



BURNETT'S EQUATIONS FOR MULTICOMPONENT MIXTURES OF POLYATOMIC GASES†

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(Received 28 August 1999)

Burnett's equations for a multicomponent gas mixture when there are external forces present which do not depend on the velocities and internal energies of the molecules are obtained using the system of kinetic equations in the quasiclassical spherically symmetrical approximation for the case of light exchanges of translational and internal energies of the molecules in the single-liquid approximation, when the system of gas-dynamic equations consists of equations for the concentration of the chemical components, the mean-mass velocity and the mean temperature. Exact and approximate formulae are obtained for the Burnett transport coefficients. Special cases, including the question of the general equations of thermal-stress and concentration-stress convection are considered. © 2000 Elsevier Science Ltd. All rights reserved.

Burnett's equations have mainly been derived (see the review [1] and later papers [2, 3]) for a simple gas [4, 5]. The most complete derivation of the expressions for the Burnett transport properties of multicomponent mixtures of monatomic gases, i.e. gases consisting of molecules with frozen internal degrees of freedom [6],‡ is refined and extended below, the results are represented in a more effective form, and both exact and approximate "working" expressions are obtained.

1. INITIAL RELATIONS

The system of kinetic equations employed here has the form [5, 7, 8]

$$\frac{\partial f_{\Omega}}{\partial t} + \xi_{i\alpha} \frac{\partial f_{\Omega}}{\partial r_{\alpha}} + \frac{F_{i\alpha}}{m_i} \frac{\partial f_{\Omega}}{\partial \xi_{i\alpha}} = L_{\Omega}(f f) \tag{1.1}$$

Here $f_{\Omega} = f(\xi_i, E_{\Omega}, \mathbf{r}, t)$ is the number of molecules of the i th chemical sort in internal state ω at the instant of time t in an element of volume of the phase space (\mathbf{r}, ξ_i) ; ξ_i and m_i are the velocity and mass of a molecule, E_{Ω} is its internal energy, $\Omega = i\omega$, L_{Ω} is the operator of elastic and inelastic binary collisions, and $i, j = 1, 2, \dots, S$, where S is the number of chemical components; the components of the radius vector \mathbf{r} are introduced by the subscripts α, β, γ , and the usual rules of summation over repeated subscripts are used.

The Chapman–Enskog method gives the expansion

$$\begin{aligned} f_{\Omega} &= f_{\Omega}^{(0)} \sum_{m=0}^{\infty} \varphi_{\Omega}^{(m)} \equiv \sum_{m=0}^{\infty} f_{\Omega}^{(m)}, \quad \varphi_{\Omega}^{(0)} = 1, \quad f_{\Omega}^{(0)} = Y_{\Omega} f_i^{(0)} \\ f_i^{(0)} &= n x_i \left(\frac{m_i}{2\pi kT} \right)^{3/2} \exp(-w_i^2), \quad x_i = \frac{n_i}{n}, \quad w_i^2 = \frac{m_i c_i^2}{2kT} \\ Y_{\Omega}(T) &= \frac{g_{\Omega}}{Q_i} \exp(-\varepsilon_{\Omega}), \quad Q_i = \sum_{\omega} g_{\Omega} \exp(-\varepsilon_{\Omega}), \quad \varepsilon_{\Omega} = \frac{E_{\Omega}}{kT} \end{aligned} \tag{1.2}$$

In (1.2) the natural velocities of the molecules $c_i = \xi_i - \mathbf{u}$ and g_{Ω} is a degeneration of the Ω -level. Henceforth we will use the following operations with $Y_{\Omega}(T)$

†Prikl. Mat. Mekh. Vol. 64, No. 4, pp. 590–604, 2000.

‡See also: Shavaliyev, M. Sh., Transport phenomena in gas mixtures in the Burnett and super-Burnett approximations, Candidate dissertation, 01.02.05, Novosibirsk, 1978.

$$\begin{aligned} \frac{dY_\Omega}{dT} &= \frac{Y_\Omega}{T} \Delta \varepsilon_\Omega, \quad \Delta \varepsilon_\Omega = \varepsilon_\Omega - \langle \varepsilon_\Omega \rangle_c, \quad \langle N \rangle_c = \sum_\omega NY_\Omega \\ \sum_\omega \varepsilon_\Omega \frac{dY_\Omega}{dT} &= \frac{c_v}{kT}, \quad \langle (\Delta \varepsilon_\Omega)^2 \rangle_c = \frac{c_v}{k}, \quad \frac{d(\Delta \varepsilon)^2}{dT} = -\frac{\Delta \varepsilon_\Omega}{T} - \frac{c_v}{kT} \\ c_v^* &= 1 + \frac{2}{3k} c_v, \quad c_v = \sum_i x_i c_{vi}, \quad E_i^* = kT \left(\frac{3}{2} + \langle \varepsilon_\Omega \rangle_c \right) \end{aligned} \quad (1.3)$$

Here and below N means any quantity on which the operator considered acts, $\langle \varepsilon_\Omega \rangle_c$ is the mean internal energy of molecules of the i th sort and c_v is the heat capacity due to the internal degrees of freedom at constant volume.

Expansion (1.2) enables us to close the system of gas-dynamic equations which, in the case of light exchanges, has the form [7.8]

$$\frac{D\rho}{Dt} + \rho \nabla \mathbf{u} = 0, \quad \frac{D}{Dt} = \frac{\partial}{\partial t} + u_\alpha \frac{\partial}{\partial r_\alpha}, \quad \nabla \mathbf{u} = \frac{\partial u_\alpha}{\partial r_\alpha} \quad (1.4)$$

$$n \frac{Dx_i}{Dt} + \frac{\partial J_{i\alpha}}{\partial r_\alpha} - x_i \sum_{j=1}^S \frac{\partial J_{j\alpha}}{\partial r_\alpha} = 0, \quad n = \sum_{i=1}^S n_i, \quad \rho = \sum_{i=1}^S m_i n_i \quad (1.5)$$

$$\rho \frac{Du_\alpha}{Dt} + \frac{\partial p}{\partial r_\alpha} + \frac{\partial \tau_{\alpha\beta}}{\partial r_\beta} = \sum_{i=1}^S n_i F_{i\alpha}, \quad \tau_{\alpha\beta} = \Pi \delta_{\alpha\beta} + \pi_{\alpha\beta} \quad (1.6)$$

$$\frac{3}{2} n k c_v^* \frac{DT}{Dt} + \frac{\partial q_\alpha}{\partial r_\alpha} + (p \delta_{\alpha\beta} + \tau_{\alpha\beta}) \frac{\partial u_\alpha}{\partial r_\beta} - \sum_{i=1}^S \left[J_{i\alpha} F_{i\alpha} + E_i^* \frac{\partial J_{i\alpha}}{\partial r_\alpha} \right] = 0, \quad p = nkT \quad (1.7)$$

In (1.7) we have used the same notation as in (1.3). System (1.5) contains $S-1$ equations. The gas-dynamic variables can be calculated from the formulae

$$n_i = (f_\Omega)_* = (f_\Omega^{(0)})_*, \quad (N)_* = \sum_\omega \int N dc_i \quad (1.8)$$

$$\mathbf{u} = \frac{1}{\rho} \sum_{i=1}^S (m_i \xi_i f_\Omega)_* = \frac{1}{\rho} \sum_{i=1}^S (m_i \xi_i f_\Omega^{(0)})_* \quad (1.9)$$

$$\left(\frac{3}{2} + \sum_{i=1}^S x_i \langle \varepsilon_\Omega \rangle_c \right) kT = \frac{1}{n} \sum_i (U f_\Omega)_* = \frac{1}{n} \sum_i (U f_\Omega^{(0)})_*, \quad U = \frac{1}{2} m_i c_i^2 + E_\Omega \quad (1.10)$$

Formula (1.10) defines the mean temperature T . By virtue of (1.8)–(1.10) perturbations $\varphi^{(r)}$, $r \geq 1$ make no contribution to the density, the mean-mass velocity and mean energy. The corresponding contributions to the transport properties, i.e. the diffusion velocity \mathbf{V}_i , the scalar and non-divergent components of the stresses Π and $\pi_{\alpha\beta}$, and the heat flux \mathbf{q} , are given by the formulae

$$\begin{aligned} \mathbf{J}_i^{(r)} &\equiv n_i \mathbf{V}_i^{(r)} = (c_i f_\Omega^{(r)})_*, \quad \mathbf{q}^{(r)} = \sum_{i=1}^S (c_i U f_\Omega^{(r)})_*, \quad r \geq 1 \\ \Pi^{(r)} &= \frac{1}{3} \sum_{i=1}^S (c_i^2 f_\Omega^{(r)})_*, \quad \pi_{\alpha\beta}^{(r)} = \sum_{i=1}^S \left[c_{i\alpha} c_{i\beta} - \frac{1}{3} \delta_{\alpha\beta} c_i^2 \right] f_\Omega^{(r)} \end{aligned} \quad (1.11)$$

