CALCULATION OF THE SHOCK-WAVE ADIABATICS FOR SOME HETEROGENEOUS MIXTURES

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UDC 534.222.2

A method has been proposed [1] for calculating shock-wave adiabatics for two-phase mixtures which does not use the additivity principle, and this is here extended to a medium consisting of n phases; the shock-wave adiabatic is derived and compared with experiment for a three-phase mixture: an alloy consisting of copper, zinc, and lead (brass). It is shown for a paraffin–tungsten mixture that the adiabatics for the individual phases deviate from ones for the corresponding solid materials. The known equations of state for aluminum and epoxide resin have been used to determine the shock-wave adiabatic for such a mixture. A comparison is made with the analogous calculation made from the additivity principle.

1. Model. Shock waves in multiphase media are involved in research on the propagation of shock waves in rocks impregnated with water or oil [2, 3], in determining the equations of state for one of the phases [1, 4], and in studying the properties of new composite materials and alloys [5, 6]. In most recently published studies [4-7], the shock-wave adiabatic of the mixture has been derived via the additive approximation, in which it is assumed that each phase is compressed in accordance with its own Hugoniot adiabatic for the solid material. However, there is another viewpoint on shock waves in heterogeneous mixtures, which has been presented [1, 8] as that the shock-wave adiabatics of the phases may deviate from those for the pure materials, with the result that at certain phase concentrations one can get an anomalous slope in the Hugoniot adiabatics, as for porous materials [9].

Let the multiphase medium consist of particles differing in nature, the state of each of which is characterized by the pressure, the density, and the temperature; these parameters are related by the equation of state for the corresponding single phase. We assume that the multiphase medium is homogeneous and isotropic on a macroscopic scale. We consider the steady-state propagation of a planar shock wave in such a medium. We assume that the wave amplitude is not too great, so that in the equation of state we do not need to take into account the electronic components for the pressure and internal energy. On the other hand, we assume also that the wave is not so weak that the hydrostatic component of the force field applied to the mixture considerably exceeds the internal shear stresses. Then the medium may be considered as a compressible liquid, and its behavior in response to shock waves is described by the equations of hydrodynamics.

The equations of motion and energy for the mixture [3] are put as follows for an n-phase mixture if one assumes that the phase pressures are equal (a two-phase mixture was considered in [1]); for phase i we have the equation of motion

$$\rho_i \alpha_i \frac{d_i w_i}{dt} = -\alpha_i \frac{\partial p}{\partial x} + R_i \tag{1.1}$$

and the equation of continuity

$$\frac{\partial (\rho_i \alpha_i)}{\partial t} + \frac{\partial (\rho_i \alpha_i w_i)}{\partial x} = 0 \tag{1.2}$$

together with the energy balance equation

Moscow. Translated from Zhurnal Prikladnoi Mekhaniki i Tekhnicheskoi Fiziki, No. 4, pp. 130-137, July-August, 1973. Original article submitted January 16, 1973.

$$\frac{\partial}{\partial t}\left\{\rho_i\alpha_i\left(\varepsilon_i+\frac{w_i^2}{2}\right)\right\}+\frac{\partial}{\partial x}\left\{\rho_i\alpha_i\left(\varepsilon_i+\frac{w_i^2}{2}\right)w_i+\alpha_i p w_i\right\}+\frac{\delta W_i}{dt}+q_i=0$$

$$\frac{\delta W_i}{dt}=p\frac{\partial\alpha_i}{\partial t}+y_i,\qquad \frac{d_i}{dt}=\frac{\partial}{\partial t}+w_i\frac{\partial}{\partial x}$$

Here ρ_i is the density of phase i, whose concentration by volume is α_i, with $\sum_{i=1}^{n}\alpha_i=1$; w_i is velocity, p is pressure, and R_i is the bulk force from the interaction between phases, which acts on phase i from the other phases, with ε_i the specific internal energy of phase i, $\delta W_i/dt$ the effective work of the forces acting from all other phases on phase i in unit time, q_i the flux of heat into phase i from all the other phases, and y_i the work of the viscous bulk forces, which is converted to heat, as performed on phase i by the other phases and arising from relative displacement of the phases. There is a zero contribution overall to the momentum and energy of the whole mixture from the internal interaction between the phases:

$$\left(\sum_{i=1}^{n}R_i=0,\qquad \sum_{i=1}^{n}q_i=0,\qquad \sum_{i=1}^{n}\delta W_i/dt=0\right)$$

