotations and vibrations of the molecules are excited, then $\omega = \alpha\beta$, $\alpha = 0, 1, 2, \ldots, N_R$, and $\beta = 0, 1, 2, \ldots, N_V$, where N_R and N_V are the numbers of rotational and vibrational levels respectively. It is assumed that the rotational energy of a molecule E_α is independent of its vibrational state [8], so that

$$\mathscr{E}^{\text{in}} = \mathscr{E}_R + \mathscr{E}_V, \quad \mathscr{E}_R = \sum_\omega E_\alpha \frac{n_\omega}{n}, \quad \mathscr{E}_V = \sum_\omega E_\beta \frac{n_\omega}{n} \tag{1.11}$$

Suppose the rotations of the molecules are rapid processes, i.e. $\tau_R/t_* \ll 1$, and the vibrations are slow processes, i.e. $\tau_V/t_* \sim 1$, where τ_R and τ_V are the rotational and vibrational relaxation times, and t_* is the gas-dynamic time.

The appearance of the small parameter $\tau_R/t_* \sim$ Kn enables us to find an approximate solution for n_ω and to transfer to a brief gas-dynamic description. Here it is sufficient to confine ourselves to the Euler approximation on the left-hand sides of Eqs (1.1) and (1.3), omitting the terms with $\mathbf{V}_\omega$, π and **q**: allowance for these terms yields higher-order terms. Remember that, in deriving equations for determining the coefficients A, B and D in expression (1.6), the convective part of the kinetic equation is transformed within the framework of the Euler approximation. Taking the above and Eq. (1.4) into account, we will sum Eqs (1.1) over the vibrational levels β. We obtain

$$n\frac{Dy_\alpha}{Dt} = R_\alpha^{(0)R} + R_\alpha^{(0)V} + R_\alpha^{(1)R} \tag{1.12}$$

where

$$y_\alpha = \frac{n_\alpha}{n},\quad n_\alpha = \sum_\beta n_\omega,\quad R_\alpha = \sum_\beta K_\omega$$

and n_α is the rotational population. The quantities with the superscript R include only rotational and translational-rotational exchanges, and the quantities with superscript V include only exchanges of vibrational energy [10]. The term $R_\alpha^{(1)V}$ is omitted as being of a higher order.

In dimensionless form, the term $R_\alpha^{(0)R} \sim 1/\mathrm{Kn}$, and the remaining terms of Eq. (1.12) are of the order of unity. We will seek a solution in the form

$$y_\alpha = y_\alpha^{(0)} + y_\alpha^{(1)},\quad y_\alpha^{(1)}/y_\alpha^{(0)} = O(\mathrm{Kn})$$

In the zeroth approximation we have

$$R_\alpha^{(0)R} = 0 \Rightarrow y_\alpha^{(0)} = y_\alpha^{\mathrm{eq}}(T_t) \tag{1.13}$$

where the Boltzmann function

$$y_\alpha^{\mathrm{eq}}(T_t) = \frac{S_\alpha}{Q}\exp(-\varepsilon_\alpha),\quad Q = \sum_\alpha S_\alpha \exp(-\varepsilon_\alpha),\quad \varepsilon_\alpha = \frac{E_\alpha}{kT_t} \tag{1.14}$$

and S_α is the statistical weight of the rotational level α.

The system of equations for the slow variables, i.e. for the relative vibrational populations

$$y_\beta = \frac{n_\beta}{n},\quad n_\beta = \sum_\alpha n_\omega$$

is obtained by summing Eqs (1.1) over α taking Eq. (1.4) into account

$$n\frac{Dy_\beta}{Dt} + \nabla\cdot n_\beta \mathbf{V}_\beta = R_\beta^{(0)V};\quad n_\beta \mathbf{V}_\beta = \sum_\alpha n_\omega \mathbf{V}_\omega,\quad R_\beta^{(0)V} = \sum_\alpha K_\omega^{(0)} \tag{1.15}$$

The right-hand side of Eq. (1.15) results from the vibrational exchanges and is calculated for $f^{(0)}$. With the assumptions made, the quantity $R_\beta^{(1)V}$ is of the order of Kn compared with $R_\beta^{(0)V}$ and is therefore omitted.

