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THE SOLUTION OF PROBLEMS OF SOUND PROPAGATION AND THE STRUCTURE OF A WEAK SHOCK WAVE IN A POLYATOMIC GAS USING BURNETT'S EQUATIONS[†]

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Expressions for the linear Burnett transport properties with transfer coefficients in the Mason-Monchik approximation are presented. Problems of sound propagation and the structure of a weak shock wave are solved using them. © 2001 Elsevier Science Ltd. All rights reserved.

The question of the significance of the effect of internal degrees of freedom of molecules on the Burnett transfer coefficients were formulated for the first time by McCoy and Dahler [1]; they derived formulae for these coefficients for classical models of molecules with rotational degree of freedom (rough sheres, loaded spheres and spherocylinders) and the problems indicated considered in the above abstract. However, these models have well-known drawbacks, and the quasi-classical approach is preferred [2, 3], by which expressions have been obtained for the Burnett transfer coefficients [4].

We emphasize that the results of this paper give, generally speaking, an upper limit of the effect of rotations of the molecules on the Burnett transfer coefficients: they are based on data [4] obtained for the case of simple exchanges of translational and internal energy of the molecules, and ignore relaxation of the rotations of the molecules.

1. LINEAR TRANSPORT PROPERTIES

Burnett's transfer coefficients of a polyatomic gas can be expressed approximately [4] in terms of the shear viscosity θ and bulk viscosity ζ , the translational thermal conductivity λ_i and the internal thermal conductivity λ_v , and the coefficient σ . For example, we have for the coefficients of the linear terms of the stress tensor and of the heat flux vector

$$\xi_{2} \approx \frac{2\eta^{2}}{p}, \quad \xi_{4} \approx \frac{4\eta}{5p}\lambda_{t}, \quad \omega_{2} \approx \frac{\varsigma}{p}(\lambda_{t} - \sigma\lambda_{v}), \quad \omega_{2} \approx \frac{3\varsigma^{2}}{2p}(1 + \sigma)$$

$$\gamma_{2} \approx -\frac{2}{5Rp} \left(\lambda_{t}^{2} + \frac{5}{2}\frac{k_{B}}{c_{v}}\lambda_{v}^{2}\right), \quad \gamma_{5} \approx \frac{4\eta\lambda_{t}}{5R\rho}, \quad \gamma_{12} \approx \frac{\varsigma}{R\rho}(\lambda_{t} - \sigma\lambda_{v})$$

$$(1.1)$$

Here we have used the notation previously employed in [4], the pressure $p = \rho RT$, $R = k_B/m$ is the gas constant, k_B is Boltzmann's constant, m is the mass of the molecule and c_v is the heat capacity due to the internal degrees of freedom at constant volume. It can be shown [2, 3] that

$$\sigma = \frac{3k_B}{2c_v} = \frac{3(\gamma - 1)}{5 - 3\gamma}, \quad \varsigma = \frac{1}{4}\pi k_B c_v \, \eta Z \left(\frac{3}{2} \, k_B + c_v\right)^{-2} \tag{1.2}$$

where γ is the ratio of the specific heat capacities and Z is the ratio of the rotational and translational relaxation times (semi-empirical Z(T) relations are known for different gases [3]).

According to the Mason-Monchik approximation, the coefficient η is the same as for the corresponding monatomic gas, and at the same time[3] we have

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$$(\lambda_{r}, \lambda_{\nu}) = \frac{15}{4} R \eta(\lambda_{r}^{*}, \lambda_{\nu}^{*}), \quad \lambda_{r}^{*} = 1 - \frac{A}{\sigma}, \quad \lambda_{\nu}^{*} = \frac{2\beta}{5\sigma} (1+A)$$

$$A = \frac{5 - 2\beta}{\pi Z} \left[1 + \frac{2}{\pi Z} \left(\frac{5}{2\sigma} + \beta \right) \right]^{-1}, \quad \beta = \frac{\rho D}{\eta} \varphi(Z) \approx 1.328 \varphi(Z)$$

$$(1.3)$$

Here we have used formula (1.2) for σ , and D is the self-diffusion coefficient of a monatomic gas. When $Z \ge 3$ we have $\varphi \approx 1$ [3]. We will henceforth assume that $\varphi = 1$; then the effect of the rotations appears via γ and Z.