In (1.11) we have used the notation from (1.2), (1.8) and (1.10)

The correction of the first approximation, corresponding to the Navier–Stokes approximation, will be sought in the form

$$\begin{aligned} f_\Omega^{(1)} &= -\frac{1}{n} f_\Omega^{(0)} \left(A_\Omega c_{i\alpha} \frac{\partial \ln T}{\partial r_\alpha} + B_\Omega c_{i\alpha} c_{i\beta} e_{\alpha\beta} + \sum_{j=1}^S D_\Omega^j c_{i\alpha} d_{j\alpha} + \Gamma_\Omega \nabla \mathbf{u} \right) \equiv \\ &\equiv A'_\Omega c_{i\alpha} \frac{\partial T}{\partial r_\alpha} + B'_\Omega c_{i\alpha} c_{i\beta} e_{\alpha\beta} + \sum_{j=1}^S D_\Omega'^j c_{i\alpha} d_{j\alpha} + \Gamma'_\Omega \nabla \mathbf{u} \end{aligned} \quad (1.12)$$

For brevity, we will mean by the Navier–Stokes approximation the linear approximations for the transport properties, and we shall mean by the Navier–Stokes equations the corresponding complete system of conservation equations [1]. The structure of solution (1.12) differs from that assumed earlier [6–8] in three terms, to determine which a more effective method is employed [5]. The following notation is used

$$d_{i\alpha} = \frac{\partial x_i}{\partial r_\alpha} + \left(x_i - \frac{\rho_i}{\rho}\right) \frac{\partial \ln p}{\partial r_\alpha} - \frac{x_i}{kT} \left(F_{i\alpha} - \frac{m_i}{\rho} \sum_{j=1}^S n_j F_{j\alpha}\right)$$

$$e_{\alpha\beta} = \left\langle \frac{\partial u_\alpha}{\partial r_\beta} \right\rangle, \quad \langle N_{\alpha\beta} \rangle = \frac{1}{2} (N_{\alpha\beta} + N_{\beta\alpha}) - \frac{1}{3} \delta_{\alpha\beta} N_{\gamma\gamma} \quad (1.13)$$

The functions, A , B , D and Γ satisfy the equations

$$\frac{1}{n} f_\Omega^{(0)} (-S_{3/2}^{(1)}(w_i^2) + \Delta \epsilon_\Omega) c_{i\alpha} = -R_\Omega(A c_\alpha) \quad (1.14)$$

$$\frac{1}{n} f_\Omega^{(0)} 2 \langle w_{i\alpha} w_{j\beta} \rangle = -R_\Omega(B \langle c_\alpha c_\beta \rangle) \quad (1.15)$$

$$\frac{1}{n} f_\Omega^{(0)} c_{i\alpha} \left(\delta_{ik} - \frac{\rho_i}{\rho} \right) = -R_\Omega(D^k c_\alpha) \quad (1.16)$$

$$\frac{1}{n} f_\Omega^{(0)} \frac{2}{3c_v^*} \left(\frac{2}{3} \frac{c_{vi}}{k} S_{1/2}^{(1)}(w_i^2) + \Delta \epsilon_\Omega \right) = R_\Omega(\Gamma) \quad (1.17)$$

Here $i, j, k = 1, 2, \dots, S$, and $R_\Omega(N)$ is the linearized collision operator [5, 7, 8] related to n^2 .

It can be seen from (1.14)–(1.17) that A , B , D and Γ depend on w_i^2 , ϵ_Ω , T , x_i and are independent of n (the latter was not taken into account earlier [6]).

The solutions of system of equations (1.14)–(1.17) are usually sought in the form of series in Sonin polynomials $S_m^{(n)}(w_i^2)$ and in polynomials which depend on ϵ_Ω ,

$$A_\Omega = -\frac{2}{5} \frac{m_i}{k^2 T x_i} \left[-\frac{5}{2} k n_i D_{Ti} + \lambda'_{ii} S_{1/2}^{(1)}(w_i^2) - \frac{5}{2} \lambda_{vi} \frac{k}{c_{vi}} \Delta \epsilon_\Omega + \dots \right]$$

$$B_\Omega = \frac{m_i \eta_i}{(kT)^2 x_i} + \dots, \quad D_\Omega^j = \frac{m_i}{kT} \left[n D_{ij} + \gamma_i^j S_{1/2}^{(1)}(w_i^2) + \dots \right] \quad (1.18)$$

$$\Gamma_\Omega = -\zeta_i (x_i kT)^{-1} \left[S_{1/2}^{(1)}(w_i^2) + \sigma_i \Delta \epsilon_\Omega + \dots \right]$$

In (1.18) η_i , ξ_{vi} , λ'_{ii} , λ_{vi} are the partial shear (dynamic) and volume viscosity coefficients and the partial translational and internal thermal conductivities, and D_{ij} and D_{Ti} are the diffusion and thermal diffusion coefficient of the multicomponent mixture of polyatomic gases (for example, the shear viscosity coefficient of the mixture $\eta = \sum_i \eta_i$).

We will write the system of equations for determining the Burnett perturbations $\varphi_\Omega^{(2)}$ in the form

$$M_\Omega = n^2 R_\Omega(\varphi^{(2)}), \quad M_\Omega = \frac{\partial_1 f_\Omega^{(0)}}{\partial t} + H_\Omega - L_\Omega(f^{(1)} f^{(1)}) \quad (1.19)$$

The inhomogeneous part of integral equation (1.19) M_Ω includes a group of terms H_Ω containing derivatives of $f_\Omega^{(1)}$, which can be conveniently expressed in terms of the natural velocities of the molecules [4, 5]

$$H_\Omega = \frac{D_0 f_\Omega^{(1)}}{Dt} + c_{i\alpha} \frac{\partial f_\Omega^{(1)}}{\partial r_\alpha} + Z_{i\alpha} \frac{\partial f_\Omega^{(1)}}{\partial c_{i\alpha}} - c_{i\beta} \frac{\partial u_\alpha}{\partial r_\beta} \frac{\partial f_\Omega^{(1)}}{\partial c_{i\alpha}}$$

$$Z_{i\alpha} = \sum_{j=1}^S \left(\delta_{ij} - \frac{\rho_j}{\rho} \right) \frac{F_{j\alpha}}{m_j} + \frac{1}{\rho} \frac{\partial p}{\partial r_\alpha}, \quad \frac{D_0}{Dt} = \frac{\partial_0}{\partial t} + u_\alpha \frac{\partial}{\partial r_\alpha} \quad (1.20)$$

In (1.19) and (1.20) we have used the expansion $\partial/\partial t = \partial_0/\partial t + \partial_1/\partial t + \dots$

This expansion is the main feature of the Chapman–Enskog method, but in a number of textbooks on kinetic theory it is not mentioned when describing the general algorithm of the method [9, 10]. Moreover, inaccuracies in describing the general algorithm occur even in well-known textbooks [4, 5] for the case of unsteady external forces. In certain sections of [4, 5] it should have been written that $f^{(m)}$ depends on \mathbf{r}, t not only in terms of the hydrodynamic variables but also in terms of $\mathbf{F}_i = \mathbf{F}_i(\mathbf{r}, t)$, beginning with $f^{(2)}$ for a simple gas and $f^{(1)}$ for a mixture of gases. It can be shown that the requirements of the method are satisfied if the partial derivatives with respect to time of the gas-dynamic variables are expanded rather than the partial derivatives with respect to time of the known functions $F_{i\alpha}(\mathbf{r}, t)$, i.e. one can use the well-known general algorithm of the Chapman–Enskog method with the additional definitions

$$\frac{\partial_0 \mathbf{F}_i}{\partial t} = \frac{\partial \mathbf{F}_i}{\partial t}, \quad \frac{\partial_n \mathbf{F}_i}{\partial t} = 0, \quad n \geq 1$$

Then, for example, we obtain

$$\begin{aligned} \frac{D_0 d_{i\alpha}}{Dt} &= \left(x_i - \frac{m_i n}{\rho} \right) \frac{D_0}{Dt} \frac{\partial \ln p}{\partial r_\alpha} + \frac{x_i}{kT^2} \left(F_{i\alpha} - m_i \sum_{j=1}^s \frac{n_j}{\rho} F_{j\alpha} \right) \frac{D_0 T}{Dt} - \\ &- \frac{x_i}{kT} \left(\frac{DF_{i\alpha}}{Dt} - m_i \sum_{j=1}^s \frac{n_j}{\rho} \frac{DF_{j\alpha}}{Dt} \right) - \frac{\partial u_\beta}{\partial r_\alpha} \frac{\partial x_i}{\partial r_\beta} \end{aligned} \quad (1.21)$$

To calculate the derivatives of the gas-dynamic variables from Eqs (1.4)–(1.7) we obtain

$$\begin{aligned} \frac{D_0 \rho}{Dt} &= -\rho \nabla \mathbf{u}, \quad \frac{D_0 x_i}{Dt} = 0, \quad \frac{D_0 u_\alpha}{Dt} = \frac{1}{\rho} \left(-\frac{\partial p}{\partial r_\alpha} + \sum_{i=1}^s n_i F_{i\alpha} \right) \\ \frac{D_0 T}{Dt} &= -\frac{2T}{3c_v^*} \nabla \mathbf{u}, \quad \frac{\partial_1 \rho}{\partial t} = 0, \quad \frac{\partial_1 x_i}{\partial t} = \frac{1}{n} \left(-\frac{\partial}{\partial r_\alpha} J_{i\alpha}^{(1)} + x_i \sum_{j=1}^s \frac{\partial}{\partial r_\alpha} J_{j\alpha}^{(1)} \right) \end{aligned} \quad (1.22)$$

etc. As in [4] we obtain D_0/D_t of the various combinations of spatial derivatives, in particular

$$\frac{D_0 \nabla \mathbf{u}}{Dt} = \frac{\partial}{\partial r_\alpha} \frac{1}{\rho} \left(\sum_{j=1}^s n_j F_{j\alpha} - \frac{\partial p}{\partial r_\alpha} \right) - \frac{\partial u_\beta}{\partial r_\alpha} \frac{\partial u_\alpha}{\partial r_\beta} \quad (1.23)$$

Finally M_Ω can be expressed in terms of well-known quantities. As is well known, it is not necessary to know $\varphi_\Omega^{(2)}$ in order to obtain the Burnett transport properties.