In the expressions for η, $\mathbf{V}_\beta$ and $\mathbf{q}$, with an error $O(\mathrm{Kn})$ compared with unity, the population $n_{\alpha\beta}$ is replaced by $y_\alpha^{\mathrm{eq}}(T_t)n_\beta$. After linearization with respect to $y^{(0)}$, the right-hand side of Eq. (1.12) will be linear in $y^{(1)}$ and contain, generally speaking, a free term (independent of $n^{(1)}$). The left-hand side of Eq. (1.12) must be set equal to

$$n\frac{Dy_\alpha^{(0)}}{Dt} = n\frac{dy_\alpha^{\mathrm{eq}}(T_t)}{dT_t}\frac{DT_t}{Dt} \tag{1.16}$$

where

$$\frac{DT_t}{Dt} = -C_v^{-1}\left(kT_t\nabla\cdot\mathbf{u} + \frac{1}{n}\sum_\beta E_\beta R_\beta^{(0)V}\right),\quad C_v = \frac{3}{2}k + c_v^R \tag{1.17}$$

The "rotational" specific heat at constant volume

$$c_v^R = \frac{d}{dT_t}\mathcal{E}_R^{\mathrm{eq}}(T_t),\quad \mathcal{E}_R^{\mathrm{eq}} = \sum_\alpha E_\alpha y_\alpha^{\mathrm{eq}}(T_t) \tag{1.18}$$

Formula (1.17) was obtained neglecting terms of the order of Kn in Eqs (1.3) and (1.15). These equations take the form

$$\frac{D}{Dt}\left(\frac{3}{2}kT_t + \mathcal{E}_R^{\mathrm{eq}} + \mathcal{E}_V\right) + kT_t\nabla\cdot\mathbf{u} = 0, \quad \frac{D\mathcal{E}_V}{Dt} = \frac{1}{n}\sum_{\beta} E_\beta R_\beta^{(0)V} \tag{1.19}$$

Equality (1.17) follows from relations (1.19).

Taking into account equalities (1.16) and (1.17), for $y_\alpha^{(1)}$ we find a system of linear algebraic equations with an inhomogeneous part that is linear in $\nabla\cdot\mathbf{u}$. As a result

$$y_\alpha^{(1)} = a_\alpha + b_\alpha\nabla\cdot\mathbf{u}$$

where the coefficients a_α and b_α are proportional to Kn.

Consequently

$$\frac{3}{2}kT_t + \mathcal{E}_R = \frac{3}{2}kT_t + \mathcal{E}_R^{\mathrm{eq}}(T_t) + Q, \quad Q = \sum_{\alpha} E_\alpha(a_\alpha + b_\alpha\nabla\cdot\mathbf{u}) \tag{1.20}$$

The quantity Q is the non-equilibrium correction to the internal energy of the gas, which is governed by translational, rotational and vibrational degrees of freedom of the molecules. Instead of equality (1.20), in the thermodynamics of irreversible processes, the following expression is used

$$\frac{3}{2}kT_t + \mathcal{E}_R = \frac{3}{2}kT + \mathcal{E}_R^{\mathrm{eq}}(T) \tag{1.21}$$

where T is the translational-rotational temperature. In order to switch from equality (1.20) to (1.21), we will perturb the translational temperature

$$T_t = T + T^{(1)}, \quad T^{(1)}/T = O(\mathrm{Kn})$$

Linearizing formula (1.2) and subtracting from the expression obtained the magnitude of the right-hand side of equality (1.21), we obtain

$$T^{(1)} = T_t - T = -C_\upsilon^{-1}Q \tag{1.22}$$

The non-equilibrium correction Q characterizes the difference in the translational and translational-rotational temperatures [11]. The quantity C_υ is defined by the final formula of system (1.17).

Taking into account relation (1.22), we reduce expression (1.8) to the form

$$\mathbf{\Pi} = (p + p_{\mathrm{rel}} - \varsigma\nabla\cdot\mathbf{u})\mathbf{I} - 2\eta\mathbf{S}, \quad p = nkT \tag{1.23}$$

The formulae for the bulk viscosity coefficient ς and the relaxation pressure p_{rel} can obviously be obtained from the previous formulae. Approximate formulae are given in Sections 2 and 3. Rigorous expressions for ς, p_{rel}, $\mathbf{V}_\beta$ and $\mathbf{q}$ are known [7].