In the case of light exchanges $Z \sim 1$. For fixed Z we obtain the case of a monatomic gas formally by assuming $c_v = 0$ ($\sigma = \infty$), in which case $\zeta = 0$, $\lambda_i^* = 1$, $\lambda_v^* = 0$. We have monatomic values of η and λ in the case of slow exchanges ($Z \gg 1$), when the temperature is determined by the kinetic energy of the molecules, there is no bulk viscosity, and the populations of the rotational levels satisfy a system of relaxation equations.

Using relations (1.1) - (1.3) and the formulae obtained previously in [4], for the one-dimensional linearized flows considered below we find the following expressions for the stress and heat flux

$$\tau \equiv \tau_{xx} = -\frac{4}{3} \eta B \frac{\partial u}{\partial x} - \frac{4}{3} \frac{\eta^2}{\rho \rho} Q_2 \frac{\partial^2 p}{\partial x^2} + \frac{2\eta^2}{T \rho} Q_3 \frac{\partial^2 T}{\partial x^2}$$
(1.4)

$$q \equiv q_x = -\frac{15}{4} R \eta \Lambda \frac{\partial T}{\partial x} - \frac{7}{4} \frac{\eta^2}{\rho} Q_1 \frac{\partial^2 u}{\partial x^2}$$
(1.5)

$$B = 1 + \frac{3}{4} \frac{\varsigma}{\eta} \approx 1 + \frac{3\pi}{32} Z(\gamma - 1)(5 - 3\gamma), \quad \Lambda = \lambda_i^* + \lambda_\nu^*$$
(1.6)

$$Q_{1} = \frac{15\sigma}{7(1+\sigma)} \left(\lambda_{t}^{*2} + \frac{5}{3}\sigma\lambda_{v}^{*2}\right) - \frac{8}{7}\lambda_{t}^{*} - \frac{20}{7}(B-1)(\lambda_{t}^{*} - \sigma\lambda_{v}^{*})$$
(1.7)

$$Q_2 = 1 + 2(1 + \sigma)(B - 1)^2, \quad Q_3 = \lambda_t^* + \frac{5}{2}(\lambda_t^* - \sigma\lambda_v^*)(B - 1)$$
(1.8)

Terms with first derivatives correspond to the Navier-Stokes approximation and terms with second derivatives correspond to Burnett's approximation, where u is the gas velocity. In the case of a monatomic gas $B = \Lambda = Q_m = 1$ (m = 1, 2, 3). The effect of the internal degrees of freedom of the molecules on the transfer coefficients manifests itself via the dependence of B, Λ and Q_m on γ and Z. The final aim is to establish a measure of this effect on Q_m and on the solution of problems (i.e. how the solutions depend on the deviations of Q_m from unity).

Henceforth we will assume the rotations are completely excited, so that $\gamma = \text{const.}$ The dependence of B, Λ and Q_m on T is then expressed in terms of the function Z(T).

The data shown in Table 1 represent the transfer coefficients as a function of Z and γ . For nitrogen

Z	γ	В	٨	Q1	Q ₂	Q3
3	1/5	1.28	1.31	0.315	1.40	1.10
2	4/3	1.29	0 1.47 0.246	1.35	1.05	
6	7/5	1.56	1.32	-0.034	2.60	1.44
0	4/3	1.59	1.49 -0.116	2.39	1.40	
10	1/5	1.94	1.33	-0.520	5.44	1.88
10	4/3	1.98	1.50	-0.619	4.86	1.86
20	1/5	2.88	1.34	-1.76	18.76	2.99
20	4/3	2.96	1.52	-1.91	16.42	3.02

Table 1

we have [3] Z = 3, 6 and 10 at $T \approx 200$, 400 and 1000 K; the value Z = 20 is close to the limit (we recall that a large spread of the existing data is characteristic for the function Z(T)).