Using the symmetry properties of the operator $R_\Omega(\varphi)$, Eqs (1.14)–(1.17) and the conditions for $\varphi_\Omega^{(2)}$ to make no contribution to (1.8)–(1.10), as in [4, 5] we obtain the following formula for Burnett's contributions to the transport properties

$$\begin{aligned} (\pi_{\alpha\beta}^{(2)}; \Pi^{(2)}; V_{k\alpha}^{(2)}; h_\alpha^{(2)}) &= \\ &= -\frac{\rho}{n^2} \sum_\Omega \int \left(B_\Omega \langle c_{i\alpha} c_{j\beta} \rangle; \Gamma_\Omega; \frac{1}{\rho} D_\Omega^k c_{i\alpha}; A_\Omega c_{i\alpha} \right) M_\Omega dc_i \end{aligned} \quad (1.24)$$

Hence, each of the transport properties can be expressed in terms of the sum of integrals with respect to c_i of M_Ω with a corresponding weight. The reduced heat flux, by definition, is

$$h_\alpha = q_\alpha - kT \sum_{i=1}^s \left(\frac{5}{2} + \langle \epsilon_\Omega \rangle_c \right) J_{i\alpha} \quad (1.25)$$

2. THE CONTRIBUTIONS OF BURNETT'S APPROXIMATION TO THE TRANSPORT PROPERTIES

To determine the contributions we will use the method described in [4], the only difference being that we will take x_i and Y_Ω (1.3) into account. Using formulae (1.12) and (1.8)–(1.25), after carrying out fairly lengthy calculations similar to those in [4] we obtain

$$\begin{aligned}
 \pi_{\alpha\beta}^{(2)} = & (\xi_1 + \xi_1^*) e_{\alpha\beta} \nabla \mathbf{u} + \xi_2 \left\langle \left[\frac{1}{\rho} \left(\sum_k n_k F_{k\beta} - p_{,\beta} \right) \right]_{,\alpha} - 2u_{\gamma,\alpha} e_{\gamma\beta} - u_{\gamma,\beta} u_{\alpha,\gamma} \right\rangle + \\
 & + (\xi_3 + \xi_3^*) \langle e_{\alpha\gamma} e_{\gamma\beta} \rangle + \xi_4 \langle T_{,\alpha\beta} \rangle + (\xi_5 + \xi_5^*) \langle T_{,\alpha} T_{,\beta} \rangle + \sum_k \{ \xi_{6k} \langle Z_{k\alpha} T_{,\beta} \rangle + \xi_{7k} \langle d_{k\beta,\alpha} \rangle + \\
 & + \langle T_{,\alpha} [\xi_{8k} x_{k,\beta} + (\xi_{9k} + \xi_{9k}^*) d_{k\beta}] \rangle \} + \sum_{kl} \langle d_{k\alpha} (\xi_{10kl} Z_{l\beta} + \xi_{11kl} x_{l,\beta} + \xi_{12kl}^* d_{l\beta}) \rangle \quad (2.1)
 \end{aligned}$$

In (2.1) we have used the symbols from (1.13) and (1.20), and summation over k and l is carried out from 1 to S . For brevity, here and below we will use the following notation for the spatial derivatives

$$u_{\alpha,\beta,\gamma} = \frac{\partial^2 u_\alpha}{\partial r_\beta \partial r_\gamma}, \quad (T_{,\alpha} T_{,\beta})_{,\gamma} = \frac{\partial}{\partial r_\gamma} \left(\frac{\partial T}{\partial r_\alpha} \frac{\partial T}{\partial r_\beta} \right) \quad (2.2)$$

etc. The coefficients with an asterisk are determined by the moments of $L_\Omega(f^{(1)}f^{(1)})$, while those without an asterisk are determined by the convective part

$$\begin{aligned}
 \xi_1 = & -\frac{2}{3} \left\{ \frac{T}{c_v^*} \frac{\partial B'_\Omega}{\partial T} + c_i^2 \frac{\partial B'_\Omega}{\partial c_i^2} + 3 \frac{\partial \Gamma'_\Omega}{\partial c_i^2} \right\}_\eta \approx \sum \frac{4}{3} \frac{\eta_i^2}{p_i} \left(\frac{7}{2} - \frac{1}{c_v^*} \partial_T \eta_i + \frac{3}{2} \frac{\zeta_i}{\eta_i} \right) \\
 \xi_2 = & \langle B'_\Omega \rangle_\eta \approx \sum \frac{2\eta_i^2}{p_i}, \quad \xi_3 = -\frac{8}{7} \left\{ c_i^2 \frac{\partial B'_\Omega}{\partial c_i^2} \right\}_\eta \approx 4\xi_2 \\
 \xi_4 = & \langle A'_\Omega \rangle_\eta \approx \sum \frac{4}{5} \frac{\eta_i}{p_i} \psi_i, \quad \xi_5 = \left\{ \frac{\partial A'_\Omega}{\partial T} \right\}_\eta \approx \sum \frac{4}{5} \frac{\eta_i}{p_i} \frac{\partial \psi_i}{\partial T}, \quad \psi_i = \lambda'_{ii} + \frac{5}{2} n_i k D_{Ti} \quad (2.3) \\
 \xi_{6k} = & 2 \left\{ \frac{\partial A'_\Omega}{\partial c_i^2} \delta_{ik} \right\}_\eta \approx -\sum \frac{2\rho_i \eta_i}{p_i T} D_{Ti} \delta_{ik} \\
 \xi_{7k} = & \langle D_{\Omega}^k \rangle_\eta \approx \sum 2\eta_i \chi_{ik}, \quad \chi_{ik} = D_{ik} - \frac{1}{n} \gamma_i^k \\
 \xi_{8k} = & \left\{ \frac{\partial A'_\Omega}{\partial x_k} \right\}_\eta \approx \sum \frac{4}{5} \frac{\eta_i}{p_i} \frac{\partial \psi_i}{\partial x_k} \\
 \xi_{9k} = & \left\{ \frac{\partial D_{\Omega}^k}{\partial T} \right\}_\eta \approx \sum \frac{2\eta_i}{T} D_{ik} \left[1 + \partial_T D_{ik} - \frac{\gamma_i^k}{n D_{ik}} (1 + \partial_T \gamma_i^k) \right] \\
 \xi_{10kl} = & 2 \left\{ \frac{\partial D_{\Omega}^{kl}}{\partial c_i^2} \delta_{il} \right\}_\eta \approx -\sum \frac{2m_i}{kT} \eta_i D_{ik} \delta_{il} \\
 \xi_{11kl} = & \left\{ \frac{\partial D_{\Omega}^{kl}}{\partial x_l} \right\}_\eta \approx \sum \frac{2\eta_i}{n_i} \frac{\partial n_i \chi_{ik}}{\partial x_l}
 \end{aligned}$$

In (2.3) A'_Ω , etc. are introduced by formula (1.12) in the same way as in [4], and δ_{ik} is the unit tensor. By definition

$$\begin{aligned}
 \langle N \rangle_\eta & \equiv -\sum \frac{8}{\Omega} \frac{(kT)^3}{15 m_i^2 n} \int B_\Omega N w_i^4 dc_i \\
 \partial_T N & = \frac{\partial \ln N}{\partial \ln T}, \quad \sum = \sum_{i=1}^S, \quad p_i = n_i kT \quad (2.4)
 \end{aligned}$$

Here and below the first expressions for the coefficients (written in terms of $\langle N \rangle_\eta$, etc.) are exact while the second expressions are approximate, obtained taking into account the terms of expansions

in polynomials given in (1.18). The transport coefficients which occur in (1.18) can be regarded as exact or corresponding to the given polynomial approximation. The final choice can be made only after making comparative calculations. In [6] a smaller number of expansion terms are retained than in (1.18), which does not enable the non-zero approximate expressions to be obtained for all the transport coefficients.

