ROZPRAWY INŻYNIERSKIE • ENGINEERING TRANSACTIONS • 25, 2, 333—347, 1977
Polska Akademia Nauk • Instytut Podstawowych Problemów Techniki

SHOCK WAVE STRUCTURE IN A BINARY MIXTURE OF GASES WITH A ROTATIONAL DEGREE OF FREEDOM AND COMPARABLE MASSES

W. FISZDON AND T. PŁATKOWSKI (WARSZAWA)

Plane stationary shock waves in a binary mixture of gases are considered. The first component of the mixture is monoatomic and the second is diatomic with a rotational degree of freedom. To obtain hydrothermodynamic quantities, the modified BGK equations are solved using the Mott-Smith assumption. To close the set of equations, two moments of the BGK set of equations are taken. The hydrothermodynamic quantities are computed numerically and shock wave profiles are found for different mass and density ratios of the two components. To investigate the influence of the rotational degree of freedom, a similar procedure is performed for the case of a binary mixture of monoatomic gases. The dependence of the shock structure on mass and density ratios as well as the rotational degree of freedom effects are shown.

1. INTRODUCTION

Although shock wave structures in gas mixtures of monoatomic components have not as yet been fully explored, it seems to be of interest to investigate the influence of the rotational degree of freedom on the shock wave structure in mixtures of different gases. Most theoretical and experimental works concerning shock waves in binary gas mixtures dealt with mixtures of monoatomic gases [1—9]. There are several papers on shock wave structures in a single diatomic gas, e.g., [10—13].

The scarcity of data on collision cross sections between monoatomic and diatomic particles and the complexity of the Boltzmann equations for mixtures of gases led us to use the simpler model kinetic equations, which proved to be successful for the case of binary gas mixtures of monoatomic gases [4—8] and for one diatomic gas [10—13]. Our considerations will be restricted to the case of mixtures of gases with comparable molecular masses, for reasons which will be further shown.

2. STATEMENT OF THE PROBLEM

We consider plane satationary shock waves in a binary mixture of gases. The first component (1) of the mixture is monoatomic and the second (2) is diatomic with a rotational degree of freedom. Both gases are assumed to be perfect and chemically inert. We denote by m_1 and m_2, respectively, the molecular masses of the components. The mixture is at room temperature, i.e., vibrational degrees of freedom are frozen and neither dissociation nor ionisation occurs. In our case the classical approach will be used.

A shock wave is propagating in the x direction with a uniform velocity u_- through a mixture of two gases. The mixture is initially in a steady uniform state of mean velocity zero and temperature T_-. The number of densities of the component gases are n_1^- and n_2^-, respectively. The x axis is in the direction opposite to that of the propagation of the shock wave and an opposite velocity u_- is imposed on the system. In that frame of reference the shock wave is at rest.

Our aim is to determine the number densities, velocities and translational temperatures of each component as well as the rotational temperature of the diatomic component as a function of position in the shock wave.

We denote by $F_1(x, \bar{v})$ and $F_2(x, \bar{v}, e)$ the particle single distribution functions of the monoatomic and diatomic gases respectively, where: x is the coordinate in the direction of the shock propagation, $\bar{v}=(v_x, v_y, v_z)$ is the velocity vector of the particle, e is the rotational energy of the diatomic particle. We denote by m_1 and m_2 the molecular masses of the monoatomic and diatomic component.

To obtain the desired hydrothermodynamical quantities, the modified BGK equations will be used. The modified BGK equations for the distribution functions of components of a binary mixture are written as follows:

$$v_x \frac{\partial F_1}{\partial x} = \nu_{11}^t (M_{11} - F_1) + \nu_{12}(M_{12} - F_1),$$

$$v_x \frac{\partial F_2}{\partial x} = \nu_{22}^t (M_{22}^t - F_2) + \nu_{22}^r (M_{22}^r - F_2) + \nu_{21}(M_{21} - F_2),$$

where the Maxwellian distribution functions M_{11}, M_{12}, M_{22} and M_{21} are defined as follows:

$$M_{11}(x, \bar{v}) = N_1(x)\,[2\pi R_1 T_1(x)]^{-3/2} \exp\left[-\frac{(\bar{v} - \bar{U}_1(x))^2}{2R_1 T_1(x)}\right],$$

$$M_{12}(x, \bar{v}) = N_1(x)\,[2\pi R_1 \tilde{T}(x)]^{-3/2} \exp\left[-\frac{(\bar{v} - \bar{U}(x))^2}{2R_1 \tilde{T}(x)}\right],$$

and

$$M_{22}^t(x, \bar{v}, e) = N_2(x)\,[2\pi R_2 T_2(x)]^{-3/2} \exp\left[-\frac{(\bar{v} - \bar{U}_2(x))^2}{2R_2 T_2(x)}\right] \times$$
$$\times \exp\left[-\frac{e}{kT_R(x)}\right] \cdot \frac{1}{kT_R(x)},$$

$$M_{22}^r(x, \bar{v}, e) = N_2(x)\,[2\pi R_2 T_c(x)]^{-3/2} \exp\left[-\frac{(\bar{v} - \bar{U}_2(x))^2}{2R_2 T_c(x)}\right] \times$$
$$\times \exp\left[-\frac{e}{kT_c(x)}\right] \cdot \frac{1}{kT_c(x)},$$

$$M_{21}(x, \bar{v}, e) = N_2(x)\,[2\pi R_2 \tilde{T}(x)]^{-3/2} \exp\left[-\frac{(\bar{v} - \bar{U}(x))^2}{2R_2 \tilde{T}(x)}\right] \times$$
$$\times \exp\left[-\frac{e}{k\tilde{T}(x)}\right] \cdot \frac{1}{k\tilde{T}(x)}.$$

The gas constants R_1 and R_2 are the ratios of the Boltzmann constant k to the molecular mass m_1 and m_2, respectively. N_1 and N_2 are the number densities of the two species, U_1 and U_2 are the flow velocities, T_1 and T_2 are the translational temperatures, T_R is the rotational temperature of the diatomic component.

