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BURNETT MODELS OF THE STRUCTURE OF A STRONG SHOCK WAVE IN A BINARY MIXTURE OF MONATOMIC GASES†

V. S. GALKIN and S. V. RUSAKOV

Zhukovskii

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The applicability of the complete and modified systems of Burnett's equations for problems on the structure of a strong shock wave in a binary mixture of monatomic gases are investigated. The results of calculations using the establishment method are compared with the results of calculations based on the Navier–Stokes equations and results obtained by direct statistical modelling. The limiting laws of intermolecular interaction (Maxwellian molecules and molecules treated as elastic spheres) are used.

Models of the structure of a shock wave and hypersonic flow, based on Burnett's equations, are widely used [1–6]. In order to suppress the so-called short-wave instability, additional damping terms have been introduced [1, 4, 5] which, however, increase the order of the system of equations and their complexity. It was found [2, 3] that the well-known "defects" of Burnett's equations can be eliminated with sufficient accuracy by simplifying and modifying them. In applications, high-temperature flows of gas mixtures are of the greatest interest [6]. The approach described earlier in [2, 3] is extended below to a binary gas mixture; Burnett's equations for this case are only applicable to certain linear problems [7, 8]. A derivation of Burnett's equations for a multicomponent mixture of monatomic gases has recently been given in [9, 10], and the necessary "working" expressions for the Burnett transport coefficients of a binary mixture of monatomic gases have been obtained [10].

The main aim of this paper is to continue the investigation of the mathematical properties, accuracies and limits of applicability of a modification of the system of Burnett's equations. The "defects" in this system of equations consist not only in the formulation of the boundary conditions (on account of the increased order of the system) and its instability: within the framework of the Navier–Stokes equations, it has been proved in [11] that, in the case of an infinitely high Mach number in front of the wave, M, there is a leading shock wave front in the gas in which the derivatives undergo discontinuities. This imposes additional requirements on the numerical algorithms in the case of large, but finite M (this is associated qualitatively with the fact that the temperature ahead of the front and, consequently, the transport coefficients are equal to zero and, therefore, what has been said also holds for other macromodels). According to kinetic theory, such a front does not exist on account of the perturbing action of "fast" molecules which create the leading "wedge" structure of a shock wave. This manifests itself to the greatest extent in the case of Maxwellian molecules and, to the least extent, in the case of elastic spheres.

In the case of flows of gas mixtures, the question of the techniques used for the macroscopic description in the case of different ratios of the masses of the molecules is important. It follows from kinetic theory [12, 13] that, generally speaking, a two-temperature (and, possibly, a two-fluid) description‡ is necessary in the case of large values of this ratio. As previously in [9, 10], single-temperature Burnett models are considered below.

1. INITIAL RELATIONS

The conservation equations for a binary mixture of monatomic gases in divergent form are

$$L_0 = \frac{\partial \rho}{\partial t} + \frac{\partial \rho u_\alpha}{\partial r_\alpha} = 0$$

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$$
\begin{aligned}
L_1 &= \frac{\partial \rho_1}{\partial t} + \frac{\partial}{\partial r_\alpha}\rho_1(u_\alpha + V_{1\alpha}) = 0 \\
L_{2\alpha} &= \frac{\partial \rho u_\alpha}{\partial t} + \frac{\partial}{\partial r_\beta}(\rho u_\alpha u_\beta + p\delta_{\alpha\beta} + \pi_{\alpha\beta}) = 0 \\
L_3 &= \frac{\partial}{\partial t}\left(\frac{\rho u^2}{2} + \frac{3}{2}p\right) + \frac{\partial}{\partial r_\alpha}\left[u_\alpha\left(\frac{\rho u^2}{2} + \frac{5}{2}p\right) + u_\beta\pi_{\alpha\beta} + h_\alpha + \frac{5}{2}p_1\left(1 - \frac{m_1}{m_2}\right)V_{1\alpha}\right] = 0
\end{aligned}
\tag{1.1}
$$

(where summation from 1 to 3 is carried out with respect to repeated Greek subscripts).

The notation from [9, 10] is used: the subscripts $i, j = 1, 2$ are the numbers of the components of the mixture, the projections of the radius vector $\mathbf{r}$ are introduced by means of the subscripts α, β ad γ, $\mathbf{u}$ is the mean mass velocity, n_i, $\rho_i = m_i n_i$, m_i, $p_i = n_i kT$, and $\mathbf{V}_i$ are the number and mass densities, the mass of the molecule, the pressure and the diffusion rate of the ith component, $\rho = \rho_1 + \rho_2$, $n = n_1 + n_2$, $p = nkT$ are the mass and number densities and the pressure of the mixture. T is the temperature, $\pi_{\alpha\beta}$ are the components of the solenoidal stress tensor and h_α is a component of the reduced heat flux. The formula $\mathbf{V}_2 = -(\rho_1/\rho_2)\mathbf{V}_1$ is used.