When writing the transport properties we will initially write a group of terms with $S = 1$ which transfer into terms for a simple gas (with coefficients $\xi_i \div \xi_6$), then the diffusion terms, equal to zero when $S = 1$ ($\xi_{7k} \div \xi_{12kl}^*$), after which the terms due solely to the multiatomicity. The latter do not occur in (2.1), and the polyatomicity only has a direct effect on ξ_1 and ξ_1^* . The vector Z_i can be expressed [6] in terms of d_i using (1.13) and (1.20), but in this case the sequence described breaks down. Note that $Z_{i\alpha} = \rho^{-1} p_{i,\alpha}$ when $S = 1$. Using the properties of isotropic tensors when carrying out the convolutions, we obtain

$$\begin{aligned} \xi_1^* &= \frac{1}{5} \{b_{\alpha\beta} \Gamma + \Gamma b_{\alpha\beta}\}_{\eta}^*, \quad \xi_3^* = \frac{12}{35} \{ \langle b_{\beta\gamma} b_{\gamma\alpha} + b_{\alpha\gamma} b_{\gamma\beta} \rangle \}_{\eta}^*, \quad \xi_5^* = \frac{1}{5} \{ \langle a_{\alpha} a_{\beta} \rangle \}_{\eta}^* \\ \xi_{9k}^* &= \frac{1}{5} \{ \langle a_{\alpha} d_{\beta}^k + d_{\alpha}^k a_{\beta} \rangle \}_{\eta}^*, \quad \xi_{12kl}^* = \frac{1}{5} \{ \langle d_{\alpha}^k d_{\beta}^l \rangle \}_{\eta}^* \\ a_{\Omega\alpha} &\equiv A_{\Omega} c_{i\alpha}, \quad b_{\Omega\alpha\beta} \equiv B_{\Omega} \langle c_{i\alpha} c_{i\beta} \rangle, \quad d_{\Omega\alpha}^k \equiv D_{\Omega}^k c_{i\alpha} \end{aligned} \quad (2.5)$$

In (2.5) we have used the operator

$$\{HN\}_{\eta}^* = \frac{kT}{n^3} \sum_{\Omega} \int b_{\Omega\alpha\beta} L_{\Omega}^* (HN) d c_i, \quad L_{\Omega}^* (n\varphi^{(1)} n\varphi^{(1)}) = n^2 L_{\Omega} (f^{(1)} f^{(1)}) \quad (2.6)$$

In (2.6) H belongs to the class of Ω -particles and N belongs to the other class of ψ -particles, and the summation is carried out over the index $\Psi = j\psi$ in L . Approximate expressions for ξ_i^* , etc. are obtained below in Section 3.

For the contribution to the scalar part of the stress tensor we obtain

$$\begin{aligned} \Pi^{(2)} &= (\omega_1 + \omega_1^*) e_{\alpha\beta} e_{\beta\alpha} + \omega_2 \nabla^2 T + (\omega_3 + \omega_3^*) (\nabla T)^2 + (\omega_4 + \omega_4^*) (\nabla u)^2 + \\ &+ \omega_5 \frac{D_0 \nabla u}{Dt} + \sum_k \{ [\omega_{6k} Z_{k\alpha} + \omega_{7k} x_{k,\alpha} + (\omega_{8k} + \omega_{8k}^*) d_{k\alpha}] T_{,\alpha} + \omega_{9k} \nabla d_k \} + \\ &+ \sum_{kl} [\omega_{10kl} Z_{l\alpha} + \omega_{11kl} x_{l,\alpha} + \omega_{12kl}^* d_{l\alpha}] d_{k\alpha} \end{aligned} \quad (2.7)$$

$$\omega_1 = -2 \left\{ B'_{\Omega} + \frac{2}{5} c_i^2 \frac{\partial B'_{\Omega}}{\partial c_i^2} \right\}_{\omega} = \sum \frac{2}{p_i} \eta_i \zeta_i$$

$$\omega_2 = \{A'_{\Omega}\}_{\omega} = \sum \frac{\zeta_i}{p_i} (\lambda'_{ii} - \sigma_i \lambda_{vi} + n_i k D_{Ti})$$

$$\omega_3 = \left\{ \frac{\partial A'_{\Omega}}{\partial T} \right\}_{\omega} = \sum \frac{\zeta_i}{p_i} \left\{ \frac{\partial \lambda'_{ii}}{\partial T} + n_i k T^{-3/2} \frac{\partial}{\partial T} (D_{Ti} T^{3/2}) - \right.$$

$$\left. - \frac{\sigma_i}{T} c_{vi} \left[n_i D_{Ti} + T^3 \frac{\partial}{\partial T} \left(\frac{\lambda_{vi}}{c_{vi}} T^{-2} \right) \right] - \lambda_{vi} \frac{\sigma_i k}{c_{vi} T} \langle (\Delta \varepsilon_{\Omega})^3 \rangle_c \right\}$$

$$\omega_4 = -2 \left\{ \frac{\partial \Gamma'_{\Omega}}{\partial c_i^2} + \frac{T}{c_i^* c_i^2} \frac{\partial \Gamma'_{\Omega}}{\partial T} \right\}_{\omega} =$$

$$= \sum \frac{\zeta_i^2}{p_i} \left\{ \frac{5}{2} + \sigma_i^2 \frac{c_{vi}}{k} - \frac{2}{3c_{vi}^*} \left[\frac{3}{2} \partial_T \zeta_i + \sigma_i^2 \frac{c_{vi}}{k} (\partial_T (\zeta_i \sigma_i) - 2) + \sigma_i^2 \langle (\Delta \varepsilon_{\Omega})^3 \rangle_c \right] \right\}$$

$$\omega_5 = \left\{ \frac{3}{c_i^2} \Gamma'_{\Omega} \right\}_{\omega} = \sum \frac{\zeta_i^2}{p_i} \left(\frac{3}{2} + \sigma_i^2 \frac{c_{vi}}{k} \right) \quad (2.8)$$

$$\omega_{6k} = 2 \left\{ \left(\frac{\partial A'_{\Omega}}{\partial c_i^2} + \frac{3}{2c_i^2} A'_{\Omega} \right) \delta_{ik} \right\}_{\omega} = - \sum \frac{p_i \zeta_i}{p_i T} D_{Ti} \delta_{ik}$$

$$\begin{aligned}
\omega_{7k} &= \left\{ \frac{\partial A'_\Omega}{\partial x_k} \right\}_\omega \approx \sum \frac{\zeta_i}{p_i} \left[\frac{\partial}{\partial x_k} (\lambda'_{vi} + n_i k D_{Ti}) - \sigma_i \frac{\partial \lambda_{vi}}{\partial x_k} \right] \\
\omega_{8k} &= \left\{ \frac{\partial D'_\Omega^k}{\partial T} \right\}_\omega \approx \sum \frac{\zeta_i}{T} \left[D_{ik} \left(\frac{5}{2} + \partial_T D_{ik} - \sigma_i \frac{c_{vi}}{k} \right) - \frac{5}{2n} \gamma_i^k (1 + \partial_T \gamma_i^k) \right] \\
\omega_{9k} &= \left\{ D'_\Omega^k \right\}_\omega \approx \sum \frac{\zeta_i}{n_i} l_{ik}, \quad l_{ik} = n_i D_{ik} - \frac{5}{2} x_i \gamma_i^k \\
\omega_{10kl} &= 2 \left\{ \left(\frac{\partial D'_\Omega^k}{\partial c_i^2} + \frac{3}{2c_i^2} D'_\Omega^k \right) \delta_{il} \right\}_\omega \approx - \sum \frac{\rho_i \zeta_i}{p_i} D_{ik} \delta_{il} \\
\omega_{11kl} &= \left\{ \frac{\partial D'_\Omega^k}{\partial x_l} \right\}_\omega \approx \sum \frac{\zeta_i}{n_i} \frac{\partial l_{ik}}{\partial x_l} \\
\omega_1^* &= \frac{1}{5} (b_{\alpha\beta} b_{\beta\alpha})_\omega^*, \quad \omega_3^* = \frac{1}{3} (a_\alpha a_\alpha)_\omega^*, \quad \omega_4^* = (\Gamma\Gamma)_\omega^* \\
\omega_{8k}^* &= \frac{1}{3} (a_\alpha d_\alpha^k + d_\alpha^k a_\alpha)_\omega^*, \quad \omega_{12kl}^* = \frac{1}{3} (d_\alpha^k d_\alpha^l)_\omega^*
\end{aligned} \tag{2.9}$$

We have used the notation from (2.5) and instead of (2.4) and (2.6) we have introduced the operators

$$\{N\}_\omega = -\frac{2}{3n} k^2 T^2 \sum_\Omega \int \frac{N}{m_i} \Gamma_\Omega w_i^2 dc_i, \quad \{HN\}_\omega^* = \frac{kT}{n^3} \sum_\Omega \int \Gamma_\Omega L'_\Omega (HN) dc_i \tag{2.10}$$