The shock-wave speed U is constant, so it is convenient in (1.1)-(1.3) to convert to the new variable $z = x - Ut$; we get the continuity integrals for the mass for each of the phases as

$$\alpha_i\rho_i u_i=d_{i0}\rho_{i0}u_{i0}=M_i\qquad(i=1,2,\ldots,n)\tag{1.4}$$

and the integrals for the conservation of the total momentum of the medium as

$$p+\sum_{i=1}^{n}M_i u_i=\sum_{i=1}^{n}M_i u_{i0}+p_0\tag{1.5}$$

and those for the overall total energy as

$$\sum_{i=1}^{n}\left\{M_i\left(\varepsilon_i+\frac{u_i^2}{2}\right)+\alpha_i u_i p\right\}=\sum_{i=1}^{n}\left\{M_i\left(\varepsilon_{i0}+\frac{u_{i0}^2}{2}\right)+\alpha_{i0}u_{i0}p_0\right\}\tag{1.6}$$

Here $u_i = w_i - U$ is the mass speed of the particles of phase i relative to the shock-wave front; subscript zero denotes quantities characterizing the state of the medium in front of the shock wave. The equations for momentum and energy balance for phase i become as follows in terms of the new variable:

$$\frac{d}{dz}(M_i w_i+\alpha_i p)-p\frac{d\alpha_i}{dz}=R_i\tag{1.7}$$

$$\frac{d}{dz}\left\{M_i\left(\varepsilon_i+\frac{w_i^2}{2}\right)+\alpha_i p w_i\right\}-Up\frac{d\alpha_i}{dz}+y_i+q_i=0\tag{1.8}$$

We multiply (1.7) by U and subtract from (1.8) to get

$$\frac{d}{dz}\left\{M_i\left(\varepsilon_i+\frac{w_i^2}{2}\right)+\alpha_i p(w_i-U)-M_i w_i U\right\}=-q_i-y_i-R_iU$$

We integrate this equation over the range $z_0 - h$, $z_0 + h$, which includes the shock-wave front, and then pass to the limit $h \to 0$, which gives us the following relationship on the assumption that the range 2h allows unlimited increase only in the derivatives, while the variables themselves w_i, ε_i, p, and the functions q_i, y_i, and R_i of these vary stepwise, but with restricted changes:

$$M_i(\varepsilon_i+u_i^2/2)+\alpha_i u_i p=M_i(\varepsilon_{i0}+u_{i0}^2/2)+\alpha_{i0}u_{i0}p_0\tag{1.9}$$

2. Mechanical Equilibrium Approximation. We write (1.4)-(1.6) and (1.9) for the case where mechanical equilibrium between the phases is attained behind the shock-wave front, i.e., we assume that immediately behind the step we have

$$u_1=u_2=\ldots=u_n=u$$

This relationship closes system (1.4)-(1.6) and (1.9).

If we define the mass phase concentrations x_i and the specific volumes v_i via

$$x_i = \alpha_i\rho_i / \sum_{i=1}^{n} \alpha_i\rho_i, \qquad v_i = 1 / \rho_i$$

then we get the specific volume for the heterogeneous multiphase mixture V as

$$V = 1 / \rho = 1 / \sum_{i=1}^{n} \alpha_i\rho_i = \sum_{i=1}^{n} x_i v_i \tag{2.1}$$

Then (1.4) and (1.5) with $u_{i0} = -U$ take the usual form for shock waves, but they apply subject to (2.1) and for mixtures:

$$u^2 / V + p = U^2 / V_0 + p_0, \qquad u / V = -U / V_0 \tag{2.2}$$

One frequently uses a different form for these equations:

$$U^2 = V_0{}^2 \frac{p - p_0}{V_0 - V}, \qquad u^2 = V^2 \frac{p - p_0}{V_0 - V} \tag{2.3}$$

Equation (1.6) gives the increment in the internal energy of the medium, and with (2.2) becomes

$$\sum_{i=1}^{n} x_i (\varepsilon_i - \varepsilon_{i0}) = {}^1/_2 (p + p_0)(V_0 - V) \tag{2.4}$$

which from (2.1) can also be put as

$$\sum_{i=1}^{n} x_i \{\varepsilon_i - \varepsilon_{i0} - {}^1/_2 (p + p_0)(v_{i0} - V)\} = 0 \tag{2.5}$$

Using (2.2), we can replace (1.9) by

$$\varepsilon_i - \varepsilon_{i0} = {}^1/_2 (p + p_0)(V_0 - V) + p(V - v_i) - p_0 (V_0 - v_{i0}) \tag{2.6}$$

Formulas (2.1)-(2.6) become the formulas of [1] for the two-phase medium.

