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Rankine–Hugoniot relations for shocks in heterogeneous mixtures

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The conservation of mass, momentum and energy are not sufficient to close a system of jump relations for shocks propagating in a heterogeneous mixture of compressible fluids. We propose here a closed set of relations corresponding to a two-stage structure of shock fronts. At the first stage, microkinetic energy due to the relative motion of mixture components is produced at the shock front. At the second stage, this microkinetic energy disappears inducing strong variations in the thermodynamical states that reach mechanical equilibrium. The microkinetic energy produced at the shock front is estimated by using an idea developed earlier for turbulent shocks in compressible fluids. The relaxation zone between the shocked state and the equilibrium state is integrated over a thermodynamic path a justification of which is provided. Comparisons with experiments on shock propagation in a mixture of condensed materials confirm the proposed theory.

1. Introduction

Knowledge of the qualitative and quantitative characteristics of shock waves propagating in heterogeneous mixtures of compressible fluids is important in many applications. The governing equations for such mixtures are hyperbolic but not in divergence form (Bedford & Drumheller 1978; Baer & Nunziato 1986; Bdzil *et al.* 1999; Kapila *et al.* 2001; Saurel & Le Metayer 2001; Gavrilyuk & Saurel 2002; Saurel, Gavrilyuk & Renaud 2003). These models can also be used for the study of high-amplitude shocks in mixtures of condensed materials since in such extreme conditions the stress tensor in solids is approximately spherical.

It is well known that shocks in realistic heterogeneous materials should be considered as fronts and not as singular interfaces where the basic flow parameters are discontinuous. By Rankine–Hugoniot relations for such shock fronts we mean algebraic relations between equilibrium states behind and ahead of the front. Formally, these relations can be implicitly obtained by studying the structure of the relaxation zone in a complete model involving pressure, velocity and temperature disequilibrium (see, for example, Fedorov & Fedorova 1992; Kapila *et al.* 1997). Such a study needs precise knowledge of the mechanical and thermal relaxation process, which

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is often known only approximatively. For the numerical treatment of shock wave dynamics approximate Riemann solvers are usually used. To formulate such Riemann solvers, explicit jump relations are needed. As was stressed by Kapila *et al.* (1997), “equilibrium with respect to even one of the process renders the mathematical model simpler, because the corresponding relaxation zone can be treated as a surface of discontinuity, across which the equilibrating quantity jumps”. In this article we will adopt this approach by assuming pressure equilibrium during the relaxation process. On the otherhand, we do not assume velocity and temperature equilibrium. This hypothesis agrees with relaxation time estimates given by Kapila *et al.* (2001). They showed that the temperature difference can be large because thermal relaxation occurs too slowly compared to mechanical relaxation. The last conclusion was also mentioned in Krueger & Vreeland (1991).

It is often assumed that components have not only equal pressures but also equal particle velocities. Even under such simplified hypotheses, the conservation of the mass, the momentum and the energy are not sufficient to close the system of jump relations. A phenomenological approach was proposed by Dremin & Karpukhin (1960), McQueen *et al.* (1970), and Alekseev, Al’tshuler & Krupnikova (1971). It is based on the use of the Hugoniots of each component under pressure and velocity equilibrium. This approach has been intensively validated (see, for example, Trunin 2001). Saurel *et al.* (2007) revisited this approach and linked it to the single pressure-and-velocity model of Kapila *et al.* (2001). They also justified this method for weak shocks by analysing the dispersive character of shocks in two-phase mixtures.