The contribution to the reduced heat flux has the form

$$\begin{aligned}
h_\alpha^{(2)} &= (\gamma_1^{(1)} + \gamma_1^{(2)} + \gamma_1^*) T_{,\alpha} \nabla \mathbf{u} + 2\gamma_2 \left[\left(\frac{T}{3c_v^*} \nabla \mathbf{u} \right)_{,\alpha} + u_{\beta,\alpha} T_{,\beta} \right] + \\
&+ \left[\sum_k \gamma_{3k} Z_{k\beta} + (\gamma_4^{(1)} + \frac{6}{5} \gamma_1^{(2)} + \gamma_4^*) T_{,\beta} \right] e_{\beta\alpha} + \gamma_5 e_{\alpha\beta,\beta} + \\
&+ \sum_k \left\{ (\gamma_{6k}^{(1)} + \gamma_{6k}^{(2)} + \gamma_{6k}^*) d_{k\alpha} \nabla \mathbf{u} + \gamma_{7k} \left(\frac{D_0 d_{k\alpha}}{Dt} - u_{\beta,\alpha} d_{k\beta} \right) + \right. \\
&+ \left. \left[\gamma_{8k} x_{k,\beta} + \left(\frac{6}{5} \gamma_{6k}^{(2)} + \gamma_{9k}^* \right) d_{k\beta} \right] e_{\alpha\beta} \right\} + \\
&+ \sum_k \left\{ \gamma_{10k} Z_{k\alpha} + \gamma_{11k} x_{k,\alpha} \right\} \nabla \mathbf{u} + \gamma_{12} (\nabla \mathbf{u})_{,\alpha} \\
\gamma_1^{(1)} &= \left\{ -\frac{2T}{3c_v^*} \frac{\partial A'_\Omega}{\partial T} + \frac{\partial \Gamma'_\Omega}{\partial T} \right\}_\gamma \approx \sum \frac{2}{5p_i} \left\{ \frac{2m_i}{3kc_v^*} \left[b_i^{(0)} n_i k T^2 \frac{\partial}{\partial T} \left(\frac{D_{Ti}}{T} \right) - \right. \right. \\
&- b_i^{(1)} \left(T \frac{\partial \lambda'_{vi}}{\partial T} + \frac{5}{2} n_i k D_{Ti} \right) + \\
&+ b_i^{(2)} \left. \left. \frac{c_{vi}}{k} \left(n_i k D_{Ti} + T^3 \frac{\partial}{\partial T} \left(\frac{k \lambda_{vi}}{T^2 c_{vi}} \right) + \lambda_{vi} \frac{k^2}{c_{vi}^2} \langle (\Delta \epsilon_\Omega)^3 \rangle_c \right) \right] \right\} + \\
&+ \zeta_i \left[-b_i^{(0)} \partial_T \zeta_i + \frac{5}{2} b_i^{(1)} \partial_T (\zeta_i T^2) + b_i^{(2)} \frac{c_{vi}}{k} (-1 + \sigma_i \partial_T (\zeta_i \sigma_i T^{-1})) + b_i^{(2)} \sigma_i \langle (\Delta \epsilon_\Omega)^3 \rangle_c \right]
\end{aligned} \tag{2.11}$$

$$\begin{aligned}
 \gamma_1^{(2)} &= -\frac{2}{3} \left\{ c_i^2 \frac{\partial A'_\Omega}{\partial c_i^2} \right\}_\gamma \approx \sum \frac{2m_i}{3kp_i} \left[\frac{7}{5} b_i^{(1)} \lambda'_{ii} - (b_i^{(0)} - b_i^{(1)}) n_i k D_{Ti} - b_i^{(2)} \lambda_{vi} \right] \\
 \gamma_2 &= -(A'_\Omega)_\gamma \approx -\sum \frac{2m_i}{5kp_i} (b_i^{(1)} \lambda'_{ii} - b_i^{(0)} n_i k D_{Ti} - b_i^{(2)} \lambda_{vi}) \\
 \gamma_{3k} &= \left\{ \left(2B'_\Omega + \frac{4}{5} c_i^2 \frac{\partial B'_\Omega}{\partial c_i^2} \right) \delta_{ik} \right\}_\gamma \approx -\sum \frac{4m_i \eta_i}{5kp_i} b_i^{(1)} \delta_{ik} \\
 \gamma_4^{(1)} &= \frac{2}{5} \left\{ c_i^2 \frac{\partial B'_\Omega}{\partial T} \right\}_\gamma \approx \sum \frac{4\eta_i}{5\rho_i} \left[b_i^{(1)} \partial_T (T^{1/2} \eta_i) - b_i^{(0)} \partial_T \eta_i - b_i^{(2)} \frac{c_{vi}}{k} \right] \\
 \gamma_5 &= \frac{2}{5} \{ c_i^2 B'_\Omega \}_\gamma \approx \sum \frac{4\eta_i}{5kn_i} (b_i^{(1)} - b_i^{(0)}) \\
 \gamma_{6k}^{(1)} &= -\frac{2}{3} \left\{ \frac{T}{c_v^*} \frac{\partial D'_\Omega^k}{\partial T} \right\}_\gamma \approx \\
 &= \sum \frac{4m_i}{15kc_v^*} \left[D_{ik} \left(b_i^{(0)} \partial_T D_{ik} - \frac{5}{2} b_i^{(1)} + b_i^{(2)} \frac{c_{vi}}{k} \right) + \frac{5}{2n} b_i^{(1)} \gamma_i^k \partial_T (T \gamma_i^k) \right] \\
 \gamma_{6k}^{(2)} &= -\frac{2}{3} \left\{ c_i^2 \frac{\partial D'_\Omega^k}{\partial c_i^2} \right\}_\gamma \approx \sum \frac{2m_i}{3k} \left[D_{ik} (b_i^{(1)} - b_i^{(0)}) - \frac{7}{2n} b_i^{(1)} \gamma_i^k \right] \tag{2.12} \\
 \gamma_{7k} &= \{ D'_\Omega^k \}_\gamma \approx -\sum \frac{m_i}{k} \left(\frac{2}{5} b_i^{(0)} D_{ik} + b_i^{(1)} \frac{1}{n} \gamma_i^k \right) \\
 \gamma_{8k} &= \frac{2}{5} \left\{ c_i^2 \frac{\partial B'_\Omega}{\partial x_k} \right\}_\gamma \approx \sum \frac{4}{5kn_i} \frac{\partial \eta_i}{\partial x_k} (b_i^{(1)} - b_i^{(0)}) \\
 \gamma_{10k} &= 2 \left\{ \delta_{ik} \frac{\partial \Gamma'_\Omega}{\partial c_i^2} \right\}_\gamma \approx -\sum \frac{m_i \zeta_i}{kp_i} \left(b_i^{(1)} + \frac{2}{5} b_i^{(2)} \sigma_i \frac{c_{vi}}{k} \right) \delta_{ik} \\
 \gamma_{11k} &= \left\{ \frac{\partial \Gamma'_\Omega}{\partial x_k} \right\}_\gamma \approx \sum \frac{2}{5n_i k} \left[\left(\frac{5}{2} b_i^{(1)} - b_i^{(0)} \right) \frac{\partial \zeta_i}{\partial x_k} + b_i^{(2)} \frac{c_{vi}}{k} \frac{\partial}{\partial x_k} (\sigma_i \zeta_i) \right] \\
 \gamma_{12} &= \{ \Gamma'_\Omega \}_\gamma \approx \sum \frac{2\zeta_i}{5n_i k} \left(\frac{5}{2} b_i^{(1)} - b_i^{(0)} + b_i^{(2)} \sigma_i \frac{c_{vi}}{k} \right) \\
 \gamma_1^* &= \frac{1}{3} \{ a_\alpha \Gamma + \Gamma a_\alpha \}_\gamma^*, \quad \gamma_4^* = \frac{1}{5} \{ b_{\alpha\beta} a_\beta + a_\beta b_{\beta\alpha} \}_\gamma^* \tag{2.13} \\
 \gamma_{6k}^* &= \frac{1}{3} \{ d_\alpha^k \Gamma + \Gamma d_\alpha^k \}_\gamma^*, \quad \gamma_{9k}^* = \frac{1}{5} \{ b_{\alpha\beta} d_\beta^k + d_\beta^k b_{\beta\alpha} \}_\gamma^*
 \end{aligned}$$

In this case, when taking (2.5) and (2.6) into account we introduced the operators

$$\{N\}_\gamma = -\frac{2}{3n} k^2 T^2 \sum_\Omega \int \frac{N}{m_i} A_\Omega w_i^2 dc_i, \quad \{HN\}_\gamma^* = \frac{kT}{n^3} \sum_\Omega \int a_{\Omega\alpha} L_\Omega^* (HN) dc_i \tag{2.14}$$