Using the equipartition assumption of translational and rotational degrees of freedom for diatomic particles, it follows that:

$$\frac{5}{2} kT_c = \frac{3}{2} T_2 + kT_R .$$

M_{12} and M_{21} can be considered as local Maxwellian reference states with unknown parameters $\tilde{U}$ and $\tilde{T}$. $\tilde{T}$ and $\tilde{U}$ are the same in the cross-collision terms M_{12} and M_{21}. This assumption is one of the important assumptions and limitations of the method used.

$\nu_{11}(x)$ and $\nu_{22}(x)$ are the frequencies for self-collisions, $\nu_{12}(x)$ and $\nu_{21}(x)$ are the frequencies for cross-collisions between the species 1 and 2. We assume that the collision frequencies are independent of molecular velocities.

The boundary conditions which have to be fulfilled can be written as follows:

$$\lim_{x \to -\infty} N_1(x) = n_1^- ,$$

$$\lim_{x \to -\infty} N_2(x) = n_2^- ,$$

$$\lim_{x \to -\infty} U_1(x) = \lim_{x \to -\infty} U_2(x) = u_- ,$$

and

$$\lim_{x \to -\infty} T_1(x) = \lim_{x \to -\infty} T_2(x) = \lim_{x \to -\infty} T_R(x) = T_- .$$

The total number of collisions between species 1 and 2 should be equal, i.e.

$$N_1 \nu_{12} = N_2 \nu_{21} .$$

Taking the $m_1 \vec{v}$ moment of the first BGK equation and the $m_2 \vec{v}$ moment of the second one and summing up, one obtains the relation

$$\nu_{11} \int (M_{11} - F_1) m_1 \vec{v} + \nu_{12} \int (M_{12} - F_1) m_1 \vec{v} + \nu_{22}^t \int (M_{22}^t - F_2) m_2 \vec{v} +$$
$$+ \nu_{22}^r \int (M_{22}^r - F_2) m_2 \vec{v} + \nu_{21} \int (M_{21} - F_2) m_2 \vec{v} = 0 ,$$

which states that the change of the total momentum is zero.

Using the relation $N_1 \nu_{12} = N_2 \nu_{21}$, the conservation of the total momentum yields the relation

$$\tilde{U}(x) = \frac{m_1 \bar{U}_1(x) + m_2 \bar{U}_2(x)}{m_1 + m_2} \quad (*) .$$

The relation (*) is the same as in Morse's paper [10], where it is required that the ratio of the momentum difference relaxation time to the temperature difference relaxation time should be the same as the one obtained from the full Boltzmann equation for Maxwell molecules.

The total energy conservation law (which is derived by taking the $m_1 v^2$ moment of the first BGK equation, $m_2 v^2+e$ moment of the second one and summing up, gives the relation between $\tilde{U}$, $\tilde{T}$, and other macroscopic quantities:

$$8k\tilde{T}=3k(T_1+T_2)+2kT_R+m_1 U_1^2+m_2 U_2^2-(m_1+m_2)\tilde{U}^2 .$$

For the self-collision frequencies we use the following expressions which can be computed using Maxwell distribution functions [17]:

$$\nu_{11}(x)=4N_1(x)\sigma_{11}^2\sqrt{\pi R_1 T_1(x)},$$

$$\nu_{22}\equiv\nu_{22}^t+\nu_{22}^r=4N_2(x)\sigma_{22}^2\sqrt{\pi R_2 T_2(x)},$$

where σ_{11}^2 and σ_{22}^2 are hard-sphere collision cross-sections between the particles 1-1 and 2-2, respectively. The ratio of translational to rotational collision frequencies is not well known in most cases and in order to obtain a quantitative indication of the influence of rotational degrees of freedom we will use the experimental value $\alpha=\nu_{22}^t/\nu_{22}^r=4.3$ corresponding to a rotational collision number $Z_R=5.3$ at temperature $T=300°\mathrm{K}$, as given in [15].

To determine the cross-collision frequencies ν_{12} and ν_{21} one additional equation (apart from the balance equation $N_1\nu_{12}=N_2\nu_{21}$) is needed. The following assumption is used:

$$\frac{\nu_{11}}{\nu_{12}}=\frac{N_1}{N_2}\frac{\sigma_{11}^2}{\sigma_{12}^2},$$

where σ_{12}^2 is the cross-section for cross-collisions and σ_{11}^2 is the cross-section for 1-1 self-collisions, obtained from hard-sphere approximation [16].