The value B increases linearly as Z increases, due to the increase in the effect of the bulk viscosity (since $Z \sim \varsigma/\eta$), while Λ tends to a value given by the modified Eucken formula [2, 3]. Rotations of the molecules have a considerably greater effect on Burnett's transfer coefficients Q_m than the on the Navier-Stokes coefficients. The coefficient Q_1 first changes sign as Z increases, and then $|Q_1|$ increases approximately linearly with respect to Z, and also Q_3 . Q_2 increases particularly strongly in view of its quadratic dependence on Z.

The effect of γ on Z is much less (with the exception of Q_1).

2. SOUND PROPAGATION

We will consider the problem of the propagation of forced plane ultrasonic oscillations with a fixed frequency ω along the x > 0 axis in a polyatomic gas. For perturbations of the gas-dynamic variables we have

$$\delta \rho = \frac{\rho - \rho_0}{\rho_0} \ll 1, \quad \delta T = \frac{T - T_0}{T_0} \ll 1, \quad u \ll c$$

$$\delta p = \frac{p - p_0}{p_0} = \delta \rho + \delta T \ll 1, \quad u \equiv u_x, \quad c = \sqrt{\gamma R T_0}$$
(2.1)

where ρ_0 , T_0 and p_0 are the mass density, temperature and pressure in the unperturbed gas and c is the velocity of sound for a Knudsen number $K_n = 0$. We will assume

$$Kn = \frac{\omega \eta_0}{p_0}, \quad \eta_0 = \eta(T_0), \quad \tau_{xx} = \tau, \quad q_x = q$$
(2.2)

The Knudsen number K_n is determined, as in a monatomic gas [5], for a clear demonstration of the effect of the internal degrees of freedom of the molecules. We will write the linearized continuity and energy equations in the variables (2.1) and (2.2)

$$\frac{\partial \delta \rho}{\partial t} = -\frac{\partial u}{\partial x}, \quad \frac{1}{\gamma - 1} \frac{\partial \delta T}{\partial t} + \frac{\partial u}{\partial x} + \frac{1}{\rho_0} \frac{\partial q}{\partial x} = 0$$
(2.3)

Hence we have

$$\frac{\partial^2 \delta \rho}{\partial t \partial x} = -\frac{\partial^2 u}{\partial x^2}$$
(2.4)

Using Eq. (2.4) and the equation of state, we can reduce the momentum equation to the form

$$\frac{\gamma}{c^2}\frac{\partial^2 u}{\partial t^2} + \frac{\partial^2 \delta T}{\partial x \partial t} - \frac{\partial^2 u}{\partial x^2} + \frac{1}{p_0}\frac{\partial^2 \tau}{\partial x \partial t} = 0$$
(2.5)

We will seek a solution in the form

$$(\delta\rho, \delta p, \delta T, u) \sim \exp(-kx^* + t^*)$$

$$k = K \frac{c}{\omega} \equiv \alpha + i\beta, \quad x^* = \frac{\omega}{c}x, \quad t^* = i\omega t$$
(2.6)

Here K is the wave number, t is the time, i is the square root of -1, α is the absorption coefficient and β is the dispersion coefficient (inversely proportional to the phase velocity).

We substitute (1.4) and (1.5) into Eqs (2.3) and (2.5), eliminating the derivative of $\delta\rho$, taking (2.4) into account, and we introduce the new variables

$$v = \frac{u}{c} \exp(-t^*), \quad \theta = \delta T \exp(-t^*)$$

assuming then that

$$\frac{\partial}{\partial t^*} = 1, \quad ()^{(n)} = \frac{d^n()}{dx^{*n}}, \quad n = 1, \dots, 5$$