In (2.12) we assumed that

$$b_i^{(0)} = -\frac{5}{2} n_i k D_{Ti}, \quad b_i^{(1)} = \lambda'_{ii}, \quad b_i^{(2)} = -\frac{5}{2} \lambda_{vi} \frac{k}{c_{vi}} \tag{2.15}$$

The expression for $V_{j\alpha}^{(2)}$ is obtained from (2.11)–(2.13) by replacing γ by δ . When calculating the coefficients δ the operators (2.14) are replaced by (2.16), and relations (2.15) are replaced by (2.17).

$$\langle N \rangle_{\delta} = -\frac{2}{3n^2} kT \sum_{\Omega} \int \frac{N}{m_i} D_{\Omega}^j N w_i^2 d\mathbf{c}_i, \quad \langle HN \rangle_{\delta}^* = \frac{1}{n^4} \sum_{\Omega} \int d_{\Omega\alpha}^j L_{\Omega}^*(HN) d\mathbf{c}_i \quad (2.16)$$

$$b_i^{(0)} = -\frac{5}{2T} x_i D_{ij}, \quad b_i^{(1)} = -\frac{5}{2nT} x_i \gamma_i^j, \quad b_i^{(2)} = 0 \quad (2.17)$$

3. THE WEAK INELASTICITY APPROXIMATION

When carrying out gas-dynamic calculations, formulae for the transport properties in the Navier–Stokes approximation are usually employed, which hold on the assumption that the contributions of the inelastic collision integrals in A_{Ω} , B_{Ω} , D_{Ω}^j are negligibly small, while the elastic collision cross-sections are averaged over the the internal variables. For the general case of non-equilibrium excitation of the internal degrees of freedom of the molecules we than have [11, 12]

$$f_{\Omega}^{(1)} = Y_{\Omega} f_i^{(0)} \varphi_{\Omega}^{(1)}, \quad \varphi_{\Omega}^{(1)} = \varphi_i^{(1)} - W_i c_{i\alpha} \frac{\partial \ln Y_{\Omega}}{\partial r_{\alpha}} + X_{\Omega}(w^2, \varepsilon) \quad (3.1)$$

Here $Y_{\Omega} = n_{\Omega}/n_i$, n_{Ω} is the population (the density of Ω -particles), and $\varphi_i^{(1)}$ and W_i are calculated from the elastic collision cross-sections and are independent of inelastic processes so that $\varphi_i^{(1)}$ is given by the well-known formula for a mixture of monatomic gases [5].

Approximation (3.1) is called the generalized non-equilibrium Eiken approximation [11, 12]. When the distribution over the internal energies is close to a Boltzmann distribution, Y_{Ω} is replaced by the equilibrium function (1.2), the quantity X_{Ω} becomes proportional to $\nabla \mathbf{u}$, and $\varphi_i^{(1)}$ reduces to the form (1.12), but now

$$B_{\Omega} = B_i, \quad D_{\Omega}^j = D_i^j, \quad A_{\Omega} = A_i^{(1)} + A_i^{(2)} \Delta \varepsilon_{\Omega}, \quad A_i^{(2)} = n W_i = \frac{n m_i}{kT} \left(\sum_{j=1}^s \frac{x_j}{\mathcal{D}_{ij}(1)} \right)^{-1} \quad (3.2)$$

In (3.2) the quantities B_i , D_i^j , $A_i^{(1)}$ and $A_i^{(2)}$ do not depend on E_{Ω} and are calculated using the elastic collision cross-sections, the expression for W_i is given to a first approximation by Sonin polynomials [12] and $\mathcal{D}_{ij}(1)$ is the binary diffusion coefficient in this approximation. The difference between (3.2) and the case of a monatomic gas lies in the occurrence of the term with the coefficient $A_i^{(2)}$. The next aim is to show how the Burnett transport coefficients are calculated both in the monatomic case and how they are calculated taking $A_i^{(2)}$ and c_{vi} into account. The coefficients, expressed in terms of Γ_{Ω} , are determined, of course, by inelastic processes.

Using relations (3.2) we will take into account the fact that

$$\sum_{\omega} Y_{i\omega} = 1, \quad \sum_{\omega} Y_{i\omega} \Delta \varepsilon_{i\omega} = 0, \quad \frac{\partial Y_{i\omega}}{\partial x_i} = 0 \quad (3.3)$$

etc. and that the operators $\{ \}^*$ are now determined from the elastic collision integrals

$$L_{\Omega}(f^{(1)} f^{(1)}) = \sum_{\Psi} \int Y_{\Omega} Y_{\Psi} f_i^{(0)} f_j^{(0)} (\varphi_{\Omega}^{(1)\prime} \varphi_{\Psi}^{(1)\prime} - \varphi_{\Omega}^{(1)} \varphi_{\Psi}^{(1)}) g_{ij} d\sigma_{ij} d\mathbf{c}_j \quad (3.4)$$

where $\Psi = j\psi$, and the collision cross-sections are independent of the “inner” indices ω and ψ , summation over which is carried out independently, since for elastic collisions of Ω -particles with ψ -particles the internal energies do not change. Properties (3.3) hold for $Y_{j\psi}$. By virtue of (3.2) we can introduce the notation

$$(B'_{\Omega}, D'_{\Omega}{}^j, A'_{\Omega}{}^{(1)}, A'_{\Omega}{}^{(2)}) = Y_{\Omega} (B'_i, D'_i{}^j, A'_i{}^{(1)}, A'_i{}^{(2)})$$

We will first consider relations (2.3)–(2.6). With the exception of ξ_1 and ξ_1^* in all the operators $\{ \}_{\eta}$ and $\{ \}_{\eta}^*$ the functions B'_{Ω} , $D'_{\Omega}{}^j$ and A'_{Ω} are replaced by the “monatomic” B'_i , $D'_i{}^j$ and $A'_i{}^{(1)}$, while the sums over Ω and Ψ are replaced by sums over i and j (after summation over ω and ψ , respectively).

For example, for ξ_5 we have

$$\frac{\partial A'_\Omega}{\partial T} = \frac{\partial Y_\Omega}{\partial T} (A_i^{(1)} + A_i^{(2)} \Delta \varepsilon_\Omega) + Y_\Omega \left(\frac{\partial A_i^{(1)}}{\partial T} + \frac{\partial A_i^{(2)}}{\partial T} \Delta \varepsilon_\Omega + A_i^{(2)} \frac{\partial \Delta \varepsilon_\Omega}{\partial T} \right) \quad (3.5)$$

Since $B_\Omega = B_i$, it is this expression that is summed over ω . After summation and taking (1.3) and (3.3) into account from (3.5) there remains

$$A_i^{(2)} \frac{c_{vi}}{kT} + \frac{\partial A_i^{(1)}}{\partial T} - A_i^{(2)} \frac{c_{vi}}{kT} = \frac{\partial A_i^{(1)}}{\partial T}$$

ξ_i depends on c_v^* and Γ_Ω and ξ_i^* depends on Γ_Ω . These conclusions transfer directly to the coefficients δ in $V_i^{(2)}$ (because $D'_\Omega = D'_i$), with the exception of $\delta_1^{(1)}$, $\delta_{10} - \delta_{12}$, δ_1^* , δ_{6k}^* . Moreover, c_v^* occurs in $\delta_{bk}^{(1)}$.

Analysis of the coefficients γ is quite complex, since $A_\Omega \neq A_i$. If only $A_i^{(1)}$ is taken into account, we obtain qualitatively the same results as for the coefficients δ . The contribution of the "non-monatomic" term $A_i^{(2)} \Delta \varepsilon_\Omega$ is non-zero when the quantity N in $\{N\}_\gamma$ contains A'_Ω or $(B'_i, D_i^{(j)}) \partial Y_\Omega / \partial T$. Instead of the operator $\{N\}_\gamma$, it is more convenient to introduce the operators $\{N\}_\gamma^{(1)}$, $\{N\}_\gamma^{(2)}$ obtained from the first formula of (2.14) by replacing A_Ω by $A_i^{(1)}$ and $A_i^{(2)}$, respectively, and the sum over Ω by a sum over i . Then

$$\{A'_\Omega\}_\gamma = \{A_i^{(1)}\}_\gamma^{(1)} + \left\{ A_i^{(2)} \frac{c_{vi}}{k} \right\}_\gamma^{(2)}, \quad \left\{ B'_i \frac{\partial Y_\Omega}{\partial T} \right\}_\gamma = \left\{ B'_i \frac{c_{vi}}{kT} \right\}_\gamma$$

etc. The coefficients ω are expressed in terms of Γ_Ω although, of course, the expressions for them are simplified using (3.2). We emphasize that when using the approximate expressions for the Burnett coefficients, given in (2.3), (2.8), (2.12), (2.15) and (2.16), it must be recalled that in this case η_i , D_{ij} , D_{Ti} , γ_i , $\lambda'_{ii} = \lambda'_i$ are calculated from formulae for a mixture of monatomic gases; at the same time [12]

$$\lambda_{vi} \approx n_i c_{vi} \left(\sum_j \frac{x_j}{\mathcal{D}_{ij}(1)} \right)^{-1} \quad (3.6)$$

Polyatomicity affects the non-divergent stress tensor weakest of all, since those of its terms $\pi_{\alpha\beta}^*$ which are due to the spatial derivatives of the temperature and concentration are given by the "monatomic" formulae. This result also holds when the internal degrees of freedom have an arbitrary non-equilibrium [13].