However, even for mixtures with approximately equal volume concentrations where the friction between components is extremely important, the hypothesis of equal particle velocities of components is far from evident. In a series of experimental and numerical works Nesterenko (2001) introduced the notion of ‘microkinetic energy’ appearing during the shock wave loading of powders. This microkinetic energy appears in a shock front, and is the exact analogue of the turbulent energy characterizing the deviation of the velocity field from the average velocity. The microkinetic energy is manifested, for example, through the formation of microjets in the vicinity of contact interfaces. The amount of this microkinetic energy depends on the amplitude of the shock wave. When the amplitude increases, this energy increases too. The microkinetic energy decreases very rapidly in the relaxation zone where it is transformed into the internal energy or plastic deformations (Bdzil *et al.* 1999). This microkinetic energy is hardly measurable in experiments but is very important to the overall material behaviour, e.g. bonding between particles in powder mixtures or the initiation of chemical reactions under shock loading (Nesterenko 2001). This is why its theoretical estimation is necessary. Using a two-dimensional computer code for mesoscale computations, a quantitative estimation of the microkinetic energy appearing under impulse loading of granular materials was obtained by Benson *et al.* (1997). Recent results on the three-dimensional measurements and simulations of shock wave propagation in granular media have been reported by Baer & Trott (2002) and Bardenhagen *et al.* (2002). The results presented in Baer & Trott (2002) confirm the presence of highly fluctuating mechanical and thermodynamical fields during the shock wave propagation. The probability distribution function data reported by these authors could provide information about the distribution of the microkinetic energy in the shock front.

The aim of this article is to determine jump conditions that account for microkinetic effects in heterogeneous mixtures. At the first stage, both components are compressed in such a way that the microkinetic energy due to the relative motion of components

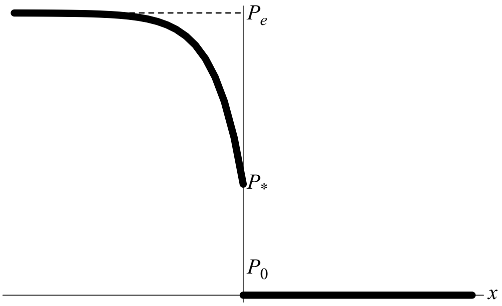

FIGURE 1. Qualitative pressure behaviour in a shock wave is shown. The initial state characterized by the pressure P_0 jumps to a state denoted by an asterisk, and then relaxes to a new equilibrium state. The microkinetic energy due to the relative motion of components appears at the asterisk state. This energy disappears in the relaxation zone.

appears at the shock front. The second stage is a stiff relaxation to the equilibrium state where this energy is zero (see figure 1). There are two unknowns in this mechanism:

(i) the amount of the microkinetic energy (we will sometimes call it 'turbulent energy') appearing in the shock front,

(ii) the distribution of the thermodynamic energy between components during the relaxation process.

We will propose a quantitative estimation of the microkinetic energy based on an idea developed earlier by Gavrilyuk & Saurel (2006) for compressible turbulent flows: the production of 'turbulent entropy', clearly linked with the 'turbulent energy', was maximal at the shock front. Then, the relaxation zone between the shocked state and the equilibrium state is integrated over a thermodynamic path a justification of which is provided. A comparison with experimental data shows the validity of this approach.

2. Reduced model

The reduced equations for the mixture mass, momentum and energy obtained by summing the phase equations of the two-phase flow model by Baer & Nunziato (1986) are

$$\frac{\partial \rho}{\partial t}+\frac{\partial}{\partial x}(\rho u)=0, \tag{2.1a}$$

$$\frac{\partial}{\partial t}(\rho u)+\frac{\partial}{\partial x}(p+\rho u^2+2k)=0, \tag{2.1b}$$

$$\frac{\partial}{\partial t}\left(\rho\varepsilon+\frac{\rho u^2}{2}+k\right)+\frac{\partial}{\partial x}\left(u\left(\rho\varepsilon+\frac{\rho u^2}{2}+3k+p\right)\right.$$
$$\left.+(\rho y_1 y_2(h_1-h_2)+k(y_2-y_1))(u_1-u_2)\right)=0. \tag{2.1c}$$

Here $\rho=\alpha_1\rho_1+\alpha_2\rho_2$ is the mixture density, ρ_i are the phase densities; $u=y_1u_1+y_2u_2$ is the mixture velocity, u_i are the phase velocities, $y_i=\alpha_i\rho_i/\rho$ are the mass fractions of each phase; $p=\alpha_1p_1+\alpha_2p_2$ is the mixture pressure, p_i are the phase pressures which are given functions of the densities ρ_i and the specific entropies η_i; $\varepsilon=y_1\varepsilon_1+y_2\varepsilon_2$ is the specific internal energy of the mixture, ε_i is the phase internal energy which is assumed to be a given function of the specific volume $v_i = 1/\rho_i$ and the pressure p_i; $k = \alpha_1\rho_1\alpha_2\rho_2\left(u_2 - u_1\right)^2/\rho$ is the microkinetic energy due to the relative motion of components, h_i are the phase enthalpies. It is assumed that the Gibbs identity for each phase is valid:

$$\theta_i \mathrm{d}\eta_i = \mathrm{d}\varepsilon_i + p_i \mathrm{d}v_i, \quad i = 1, 2, \tag{2.2}$$

where θ_i are the temperatures of the pure components.