3. SOLUTION OF THE SET OF EQUATIONS

To solve the set of the two BGK equations, the Mott-Smith assumption for the gas distribution functions is used [14]:

$$F_1(x,\bar{v})=w_1(x)f_1^-(\bar{v})+w_2(x)f_1^+(\bar{v}),$$

$$F_2(x,\bar{v},e)=w_3(x)f_2^-(\bar{v},e)+w_4(x)f_2^+(\bar{v},e),$$

where $f_i^-(\bar{v})$ and $f_i^+(\bar{v})$ are the upstream (−) and downstream (+) Maxwell distribution functions for i species ($i=1,2$)

$$f_1^-(\bar{v})=(2\pi R_1 T_-)^{-3/2}\exp\left[-\frac{(\bar{v}-u_-)^2}{2R_1 T_-}\right],$$

$$f_1^+(\bar{v})=(2\pi R_1 T_+)^{-3/2}\exp\left[-\frac{(\bar{v}-u_+)^2}{2R_1 T_+}\right],$$

$$f_2^-(\bar{v},e)=(2\pi R_2 T_-)^{-3/2}\exp\left[-\frac{(\bar{v}-u_-)^2}{2R_2 T_-}\right]\exp\left[-\frac{e}{kT_-}\right]\cdot\frac{1}{kT_-},$$

$$f_2^+(\bar{v},e)=(2\pi R_2 T_+)^{-3/2}\exp\left[-\frac{(\bar{v}-u_+)^2}{2R_2 T_+}\right]\exp\left[-\frac{e}{kT_+}\right]\cdot\frac{1}{kT_+}.$$

$w_k(x)$ $(k=1, 2, 3, 4)$ are unknown functions of position in the shock wave, with suitable boundary conditions:

$$\lim_{x\to-\infty} w_1(x)=n_1^-, \quad \lim_{x\leftarrow-\infty} w_3(x)=n_2^-,$$

$$\lim_{x\to+\infty} w_1(x)=\lim_{x\to+\infty} w_3(x)=0.$$

The parameters T_+, u_+, n_1^+, and n_2^+ in downstream Maxwell steady state have to be determined from the Rankine-Hugoniot's type conditions for the mixture. To obtain Rankine-Hugoniot's type conditions, we write mass, total momentum and total energy conservation equations for the upstream and downstream steady equilibrium states; the resulting equations are then solved and yield the following relations:

$$n_2^+=s_1 n_2^-, \quad n_1^+=s_1 n_1^-,$$

$$u_+=\frac{1}{S_1}u_-, \quad T_+=S_2 T_-,$$

where

$$S_1^{-1}=\frac{\gamma-1}{\gamma+1}\left[\frac{2}{(\gamma-1)M^2}+1\right],$$

$$S_2=\frac{2\gamma(\gamma-1)}{(\gamma+1)^2}\left(M^2+\frac{2}{\gamma-1}\right)\left(M^2-\frac{\gamma-1}{2\gamma}\right)\frac{1}{M^2},$$

$$\gamma=\frac{7\kappa+5}{5\kappa+3},$$

$$\kappa=\frac{n_2^-}{n_1^-}$$

and the upstream Mach number is defined:

$$M^2=\frac{(m_1+\kappa m_2)u_-^2}{\gamma\cdot kT^-}.$$

To make all variables nondimensional we introduce the following notation:

$$\tilde{x}=\frac{x}{\lambda_-}, \quad \tilde{N}_1=\frac{N_1}{n_1^-}, \quad \tilde{N}_2=\frac{N_2}{n_2^-}, \quad \tilde{w}_1=\frac{w_1}{n_1^-}, \quad \tilde{w}_2=\frac{w_2}{n_1^-},$$

$$\tilde{w}_3=\frac{w_3}{n_2^-}, \quad \tilde{w}_4=\frac{w_4}{n_2^-}, \quad \tilde{T}_1=\frac{T_1}{T_-}, \quad \tilde{T}_2=\frac{T_2}{T_-}, \quad \tilde{T}_R=\frac{T_R}{T_-}, \quad \tilde{T}_c=\frac{T_c}{T_-},$$

$$\tilde{\tilde{T}}=\frac{\tilde{T}}{T^-}, \quad \tilde{U}_1=\frac{U_1}{u_-}, \quad \tilde{U}_2=\frac{U_2}{u_-}, \quad \tilde{\tilde{U}}=\frac{\tilde{U}}{u_-},$$

$$\tilde{\alpha}_1=\frac{\alpha_1}{kT_-}, \quad \tilde{\alpha}_2=\frac{\alpha_2}{kT_-}, \quad \tilde{A}_1=\frac{A_1}{kT_-}, \quad \tilde{A}_2=\frac{A_2}{kT_-}, \quad \tilde{B}_1=\frac{B_1}{kT_-}, \quad \tilde{B}_2=\frac{B_2}{kT_-},$$

$$C_1 = \frac{\gamma \cdot M^2 (1+\kappa)}{1+\kappa m}, \qquad C_2 = \frac{\gamma \cdot M^2 (1+\kappa)}{\frac{1}{m}+\kappa'}, \qquad m = \frac{m_2}{m_1},$$

$$\tilde{a}_1 = \frac{\nu_{22}^t}{\lambda_-}, \qquad \tilde{a}_2 = \frac{\nu_{22}^r}{\nu_-}, \qquad \tilde{a}_3 = \frac{\nu_{21}}{\lambda_-}, \qquad \tilde{a}_4 = \frac{\nu_{11}}{\lambda_-}, \qquad \tilde{a}_5 = \frac{\nu_{12}}{\lambda_-},$$

where

$$A_1 = 3kT_- + m_1 u_-^2,$$

$$A_2 = 3kT_+ + m_1 u_+^2,$$

$$\alpha_1 = A_1 - A_2,$$

$$\alpha_2 = kT_- - kT_+,$$

$$B_1 = kT_- + m_1 u_-^2,$$

$$B_2 = kT_+ + m_1 u_+^2.$$

The upstream mean free path for the mixture of hard spheres λ_- is defined as follows [6]:

$$(n_1^- + n_2^-)\lambda_- = \lambda_-^1 n_1^- + \lambda_-^2 n_2^-,$$

where

$$\lambda_-^1 = \pi^{-1}\{n_1^- \sigma_{11}^2 \sqrt{2} + n_2^- \sigma_{12}^2 \sqrt{1+m^{-1}}\}$$

and

$$\lambda_-^2 = \pi^{-1}\{n_2^- \sigma_{22}^2 \sqrt{2} + n_1^- \sigma_{21}^2 \sqrt{1+m}\}.$$

The mass conservation of each species in the shock wave gives us two relations between the $w_k(x)$ functions:

$$w_2(x) = [n_1^- - w_1(x)]\, S_1^-,$$

$$w_4(x) = [n_2^- - w_3(x)]\, S_1^-.$$

To close the set of equations two additional moments of the considered equations are arbitrarily chosen: we take the $m_1 v_x^2$ moment of the first equation and the e moment of the second one. We then obtain a set of two first-order ordinary differential equations for $w_1(x)$ and $w_3(x)$.