Putting

$$
(V_{1\alpha}, \pi_{\alpha\beta}, h_\alpha) = (V_{1\alpha}^{(1)}, \pi_{\alpha\beta}^{(1)}, h_\alpha^{(1)}) \tag{1.2}
$$

in the first three equations of (1.1), we obtain a system of conservation equations in the Navier–Stokes approximation (for brevity, simply the Navier–Stokes equations). Here,

$$
\begin{aligned}
V_{1\alpha}^{(1)} &= -\frac{m_2 n}{x_1 \rho}\mathscr{D}_{12}\left(d_{1\alpha} + k_T\frac{\partial \ln T}{\partial r_\alpha}\right), \quad d_{1\alpha} = \frac{\partial x_1}{\partial r_\alpha} + k_p\frac{\partial \ln p}{\partial r_\alpha} \\
\pi_{\alpha\beta}^{(1)} &= -2\eta e_{\alpha\beta}, \quad h_\alpha^{(1)} = -\lambda\frac{\partial T}{\partial r_\alpha} + p\frac{\rho}{\rho_2}k_T V_{1\alpha}^{(1)} \\
k_p &= x_1 x_2(m_2 - m_1)\frac{n}{\rho}, \quad x_i = \frac{n_i}{n} \\
e_{\alpha\beta} &= \left\langle\frac{\partial u_\alpha}{\partial r_\beta}\right\rangle, \quad \langle N_{\alpha\beta}\rangle = \frac{1}{2}(N_{\alpha\beta} + N_{\beta\alpha}) - \frac{1}{3}\delta_{\alpha\beta}N_{\gamma\gamma}
\end{aligned}
\tag{1.3}
$$

In relations (1.3), $\mathscr{D}_{12}$, η, λ and k_T are the coefficients of binary diffusion, viscosity, heat transfer and thermal diffusion ratio, respectively [10], and k_p is the coefficient of barodiffusion.

We obtain Burnett's equations by putting [10]

$$
(V_{1\alpha}, \pi_{\alpha\beta}, h_\alpha) = (V_{1\alpha}^{(1)} + V_{1\alpha}^{(2)}, \pi_{\alpha\beta}^{(1)} + \pi_{\alpha\beta}^{(2)}, h_\alpha^{(1)} + h_\alpha^{(2)}) \tag{1.4}
$$

Following a previously described procedure [3], we decompose the Burnett contributions into the transport properties

$$
(V_{1\alpha}^{(2)}, \pi_{\alpha\beta}^{(2)}, h_\alpha^{(2)}) = (V_{1\alpha}^{A} + V_{1\alpha}^{B}, \pi_{\alpha\beta}^{A} + \pi_{\alpha\beta}^{B}, h_\alpha^{A} + h_\alpha^{B}) \tag{1.5}
$$

We then write the Burnett contributions to the stresses in the form

$$
\pi_{\alpha\beta}^{A} = \xi_1 e_{\alpha\beta}\nabla\mathbf{u} - \xi_2\left\langle 2\frac{\partial u_\gamma}{\partial r_\alpha}e_{\gamma\beta} + \frac{\partial u_\gamma}{\partial r_\beta}\frac{\partial u_\alpha}{\partial r_\gamma}\right\rangle + \xi_3\langle e_{\alpha\gamma}e_{\gamma\beta}\rangle \tag{1.6}
$$

$$
\begin{aligned}
\pi_{\alpha\beta}^{B} &= -\xi_2\left\langle\frac{\partial}{\partial r_\alpha}\left(\frac{1}{\rho}\frac{\partial p}{\partial r_\beta}\right)\right\rangle + \xi_4\left\langle\frac{\partial^2 T}{\partial r_\alpha \partial r_\beta}\right\rangle + \xi_5\left\langle\frac{\partial T}{\partial r_\alpha}\frac{\partial T}{\partial r_\beta}\right\rangle + \xi_6\left\langle\frac{\partial p}{\partial r_\alpha}\frac{\partial T}{\partial r_\beta}\right\rangle + \\
&+ \xi_7\left\langle\frac{\partial d_{1\beta}}{\partial r_\alpha}\right\rangle + \left\langle\frac{\partial T}{\partial r_\alpha}\left(\xi_8\frac{\partial x_1}{\partial r_\beta} + \xi_9 d_{1\beta}\right)\right\rangle + \left\langle d_{1\alpha}\left(\xi_{10}\frac{\partial p}{\partial r_\beta} + \xi_{11}\frac{\partial x_1}{\partial r_\beta} + \delta\xi_{12}^{*}d_{1\beta}\right)\right\rangle
\end{aligned}
\tag{1.7}
$$