Finally, the search for a solution in the form (2.6) leads to the following system of equations

$$v + \frac{1}{\gamma} \left(1 + \frac{4}{3} i \operatorname{Kn} B_0 \right) v^{(2)} - \frac{4}{3\gamma^2} \operatorname{Kn}^2 Q_{20} v^{(4)} - \frac{i}{\gamma} \theta^{(1)} - \frac{2i}{3\gamma^2} \operatorname{Kn}^2 S \theta^{(3)} = 0$$

$$\frac{2}{3} v^{(1)} - \frac{7}{6\gamma} \operatorname{Kn}^2 Q_{10} v^{(3)} + \frac{2i}{3(\gamma - 1)} \theta - \frac{5}{2\gamma} \operatorname{Kn} \Lambda_0 \theta^{(2)} = 0, \quad S = 3Q_{30} - 2Q_{20}$$
(2.7)

We obtain B_0 , Λ_0 and Q_{m0} using relations (1.3) and (1.6) – (1.8), by replacing Z by $Z_0 = Z(T_0)$. From system (2.7) we have the dispersion equation

$$k^{6} \frac{\gamma - 1}{6\gamma^{3}} \operatorname{Kn}^{3} (7 \operatorname{Kn} Q_{10} S - 30i \Lambda_{0} Q_{20}) + + k^{4} \frac{\operatorname{Kn}}{12\gamma^{2}} \{ \operatorname{Kn} [3(\gamma - 1)(8Q_{30} - 7Q_{10} - 20B_{0}\Lambda_{0}) - 16Q_{20}\gamma] + 45i(\gamma - 1)\Lambda_{0} \} + + k^{2} \frac{1}{12\gamma} \{ i \operatorname{Kn} [45(\gamma - 1)\Lambda_{0} + 16B_{0}] + 12\gamma \} + 1 = 0$$
(2.8)

Henceforth we will only consider the sonic mode [5]. When $Kn \ll 1$ it follows from (2.8) that

$$\alpha = \alpha_1 \operatorname{Kn} + O(\operatorname{Kn}^3), \quad \beta = 1 - \beta_2 \operatorname{Kn}^2 + O(\operatorname{Kn}^4), \quad \beta_2 = \varkappa_1 + \varkappa_2$$
 (2.9)

Expansion (2.9) was discussed in [5] in the case of a monatomic gas.

The quantity α_1 is given by the Navier–Stokes approximation

$$\alpha_{1} = \frac{2B_{0}}{3\gamma} + \frac{15}{8\gamma^{2}} \Lambda_{0} (\gamma - 1)^{2}$$
(2.10)

At the same time both the Navier–Stokes approximation (x_1) and the Burnett approximation (x_2) make a contribution to β_2

$$\kappa_{1} = \frac{2B_{0}^{2}}{3\gamma^{2}} + \frac{25B_{0}}{4\gamma^{3}}\Lambda_{0}(\gamma - 1)^{2} + \frac{225\Lambda_{0}^{2}}{128\gamma^{4}}(\gamma - 1)^{3}(3\gamma - 7)$$

$$\kappa_{2} = \frac{\gamma - 1}{\gamma^{2}} \left(\frac{7}{8}Q_{10} - Q_{30}) + \frac{2Q_{20}}{3\gamma}\right)$$
(2.11)

Formulae (2.9) – (2.11) are the asymptotic solution $(K_n \rightarrow 0)$ of the problem in the Burnett approximation, and higher approximations of the Chapman-Enskog method make a contribution to the following terms of the series.

In Tables 2 and 3 we show some results of calculations for this and the following sections. Case 9° corresponds to a monatomic gas ($\gamma = 5/3$). Naturally, for the same γ and $Z_0 = Z$, the values of the transfer coefficients B_0 , Λ_0 and Q_{m0} are equal to the values of the coefficients B, Λ and Q_m given in Table 1. The quantities B_2 and x_1/x_2 represent the dispersion and comparative contribution of the

The quantities B_2 and x_1/x_2 represent the dispersion and comparative contribution of the Navier-Stokes and Burnett approximations. The ratio x_1/x_2 decreases as Z increases, i.e. the relative contribution of the Burnett approximation to the dispersion coefficient increases.