After introducing nondimensional variables the set of equations can be written as follows:
(we omit the tyldas for convenience):

$$\alpha_1 \frac{dw_1}{dx} = -(a_4+a_5)(B_1 w_1 + B_2 w_2) + a_4 N_1 (C_1 U_1^2 + T_1) + a_5 N_1 (C_1 \tilde{U}^2 + \tilde{T}),$$

$$\alpha_2 \frac{dw_3}{dx} = -(a_1+a_2+a_3)(w_3 + w_4 S_2) + a_1 N_2 T_R + a_2 N_2 T_c + a_3 N_2 \tilde{T}$$

with the boundary conditions

$$w_1(-\infty)=w_3(-\infty)=1\,,\qquad w_1(+\infty)=w_3(+\infty)=0\,.$$

This set of equations was solved numerically, using the fourth-order Runge-Kutta's procedure on the CDC-Cyber computer. The typical computation time for one set of initial data was about 1 minute.

Once the $w_1(x)$ and $w_3(x)$ functions are found, all required macroscopic quantities can be computed by taking adequate moments of the distribution functions which, in accordance to the Mott-Smith assumption, are linear combinations of the $w_k(x)$ functions. By definitions we have:

$$N_1(x)=\int_{-\infty}^{+\infty} d\bar{v}F_1(x,\bar{v})\,,$$

$$N_2(x)=\int_{-\infty}^{+\infty} d\bar{v}\int_0^{\infty} deF_2(x,\bar{v},e)\,,$$

$$N_1(x)\,U_1(x)=\int_{-\infty}^{\infty} d\bar{v}\bar{v}F_1(x,\bar{v})\,,$$

$$N_2(x)\,U_2(x)=\int_{-\infty}^{\infty} d\bar{v}\int_0^{\infty} de\,F_2(x,\bar{v},e)\,,$$

$$\frac{3}{2}N_1(x)kT_1(x)=\int_{-\infty}^{\infty} d\bar{v}\,\frac{m_1 v_c^2}{2}F_1(x,\bar{v})\qquad\text{where}\qquad \bar{v}_c=\bar{v}-\bar{U}_1\,,$$

$$\frac{3}{2}N_2(x)kT_2(x)=\int_{-\infty}^{\infty} d\bar{v}\int_0^{\infty} de\frac{m_1 v_c^2}{2}F_2(x,\bar{v},e)\quad\text{where}\quad \bar{v}_{cc}=\bar{v}-\bar{U}_2\,,$$

$$N_2(x)kT_R(x)=\int_{-\infty}^{\infty} d\bar{v}\int_0^{\infty} de\,e\,F_2(x,\bar{v},e)\,.$$

The results of numerical computations will be shown on diagrams.

4. BINARY MIXTURE OF MONOATOMIC GASES

The BGK set of equations for that case can be written as follows:

$$v_x\frac{\partial F_1}{\partial x}=\nu_{11}(-F_1+M_{11}^0)+\nu_{12}(-F_1+M_{11}^0),$$

$$v_x\frac{\partial F_2}{\partial x}=\nu_{22}(-F_2+M_{22}^0)+\nu_{21}(-F_2+M_{21}^0).$$

The notation is the same as in the previous case. The internal state variable does not come in now, and

$$M^0_{11}(x, \bar{v}) = N_1(x)\,[2\pi R_1 T_1(x)]^{-3/2} \exp\left[-\frac{m_1(\bar{v} - U_1(x))^2}{2R_1 T_1(x)}\right],$$

$$M^0_{12}(x, \bar{v}) = N_1(x)\,[2\pi R_1 \tilde{T}(x)]^{-3/2} \exp\left[-\frac{(\bar{v} - \tilde{U}(x))^2}{2R_1 \tilde{T}(x)}\right],$$

$$M^0_{22}(x, \bar{v}) = N_2(x)\,[2\pi R_2 T_2(x)]^{-3/2} \exp\left[-\frac{(\bar{v} - \bar{U}_2(x))^2}{2R_2 T_2(x)}\right],$$

$$M^0_{21}(x_1, \bar{v}) = N_2(x)\,[2\pi R_2 \tilde{T}(x)]^{-3/2} \exp\left[-\frac{(\bar{v} - \tilde{U}(x))^2}{2R_2 \tilde{T}(x)}\right].$$

For that mixture $\gamma = 53$ for both gases, and Rankin-Hugoniot's type conditions can be written as follows:

$$\frac{T_+}{T_-} \equiv S_2 = \frac{(M^2+3)(5M^2-1)}{16M^2}, \qquad \frac{u_-}{u_+} = S_1 = \frac{M^2+3}{4M^2}.$$

The total momentum conservation equation is the same as in the previously considered case. As shown in [16], the existence of the rotational degree of freedom doesn't influence the diffusion coefficient.