As previously in [10], we combine the expressions for the contributions to the vector transport properties, writing them more compactly as

$$\Lambda_\alpha^A = \left(\varphi_1 + \frac{\varphi_2}{3}\right)\frac{\partial T}{\partial r_\alpha}\nabla\mathbf{u} + \left(\varphi_2\frac{\partial T}{\partial r_\beta} - 2\varphi_7\frac{\partial x_1}{\partial r_\beta}\right)\frac{\partial u_\beta}{\partial r_\alpha} + \\ + \left(\varphi_4\frac{\partial T}{\partial r_\beta} + (\varphi_8 + \varphi_9 + \delta\varphi_9^*)\frac{\partial x_1}{\partial r_\beta}\right)e_{\beta\alpha} + \varphi_6\frac{\partial x_1}{\partial r_\alpha}\nabla u \tag{1.8}$$

$$\Lambda_\alpha^B = \left(\frac{\varphi_2}{3}T - \varphi_7\frac{5}{3}k_p\right)\frac{\partial\nabla\mathbf{u}}{\partial r_\alpha} + \left[\varphi_3 + (\varphi_9 + \delta\varphi_9^*)\frac{k_p}{p}\right]\frac{\partial p}{\partial r_\beta}e_{\beta\alpha} + \\ + \varphi_5\frac{\partial e_{\alpha\beta}}{\partial r_\beta} + \left(\varphi_6\frac{\nabla p}{\partial r_\alpha}\nabla\mathbf{u} - 2\varphi_7\frac{\partial p}{\partial r_\beta}\frac{\partial u_\beta}{\partial r_\alpha}\right)\frac{k_p}{p} \tag{1.9}$$

Definitions (1.3) for the operator $\langle\cdot\rangle$ and the coefficient k_p, and the expressions $x_2 = 1 - x_1$, $d_{2\alpha} = -d_{1\alpha}$, $\nabla\mathbf{u} = \partial u_\alpha/\partial r_\alpha$ have been used in formulae (1.6)–(1.9).

The expressions for h_α^A and h_α^B, are obtained from expressions (1.8) and (1.9) by means of the substitution [10]

$$(\Lambda_\alpha^A, \Lambda_\alpha^B) \to (h_\alpha^A, h_\alpha^B), \quad \varphi_m \to \gamma_m, \quad \delta\varphi_9^* \to \delta\gamma_9^*, \quad m = 1, 2, \ldots, 9 \tag{1.10}$$

(the magnitude of $\delta\gamma_9^*$ is given by formula (4.4) in [9]) and the expressions for $V_{1\alpha}^A$ and $V_{1\alpha}^B$ are obtained by means of the substitution

$$(\Lambda_\alpha^A, \Lambda_\alpha^B) \to (V_{1\alpha}^A, V_{1\alpha}^B), \quad \varphi_m \to \delta_m, \quad \delta\varphi_9^* \to 0 \tag{1.11}$$

The system of truncated Burnett equations, taking account of relations (1.1)–(1.11), has the form

$$L_0 = 0, \quad L_1^0 = 0, \quad L_{2\alpha}^0 = 0, \quad L_3^0 = 0 \tag{1.12}$$

The expressions for L_1^0, $L_{2\alpha}^0$ and L_3^0 are obtained from L_1, $L_{2\alpha}$ and L_3, defined by formulae (1.1), by means of the substitution

$$(V_{1\alpha}, \pi_{\alpha\beta}, h_\alpha) = (V_{1\alpha}^{(1)} + V_{1\alpha}^A, \pi_{\alpha\beta}^{(1)} + \pi_{\alpha\beta}^A, h_\alpha^{(1)} + h_\alpha^A) \tag{1.13}$$

Hence, only those terms of the Burnett transport properties containing paired products of the first derivatives of the components of the velocity vector, temperature and concentrations, which do not increase the order of the system compared with order of the Navier–Stokes equations, are included in the system of truncated Burnett equations.

The system of inhomogeneous truncated Burnett equations has the form

$$L_0 = 0, \quad L_1^0 = -\left(\frac{\partial}{\partial r_\alpha}\rho_1 V_{1\alpha}^B\right)_0, \quad L_{2\alpha}^0 = -\left(\frac{\partial}{\partial r_\beta}\pi_{\alpha\beta}^B\right)_0 \\ L_3^0 = -\left(\frac{\partial}{\partial r_\alpha}\left(u_\beta\pi_{\alpha\beta}^B + h_\alpha^B + \frac{5}{2}p_1\left(1 - \frac{m_1}{m_2}\right)V_{1\alpha}^B\right)\right)_0 \tag{1.14}$$

The right-hand sides of Eqs (1.14) are calculated for the solution of system (1.12). The complete system of Burnett equations is obtained if the zero subscript in the last three equations of (1.14) is omitted.

In the one-dimensional case, we use the notation $r_1 = x$, $u_x = u$. The x axis is directed along the flow and the conditions $x = -\infty$ correspond to the conditions in front of the shock wave.