The change in the internal energy of phase i on passage of the shock wave can be put as a sum of increments in the elastic energy ε_x and the thermal energy [9]:

$$\varepsilon_i - \varepsilon_{i0} = \varepsilon_x (v_i) + v_i (p - p_x (v_i)) / \gamma (v_i) \tag{2.7}$$

where $p_x(v_i)$ is the cold pressure on phase i, and $\gamma(v_i)$ is the Grüneisen parameter; we eliminate $\varepsilon_i - \varepsilon_{i0}$ from (2.6) and (2.7) to get the equation for the Hugoniot adiabatic in the form

$$p = \frac{(h - 1)\, p_x (v_i) - 2\varepsilon_x (v_i) / v_i}{h + 1 - (V + V_0) / v_i} \tag{2.8}$$

where $h = 1 + 2/\gamma(v_i)$, while p_0 has been omitted, because $p_0 \ll p$.

If $V = v_i$ and $v_0 = v_0$, (2.8) becomes the adiabatic equation for solid phase i, which has been given [9]:

$$p = \frac{(h - 1)\, p_x (v_i) - 2\varepsilon_x (v_i) / v_i}{h - v_{i0} / v_i} \tag{2.9}$$

If we formally extend (2.8) to high-amplitude shock waves, we get the condition for the limiting compression of the multiphase medium: $(V_0 + v)/V_i < h + 1$.

If the pressure and specific volume of the mixture are known, (2.8) allows one to find the specific volume of phase i and hence to construct the shock-wave adiabatic for this phase.

Similarly, one handles the inverse problem of constructing the shock-wave adiabatic for the mixture from the known equations of space for the phase shift; for this purpose we draw up a system of n+ 1 algebraic equations in the form

$$V = \sum_{i=1}^{n} x_i v_i, \quad p = p(V, v_i) \quad (i = 1, 2, \ldots, n) \tag{2.10}$$

where $p(V, v_i)$ is the right side of (2.8); this system becomes closed if the pressure is given, and we can solve it for the specific volume and thus construct the shock-wave adiabatic for the mixture.

3. Working Approximations. In the calculations given below for heterogeneous mixtures, we use the equations of state for the following substances: copper, zinc, lead, tungsten, aluminum, and epoxide resin. We use the following form [10] for the elastic components of the pressure for the metals except for aluminum:

$$\begin{aligned} &p_x(v_i) = p_H - \gamma(v_i)(\varepsilon_H - \varepsilon_x(v_i))/v_i \\ &p_H = a^2 (v_{i0} - v_i) / [v_{i0} - b(v_{i0} - v_i)]^2, \qquad \varepsilon_H = {}^1/_2 p_H (v_{i0} - v_i) \end{aligned} \tag{3.1}$$

where a and b are coefficients determined by the linear relationship between the shock-wave speed in solid phase i on the mass velocity ($U = a + bw$); the numerical values for these coefficients are given in Table 1. We use the following form [16] for the elastic pressures of aluminum and epoxide resin:

$$p_x(v_i) = C\mu_i + D\mu_i^2 + S\mu_i^3 \quad (\mu_i = v_{i0}/v_i - 1) \tag{3.2}$$

where Table 2 gives the values of C, D, and S; the specific energy of cold compression was calculated for all substances from

$$\varepsilon_x(v_i) = -\int_{v_{i0}}^{v_i} p_x(v)\,dv \tag{3.3}$$

The function $\gamma(v_i)$ was considered as proportional to v_i, i.e.,

$$\gamma(v_i) = \gamma_0 v_i / v_{i0} \tag{3.4}$$

where γ_0 is the Grüneisen coefficient under normal conditions, which is given in Tables 1 and 2; approximations (3.1), (3.3), and (3.4) have been used [10] in calculating the shock-wave curves for porous aluminum.

We evaluated the accuracy of (3.1)-(3.4) and of the constants in them by comparing the calculated adiabatics for metals given by (2.9) with the measurements of [11], and also with the adiabatics calculated by a more complex method [12].