The total energy conservation law yields the equation

$$6k\tilde{T} = 3(kT_1 + kT_2) + m_1 U_1^2 + m_2 U_2^2 - (m_1 + m_2)\tilde{U}^2.$$

The Mott-Smith assumption results in:

$$F_1(x, \bar{v}) = f_1^-(\bar{v})\, w_1(x) + f_1^+(\bar{v})\, w_2(x),$$

$$F_2(x, \bar{v}) = f_2^{0-}(\bar{v})\, w_3(x) + f_2^{0+}(\bar{v})\, w_4(x),$$

where

$$f_2^{0-}(\bar{v}) = (2\pi R_2 T_-)^{-3/2} \exp\left[-\frac{(\bar{v} - \bar{u}_-)^2}{2R_2 T_-}\right],$$

$$f_2^{0+}(\bar{v}) = (2\pi R_2 T_+)^{-3/2} \exp\left[-\frac{(\bar{v} - \bar{u}_+)^2}{2R_2 T_+}\right].$$

The resulting set of equations was, after nondimensionalisation, solved numerically as in the previous case.

5. RESULTS

First, we focusses out attention on the separation of the gas mixture components in a shock wave. We found that when the difference between masses of components is too big, the method used didn't give any reasonable shock structure. This is probably due to the assumption that the cross-collision parameters $\tilde{U}$ and $\tilde{T}$ are the same in both cross-referrence Maxwellian functions M_{12} and M_{21}.

This assumption should correspond to an easy transfer of energy in cross collisions, which is not the case in disparate-mass cases.

We investigated cases of four density ratios $\kappa \equiv n_2^-/n_1^- = 10.0$, 2.0, 1.0, 0.1, and three different mass ratios $m = 1.5$, 0.72 and 0.22, which correspond to the mixtures of O_2/Ne, N_2/Ar and N_2/Xe, respectively. Some of the results will be reported below. All results are computed for the shock wave Mach number $M = 2.0$.

It was noted that the position of maximum separation in the shock wave (as well as the magnitude of separation) depends on the mass and density ratios of the components, as can be seen in Figs. 1 and 2.

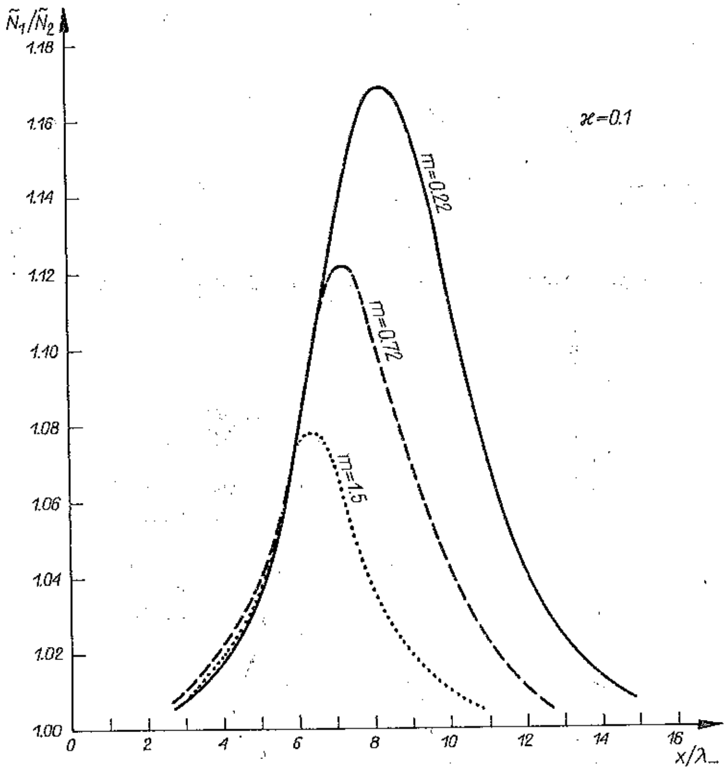

FIG. 1. Separation of gas mixture in shock wave for $\kappa = \frac{n_2}{n_1} = 0.1$("rotational" case), $m = \frac{m_2}{m_1}$.

Comparing the magnitude of separation obtained for a mixture having an internal degree of freedom with that for a mixture of monoatomic gases, it can be seen that the magnitude of the separation depends on the existence of a rotational degree of freedom. Fig. 3 shows this dependence for the case of density and mass ratios, $\kappa = 1.0$ and $m = 1.5$.

Figures 4, 5, 6, 7, 8 show density profiles for mixtures with and without a rotational degree of freedom. We see a broadening of the shock wave thickness measured, for example from the "maximum slope" definition for the mixture with rotation, when compared with the monoatomic gas mixture.

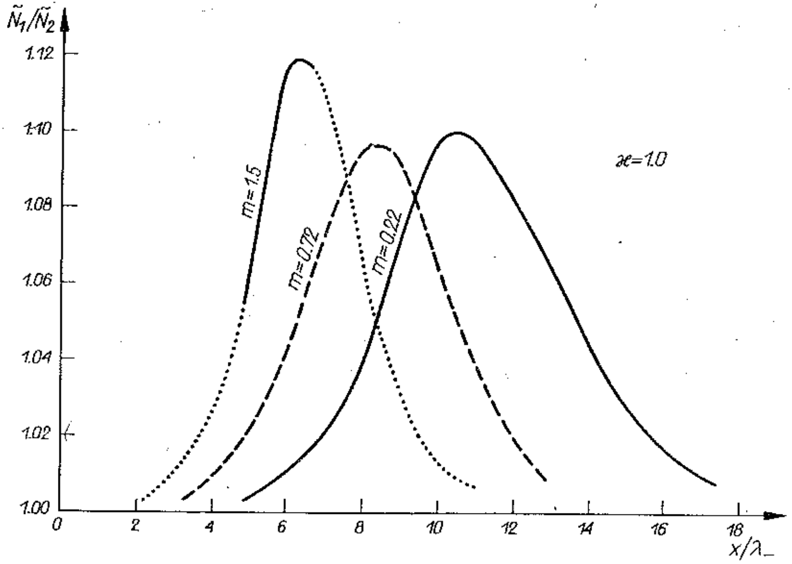

FIG. 2. Separation of gas mixture in shock wave for $\kappa=1.0$ ("rotational" case) $\kappa=\frac{n_2^-}{n_1^-}$, $m=\frac{m_2}{m_1}$.