A formal averaging of system (2.1), in which the odd moments of $w = u_2 - u_1$ are assumed to be zero, gives equations reminiscent of the equations of turbulent compressible flows (we will use the same notation for the averaged variables):

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho u) = 0, \tag{2.3a}$$

$$\frac{\partial}{\partial t}(\rho u) + \frac{\partial}{\partial x}(p + \rho u^2 + 2k) = 0, \tag{2.3b}$$

$$\frac{\partial}{\partial t}\left(\rho\varepsilon + \frac{\rho u^2}{2} + k\right) + \frac{\partial}{\partial x}\left(u\left(\rho e + \frac{\rho u^2}{2} + 3k + p\right)\right) = 0. \tag{2.3c}$$

We add two evolution equations to complete system (2.3). The first is the conservation of the mass fraction along the trajectories related to the average mixture velocity, and the second is the conservation of the ‘turbulent entropy’ $\varkappa = k/\rho^3$ along the trajectories:

$$\frac{\partial y_2}{\partial t} + u\frac{\partial y_2}{\partial x} = 0, \quad \frac{\partial}{\partial t}\left(\frac{k}{\rho^3}\right) + u\frac{\partial}{\partial x}\left(\frac{k}{\rho^3}\right) = 0. \tag{2.4}$$

The equation for the turbulent entropy $\varkappa = k/\rho^3$ is a consequence of the energy equation, the pressure equilibrium condition ($p_1 = p_2 = p$), and the condition that the flow is isentropic:

$$\frac{\mathrm{d}\eta_i}{\mathrm{d}t} = 0, \quad i = 1, 2. \tag{2.5}$$

3. Non-equilibrium multi-dimensional model

We present here a multi-dimensional analogue of system (2.3)–(2.5), and introduce relaxation terms compatible with the second law of thermodynamics. The governing equations are:

$$\frac{\partial \rho}{\partial t} + \nabla\cdot(\rho\boldsymbol{u}) = 0, \quad \frac{\partial(y_i\rho)}{\partial t} + \nabla\cdot(y_i\rho\boldsymbol{u}) = 0, \quad i = 1, 2, \tag{3.1a,b}$$

$$\frac{\partial \rho\boldsymbol{u}}{\partial t} + \nabla\cdot(\rho\boldsymbol{u}\otimes\boldsymbol{u} + P\boldsymbol{I}) = 0, \tag{3.1c}$$

$$P = p + (\Gamma - 1)k, \quad p = p_1(\rho_1, \eta_1) = p_2(\rho_2, \eta_2), \quad k = \varkappa\rho^{\Gamma}, \tag{3.1d–f}$$

$$\frac{\partial}{\partial t}\left(\rho\varepsilon + \frac{\rho\left|\boldsymbol{u}\right|^2}{2} + k\right) + \nabla\cdot\left(\boldsymbol{u}\left(\rho\varepsilon + \frac{\rho\left|\boldsymbol{u}\right|^2}{2} + k + P\right)\right) = 0, \tag{3.1g}$$

$$\frac{\mathrm{d}\varkappa}{\mathrm{d}t} = \dot{\varkappa}, \quad \frac{\mathrm{d}\eta_i}{\mathrm{d}t} = \dot{\eta}_i, \quad i = 1, 2, \quad \frac{\mathrm{d}}{\mathrm{d}t} = \frac{\partial}{\partial t} + \boldsymbol{u}\cdot\nabla. \tag{3.1h–j}$$

Here $\varkappa = k/\rho^{\Gamma}$ is the ‘turbulent entropy’. The parameter Γ is the ‘turbulent’ polytropic exponent defined by the space geometry ($\Gamma = 5/3$, 2 or 3 depending whether the velocity fluctuations are three-dimensional, two-dimensional or one-dimensional, respectively). For example, for the mixture of solids in the one-dimensional case we usually take $\Gamma = 3$ (the relative velocity of components which is considered as a fluctuation is essentially one-dimensional). This is different from the turbulent motion of gas where one usually takes $\Gamma = 5/3$ (the fluctuation velocity components are isotropic). Finally, $\dot{\eta}_i$ and $\dot{\varkappa}$ are unknown production terms which will be determined later.