The two calculations and the experimental figures were in close agreement for all the metals; as we have no published experimental data for the shock-wave adiabatic of epoxide resin, no such check was pos-

TABLE 1

Material	ρ_0, g/cm^3	a km/sec	b	γ_0	Ref.
Cu	8.90	3.958	1.497	2.00	[11]
Zn	7.14	3.050	1.559	2.45	[11]
Pb	11.34	2.028	1.517	2.77	[11]
W	19.35	4.000	1.285	1.54	[7,11]

TABLE 2

Material	C, Mbar	D, Mbar	S, Mbar	γ_0	ρ_0, g/cm^3
Al	0.761888	0.778860	1.19871	2.13	2.785
epoxide resin	0.098842	0.059183	0.16653	0.79	1.190

sible for this substance.

4. Shock-Wave Adiabatic of a Three-Phase Mixture. We used the above method to determine this adiabatic for a mixture of three phases, for which purpose we took brass, which consists of copper, zinc, and lead with weight proportions of the components respectively 61.5, 36, and 2.5% [13]. We wrote system (2.10) for n=3 and substituted for $p_x(v_i)$, $\varepsilon_x(v_i)$, and $\gamma(v_i)$ from (3.1), (3.3), and (3.4) to get a system of algebraic nonlinear equations for the unknown v_i and V; this system was solved by computer using a gradient method. As our initial approximation we took the values of the v_i corresponding to normal conditions. The computation was terminated when the differences of the v_i in two successive iterations were less than 0.0001 cm³/g.

Figure 1 shows the calculated shock-wave adiabatic for brass (full line) together with the measurements of [13], which agree well; brass has a partly ordered CuZn structure, so at zero pressure the observed density of 8.41 g/cm³ is greater than the 8.22 given by the mixtures rule [13]. A simple displacement of the predicted Hugoniot curve to the point for the observed initial density results in improved agreement with experiment for all densities.

5. Two-Phase Mixtures. We show for the paraffin–tungsten mixture how to use the experimental shock-wave adiabatic [7] and the known equation of state for one of the phases to find the shock-wave adiabatics for these phases. For this purpose it is sufficient to find the specific volume of one of the phases from (2.8), since that for the other phase is defined by (2.1). In our calculations we used previously checked parameters for tungsten.

Table 3 and Figs. 2 and 3 show the calculated curves for tungsten (curve 2) and paraffin (curve 4), together with the experimental data of [7] (point 1) for a paraffin–tungsten mixture containing respectively 66.2% ($x_1=0.662$) and 84% ($x_1=0.84$) tungsten by weight (curve 3). It is clear from these figures that the shock-wave adiabatics for the tungsten and paraffin phases deviate from those for the pure materials (curves 1 and 5 respectively for tungsten and paraffin). The experimental points 2 in Figs. 2 and 3 were taken from [11]. The heavy phase (tungsten) expands in a mixture with a light one, as in the case of porous metals [9], which leads to an anomalous slope in the curve. This behavior in shock waves may be explained if we consider the mixture as a porous material, for instance, of the heavy phase with pores filled by the light phase. Although the mixture is overall compressed behind the shock wave, the heavy phase may enter into the pores, and there may therefore be an effective expansion of this phase, with additional compression of the light one.

It has been shown for shock waves in paraffin–tungsten mixtures [7] that one can use an additive approximation with the known Hugoniot adiabatics of tungsten and the mixture to determine the adiabatic for paraffin. From this it was concluded [7] that mixture shock-wave adiabatics satisfy the additivity principle. Our calculation shows that the measured adiabatic for the mixture can be represented as a sum of displaced adiabatics for the individual phases.

We can compare the calculations of the mixture by our method with those from the additive approximation [4, 7], the latter for the binary mixture being

$$V(p) = x_1 v_1(p) + x_2 v_2(p)$$
$$\varepsilon_1 = {}^1/_2 p\,(v_{10} - v_1), \qquad \varepsilon_2 = {}^1/_2 p\,(v_{20} - v_2)$$

To close a system one has to add the equations of state for the individual phases; as an example we calculated the shock-wave adiabatic for a mixture consisting of aluminum and epoxide resin [16]. There is no reliable evidence on the equation of state for paraffin, so one cannot perform an analogous calculation for a paraffin–tungsten mixture. Table 4 gives the results from calculations via the schemes of [1] and [7], together with the experimental data of [16], and it is clear that both calculations agree closely with the experimental figures.

These calculations therefore do not enable one to judge definitively whether the additivity principle is correct [4, 7]; major difficulties have been encountered [14] in applying this principle to detonation in a mixture of explosive with tungsten. When one transfers to porous materials (one of the phases consists of gas or cavities), one is certain that the additivity principle does not apply, whereas essentially this principle is used to derive semiempirical equations of state for condensed media away from the Hugoniot adiabatic for solid materials.