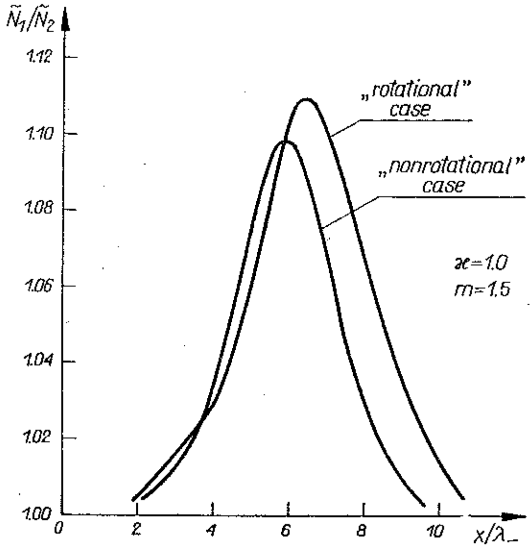

FIG. 3. Comparison of the separation of gas mixture for "rotational" and "nonrotational" case ($\kappa=1.0$, $m=1.5$).

The existence of a rotational degree of freedom is obviously responsible for the slow relaxation to downstream equilibrium conditions and, what follows, for an increase of the shock wave thickness. The increase of the shock thickness depends on the mass and density ratios, as can be easily seen from Figs. 5—8. The shock wave thickness increases when the density ratio $\kappa=n_2^-/n_1^-$ increases and when the mass ratio increases, i.e. when the diatomic gas is prevailing and is heavier.

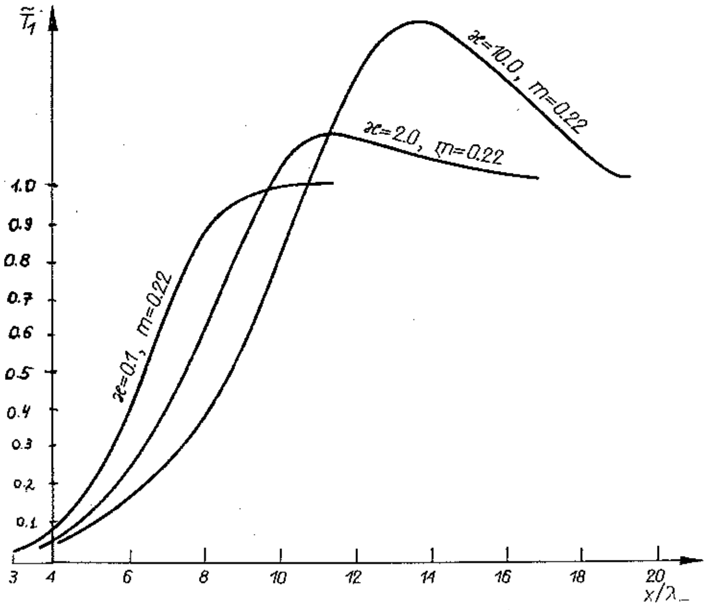

FIG. 4. Translational temperatures of monoatomic gas in mixture with diatomic gas ("rotational" case).

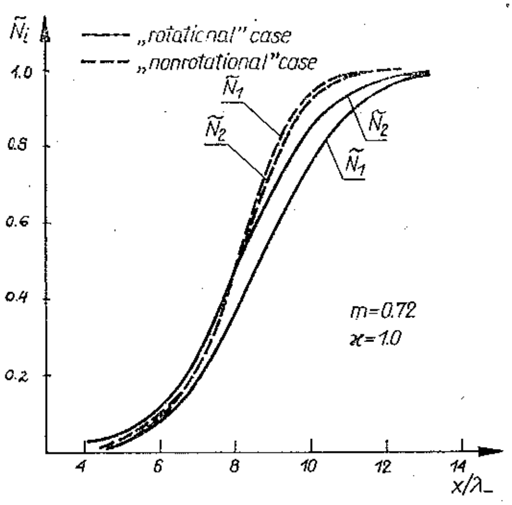

FIG. 5. Profile densities in shock wave.

As an example of calculations we choose $\kappa=10.0$ and $(m=m_2/m_1)$ $m=0.22$, i.e. the case where the diatomic gas is prevailing and the monoatomic gas is heavier. The resulting density and temperature profiles are presented in Figs. 9 and 10. For comparison we plotted on the same diagrams the case of a mixture of monoatomic gases (we shall call these two cases "nonrotational" and "rotational", respectively.

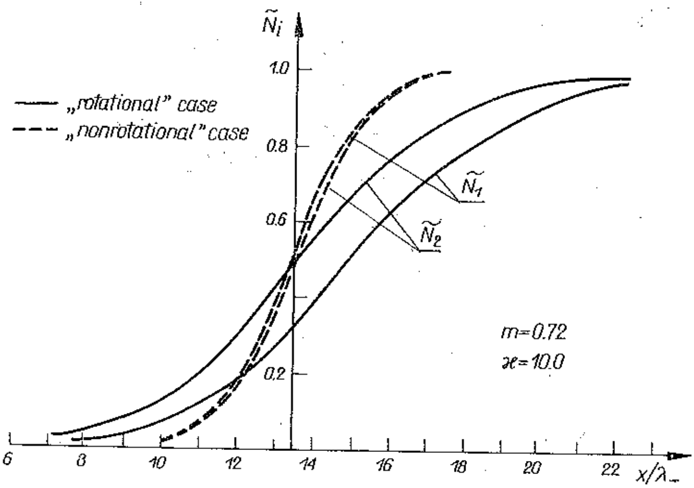

FIG. 6. Density profiles in shock wave.