Formulae (1.6) and (1.7) reduce to the form (a prime denotes a partial derivative with respect to x)

$$\pi_{xx}^A = \frac{2}{3}\left(\xi_1 - \frac{7}{3}\xi_2 + \frac{1}{3}\xi_3\right)u'^2$$

$$\pi_{xx}^B = \frac{2}{3}\left\{-\xi_2\left(\frac{p'}{\rho}\right)' + \xi_4 T'' + \xi_5 T'^2 + \xi_6 p' T' + \xi_7 d_{1x}' + \right. \tag{1.15}$$

$$\left. + (\xi_8 x_1' + \xi_9 d_{1x}) T' + (\xi_{10} p' + \xi_{11} x_1' + \delta\xi_{12}^* d_{1x}) d_{1x} \right\}$$

The "working" expressions for $\xi_n (n = 1, 2, \ldots, 12)$ are given by the right-hand sides of formulae (3.2) in [10]. The quantity $\delta\xi_{12}^*$ is calculated using formulae (4.4) of [9]. Formulae (1.8) and (1.9) reduce to the form

$$\begin{Vmatrix} h_x^A \\ V_{1x}^A \end{Vmatrix} = \begin{Vmatrix} \Phi_1^h \\ \Phi_1^V \end{Vmatrix} u'T' + \begin{Vmatrix} \Phi_2^h + \delta\gamma_9^* \\ \Phi_2^V \end{Vmatrix} u' x_1'$$

$$\begin{Vmatrix} h_x^B \\ V_{1x}^B \end{Vmatrix} = \begin{Vmatrix} \Phi_3^h \\ \Phi_3^V \end{Vmatrix} u'' + \begin{Vmatrix} \Phi_4^h + \dfrac{k_p}{p}\delta\gamma_9^* \\ \Phi_4^V \end{Vmatrix} u' p' \tag{1.16}$$

$$\Phi_1^h = \gamma_1 + \frac{2}{3}(2\gamma_2 + \gamma_4), \quad \Phi_2^h = \gamma_6 - 2\gamma_7 + \frac{2}{3}(\gamma_8 + \gamma_9)$$

$$\Phi_3^h = \frac{T}{3}\gamma_2 + \frac{2}{3}\gamma_5 - \frac{5}{3}\gamma_7 k_p, \quad \Phi_4^h = \frac{2}{3}\gamma_3 + \left(\gamma_6 - 2\gamma_7 + \frac{2}{3}\gamma_9\right)\frac{k_p}{p} \tag{1.17}$$

In order to obtain $\Phi_k^V (k = 1, 2, 3, 4)$, it is necessary to replace γ_m and δ_m in expressions (1.17) in accordance with (1.10) and (1.11). The "working" expressions for the coefficients γ and δ are calculated using the right-hand sides of formulae (3.4) and formulae (3.6) and (3.10) of [10]. The final formulae for Φ_k^h, Φ_k^V and the coefficients in (1.15) are lengthy and are not presented here.

2. NUMERICAL METHODS

Earlier in [2], in order to calculate the structure of a strong shock wave in a simple gas, steady-state systems of one-dimensional modified Burnett equations were integrated upwards along the flow from the neighbourhood of the singular point when $x = \infty$. However, this technique is inapplicable in the case of the complete system of Burnett equations on account of the well-known properties of its singular points, and the establishment method [1, 4] is therefore used. Moreover, the analysis of the singular points is significantly more difficult in the case of a gas mixture.

The numerical solution is constructed in a uniform, one-dimensional mesh. The following procedures are used when choosing the initial approximation. In the case of the system of Navier–Stokes equations when $t = 0$, a shock wave in the form of a compression shock of infinitesimal thickness is placed in the middle of the control volume (the number of cells is chosen to be even). The solution of this system is used as the initial approximation for the system of truncated Burnett equations (1.12) (here and below, the corresponding systems of one-dimensional equations must be borne in mind) with the same boundary conditions. It is possible to use both approaches in the case of the complete system of Burnett equations (or for system (1.14) when $M < 11$) but the calculations are carried out in several stages: a coarse mesh is used in the first stage and the solution obtained in the first stage is used as the initial solution in the second stage but the number of cells is increased by a factor of two, and so on (see Section 3). An analogous procedure is used to solve the system of truncated Burnett equations (1.14) when $M \geqslant 11$, but the solution of system (1.12) is chosen as the initial solution. Boundary conditions, corresponding to the free stream, are imposed on the boundary of the computational domain, the pressure is fixed on the other boundary and an extrapolation of the boundary conditions is used for the other parameters (the temperature, velocity, density and concentration of a component).

A "kinetically matched" difference scheme [14], employing well-known procedures for correcting flows which are used to construct schemes analogous to that described previously in [15], was used to approximate the convective terms of the system of equations. For smooth solutions, the scheme, which has been corrected in this manner, has an increased (above the first) order of approximation. A central

difference scheme of the second order of accuracy was used to approximate the viscous terms of the equations but, in certain calculations, the order of approximation was increased up to the fourth order in order to ensure the stability of the system of inhomogeneous truncated Burnett equations (1.14). The empirical formula [16].

$$\Delta t \leq \alpha \frac{\Delta x \mathrm{Cu}}{u(1 + 2\mathrm{Re}^{-1})}, \quad \mathrm{Re} = \frac{\rho u \Delta x}{\eta}$$

was taken as the stability condition for the proposed scheme, where the safety factor $\alpha = 0.7$, the Courant number $\mathrm{Cu} \leqslant 1/2$, the spatial step $\Delta x \leqslant 1/3l$, l is the minimum mean free path in the computational domain, u is the local velocity in the cell and Re is the mesh Reynolds number.