To analyse the significance of the difference of the Burnett transfer coefficients Q_{m0} from unity for different K_m , Z and γ , Table 3 gives the following quantities

$$\Delta_{\alpha} = \frac{\alpha}{\alpha_{\star}}, \quad \Delta_{\beta} = \frac{\beta}{\beta_{\star}}, \quad \alpha_{\star} = \alpha(\gamma, B_0, \Lambda_0, Q_{m0} = 1), \quad \beta_{\star} = \beta(\gamma, B_0, \Lambda_0, Q_{m0} = 1)$$

N₂	γ	Z ₀	β ₂	x1/x2	<i>G</i> 1	<i>G</i> ₂	<i>G</i> ₃	G	Δ_G
1°	1/5	3	1.53	2.07	-239	25	449	235	1.22
2°	1/5	6	2.38	1.54	-309	34	723	448	3.39
3°	1/5	10	4.20	0.985	-424	49	1367	992	30.4
4°	7/5	20	12.10	0.511	-818	96	4378	3656	-11.6
5°	4/3	3	1.57	2.04	-211	19	363	171	1.16
6°	4/3	6	2.42	1.65	-283	26	573	316	3.85
7°	4/3	10	4.18	1.12	-400	38	1066	704	-30.7
8°	4/3	20	11.80	0.609	-806	77	3370	2641	-6.78
9°	5/3	-	1.08	1.90	-353	51	756	454	-

Tal	ble	3

№	Kn = 0.1	0.3	0.5	0.7	0.9	1.1	1.3		
$\Delta_{\alpha} \cdot 10^3$									
10	996	980	968	957	945	930	912		
, 20	976	889	830	789	755	727	704		
3°	930	739	641	587	553	532	517		
4°	774	470	384	350	335	329	329		
5°	997	983	972	961	949	933	914		
6°	979	901	850	814	785	760	739		
7°	937	764	675	625	594	573	560		
8°	792	505	420	387	372	367	369		
			Δ _β .	10 ³		•			
10	1 1000	1000	1006	1015	1028	1044	1063		
20	996	989	997	1012	1028	1045	1062		
30	987	967	973	985	998	1011	1023		
40	955	908	911	923	936	949	962		
5°	1000	1000	1006	1014	1025	1039	1055		
6°	996	991	1000	1015	1032	1050	1067		
7°	989	973	984	1000	1015	1030	1044		
8°	960	927	940	958	976	992	1007		
	•		α.	10 ³		•	•		
1°	78	186	237	260	271	276	279		
2°	90	209	259	279	285	286	284		
3°	106	235	281	295	296	292	286		
4°	144	283	314	315	308	297	286		
5°	79	186	236	258	268	272	275		
6°	92	212	261	279	285	286	283		
7°	110	240	285	298	298	294	287		
8°	151	290	319	319	310	298	287		
β, 10 ³									
10	986	908	825	755	699	651	610		
2°	982	888	794	717	657	607	565		
<u>3</u> °	976	862	754	672	610	560	520		
4°	960	795	668	581	518	471	435		
5°	986	906	822	753	696	650	610		
6°	981	885	789	713	652	603	561		
7°	975	856	747	664	602	552	512		
8°	956	784	653	565	503	456	420		

Table 2

Here $\alpha *$ and $\beta *$ are the solutions of Eq. (2.8) for $Q_{m0} = 1$ (but $B_0 \neq 1$, $\Lambda_0 \neq 1$, $\gamma \neq \frac{5}{3}$). (Detailed data are given in [6] for a monatomic gas.)

The differences of the quantities Δ_{α} and Δ_{β} from unity represent the degree of influence of changes in the Burnett coefficients Q_{m0} , due to rotation of the molecules, on the solution of the problem of sound propagation. This influence increases as K_n and Z increase, particularly for the absorption coefficient α .