It can be seen from the above figures that for the "nonrotational" case there is a retardation of the heavier monoatomic component in the shock wave, which is obvious from the physical point of view.

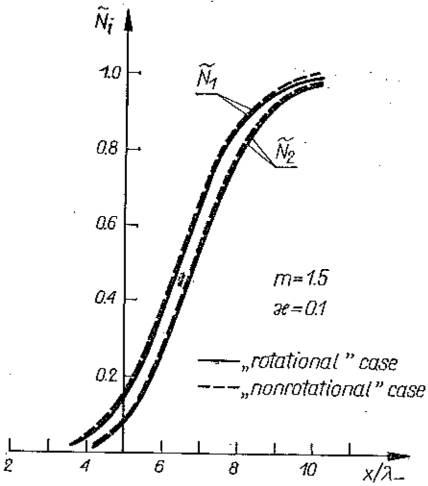

FIG. 7. Density profiles in shock wave.

The "rotational" case is quite different. For comparable molecular masses of gases, the diatomic component lags behind the monoatomic component. This may be due to the large proportion of the shock wave energy contained in the rotational degree of freedom. In the "nonrotational" case the whole shock wave energy increased the translational temperatures of the mixture.

For comparison we considered the case $m=1.5$ and $\kappa=10.0$ (see Fig. 8). In this case the "nonrotational" profiles show retardation of the heavier (m_2) component.

For the case of $\kappa=0.1$, i.e., when the monoatomic gas is prevailing, the difference between the shock profiles obtained for different investigated mass ratios is small. This corresponds to the negligible role of the rotational degree of freedom in these cases, independently of the mass ratios(*).

---

*) The negligible role of rotation in that case can also be clearly seen from a comparison between "rotational" and "nonrotational" cases. There is good agreement between the density profiles in the "rotational" and "nonrotational" cases.

Figure 4 shows translational temperatures of the monoatomic gas as functions of position in the shock wave for the "rotational" case. We note a translational temperatures overshoot of the heavier gas for $\kappa=10.0$ and $\kappa=2.0$. It decreases with the decrease of the density ratio. For $\kappa=0.1$, i.e., when the monoatomic gas is prevailing, there is no temperature overshoot, independently of the considered mass ratios.

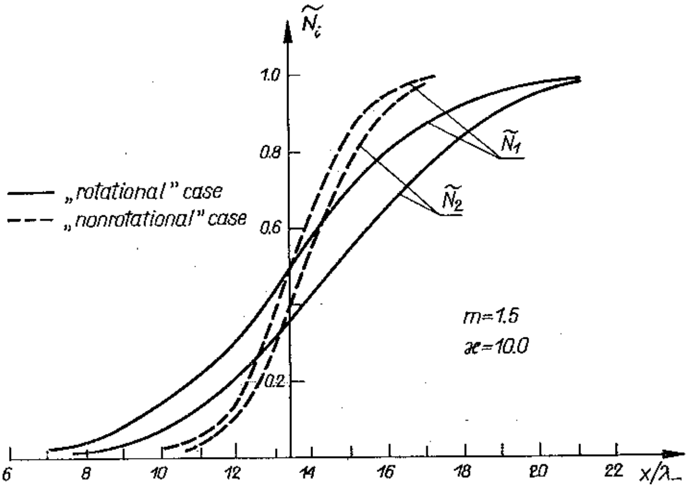

FIG. 8. Density profiles in shock wave.

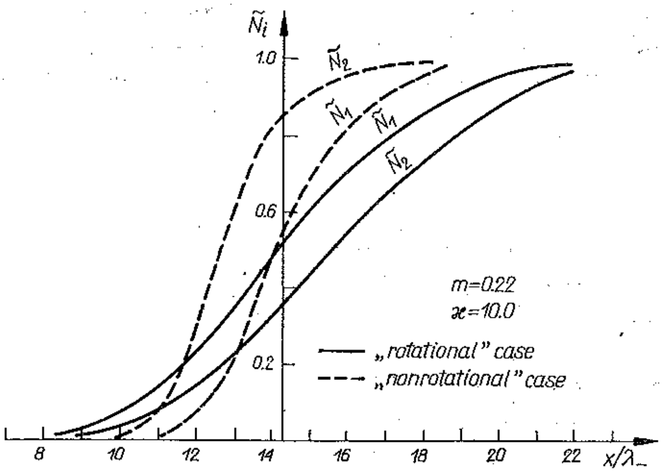

FIG. 9. Density profiles in shock wave.

The magnitude of temperature overshoot also depends on mass ratio. For $m=1.5$ and $m=0.72$ there is no temperature overshoot (for comparable number densities). This probably results from a quicker energy transfer in these cases, compared with the case of mass ratio $m=0.22$.

For the case of a monoatomic gas mixture there is no temperature overshoot $m=0.72$ and $m=1.5$ as it is expected for mixtures with comparable molecular masses of components.