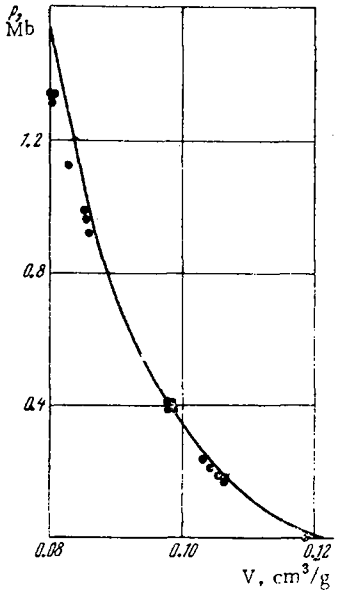

Fig. 1

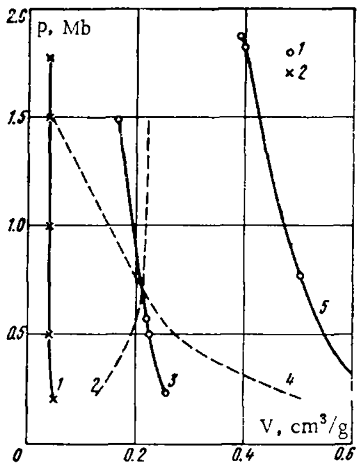

Fig. 2

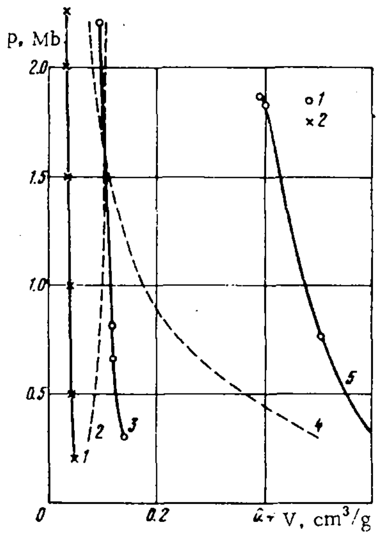

Fig. 3

TABLE 3

x_1	V, cm³/g	p, Mbar	V_W, cm³/g	V_n, cm³/g	$\varepsilon \cdot 10^{-10}$, erg/g	$\varepsilon_W \cdot 10^{-10}$, erg/g	$\varepsilon_n \cdot 10^{-10}$, erg/g
0.662	0.252	0.231	0.129	0.494	1.826	4.680	−3.762
	0.221	0.500	0.195	0.272	4.728	6.025	2.187
	0.217	0.574	0.204	0.243	5.543	6.306	4.049
	0.165	1.495	0.224	0.049	18.327	9.486	35.643
0.840	0.140	0.310	0.072	0.495	1.265	3.368	−9.77
	0.119	0.656	0.089	0.276	3.365	5.334	−6.97
	0.115	0.816	0.094	0.223	4.349	6.041	−4.53
	0.090	2.200	0.106	0.007	14.481	11.007	32.71

TABLE 4

Vol. of Al, %	p, Mbar	Experiment			Additive calcu.	Calc. from [1]			
		w, km/sec	U, km/sec	V, cm³/g	V, cm³/g	V, cm³/g	$\varepsilon \cdot 10^{-10}$, erg/g	$\varepsilon_{Al} \cdot 10^{-10}$, erg/g	$\varepsilon_p \cdot 10^{-10}$, erg/g
25	0.242	2.28	6.63	0.41	0.407	0.406	2.70	0.048	4.82
40	0.281	2.21	6.97	0.374	0.367	0.368	2.52	0.415	5.81
60	0.328	2.23	7.25	0.330	0.330	0.328	2.32	0.965	7.07

Calculation from (2.6) results in negative increments in the specific internal energy of the light phase ε_n at certain pressures in the case of a paraffin–tungsten mixture (Table 3); this was considered [7] as a paradoxical result, since in calculations for other mixtures the increment was always positive (Table 4). This distribution of the internal energy between the phases may arise because the conditions for mechanical equilibrium and a thermally metastable state may not be met simultaneously behind the shock wave in the measurements, or else it may arise from the inadequacy of the linear approximation for the relation between the mass velocity and the shock-wave speed [15].

I am indebted to V. N. Nikolaevskii for suggesting the topics and for useful discussion.

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