The reduced system of equations consists of Eqs (1.2)–(1.4) and $N_V - 1$ equations (1.15) for the relative vibrational populations y_β. The stress tensor is given by formula (1.23). The internal energy of the gas

$$\mathcal{E} = \frac{3}{2}kT + \mathcal{E}_R^{\mathrm{eq}}(T) + \mathcal{E}_V, \quad \mathcal{E}_V = \sum_{\beta} E_\beta y_\beta \tag{1.24}$$

In all instances, T_t is replaced by T. If the vibrations are frozen, system (1.2)–(1.4) holds and the quantities p_{rel}, $\mathbf{V}_\beta$ and $\mathcal{E}_V$ are omitted. The heat flux vector takes the form

$$\mathbf{q} = -\lambda\nabla T \tag{1.25}$$

where λ is the thermal conductivity.

2. MODEL OF THE RELAXATION OF ROTATIONAL ENERGY

Here and in the following section, the general theory of bulk viscosity and relaxation pressure described above will be illustrated on gas dynamic models, avoiding kinetic theory. As stated in Section 1, the balance equations in the Euler approximation are used. The trace of the stress tensor

$$P = nkT_t \tag{2.1}$$

We will consider a gas with relaxing rotational degrees of freedom of the molecules, and the vibrations frozen. The energy equation (1.3) takes the form

$$\frac{D\mathscr{E}}{Dt} + kT_t\nabla\cdot\mathbf{u} = 0, \quad \mathscr{E} = \frac{3}{2}kT_t + \mathscr{E}_R \tag{2.2}$$

where $\mathscr{E}$ is the internal energy of the gas, referred to the number of particles per unit volume.

For the rotational energy $\mathscr{E}_R$, we will use the simplest relaxation equation [8, 12]

$$\frac{D\mathscr{E}_R}{Dt} = \frac{1}{\tau_R}[\mathscr{E}_R^{\text{eq}}(T_t) - \mathscr{E}_R] \tag{2.3}$$

where τ_R is the rotational relaxation time, and $\mathscr{E}_R^{\text{eq}}$ is the known equilibrium function T_t (see formulae (1.14) and (1.18)). Equation (2.3) is obtained from Eq. (1.12), if we omit $R_\alpha^{(0)V}$ (the vibrations are frozen), assume the term $R_\alpha^{(1)R}$ to be negligibly small, multiply by E_α, sum in terms of α and approximate the right-hand side with the simplest relaxation expression.

Local equilibrium (i.e. completely excited rotations) occurs in the limit as $\tau_R/t_* \to 0$. We will write the solution of Eq. (2.3) for this case in the form of a series power of τ_R

$$\mathscr{E}_R = \mathscr{E}_R^{(0)} + \tau_R\mathscr{E}_R^{(1)} + \ldots \tag{2.4}$$

In the zeroth approximation, we have the equilibrium solution

$$\mathscr{E}_R^{(0)} = \mathscr{E}_R^{\text{eq}}(T_t) \tag{2.5}$$

In the following approximation, taking (1.4) and (2.2)–(2.5) into account, we obtain

$$-\mathscr{E}_R^{(1)} = \frac{D\mathscr{E}_R^{\text{eq}}(T_t)}{Dt} = c_\upsilon^R\frac{DT_t}{Dt} = -kT_tc_\upsilon^RC_\upsilon^{-1}\nabla\cdot\mathbf{u} \tag{2.6}$$

The quantities C_υ and c_υ^R are given by formulae (1.7) and (1.18). Using relations (2.6), we reduce the second formula of system (2.2) to the form

$$\mathscr{E} = \frac{3}{2}kT_t + \mathscr{E}_R^{\text{eq}}(T_t) + A(T_t)\nabla\cdot\mathbf{u} \tag{2.7}$$

$$A(T_t) = \tau_Rc_\upsilon^RkT_tC_\upsilon^{-1} \tag{2.8}$$

We omit quantities proportional to τ_R^n, $n \geq 2$ everywhere.

We emphasize that the term $A\nabla\cdot\mathbf{u}$ is the relaxation contribution to the energy of the gas. Here, according to formula (2.1), the hydrostatic pressure nkT_t is calculated from the translational temperature T_t. We will introduce the translational-rotational temperature T by the equality

$$\mathscr{E} = \frac{3}{2}kT + \mathscr{E}_R^{\text{eq}}(T) \tag{2.9}$$

where for $\mathscr{E}$, formula (2.7) also holds.