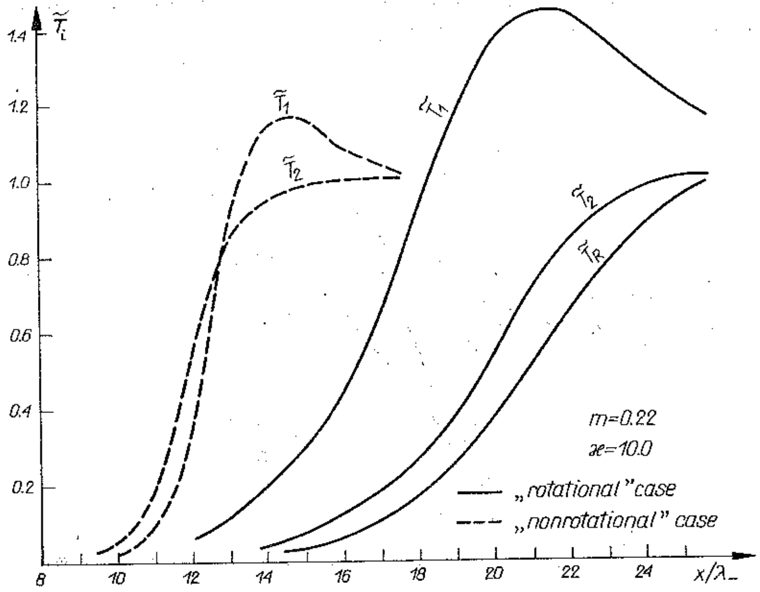

FIG. 10. Temperature profiles in shock wave.

Further investigations of this model are in progress. We are exploring the possibilities of introducing different "velocities" and "temperatures" in cross-collision Maxwellian functions which would hopefully allow to investigate the strongly disparate — mass cases.

REFERENCES

1. F. SHERMAN, J. Fluid Mech., **8**, 465, 1960.
2. L. SIROVICH, Phys. of Fluids, **8**, 908, 1962.
3. GOLDMAN, L. SIROVICH, J. Fluid Mech., **35**, 575, 1969.
4. OBERAI, Phys. of Fluids, **8**, 826, 1966.
5. WU, LEE, Phys. of Fluids, **14**, 313, 1970.
6. G. BIRD, J. Fluids Mech., **31**, 657, 1968.
7. ABE, OGUCHI, ISAS Report No. 511, **39**, 1974.
8. B. HAMEL, Phys. of Fluids, **8**, 418, 1965.
9. W. FISZDON, Z. WALENTA, HARASIMOWICZ, [to be published in Reports of IFTP, Polish Acad. of Sci.].
10. T. F. MORSE, Phys. of Fluids, **7**, 2020, 1964.
11. BRAU, JONKMAN, J. Chem. Phys., **52**, 477, 1970.
12. L. HOLWAY, Phys. of Fluids, **9**, 1958, 1966.
13. VENKATARAMAN, MORSE, 6 RGD, 477, 1968.

14. Mott-Smith, Phys. Rev., **82**, 885, 1951.
15. Lordi, Mates Phys. of Fluids, **13**, 291, 1970.
16. Chapman, Cowling, The mathematical theory of non-uniform gases, Cambridge Univ. Press, 1970.
17. Hirschfelder, Curtiss, Bird, Molecular theory of gases and liquids, Wiley, New York 1954.

Streszczenie

STRUKTURA FALI UDERZENIOWEJ W DWUSKŁADNIKOWEJ MIESZANINIE GAZÓW POSIADAJĄCYCH OBROTOWE STOPNIE SWOBODY I PORÓWNYWALNE MASY

Rozważane są płaskie stacjonarne fale uderzeniowe w dwuskładnikowej mieszaninie gazów. Jednym ze składników mieszaniny jest jednoatomowy gaz, drugi natomiast gaz dwuatomowy z obrotowymi stopniami swobody. W celu otrzymania wielkości hydrotermodynamicznych rozwiązane są zmodyfikowane równania BGK wykorzystując założenie Mott-Smith'a. Pełny układ równań otrzymuje się biorąc dwa momenty układu równań BGK. W wyniku obliczeń numerycznych znalezione zostały wielkości hydrotermodynamiczne oraz profile fal uderzeniowych dla różnych stosunków mas i gęstości składników. W podobny sposób określono wpływ obrotowych stopni swobody dla dwuskładnikowej mieszaniny jednoatomowych gazów. Pokazana jest zależność struktury fali uderzeniowej od stosunku mas i gęstości oraz od efektów wywołanych obrotowymi stopniami swobody.

Резюме

СТРУКТУРА УДАРНОЙ ВОЛНЫ В ДВУХКОМПОНЕНТНОЙ СМЕСИ ГАЗОВ ОБЛАДАЮЩИХ ВРАЩАТЕЛЬНЫМИ СТЕПЕНЯМИ СВОБОДЫ И СРАВНИТЕЛЬНЫМ МАССАМИ

Рассматриваются плоские стационарные ударные волны в двухкомпонентной смеси газов. Одним из компонентов смеси является одноатомный газ, вторым же двухатомный газ с вращательными степенями свободы. С целью получения гидротермодинамических величин решены модифицированные уравнения БГК, используя предположение Мотт-Смита. Полная система уравнений получается принимая два момента системы уравнений БГК. В результате численных расчетов найдены гидротермодинамические величины, а также профили ударной волны для разных отношений масс и плотностей компонентов. Аналогичным образом определено влияние вращательных степений свободы для двухкомпонентной смеси одноатомных газов. Показана зависимость структуры ударной волны от отношения масс и плотностей, а также от эффектов вызванных вращательными степенями свободы.

POLISH ACADEMY OF SCIENCES
NSTITUTE OF FUNDAMENTAL TECHNOLOGICAL RESEARCH

Received October 29, 1976.