The problem being treated was also solved by the method of direct statistical modelling using a well-known algorithm [17]. At the initial instant of time, the shock wave in the form of a compression shock of infinitesimal is placed in the middle of the control volume. The steady-state distribution of all the parameters of the medium is calculated after the establishment of the process in time. In order that the shock should be steady, new particles are introduced into the control volume through a given segment of the boundary such that, in this segment, the time-averaged flows of the substance, the momentum and energy are equalized to their theoretical values [17]. In order to model the collisions of the particles, an algorithm [18] was used which ensures the necessary frequency of the collisions and minimization of the volume of the calculations. In order to test the proposed techniques, comparisons with known results [2, 3, 17] were made. For the case of Maxwellian molecules, the VHS-model [17] (the molecules are elastic spheres of variable diameter) was used for a characteristic temperature equal to 273 K. The mean free path ahead of the shock wave

$$l = \sum_{i=1}^{2} x_i \left[\sum_{j=1}^{2} \pi d_{ij}^2 n_j \left(\frac{m_1 + m_2}{m_j} \right)^{1/2} \right]^{-1} \tag{2.1}$$

The diameter of the "pseudosphere", d_{ij}, of the VHS-model is expressed in terms of its parameters [17]. The Mach number in front of the wave

$$M = \frac{u_-}{a}, \quad a^2 = \frac{5n_-}{3\rho_-} kT_-, \quad T_- \equiv T(x = -\infty) = 273 \text{ K} \tag{2.2}$$

The dimensionless variables

$$x^* = \frac{x}{l}, \quad T^* = \frac{T(x^*) - T(-\infty)}{T(\infty) - T(-\infty)}, \quad \rho^* = \frac{\rho(x^*) - \rho(-\infty)}{\rho(\infty) - \rho(-\infty)}, \quad x_1^* = \frac{x_1(x^*) - x_1(-\infty)}{x_1(-\infty)} \tag{2.3}$$

are used.

3. THE MATHEMATICAL FEATURES OF BURNETT MODELS

The mathematical theory of Burnett's equations and their modifications has not been developed and proofs are of a semi-empirical numerical character. In particular, a sufficiently complete analysis of questions concerning stability has not been carried out.

The short-wave instability of Burnett's equations has been discussed in which the numerical establishment method has been used [4]. When the mesh is finely subdivision, pulsations set in and the solution breaks up. In order to suppress this instability, semi-empirical damping terms were introduced, which have only an insignificant effect on the solution, and, as a result, a system of modified Burnett equations was obtained. Results of calculations using this system on a fine mesh and the initial system of Burnett's equations on a coarse mesh, that is, on a mesh which is close to an "unstable" mesh, have been presented in [4]. The data are practically identical throughout the thickness of shock wave up to $M = 50$, and with respect to the temperature profile along the critical line for hypersonic flow about a circular cylinder in the case of a small rarefaction. These and other data are responsible for the assertion that the inclusion of additional damping terms in Burnett's equations was mainly due to the transition to two- and three-dimensional flow problems [4].

The systematic calculations carried out using the techniques employed here demonstrated the practical convergence of the solution of Burnett's equations on the coarse mesh. For example, in the case of Maxwellian molecules when $M = 25$, $m_2 = 2m_1$, $d_{11} = d_{22}$, $x_1(-\infty) = 1/2$, we have

$$T^* = (0.07, 0.03, 0.00), (0.21, 0.16, 0.14), (0.39, 0.38, 0.37)$$

for $x^* = -50, -40, -30$ respectively. The last of the values enclosed in brackets were obtained for a value of the step size $\Delta_* x$, which is close to the "unstable" value, the second values were obtained for $\Delta x = 2\Delta_* x$ and the first for $\Delta x = 4\Delta_* x$. Changes occur in the third symbol. In the remaining part of the shock wave, the convergence is approximately the same as for $x^* = -30$.

By virtue of what has been said, we shall assume, for qualitative purposes, that the "established" results of calculations on a coarse mesh, close to an unstable mesh, are the solution of the system of Burnett equations.

However, the fact (see the introductory part of this paper) that, when $M = \infty$, the domain of the perturbed flow is separated from the uniform free stream by a front on the surface of which the derivatives are discontinuous, that is fundamental in the theory of macromodels of the structure of a shock wave, has not been discussed. The position of the front is different for different models. If the x coordinate is measured from the front along the flow, then, up to the front (when $x < 0$), the temperature T and the pressure p are equal to zero and, when $x = +0$, we have [11] $(T, p) \sim x^{1/n}$, where n is exponent for the temperature-dependence of the gas viscosity coefficient. This feature is most significant in the case of Maxwellian molecules when $n = 1$ (for molecules which are elastic spheres, $n = 1/2$).

At higher, but finite, values of M, this surface becomes blurred, passing into a zone where there sharp increase in the derivatives, which is more pronounced the greater the order of the derivatives.