Equations (3.1) and the Gibbs identities (2.2) imply the entropy equation

$$\rho \sum_{i=1}^{2} \theta_i \frac{\mathrm{d}(y_i \eta_i)}{\mathrm{d}t} + \rho^{\Gamma} \frac{\mathrm{d}\varkappa}{\mathrm{d}t} = 0. \tag{3.2}$$

When one of the phases is absent, equations (3.1) are reduced to the classical dissipation-free turbulent k-model (Mohammadi & Pironneau 1994; Wilcox 1998). The two-velocity effects are incorporated into model (3.1) in the simplest manner.

System (3.1) is hyperbolic. The sound speed is

$$c_T^2 = c_W^2 + \Gamma(\Gamma - 1)\varkappa\rho^{\Gamma-1}, \qquad \frac{1}{\rho c_W^2} = \frac{\alpha_1}{\rho_1 c_1^2} + \frac{\alpha_2}{\rho_2 c_2^2},$$

where c_W is the Wood sound speed (Wood 1930), and c_i^2 are the sound speed of each component.

To study the evolution of physical parameters in the relaxation zone, we need to know the production terms $\dot{\varkappa}$ and $\dot{\eta}_i$, $i = 1, 2$. Note that $\varkappa$ does not have the same dimension and the behaviour as the classical thermodynamic entropy. It increases immediately in a shock front, but, unlike the thermodynamic entropy, disappears in the relaxation zone by transforming to internal energies of components or irreversible deformations. The simplest expression for $\dot{\varkappa}$ in the relaxation zone is

$$\dot{\varkappa} = -\frac{\varkappa}{\tau_{rel}},$$

where τ_{rel} is a characteristic relaxation time. The entropy equation (3.2) will then become

$$\rho \sum_{i=1}^{2} \theta_i \frac{\mathrm{d}(y_i \eta_i)}{\mathrm{d}t} = \rho^{\Gamma} \frac{\varkappa}{\tau_{rel}} \geqslant 0.$$

Below, we will give physical arguments for the choice of the entropy production terms $\dot{\eta}_i$ based on the assumption that thermal exchanges between mixture components are negligible (Krueger & Vreeland 1991; Kapila *et al.* 2001).

4. Rankine–Hugoniot relations for the non-equilibrium model

Consider a stationary one-dimensional shock front (see figure 1) with zero turbulent entropy ahead of the front. The conservation of the mass, the momentum and the energy are

$$y_2 = y_{20}, \quad \rho(u - D) = \rho_0(u_0 - D) = -\rho_0 D = m = \text{const}, \tag{4.1a,b}$$

$$P - P_0 + m^2(v - v_0) = 0, \quad P = p + (\Gamma - 1)\varkappa\rho^{\Gamma}, \tag{4.1c,d}$$

$$p = p_1 = p_2, \quad p_i = p_i\left(\frac{y_i\rho}{\alpha_i}, \eta_i\right), \quad i = 1, 2, \tag{4.1e,f}$$

$$\varepsilon + \varkappa\rho^{\Gamma-1} - \varepsilon_0 + \tfrac{1}{2}(P + P_0)(v - v_0) = 0. \tag{4.1g}$$