3. STRUCTURE OF A WEAK SHOCK WAVE

The conservation equations take the form

$$\rho u = C_1, \quad p = C_1 \frac{RT}{u}$$

$$\rho + \rho u^2 + \tau = C_2, \quad C_1 \left(u^2 + \frac{2R\gamma}{\gamma - 1}T \right) + 2u\tau + 2q = C_3$$
(3.1)

where C_m (m = 1, 2, 3) are integration constants. Introducing the variables

2

$$u_{\star} = \frac{C_1}{C_2} u, \quad T_{\star} = \left(\frac{C_1}{C_2}\right)^2 RT, \quad \tau_{\star} = \frac{\tau}{C_2}, \quad q_{\star} = \frac{C_1}{C_2^2} q$$

eliminating ρ and p using the first two equations of (3.1) and subtracting the momentum equation from the energy equation, we obtain instead of the last two equations of (3.1)

$$u_{*}^{2} + T_{*} - u_{*} + u_{*}\tau_{*} = 0$$

$$\frac{\gamma + 1}{\gamma - 1}T_{*} + u_{*} + u_{*}\tau_{*} + 2q_{*} = C, \quad C = \frac{C_{1}C_{3}}{C_{2}^{2}}$$
(3.2)

We will use a method similar to that employed earlier in [7] for a mixture of monatomic gases, choosing as the small parameter

$$\varepsilon = u_{\bullet}^{-} - u_{\bullet}^{+} = \frac{2\gamma(M^{2} - 1)}{(\gamma + 1)(\gamma M^{2} + 1)}; \quad u^{-} = u(x = -\infty), \quad u^{+} = u(x = \infty)$$
(3.3)

where M is the Mach number in front of the shock wave $(x = -\infty)$. Multiplying both sides of the first equation of (3.3) by $(\gamma + 1)/(\gamma - 1)$, we obtain a parameter, the effectiveness of which was demonstrated in [8]. The advantage of this kind of parameters compared with the parameter $[1] y = M - 1 \ll 1$ is the fact that they are finite as M increases and accelerate the convergence of the series with respect to the small parameter. The parameter C is expressed in terms of ε by the formula

$$C = \frac{\gamma^2}{\gamma^2 - 1} - \frac{\gamma + 1}{\gamma - 1} \frac{\varepsilon^2}{4}$$

We will introduce the following variables which depend on w and v and are independent of ξ

$$u_* = \frac{\gamma}{1+\gamma} + \frac{\varepsilon}{2} w, \quad T_* = \frac{\gamma}{(1+\gamma)^2} + \frac{\gamma-1}{2(\gamma+1)} \varepsilon \vartheta - \frac{\varepsilon^2}{4}, \quad x = \frac{\eta_0 \xi}{C_1 \varepsilon}$$

$$w(0) = 0, \quad w^- = 1, \quad w^+ = -1, \quad \vartheta^- = -1, \quad \vartheta^+ = 1$$
(3.4)

The quantity η_{θ} is defined below (see (3.6)). We can now write the system of equations (3.2) in the form

$$\varepsilon(w+\vartheta)+\varepsilon^2\frac{\gamma+1}{2(\gamma-1)}(w^2-1)+[2\gamma+(\gamma+1)\varepsilon w]\frac{\tau_*}{\gamma-1}=0$$

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$$\varepsilon(w+\vartheta) + \varepsilon^2 \frac{\gamma+1}{2(\gamma-1)} (w^2 - 1) + [2\gamma + (\gamma+1)\varepsilon w] \frac{\tau_*}{\gamma-1} = 0$$
(3.5)

We will seek a solution of system (3.5) in the form

$$w = w_0 + \varepsilon w_1 + \dots, \quad \vartheta = \vartheta_0 + \varepsilon \vartheta_1 + \dots$$

so that

$$\tau_* \approx \tau_2 \varepsilon^2 + \tau_3 \varepsilon^3, \quad q_* \approx q_2 \varepsilon^2 + q_3 \varepsilon^3$$

In the Burnett approximation we need to take into account perturbations of the Navier–Stokes transfer coefficients. Here (see (1.4)-(1.6)), as in the well-known approach [8], we have

$$\eta B \approx \eta_0 \left[B_0 + (\eta B)_T \frac{\gamma - 1}{2(\gamma + 1)} \varepsilon \vartheta_0 \right], \quad (\eta B)_T = \frac{1}{\eta} \frac{\partial(\eta B)}{\partial T_*} \bigg|_{T_* = T_{*0}}$$
(3.6)
$$\eta_0 = \eta(T_0), \quad T_0 = \frac{C_2^2}{RC_1^2} T_{*0} = T^- \left[\frac{\gamma M}{\gamma + 1} \left(1 + \frac{1}{\gamma M^2} \right) \right]^2, \quad T_{*0} = \frac{\gamma}{(1 + \gamma)^2}$$

and similarly for $\eta \Lambda$. Here T^- is the gas temperature in front of the shock wave.