We will perturb [5] the translational temperature $T_t = T + \tau_RT^{(1)}$. Linearizing the right-hand side of formula (2.7) with respect to τ_R, and equating it to the right-hand side of formula (2.9), we find

$$C_\upsilon\tau_RT^{(1)} + A\nabla\cdot\mathbf{u} = 0$$

such that

$$T_t - T = \tau_R T^{(1)} = -A(T) C_v^{-1} \nabla \cdot \mathbf{u} \equiv -\frac{1}{nk} \varsigma \nabla \cdot \mathbf{u} \tag{2.10}$$

Substituting the expressions (2.8) and (2.10) into the right-hand side of equality (2.1), we "convert" the relaxation term into the stress tensor such that its trace

$$P = nkT_t = p - \varsigma \nabla \cdot \mathbf{u}, \quad p = nkT \tag{2.11}$$

where the pressure p is calculated from the translational-rotational temperature T. Taking into account formulae (2.8) and (2.10), we write the expression for the bulk viscosity coefficient

$$\varsigma = nk^2 T \tau_R c_v^R(T) \left(\frac{3}{2} k + c_v^R(T) \right)^{-2} \tag{2.12}$$

For the coefficient A, in the non-equilibrium correction to the specific internal energy (2.7), we obtain the expression

$$A(T_t) = \frac{C_v(T_t)}{nk} \varsigma(T_t) \tag{2.13}$$

The quantity $\varsigma(T_t)$ is given by formula (2.12) with T replaced by T_t.

By virtue of relations (2.10), the difference between the translational and translational-rotational temperatures is proportional [11] to the bulk viscosity: $\varsigma \nabla \cdot \mathbf{u}$.

3. MODEL OF ROTATIONAL–VIBRATIONAL RELAXATION

Suppose that, apart from rotations, vibrations of the molecules are also excited in the gas. The energy equation is given by the first formula of system (2.2), but vibrational energy $\mathscr{E}_V$ is added to the expression for the specific internal energy of the gas, i.e.

$$\mathscr{E} = \frac{3}{2} kT_t + \mathscr{E}_R + \mathscr{E}_V \tag{3.1}$$

The rotational energy $\mathscr{E}_R$ satisfies Eq. (2.3), and for the energy $\mathscr{E}_V$ we consider the relaxation equation

$$\frac{D\mathscr{E}_V}{Dt} = \frac{1}{\tau_V} [\mathscr{E}_V^{\mathrm{eq}}(T_t) - \mathscr{E}_V] \tag{3.2}$$

to hold, where τ_V is the vibrational relaxation time.

Equation (3.2) is obtained from Eq. (1.15) in the Euler approximation (when $\mathbf{V}_\beta = 0$) by multiplying by E_β and summing over β for a model of the molecules – harmonic oscillators with single-quantum transitions [4].

Suppose, as in Section 2, that $\tau_R/t_* \to 0$. We will consider the case of slowed exchanges of vibrational energy of the molecules: $\tau_V/t_* = O(1)$. Again, we expand the solution of Eq. (2.3) in series (2.4). As above, we obtain

$$\mathscr{E}_R^{(0)} = \mathscr{E}_R^{\mathrm{eq}}(T_t), \quad -\mathscr{E}_R^{(1)} = c_v^R \frac{DT_t}{Dt}$$

Using the energy equation (the first formula of system (2.2)), expression (3.1) for the specific internal energy of the gas and relaxation equation (3.2), we find

$$\frac{DT_t}{Dt} = -C_v^{-1} \left(kT_t \nabla \cdot \mathbf{u} + \frac{\mathscr{E}_V^{\mathrm{eq}}(T_t) - \mathscr{E}_V}{\tau_V} \right)$$

The quantity C_v is defined by formulae (1.17) and (1.18).

Perturbing T_t with respect to the rotational-translational temperature T, in much the same way as in Section 2, we obtain formula (1.24) for the specific internal energy of the gas, and instead of formula (2.11) we obtain the expression

$$P = p + p_{\text{rel}} - \varsigma\nabla \cdot \mathbf{u}, \quad p = nkT$$

The gas flow is described by the system of equations shown at the end of Section 1. The bulk viscosity coefficient ς is given by formula (2.12).