Here D is the front velocity, and subscript 0 denotes the initial state. For each $\varkappa \geqslant 0$ consider *the turbulent Hugoniot surface* $H_\varkappa(v, \alpha_2, P; v_0, \alpha_{20}, P_0, y_{20}) = 0$ *of centre* $(v_0, \alpha_{20}, P_0, y_{20})$ where

$$H_\varkappa(v, \alpha_2, P; v_0, \alpha_{20}, P_0, y_{20}) = E(v, \alpha_2, P, \varkappa) - E(v_0, \alpha_{20}, P_0, 0) + \tfrac{1}{2}(P + P_0)(v - v_0),$$

$$E(v, \alpha_2, P, \varkappa) = y_1 \varepsilon_1 \left(\frac{\alpha_1 v}{y_1}, P - (\Gamma - 1)\varkappa v^{-\Gamma} \right) + y_2 \varepsilon_2 \left(\frac{\alpha_2 v}{y_2}, P - (\Gamma - 1)\varkappa v^{-\Gamma} \right) + \varkappa v^{-(\Gamma-1)}$$

and *the turbulent Rayleigh plane* $M(v, P; v_0, P_0) = 0$ where

$$M(v, P; v_0, P_0) = P - P_0 + m^2(v - v_0).$$

The initial and final equilibrium states corresponding to $\varkappa = 0$ belong to the curve which is the intersection of the Hugoniot surface $H_0 = 0$ and the Rayleigh plane $M = 0$ in the space (v, α_2, P). The intermediate state * belongs to the intersection of $H_{\varkappa_*} = 0$ and $M = 0$ where $\varkappa_*$ should be determined somehow.

Let us suppose that

$$\left. \frac{\partial E}{\partial \varkappa} \right|_{v, \alpha_2, P} < 0. \tag{4.2}$$

In the case of a single component we have called this inequality the condition of ‘exothermic turbulence’ (Gavrilyuk & Saurel 2006) by analogy with detonation theory (Fickett & Davis 1979). For a mixture of materials where each phase is governed by the stiffened gas equation of state

$$\varepsilon_i(v_i, p_i) = \frac{(p_i + \gamma_i p_{\infty,i})\, v_i}{\gamma_i - 1}, \quad \gamma_i = \text{const} > 1, \quad p_{\infty,i} = \text{const} > 0 \tag{4.3}$$

condition (4.2) is satisfied if

$$\gamma_i < \Gamma, \quad i = 1, 2. \tag{4.4}$$

For a given $\varkappa$, the Hugoniot surface in the space (P, v, α_2) is given by

$$\sum_{i=1}^{2} y_i \left(\varepsilon_i(v_i, P - (\Gamma - 1)\varkappa v^{-\Gamma}) + \varkappa v^{-\Gamma} v_i - \varepsilon_{i0} + \tfrac{1}{2}(P + P_0)(v_i - v_{i0}) \right) = 0. \tag{4.5}$$

4.1. *Remarks about closure relations for the equilibrium model*

When the two-velocity effects are ignored ($\varkappa = 0$), Dremin & Karpukhin (1960), McQueen *et al.* (1970), and Alekseev *et al.* (1971) proposed replacing the total energy equation by the energy equations for each component, i.e. to assume that each component follows its own Hugoniot. The equilibrium state, in the absence of microkinetic energy, is determined as a solution of the following system:

$$\varepsilon_i\,(v_i, p) - \varepsilon_i\,(v_{i0}, p_0) + \tfrac{1}{2}(p + p_0)(v_i - v_{i0}) = 0, \quad i = 1, 2, \tag{4.6a}$$

$$y_2 = y_{20}, \quad \rho(u - D) = \rho_0(u_0 - D) = -\rho_0 D = m = \text{const}, \tag{4.6b,c}$$

$$p - p_0 + m^2(v - v_0) = 0. \tag{4.6d}$$

Relations (4.6) imply conservation of the total energy. This method which is usually called the ‘additivity principle’ can easily be generalized to the case of many components. This approach has been intensively validated on more than 200 tests involving mixtures of materials with varying density ratio and acoustic impedance, weak and very strong shock waves (Trunin 2001). The same type of validation was done in Saurel *et al.* (2007) where a theoretical justification of this method for weak shocks was given. It was shown that if phase transitions or internal damage do not occur during shock loading, the additivity principle describes with a very good accuracy equilibrium mechanical characteristics of shocked components (pressure, particle velocity etc.).