The simplifications considered enable us to complete the calculations of the coefficients ξ^* , ω^* , γ^* , δ^* . In the general case the expressions for these have a formal form in view of the insufficiency of the information on the inelastic collisions. When only the elastic collisions are taken into account, even within the framework of the main approximations in terms of Sonin polynomials, very complex formulae are obtained and they are only accurate in the case of Maxwell molecules. Hence, we will immediately consider the case of Maxwell molecules and we will write the results in a form suitable for arbitrary intermolecular potentials [6]. For a simple gas the coefficients ξ^* and γ^* turn out to be zero, and in the general case they can be neglected [4]. For mixtures the majority of the coefficients ξ^* , ω^* , γ^* , δ^* are also zero and, as in [4-6], they can be neglected. Only the following coefficients are non-zero

$$\xi_{12kl}^* = \sum_{ij} \frac{2\eta_i x_j}{\mathcal{D}_{ij}(1)} (M_i - M_j + 3A_{ij} M_j) D_{ki} D_{lj} \quad (3.7)$$

$$\omega_{12kl}^* = \sum_{ij} \frac{\zeta_i x_j}{\mathcal{D}_{ij}(1)} (M_i - M_j) D_{ki} D_{lj} \quad (3.8)$$

$$\begin{aligned} \gamma_{6k}^* = & \sum_{ij} \frac{D_{ki} \zeta_j x_i}{kn \mathcal{D}_{ij}(1)} \left\{ 2M_i (M_i - M_j + 2A_{ij} M_j) \frac{\lambda_i}{x_i} + \right. \\ & \left. + \left[(M_i - M_j)^2 + 4A_{ij} M_i M_j \right] \frac{\lambda_j}{x_j} - \frac{\lambda_{vj} \sigma_j}{x_j} \right\} \quad (3.9) \end{aligned}$$

$$\begin{aligned} \gamma_{9k}^* = & \sum_{ij} \frac{4}{5} \frac{D_{ki} \eta_j x_i}{kn \mathcal{D}_{ij}(1)} \left\{ (M_i - M_j) \left[(M_i - M_j) \frac{\lambda_j}{x_j} + 2M_i \frac{\lambda_i}{x_i} \right] + \right. \\ & \left. + A_{ij} M_i (M_j - 3M_i) \left(\frac{\lambda_j}{x_j} + \frac{\lambda_i}{x_i} \right) \right\} \end{aligned} \quad (3.10)$$

In deriving formulae (3.7)–(3.10) we used formulae (1.18), (2.5), (2.6), (2.9), (2.10), (2.13), (2.14), (2.16) and (3.4) and the notation

$$(M_i, M_j) = \frac{(m_i, m_j)}{m_i + m_j}, \quad A_{ij} = \frac{1}{5} \frac{\Omega_{ij}^{(2)}(2)}{\Omega_{ij}^{(1)}(1)}, \quad \mathcal{D}_{ij}(1) = \frac{3kT}{16nm_i M_j \Omega_{ij}^{(1)}(1)} \quad (3.11)$$

The quantities Ω are defined in [4], the coefficients $\eta_i, \lambda_i, D_{ij}$ are calculated from formulae for a mixture of monatomic gases [5]; and λ_{vi} is calculated from (3.6).

4. APPROXIMATE FORMULAE FOR A BINARY MIXTURE OF MONATOMIC GASES

We will neglect external forces and thermal and barodiffusion. Then

$$\begin{aligned} D_{T_i} = 0, \quad \gamma_i^j = 0, \quad d_{i\alpha} = x_{i,\alpha}, \quad \frac{D_0 d_{i\alpha}}{Dt} = -u_{\beta,\alpha} x_{i,\beta}, \quad c_v^* = 1, \quad \lambda_{ii}^* = \lambda_i \\ Z_{i\alpha} = \rho^{-1} p_{,\alpha}, \quad \mathcal{D}_{ij}(1) = \mathcal{D}_{ij} \end{aligned} \quad (4.1)$$

From (2.3) and (2.12), taking (2.4) and (4.1) into account, we obtain

$$\begin{aligned} \xi_1 & \approx \sum \frac{4}{3} \frac{\eta_i^2}{p_i} \left(\frac{7}{2} - \partial_T \eta_i \right), \quad \xi_2 \approx \sum 2 \frac{\eta_i^2}{p_i} = \frac{1}{4} \xi_3 \\ \xi_4 & \approx \sum \frac{4}{5} \frac{\eta_i}{p_i} \lambda_i = \frac{\gamma_5}{T}, \quad \xi_5 \approx \sum \frac{4}{5} \frac{\eta_i}{p_i} \frac{\partial \lambda_i}{\partial T}, \quad \xi_6 = 0 \\ \gamma_1 & \approx \sum \frac{4}{15} \frac{m_i}{kp_i} \lambda_i^2 \left(\frac{7}{2} - \partial_T \lambda_i \right), \quad \gamma_2 \approx -\sum \frac{2}{5} \frac{m_i}{kp_i} \lambda_i^2 \\ \gamma_3 & \approx -\sum \frac{4}{5} \frac{m_i \eta_i \lambda_i}{kp_i}, \quad \gamma_4 \approx \sum \frac{4}{5} \frac{\lambda_i}{p_i} \left[\eta_i \left(\frac{7}{2} + \partial_T \eta_i \right) + \frac{7}{5} \frac{m_i}{k} \lambda_i \right] \end{aligned} \quad (4.2)$$

(the summation over i is from 1 to 2).

Terms in which the other coefficients ξ and γ occur can be combined using (4.1), the representation of D_{ij} in terms of the binary diffusion coefficient D_{12} [5], which is inversely proportional to n , and the equality $x_{1,\alpha} = -x_{2,\alpha}$. Finally, these terms $\pi_{\alpha\beta}^{(2)}$ and $h_\alpha^{(2)}$ take the form

$$\begin{aligned} \delta\pi_{\alpha\beta}^{(2)} & = \alpha_1 \langle x_{1,\alpha\beta} \rangle + \left[\frac{\alpha_1}{T} (1 + \partial_T \mathcal{D}_{12}) + \sum \frac{8}{5} \frac{\eta_i}{p_i} \frac{\partial \lambda_i}{\partial x_i} \right] \langle T_{,\alpha} x_{1,\beta} \rangle - \\ & - \frac{\alpha_1^* m_1 m_2}{\rho k T} (\eta_1 n_2 - \eta_2 n_1) \langle p_{,\alpha} x_{1,\beta} \rangle + \left\{ 2\alpha_1 \frac{n}{\rho} (m_2 - m_1) + \delta\xi_{12}^* \right\} \langle x_{1,\alpha} x_{1,\beta} \rangle \\ \delta h_\alpha^{(2)} & = \frac{2}{5k} \left[\alpha_1^* m_1 m_2 (\lambda_1 n_2 - \lambda_2 n_1) + \sum 4 \frac{\lambda_i}{n_i} \frac{\partial \eta_i}{\partial x_i} + \delta\gamma_9^* \right] e_{\alpha\beta} x_{1,\beta} \\ \alpha_1 & = \alpha_1^* (\eta_1 \rho_2 - \eta_2 \rho_1), \quad \alpha_1^* = \frac{2\mathcal{D}_{12}}{x_1 x_2 \rho} \end{aligned} \quad (4.3)$$

The coefficients $\delta\xi_{12}^*$ and $\delta\gamma_9^*$ in (4.3) are obtained by a corresponding combination of the coefficients

(3.7) and (3.10). Using (3.11) we have

$$\begin{aligned} \delta\xi_{12}^* &= 2\left(\frac{n}{\rho}\right)^2 \mathcal{D}_{12} m_1 m_2 \sum' \frac{\eta_i}{x_i} \left[3A_{ii} \frac{\mathcal{D}_{12}}{\mathcal{D}_{ii}} M_j - M_i + M_j - 3A_{12} M_j \right] \\ \delta\gamma_9^* &= \frac{8}{5} \frac{m_1 m_2}{k\rho} \sum' \frac{\eta_i}{m_j} (-1)^i \left\{ 4A_{ii} \frac{\mathcal{D}_{12}}{\mathcal{D}_{ii}} M_1 M_2 \frac{\lambda_i}{x_i} + \left[(M_j - M_i) \frac{\lambda_i}{x_i} + \right. \right. \\ &\quad \left. \left. + 2M_j \frac{\lambda_j}{x_j} \right] (M_j - M_i) + A_{12} M_j (M_i - 3M_j) \left(\frac{\lambda_1}{x_1} + \frac{\lambda_2}{x_2} \right) \right\} \end{aligned} \quad (4.4)$$