Taking relations (3.4) and (3.6) into account, we obtain (the prime denotes a derivative with respect to ξ)

$$\tau_2 = -\frac{2}{3} B_0 w'_0, \quad q_2 = -\frac{15}{4} \Lambda_0 \frac{\gamma - 1}{2(\gamma + 1)} \vartheta'_0 \tag{3.7}$$

Using relations (3.7), in the Navier-Stokes approximation from system (3.5) we obtain

$$\vartheta_0 = -w_0, \quad w_0^2 - 1 = bw_0', \quad b = \frac{4\gamma}{(\gamma+1)^2} \left[\frac{4}{3} B_0 + \frac{(\gamma-1)^2}{\gamma} \frac{15}{4} \Lambda_0 \right]$$
 (3.8)

and, consequently

$$w_0 = -\operatorname{th}\left(\xi/b\right) \tag{3.9}$$

Taking relations (1.4), (1.5), (3.2), (3.4), (3.6) and (3.8) into account we have

$$\tau_{3} = -\frac{2}{3} B_{0} w_{1}' + w_{0}'' \left[(\eta B)_{T} \frac{(\gamma - 1)b}{6(\gamma + 1)} + \frac{2}{3} \gamma Q_{20} - (\gamma - 1)Q_{30} \right]$$

$$q_{3} = -\frac{1}{2(\gamma + 1)} \left\{ \frac{15}{4} \Lambda_{0} (\gamma - 1)\vartheta_{1}' + \frac{1}{4} w_{0}'' \left[\frac{15}{4} (\eta \Lambda)_{T} \frac{(\gamma - 1)^{2}}{\gamma + 1} b + 7\gamma Q_{10} \right] \right\}$$
(3.10)

In the next approximation

$$\vartheta_1 = -w_1 + bdw'_0, \quad d = \frac{2}{b(\gamma+1)} \left[\frac{2}{3} \gamma B_0 - (\gamma-1) \frac{15}{4} \Lambda_0 \right]$$
 (3.11)

$$2w_0w_1 + \frac{8}{(\gamma+1)^2} \left[\gamma \tau_3 - (\gamma^2 - 1)q_3 + \frac{\gamma+1}{2}w_0\tau_2 \right] = 0$$
(3.12)

Using relations (3.7), (3.10) and (3.11) we reduce Eq. (3.12) to the form

$$w_1'b - 2w_0w_1 = \frac{G}{9(\gamma+1)^3}w_0''$$
(3.13)

Using expression (3.9) we will write the solution of Eq. (3.13) in the form

$$w_1 = FG \frac{\ln \operatorname{ch} X}{\operatorname{ch}^2 X}; \quad F = \frac{2}{9(\gamma + 1)^3 b^2}, \quad X = \frac{\xi}{b}$$
 (3.14)

and using relations (3.9), (3.11) and (3.14) we obtain

$$\vartheta_1 = -\frac{1}{\operatorname{ch}^2 X} (d + FG \ln \operatorname{ch} X)$$
(3.15)

In (3.13)-(3.15)

$$G = G_{1} + G_{2} + G_{3}$$

$$G_{1} = -8 \left\{ B_{0}^{2} [8\gamma - (\gamma - 1)^{3}] + (\gamma - 1)^{3} \left(\frac{45}{4}\Lambda_{0} - B_{0}\right)^{2} \right\}$$

$$G_{2} = 12\gamma(\gamma - 1)b \left[(\eta B)_{T} + \frac{45}{16\gamma}(\gamma - 1)^{2}(\eta \Lambda)_{T} \right]$$

$$G_{3} = 3\gamma(\gamma + 1) [16\gamma Q_{20} + 3(\gamma - 1)(7Q_{10} + 8Q_{30})]$$
(3.16)

The quantity G_1 is found by the approximate Navier-Stokes approximation with unperturbed values of the transfer coefficients, G_2 is determined by the contribution of the perturbations of these coefficients and G_3 is determined by the Burnett approximation.