The stress tensor contained the relaxation pressure

$$p_{\text{rel}} = -\frac{\varsigma}{kT}\frac{\mathscr{E}_V^{\text{eq}}(T) - \mathscr{E}_V}{\tau_V} \tag{3.3}$$

Expression (3.3) is identical with the expression obtained earlier [10] by the modified Chapman–Enskog method.

Relaxation pressure occurs in the case of simultaneous rapid (rotations) and slow (vibrations) exchanges of internal energy of the molecules [4, 7, 10]. The role of chemical reactions is similar to the role of vibrations: if their relaxation time $\tau_c \to 0$, then they make a contribution to ς, and if $\tau_c = O(1)$, the contribute to the relaxation pressure [7].

4. THE DEFINITION OF TEMPERATURE IN THE CHAPMAN-ENSKOG METHOD

The bulk viscosity coefficient and the relaxation pressure are normally calculated for specific limit situations [7], and not on the basis of the relaxation description given above (an approach similar to that described in Section 2 and 3 was used when Grad's method was employed [8]). The solution of the system of kinetic equations is sought in the form of the series $f_\omega^{(0)} + f_\omega^{(1)} + \dots$, where the distribution function $f_\omega^{(0)}$ is locally equilibrium with respect to the velocities of the molecules and with respect to part of their internal energy, taking into account of which the temperature T is defined. The solution of systems of integral equations for the constituents of the function $f_\omega^{(1)}$ becomes unique when the conditions of [3] are added, one of which is simplified when the temperature is defined basing on the translational degrees of freedom. As a result, the system of equations for determining the scalar constituent of the function $f_\omega^{(1)}$ becomes simpler.

We will illustrate the above using the simplest example [3]. A gas with excited rotational degrees of freedom is examined (as above, the rotational levels are denoted by α, and the vibrations are frozen). The scalar component of the function $f_\alpha^{(1)}$ has the form

$$-(1/n)f_\alpha^{(0)}\Gamma_\alpha\nabla \cdot \mathbf{u} \tag{4.1}$$

where $f_\alpha^{(0)}$ is the Maxwell–Boltzmann distribution function, and Γ_α is a function of hc^2 and $E_\alpha/(kT)$.

The system of equations for the scalar quantity Γ_α is solved under the conditions [3]

$$\sum_\alpha \int f_\alpha^{(0)}\Gamma_\alpha d\mathbf{c} = 0, \quad \sum_\alpha \int f_\alpha^{(0)}\Gamma_\alpha(mc^2/2 + E_\alpha)d\mathbf{c} = 0 \tag{4.2}$$

following from the requirements that with respect to $f_\alpha^{(0)}$ the numerical density and translational-rotational energy of the gas (2.9) are determined. The solution is sought in the form of a series in orthogonal polynomials, and the simplest approximation, enabling us to satisfy conditions (4.2), has the form [3]

$$\Gamma_\alpha = \gamma_1(hc^2 - 3/2) + \gamma_2(\mathscr{E}_R^{\text{eq}}(T) - E_\alpha) \tag{4.3}$$

From the second condition of (4.2) we obtain a linear relation between the coefficients γ_1 and γ_2 [3], and it follows that the perturbation (4.1) contributes $-\varsigma\nabla \cdot \mathbf{u}$ to the trace of the stress tensor (2.11), and the bulk viscosity coefficient ς is proportional to γ_1 [3].

If the temperature is defined basing on the translational degrees of freedom, then, instead of the second condition of (4.2), we will have the simpler condition

$$\sum_\alpha \int f_\alpha^{(0)}\Gamma_\alpha c^2 d\mathbf{c} = 0 \tag{4.4}$$

and consequently the simpler approximation

$$\Gamma_\alpha = \gamma_3(\mathscr{E}_R^{\mathrm{eq}}(T_t) - E_\alpha) \tag{4.5}$$

We recall that the coefficients γ_k are constant quantities ($k = 1, 2, 3$). By virtue of condition (4.4), the perturbation (4.1) and (4.5) makes a contribution only to the expression for the specific internal energy (2.7). By using equations given in [3], it is easy to prove the validity of formula (2.13).

The computing advantages of introducing T_t increase on changing to more complex cases (for example, a mixture of gases with quasi-stationary vibrational states [7]).