In (4.4) \sum' means the sum over i from 1 to 2 when $j \neq i$, and \mathcal{D}_{ij} is the self-diffusion coefficient of the i th component. The greatest simplifications occur for the diffusion velocity

$$\begin{aligned} V_{1\alpha}^{(2)} &= \alpha_2 \left(\frac{\partial \eta_1}{\partial T} \rho_2 - \frac{\partial \eta_2}{\partial T} \rho_1 \right) T_{,\beta} e_{\alpha\beta} + \alpha_1 \frac{\rho_2}{\rho\rho} e_{\alpha\beta,\beta} + \frac{5}{3} \alpha_3 \left(1 - \frac{2}{5} \partial_T \mathcal{D}_{12} \right) x_{1,\alpha} \nabla \mathbf{u} - \\ &\quad - 2\alpha_3 u_{\beta,\alpha} x_{1,\beta} + 2 \left\{ \alpha_3 + \alpha_2 \left(\frac{\partial \eta_1}{\partial x_1} \rho_2 - \frac{\partial \eta_2}{\partial x_1} \rho_1 \right) \right\} e_{\beta\alpha} x_{1,\beta} \\ \alpha_2 &= \frac{2m_2 n \mathcal{D}_{12}}{\rho_1 \rho^2}, \quad \alpha_3 = \frac{m_1^2 m_2^2 n^4 \mathcal{D}_{12}^2}{\rho \rho^3} \left(\frac{\rho_2}{\rho_1} - 1 \right) \end{aligned} \quad (4.5)$$

The partial quantities η_i and λ_i , occurring in (4.2)–(4.5), are calculated from the formulae

$$\begin{aligned} \eta_i &= x_i \left(x_i H_{jj}^{00} - x_j H_{ij}^{00} \right) \left(H_{ii}^{00} H_{jj}^{00} - H_{ij}^{00} H_{ji}^{00} \right)^{-1} \\ \lambda_i &= x_i \left(x_i \Lambda_{jj}^{11} - x_j \Lambda_{ij}^{11} \right) \left(\Lambda_{ii}^{11} \Lambda_{jj}^{11} - \Lambda_{ij}^{11} \Lambda_{ji}^{11} \right)^{-1} \end{aligned}$$

Here, as in (4.4), $i, j = 1, 2, j \neq i$. The functions H and Λ are defined in [5].

5. THE EQUATIONS OF THERMAL AND CONCENTRATION-STRESS CONVECTION

For slow flows, by definition, the following estimates hold

$$\begin{aligned} u &\sim \text{Kn}, \quad D/Dt \sim \text{Kn}, \quad p = p_0(1 + \delta p), \quad p_0 = nkT = \text{const} \\ \text{Kn} &\approx M \text{Re}^{-1} \rightarrow 0, \quad \text{Re} = O(1), \quad \delta p = O(\text{Kn}^2) \end{aligned} \quad (5.1)$$

where Kn , M and Re are the Knudsen, Mach and Reynolds numbers and δp is the dimensionless variable part of the pressure. If in this case, due to the boundary conditions, the characteristic relative temperature and concentration drops are of the order of unity, in the momentum equation and in the expression for the local force acting on an element of the surface of the body around which the flow occurs, we must take into account $\pi_{\alpha\beta}^*$, i.e. those terms of the stress tensor which contain derivatives of the temperature and concentration. Consequently, the Navier–Stokes equations in this continuous-mean limit are invalid, and the stresses $\pi_{\alpha\beta}^*$ cause new effects, in particular, new types of free convection when there are no external forces (see the review [1]).

For simplicity and clarity the analysis of these effects has been confined to slow steady flows of a simple gas [14] and an isothermal binary mixture of monatomic gases [15].

We will consider the more general case, following from Eqs (1.4)–(1.7), taking all the stresses due to the variability to T and x_i into account. We will assume, naturally, that the transient effects and the action of external forces do not change the defining estimates (5.1). The conservation equations are then simplified as described previously in [14, 15]: we assume $p = p_0$ in the coefficients of the equations, Eqs (1.4), (1.5) and (1.7) are simplified within the framework of the Navier–Stokes approximation, and in the energy equation terms with external forces and viscous stresses are dropped, i.e. $(p\delta_{\alpha\beta} + \tau_{\alpha\beta})u_{\alpha,\beta} \approx p_0 \nabla \mathbf{u}$. (We recall that in the case considered the coefficients of dynamic viscosity, η and volume viscosity S are commensurable; we will use the notation (2.2) for the spatial derivatives.)

The variable part of the complete stress tensor will only occur in the momentum equation and the expression for the local force. Using the fact that δp is small, as in the approach described earlier [14, 15], we will write it in the form

$$\begin{aligned} p_0 \delta p \delta_{\alpha\beta} + \tau_{\alpha\beta} &\equiv X \delta_{\alpha\beta} + R \pi_{\alpha\beta}, \quad X = p_0 \delta p + \Pi + \Theta \\ R \pi_{\alpha\beta} &\equiv \pi_{\alpha\beta} - \Theta \delta_{\alpha\beta} = R \pi_{\alpha\beta}^{(1)} + R \pi_{\alpha\beta}^* + \dots, \quad \Theta = \frac{2}{3} \eta \nabla \mathbf{u} + \dots \end{aligned}$$

Hence, X includes, in particular, the volume viscosity and the Burnett terms of the scalar Π , due to multiatomicity polyatomicity and those terms of the tensor $\pi_{\alpha\beta}$ which contain $\delta_{\alpha\beta}$ and which are not taken into account in $R \pi_{\alpha\beta}$. The specific features of the problem are such that X can be assumed to be a new gas-dynamic variable, whose structure it is not necessary to know.

After this from the derivatives $(R \pi_{\alpha\beta}^*)_{,\beta}$ occurring in the momentum equation we separate the third derivatives of T and x_i and we combine them with ∇X , which leads to a reduction in the order of the system of equations. For example.

$$(\xi_4 T_{,\alpha\beta})_{,\beta} = (\xi_4 T_{,\beta})_{,\alpha\beta} - (\xi_{4,\alpha} T_{,\beta})_{,\beta}$$

Finally, neglecting quantities $O(Kn^2)$ compared with unity, we can reduce the divergence of the total stress tensor, occurring in momentum equation (1.6), to the form

$$\begin{aligned} (p \delta_{\alpha\beta} + \tau_{\alpha\beta})_{,\beta} &= \Lambda_{,\alpha} - \left[\eta (u_{\alpha,\beta} + u_{\beta,\alpha}) \right]_{,\beta} + W_{\alpha\beta,\beta} \\ \Lambda &= X + \nabla(\xi_4 \nabla T) + \sum_j \nabla(\xi_{7j} \nabla x_j) \\ W_{\alpha\beta} &= -\xi_{4,\alpha} T_{,\beta} + (\xi_5 + \xi_5^*) T_{,\alpha} T_{,\beta} + \\ &+ \sum_k \left\{ -\xi_{7k,\alpha} x_{k,\beta} + \frac{1}{2} (\xi_{8k} + \xi_{9k} + \xi_{9k}^*) (T_{,\alpha} x_{k,\beta} + T_{,\beta} x_{k,\alpha}) \right. \\ &\left. + \frac{1}{2} \sum_l (\xi_{11kl} + \xi_{12kl}^*) (x_{k,\alpha} x_{l,\beta} + x_{k,\beta} x_{l,\alpha}) \right\} \end{aligned} \quad (5.2)$$

The quantity Λ is the new dependent variable of the system of conservation equations. In the cases considered previously in [14, 15] one can make a further simplification of expressions (5.2) and (5.3). In the approximation considered in Section 3, the coefficients ξ in (5.2) and (5.3) are calculated as for a mixture of monatomic gases.

6. CONCLUSION

The expressions for the Burnett transport coefficients are operators of scalar functions of the velocities and internal energies of the molecules A , B , D and Γ , specified by the first approximation of the Chapman–Enskog method. In the general case these expressions have a formal form, which is due to the insufficiency of the information on the inelastic collision cross-sections and purely mathematical difficulties. However, the latter are not a very serious obstacle in the present state of computational techniques, at least for the case of a mixture of monatomic gases. The results of the corresponding numerical solution could be very important for analysing the applicability of approximate analytic expressions for the Burnett coefficients, obtained by representing the functions A , B , D and Γ by sections of series in polynomials. The convergence of the series for the Burnett coefficients, even in the case of a simple gas, is very much slower, generally speaking, than for the Navier–Stokes transport coefficients. This is even more true for a mixture of monatomic gases, when there are only separate results [1, 6], a sufficiently complete analysis has not been carried out, but there is a fact that supports this conclusion, namely, the approximate expressions are exact for Maxwell molecules and, consequently, can be used in the case of “soft” intermolecular potentials.

I wish to thank V. A. Zharov for his help and M. Sh. Shavaliyev for comments on the manuscript.

This research was supported financially by the Russian Foundation for Basic Research (99-01-60409) and the “State Support for Leading Scientific Schools” programme (96-15-96063).

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Translated by R.C.G.