Using solutions (3.8), (3.9) and (3.14)–(3.16), we obtain the asymmetry parameters of the profiles of the density Q_0 and the temperature Q_1 in the shock wave. By definition

$$\mathcal{Q}_{\rho} = \int_{-\infty}^{X_{\rho}} W_{\rho} dX \left[\int_{X_{\rho}}^{\infty} (1 - W_{\rho}) dX \right]^{-1}, \quad W_{\rho} = \frac{\rho(X) - \rho^{-1}}{\rho^{+} - \rho^{-1}}$$

where the centre of the density profile X_{ρ} is the root of the equation $W_{\rho}(X) = \frac{1}{2}$. Formulae for the asymmetry parameter Q_T are hence obtained by replacing ρ by T. As in the well-known approach [7] we obtain

$$X_{\rho} = \varepsilon \frac{\gamma + 1}{2\gamma} + O(\varepsilon^2), \quad X_T = \varepsilon d + O(\varepsilon^2)$$
(3.17)

after which we obtain

$$Q_{0} = Q_{T} = 1 - \varepsilon FG(1/\ln 2 - 1) + O(\varepsilon^{2})$$
(3.18)

The coefficients d, F and G are found from (3.11), (3.14) and (3.16).

Note that the formulae in [7], like (3.6), (3.13), (3.14), (3.16) and (3.17), need refinement.

To analyse G_1 , G_2 and G_3 we will consider the linear relationship between the transfer coefficients and the temperature, when $(\eta B)_T = B_0$ and $(\eta \Lambda)_T = \Lambda_0$. For actual intermolecular potentials these relations are less pronounced and G_2 will be even less.

Characteristic values of these quantities are given in Table 1, where

$$\Delta_G = \frac{G(\gamma, B_0, \Lambda_0, Q_{m0})}{G(\gamma, B_0, \Lambda_0, Q_{m0} = 1)}$$

represents the contribution to G of changes in the Burnett transfer coefficients due to rotations of the molecules (like Δ_{α} and Δ_{β} in Section 2).

The solution changes qualitatively if the Burnett terms are taken into account: in the Navier-Stokes approximation $G = G_1 + G_2 < 0$, but in the Burnett approximation $G = G_1 + G_2 = G_3 > 0$. This is of basic importance for the asymmetry parameters (3.18). Here the Burnett equations give the correct result, unlike the Navier-Stokes equations. Experimental and numerical investigations have shown that when M < 1.8 the parameter Q_{ρ} is less than unity. It follows from the Navier–Stokes equations that for any M we have $\hat{Q}_0 > 1$ [7, 9].

In this connection, it is of considerable importance to take into account the effect of rotations on the Burnett transfer coefficients. The denominator in the expression for Δ_G for small Z is positive, it passes through zero as Z increases and then becomes negative. This is explained by the "behaviour" of Δ_G in Table 2.

4. CONCLUSION

The effect of rotations of the molecules on the Burnett transfer coefficients is much greater than the effect on the Navier-Stokes transfer coefficients. It increases with temperature and is determined by the increase in the significance of the bulk viscosity. The part played by changes in the Burnett transfer coefficients, due to rotations of the molecules, in the problem of sound propagation increases when the Knudsen number and the temperature increase, and is much greater for the absorption coefficient than for the dispersion coefficient. The dependence of the Burnett transfer coefficients on the polyatomicity considerably changes the asymmetry parameters of the density and temperature profiles in a shock wave (if this relationship is not taken into account, the results will be qualitatively incorrect).

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