The following remarks are associated with the selection of the basis in which the iterative method for solving the system of Burnett's equations is set up [2, 3], that is, with the solution of the problem of which Burnett terms have to be retained in Eqs (1.12).

It was initially proposed in [2] not to include only the terms π_{xx} and q_x, which contain the second derivatives of T and u (in order to eliminate short-wave instability and to reduce the order of the system of equations to the order of the Navier–Stokes equations; the density was eliminated in the once integrated steady-state Burnett equations). However, in the case of integration upstream along the flow adopted in [2, 3], the values of x, where the state of the flow is sufficiently close to the limiting state, could sometimes not be successfully reached. This "defect" was removed by the transfer of the term π_{xx}, containing T'^2, into the inhomogeneous part [2]. This approach was refined and generalized in [3]. The question concerning this transfer was analysed again using the establishment method, employed here. The term $2/3\xi_5 T'^2$ was taken into account in π_{xx}^A, that is, in the truncated Burnett equations, which led to the occurrence of pulsations in the leading part of the shock wave, As M increases, the extent of the pulsation domain becomes larger and a monotonic solution is only obtained on a coarse mesh. Meanwhile, the term being considered has a weak effect on the solution. The transfer of the term into the inhomogeneous part liquidates the pulsations.

Analogous effects also occur in the case of Eq. (1.14) due to the extreme non-linearity of the right-hand sides of these equations.

The transfer of the term containing $x_1'^2$ into π_{xx}^B is not of great significance since the changes in x_i within the shock wave are small compared with the change in T or ρ. The terms Λ_x^A, containing x_1', have only a small effect on the solution. The results of the calculations presented here were obtained without taking account of these terms in Λ_x^A.

When the damping terms [4, 5] are added to Burnett's equations, not only is the short-wave instability liquidated but, also, the indicated domain of pulsations is apparently "smeared out", although this latter fact was not even discussed. The numerical techniques adopted are sufficient for the purposes of this paper.

4. THE APPLICABILITY OF BURNETT MODELS

The results of calculations, obtained for the cases of Maxwellian molecules (a) and molecules which are elastic spheres (b) using the method of direct statistical modelling (the small crosses), the systems of Navier–Stokes equations (the dark points), Burnett's equations (the small circles), the truncated Burnett equations (the solid curves) and the inhomogeneous truncated Burnett equations (the dashed curves) are shown in Figs 1–3. The notation is given by formulae (2.1)–(2.3). Everywhere, $M = 11$ (the