5. THE BULK VISCOSITY COEFFICIENT AND THERMAL CONDUCTIVITY

Consider the transport properties of a gas with rotational degrees of freedom of the molecules close to local equilibrium (the case of rapid exchanges of rotational energy of the molecules). The vibrations of the molecules are frozen, and there are no chemical reactions. The stress tensor is given by formula (1.23), where, in the given case, $p_{\mathrm{rel}} = 0$. We will ignore the dependence of the dynamic viscosity coefficient η on the rotational degrees of freedom [3], and for the function $\eta(T)$ there are reliable experimental data.

We will write formula (2.12) for the bulk viscosity coefficient ς in the form

$$\varsigma = \frac{1}{4}\pi k c_v^R \eta Z\left(\frac{3}{2}k + c_v^R\right)^{-2}; \quad Z = \frac{\tau_R}{\tau_t}, \quad \tau_t = \frac{\pi\eta}{4p} \tag{5.1}$$

where τ_t is the relaxation time of the translational degrees of freedom of the molecules.

The same expression for ς is obtained by the Chapman–Enskog method in the main approximation in terms of Sonine and Waldmann–Trübenbacher polynomials in [8]. Below, the specific heat capacity c_v^R, governed by the rotational degrees of freedom of the molecules, is assumed to be equal to k (a diatomic gas; here, the specific-heat ratio $\gamma = 7/5$, $\mathscr{E}_R^{\mathrm{eq}} = kT$). For the ratio of the rotational and translational relaxation times Z, Parker's approximation formula

$$Z = Z_\infty\left[1 + \frac{\pi^{3/2}}{2}\theta^{1/2} + \left(\frac{\pi^2}{4} + 2\right)\theta\right]^{-1}, \quad \theta = \frac{T_*}{T} \tag{5.2}$$

is often used and also a revised formula [8] differing from (5.2) by the presence in square brackets of the additional term $\pi^{3/2}\theta^{3/2}$.

For nitrogen, $T_* = 91.5$ K and $Z_\infty = 18.2$.

Figure 1 shows graphs of the ratio ς/η against T, calculated for nitrogen from formula (5.1) using Parker's formula (5.2) (the continuous curve) and using the revised formula [8] (the dashed curve). The limit value (as $T \to \infty$) of this ratio is equal to 2.23. For $T > 900$ K, the relative contribution of the vibrational degrees of freedom to the specific heat becomes substantial.

The heat flux vector is given by formula (1.25). We will write the thermal conductivity in the form [13]

$$\lambda = \frac{15}{4}R\eta\Lambda, \quad \Lambda = \lambda_t^* + \lambda_R^*, \quad R = \frac{k}{m} \tag{5.3}$$

where λ_t^* and λ_R^* are due to the translational and rotational degrees of freedom respectively. In practice, one is usually limited to the modified Eucken approximation [3]. Here

$$\lambda_t^* = 1, \quad \lambda_R^* = \frac{4}{15}\beta_t \approx \frac{4}{15}1.328, \quad \beta_t = \frac{\rho\mathscr{D}}{\eta} \tag{5.4}$$

where $\mathscr{D}$ is the self-diffusion coefficient of the gas, ignoring rotational degrees of freedom. The quantity β_t depends slightly on the intermolecular potentials, and therefore its average value, given in the second formula of system (5.4), is used [3]. In this approximation, the Prandtl number $\mathrm{Pr} = \gamma C_v\eta/\lambda = \mathrm{const}$

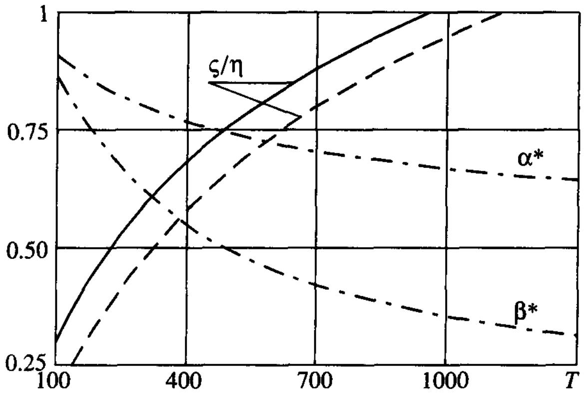

Fig. 1

(recall that γ and C_υ are constant quantities). At low T, the accuracy of approximation (5.4) is inadequate, and the Mason–Monchic approximation [8] is used, namely