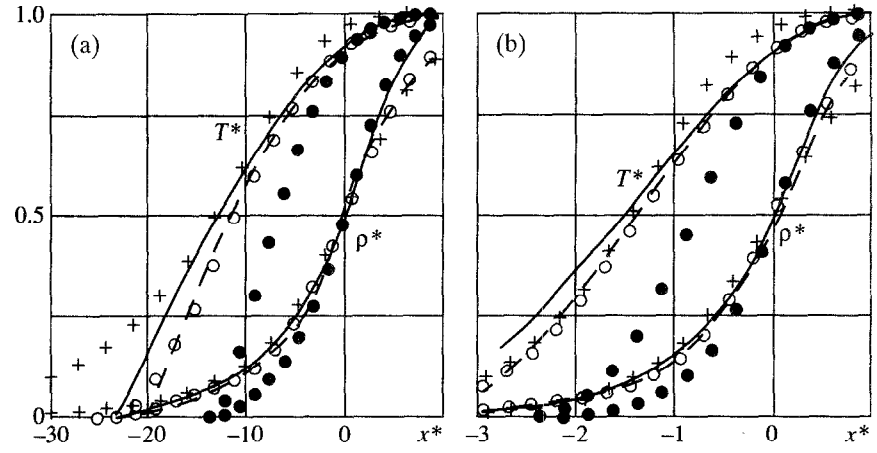

Fig. 1

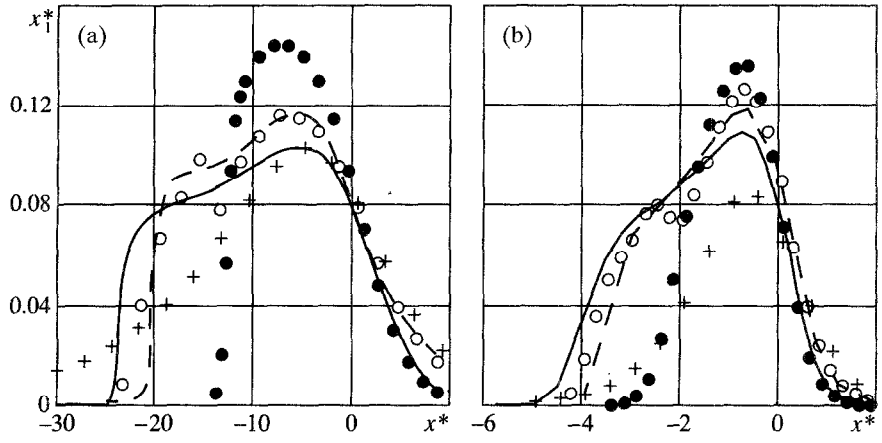

Fig. 2

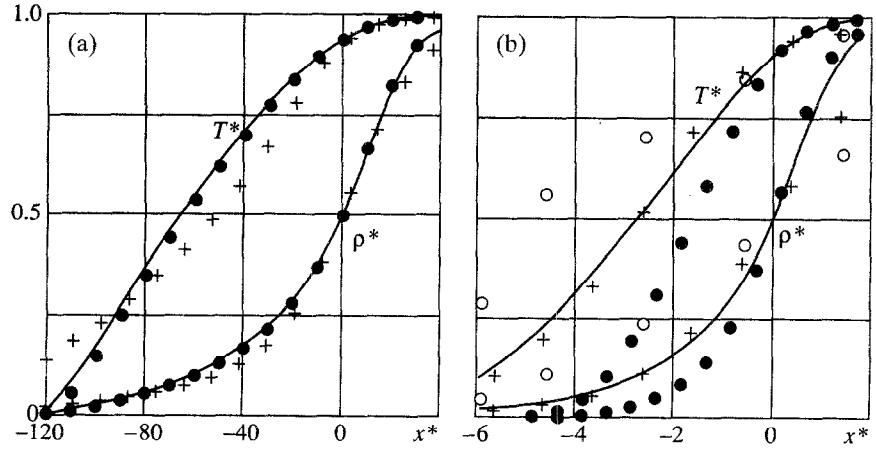

Fig. 3

traditional value for this problem [1–3]), $d_{11} = d_{22}$ and $x_i(-\infty) = 1/2$. Calculations were carried out for different values of the parameters and the most characteristic results are presented. A change in M from five and above has no effect on the conclusions reached.

The data in Figs 1 and 2 were obtained for $m_2/m_1 = 2$. These and the other results of the calculations enable us to draw the following conclusion (we recall that $u \sim 1/\rho$): in the case of small relative differences in the masses and diameters of the molecules, the conclusions concerning the accuracy of the models for the T^* and ρ^* profiles are qualitatively the same as in the case of a simple gas [2, 3]: Burnett's equations basically refine the Navier–Stokes equations, that is, they give results which are far closer to the results obtained using the method of direct statistical modelling. The results of calculations carried out within the framework of the inhomogeneous truncated Burnett equations (1.14) and within the framework of Burnett's equations are found to be close.

The fact that the data presented here were obtained using the truncated Burnett equations (1.12) is the principal difference from the results obtained previously [2, 3]. In the case of Maxwellian molecules, the truncated Burnett equations are even more accurate than the complete system of Burnett's equations in the leading part of the shock wave (Fig. 1). In the dense part of the shock wave, they are close to the Navier–Stokes equations. However,here, the difference between the results of calculations using the truncated Burnett equations and a calculation using the method of direct statistical modelling is about 10%. The fact [4, 5] that, in the flow problems, the results provide Burnett's equations are considerably more accurate than the results of calculations using the Navier–Stokes equations for the temperature precisely in the leading part of the wave is important. The above-mentioned "defects" in the stability and action of the domain of pulsations are not characteristic of the truncated Burnett equations. In the case of a simple gas, the singular points and, in general, the phase pattern of the structure of the shock wave are the same as in the case of Navier–Stokes equations [3]. In other words, the fundamental properties of the truncated Burnett equations are close to those of the Navier–Stokes equations.

In the light of what has been said, it is possible to simplify the algorithm [3] for constructing non-Navier–Stokes models by separating out the truncated Burnett equations as the basic model and simplifying it by transferring a number of the terms (containing derivative of x_1) to the following iteration. Of course, a somewhat different structure of the basic system of truncated Burnett equations may be more effective for other classes of problems.

The relative changes in the concentrations are far smaller than the changes in T^* and ρ^*, and, moreover, they depend strongly on the parameters of the problem. Increased requirements on the accuracy of the calculation of $x_i(x^*)$, including also on the method of direct statistical modelling, are necessary. The data obtained for the case of Maxwellian molecules in Fig. 2(a) demonstrate the advantages of Burnett models compared with Navier–Stokes modelling in the leading part of the shock wave. However, in the case of molecules which are elastic spheres (Fig. 2b), there are in fact no such advantages. The distinguishing feature of Burnett models is the non-monotonicity of the concentration profiles, which is particularly pronounced in the case of the complete system of Burnett's equations.

As m_2/m_1 increases the conclusions which have been reached concerning the advantages of Burnett models no longer hold (Fig. 3). In the case of Maxwellian molecules when $m_2/m_1 = 100$, the Burnett and Navier–Stokes profiles of T^* and ρ^* almost merge (hence only the results of calculations within the framework of the truncated Burnett equations and the Navier–Stokes equations are therefore shown in Fig. 3a). The difference between the Navier–Stokes profiles and the result of a calculation using the method of direct statistical modelling is significantly less than in Fig. 1.