$$\lambda_t^* = 1-\frac{A}{\sigma},\quad \lambda_R^* = \frac{2\beta_R}{5\sigma}(1+A),\quad \beta_R = \frac{\rho\mathcal{D}_R}{\eta} = \beta_t\varphi(T)$$
$$A = \frac{5-2\beta_R}{\pi Z}\left[1+\frac{2}{\pi Z}\left(\frac{5}{2\sigma}+\beta_R\right)\right]^{-1},\quad \sigma = \frac{3}{2}\frac{k}{c_\upsilon^R} \tag{5.5}$$

where $\mathcal{D}_R$ is the self-diffusion coefficient of the gas, taking into account the rotational degrees of freedom. The ratio $\mathcal{D}_R/\mathcal{D}$ will be estimated using Sandler's approximate formula [8]

$$\mathcal{D}_R/\mathcal{D} \equiv \varphi(T) = 1+0.27Z^{-1}-0.44Z^{-2}-0.90Z^{-3} \tag{5.6}$$

In approximation (5.5), (5.6), the Prandtl number depends on the temperature T.

6. THE ABSORPTION AND DISPERSION OF SOUND

The bulk viscosity is important if it is of the order of the dynamic viscosity and must be taken into account mainly by the Kn $\ll$ 1 approximation. An example is the propagation of small perturbations in a molecular gas with excited rotational degrees of freedom. The dimensionless absorption coefficient

$$\alpha = \alpha_1\mathrm{Kn}+O(\mathrm{Kn}^3),\quad \mathrm{Kn} = \omega\eta/p \ll 1 \tag{6.1}$$

where ω is the frequency. We emphasize that all the quantities (i.e. p, η, ς, etc.) occurring in formula (6.1) and formulae (6.2)–(6.4) given below are equal to their values in a stationary gas.

The coefficient α_1 is well known [2], since it is given by the Navier–Stokes approximation

$$\alpha_1 = \frac{2B}{3\gamma}+\frac{15}{8\gamma^2}\Lambda(\gamma-1)^2,\quad B = 1+\frac{3\varsigma}{4\eta} \tag{6.2}$$

Much less familiar is the fact that dispersion of sound should be investigated within the framework of Burnett's approximation, since the Navier–Stokes and Burnett terms of the transport properties make a contribution of the same order of magnitude to the deviation of the dispersion coefficient from the limit value as Kn → 0 (see, for example, [13]).

The dimensionless dispersion coefficient

$$\beta = 1-\beta_2\mathrm{Kn}^2+O(\mathrm{Kn}^4),\quad \beta_2 = \kappa_1+\kappa_2 \tag{6.3}$$

characterizes the change in the phase velocity as Kn increases. The coefficient

$$\kappa_1 = \frac{2B^2}{3\gamma^2} + \frac{25B}{4\gamma^3}\Lambda(\gamma-1)^2 + \frac{225}{128\gamma^4}\Lambda^2(\gamma-1)^3(3\gamma-7) \tag{6.4}$$

is given by the Navier–Stokes approximation, while the coefficient

$$\kappa_2 = \frac{\gamma-1}{\gamma^2}\left(\frac{7}{8}Q_1 - Q_3\right) + \frac{2Q_2}{3\gamma} \tag{6.5}$$

is governed by the Burnett terms of the transport properties [13], where

$$\begin{aligned} Q_1 &= \frac{15\sigma}{7(1+\sigma)}\left(\lambda_t^{*2} + \frac{5}{3}\sigma\lambda_R^{*2}\right) - \frac{8}{7}\lambda_t^* - \frac{20}{7}(B-1)(\lambda_t^* - \sigma\lambda_R^*) \\ Q_2 &= 1 + 2(1+\sigma)(B-1)^2, \quad Q_3 = \lambda_t^* + \frac{5}{2}(\lambda_t^* - \sigma\lambda_R^*)(B-1) \end{aligned} \tag{6.6}$$

The quantities in expressions (6.2) and (6.4)–(6.6) will be calculated using the formulae from the previous section for nitrogen ($c_\upsilon^R = k$, $\gamma = 7/5$). The quantity B is defined by the second formula of system (6.2).

We will denote by

$$\alpha^* = \alpha_1(\varsigma = 0)/\alpha_1(\varsigma \neq 0), \quad \beta^* = \beta_2(\varsigma = 0)/\beta_2(\varsigma \neq 0)$$

the ratios defining the contribution of the bulk viscosity to the absorption and dispersion coefficients. The values of the quantities in the numerators are obtained if we put $B = 1$ in formulae (6.2), (6.4) and (6.6).