The applicability of Burnett models deteriorates in the case of molecules which are elastic spheres. According to the complete system of Burnett's equations, the domain of perturbed flow has expanded considerably when $m_2/m_1 = 10$ (Fig. 3b). The truncated Burnett equations give acceptable results here. However, when $m_2/m_1 = 100$, they give much worse agreement with the results of the method of direct statistical modelling than the Navier–Stokes equations (particularly, for T^*).

For x_1^* at high m_2/m_1, similar conclusions on the accuracy of Burnett models hold.

Hence, using the limiting laws of intermolecular interaction, general conclusions have been drawn regarding the accuracy of Burnett models when there are small relative differences in the masses of the molecules (in particular, when $m_2/m_1 = 2$) which are similar to the case of a simple gas. When there are considerable differences in the masses of the molecules, the areas of applicability of macromodels depend fundamentally on the interaction law adopted, and a corresponding analysis for actual gas mixtures is required.

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REFERENCES

1. GALKIN, V. S. and SHAVALIYEV, M. Sh., Gas dynamic equations for higher approximations of the Chapman–Enskog method. *Izv. Ross. Akad. Nauk. MZhG*, 1998, 4, 8–28.
2. BUZYKIN, O. G., GALKIN, V. S. and NOSIK, V. I., Modification of Burnett's equations and the structure of a shock wave. Izv. Ross., *Akad. Nauk. MZhG*, 1998, 3, 164–176.
3. BUZYKIN, O. G. and GALKIN, V. S., Modifications of the gas dynamic equations of higher approximations of the Chapman–Enskog method. *Izv. Ross., Akad. Nauk, MZhG*, 2001, 3, 185–199.
4. ZHONG, X., MACCORMACK, R. W. and CHAPMAN, D. R., Stabilization of the Burnett equations and application to hypersonic flows. *AIAA J.*, 1993, **31**, 1036–1043.
5. AGARWAL, R., YUN, K.-Y. and BALAKRISHNAN, R., Beyond Navier–Stokes: Burnett equations for flows in the continuum–transition regime. *Phys. Fluids*, 2001, **13**, 3061–3085.
6. CHENG, H. K. and EMANUEL, G., Perspective on hypersonic nonequilibrium flow. *AIAA J.*, 1995, **33**, 386–400.
7. ZHDANOV, V. M. and ROLDUGIN, V. I., Non-equilibrium thermodynamics and the kinetic theory of rarefied gases. *Uspekhi Fiz. Nauk*, 1998, **168**, 4, 407–438.
8. SHAVALIYEV, M. Sh., Investigation of the structure of a weak shock wave and the propagation of small perturbations in gas mixtures using Burnett's equations. *Prikl. Mat. Mekh.*, 1999, **63**, 3, 444–456.
9. GALKIN, V. S., Burnett's equations for multicomponent mixtures of monatomic gases. *Prikl. Mat. Mekh.*, 2000, **64**, 4, 590–604.
10. GALKIN, V. S. and ZHAROV, V. A., The transport properties of gases in the Burnett approximation. *Prikl. Mat. Mekh.*, 2002, **66**, 3, 434–447.
11. SYCHEV, V. V., Hypersonic flows of a viscous, heat-conducting gas. *Prikl. Mat Mekh.*, 1961, **25**, 4, 600–610.
12. GALKIN, V. S. and MAKASHEV, N. K., The kinetic derivation of the equations of gas dynamics of multicomponent mixtures of light and heavy particles. *Izv. Ross. Akad. Nauk. MZhG*, 1994, 1, 180–200.
13. GORBACHEV, Yu. Ye., Multivelocity models in the theory of heterogeneous media, *Izv. Akad. Nauk. SSSR. MZhG*, 1991, 3, 54–66.
14. VORONICH, I., VOIKOV, V. and KHLOPKOV, Yu., Application of kinetic models for the construction of finite difference schemes in gas dynamics. *Proc. 3rd Seminar on RRDPAE.*, Warsaw, 1999, 163–166.
15. KOLGAN, V. P., The use of the principle of minimum values of a derivative to construct finite – difference schemes for calculating discontinuous solutions in gas dynamics. *Uchen. Zap. Tsentr. Aero-Gidrodinam. Inst.*, 1972, **3**, 6, 68–77.
16. ANDERSON, D. A., TANNEHILL, I. C. and PLETCHER, R. H., Computational Fluid Mechanics and Heat Transfer. Hemisphere, New York, 1984.
17. BIRD, G. A., *Molecular Gas Dynamics and the Direct Simulation of Gas Flow*. Clarendon Press, Oxford, 1994.
18. BELOTSERKOVSKII, O. M. and YANITSKII, V. Ye., The statistical method of particles in cells for solving problems in the dynamics of a rarefied gas. 1. Foundations of the construction of the method. *Zh. Vychisl. Mat. Mat. Fiz.*, 1975, **15**, 5, 1195–1208. 2. Computational aspects of the method. *Ibid.*, 6, 1553–1567.
19. LUKSHIN, A. V. and SMIRNOV, S. N., A stochastic method for solving Boltzmann's equation. *Zh. Vyschisl. Mat. Mat. Fiz.*, 1988, **28**, 2, 293–297.

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