The results of calculations of these ratios are given in Fig. 1. The bulk viscosity has a particularly strong effect on the dispersion coefficient β_2; the quantity Q_2 is quadratic in ς. We emphasize, however, that, when the bulk viscosity has a considerable influence, it might be necessary to change to a relaxation description [8], i.e. τ_R/t_* must not be assumed to be a small quantity.

7. THE SHOCK-WAVE STRUCTURE

As noted in the introductory part of this paper, the relative magnitude of the bulk viscosity gradient in the equation of motion of a compressible fluid in general is of the order of Re^{-1}. However, this is valid if the gas temperature is sufficiently high, such that $\varsigma \sim \eta$, and if the velocity divergence is not small. An upper estimate of this influence is obtained if we consider the question of the influence of the bulk viscosity on the shock wave structure, since here $\text{Re} \sim 1$, $\varsigma \sim \eta$ and $\nabla \cdot \mathbf{u} \sim u/L$. The problem of the structure of a weak shock wave in a molecular gas was solved earlier in [13]. We will denote by u^* and T^* the reduced valves of the velocity and temperature in a shock wave

$$u^* = \frac{u(\xi) - u(-\infty)}{u(\infty) - u(-\infty)}, \quad T^* = \frac{T(\xi) - T(-\infty)}{T(\infty) - T(-\infty)} \tag{7.1}$$

where ξ is the dimensionless streamwise coordinate [13]. The first approximation with respect to the parameter of the shock wave intensity is given by the Navier–Stokes approximation (in the following approximation, allowance for the Burnett transport properties is necessary [13]). Here

$$u^* = T^* = (1 + \text{th}(\xi/b))/2, \quad b = 8\gamma^2\alpha_1(\gamma+1) \tag{7.2}$$

The absorption coefficient α_1 is defined by the first formula of system (6.2) and is calculated from data for unperturbed flow. When the ratio ς/η increases, the coefficient b increase. Consequently, the region of perturbed flow expands in terms of ξ.

In applications, the question of the influence of bulk viscosity on the T and ρ profiles in shock waves of moderate and high intensity is of greater interest. The equations

$$\Delta_T = T(\varsigma = 0)/T(\varsigma \neq 0), \quad \Delta_\rho = \rho(\varsigma = 0)/\rho(\varsigma \neq 0)$$

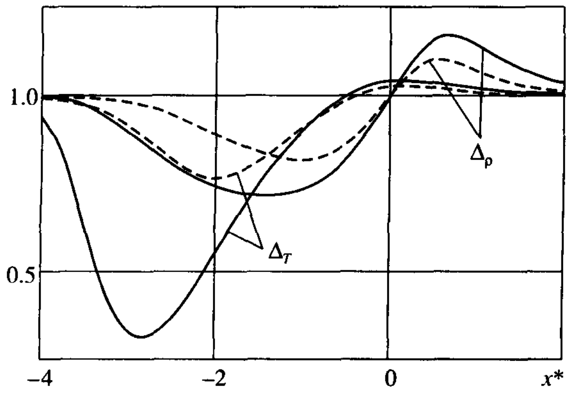

Fig. 2

denote the ratios of the values of temperature and density calculated using the Navier–Stokes equations by the method proposed in [14] for $\varsigma = 0$ and $\varsigma \neq 0$ (we recall that, in a shock wave, $\rho \sim 1/u$). The data in Fig. 2 were obtained for $T(-\infty) = 100$ K, the Mach number upstream of the wave $M = 5$ (the dashed curves) and $M = 11$ (the continuous curves), the streamwise coordinate x^* is referred to the mean free path upstream of the wave, and the value of the reduced density $\rho^* = 1/2$ corresponds to the value $x^* = 0$ [14].

The formulae from Section 4 are used, and, in particular, formula (5.2) for Z.

The bulk viscosity changes the density and temperature profiles considerably, especially in the front zone of the shock wave. Its influence increases as the Mach number increases.

We wish to thank G. A. Tirskii for helpful comments.

This research was supported financially by the Russian Foundation for Basic Research (02-01-00501), by the "State Support for Leading Scientific Schools" programme (NSh-1984.2003.1), and by the Russian Ministry of Education (E02-40-52).

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Translated by P.S.C.