4.2. *Additivity principle for the non-equilibrium model*

We propose the analogue of the additivity principle (4.6) for the closure of Rankine–Hugoniot relations when the microkinetic energy is present. The total energy equation (4.5) is satisfied, if we take the energy equation for each component in the form

$$\varepsilon_i(v_i, P-(\Gamma-1)\varkappa v^{-\Gamma}) + \varkappa v^{-\Gamma} v_i - \varepsilon_{i,0} + \tfrac{1}{2}(P+P_0)(v_i - v_{i0}) = 0, \quad i = 1, 2. \tag{4.7}$$

However, this does not solve the closure problem completely. Indeed, the value of the turbulent entropy $\varkappa$ generated in the shock front is unknown. For a given $\varkappa$, equations (4.7) allow us to obtain the total pressure P as a function of v and $\varkappa$:

$$P = P^H(v, \varkappa)$$

or the specific volume v as a function of P and $\varkappa$:

$$v = v^H(P, \varkappa).$$

As an example, consider the equation of state of stiffened gas (4.3). Equations (4.7) for shocks of high amplitude (p_0 is negligible with respect to P and $p_{\infty,i}$) are:

$$\frac{(P+\gamma_i p_{\infty,i})v_i}{\gamma_i - 1} - \frac{\gamma_i p_{\infty,i} v_{i0}}{\gamma_i - 1} + \tfrac{1}{2}P(v_i - v_{i0}) - \frac{\Gamma - \gamma_i}{\gamma_i - 1}\varkappa v^{-\Gamma} v_i = 0.$$

This allows to obtain $v = v^H(P, \varkappa)$ implicitly from the relation

$$v = \sum_{i=1}^{2} y_i v_i = \sum_{i=1}^{2} \frac{y_i v_{i0}\left(\dfrac{P}{2} + \dfrac{\gamma_i p_{\infty,i}}{\gamma_i - 1}\right)}{\dfrac{P(\gamma_i+1)}{2(\gamma_i-1)} + \dfrac{\gamma_i p_{\infty,i}}{\gamma_i - 1} - \dfrac{\Gamma-\gamma_i}{\gamma_i - 1}\varkappa v^{-\Gamma}}. \tag{4.8}$$

It can be found from (4.8) that

$$\left.\frac{\partial v^H}{\partial \varkappa}\right|_{P=const} > 0$$

if inequalities (4.4) are satisfied. Hence, the mixture Hugoniots for the stiffened gas equation of state form a monotonic family of curves in the plane (v, P) (see figure 2).

4.3. *Turbulent energy creation in a shock*

The first step is to determine the production of the turbulent entropy in the shock front. For this, we exploit the idea proposed in Gavrilyuk & Saurel (2006) for turbulent gas flows. If the family of Hugoniots is monotonic, there exists a critical value of the turbulent entropy $\varkappa_*$ such that the Rayleigh line is tangent to the critical Hugoniot curve. This tangent point is denoted CJ in figure 2. The condition of tangency is reminiscent of the Chapman–Jouget condition in detonation theory (Fickett & Davis 1979).

We will assume that the turbulent energy which is created in the shock front is equal to the turbulent energy corresponding to this maximal value of the turbulent entropy.

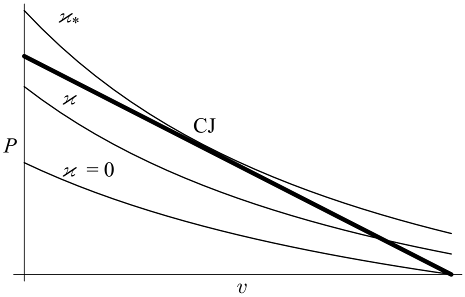

FIGURE 2. The family $P^H(v, \varkappa)$ is monotonic with respect to $\varkappa$. For the stiffened gas equation of state a sufficient condition of that is given by (4.4). This implies the existence of a point (denoted by CJ in the figure) where the turbulent Hugoniot curve is tangent to the Rayleigh line. The initial pressure p_0 is taken as zero.

Then the state behind the shock front is completely determined: when the turbulent entropy is equal to the critical value $\varkappa = \varkappa_*$, we can determine the specific volume v_*, the critical total pressure P_* and the volume concentration α_{2*} corresponding to the CJ point.

The equations determining the critical state are

$$P - P_0 + m^2(v^H(P, \varkappa) - v_0) = 0, \quad m^2 \frac{\mathrm{d}v^H(P, \varkappa)}{\mathrm{d}P} + 1 = 0, \tag{4.9}$$

where $v^H(P, \varkappa)$ is the mixture Hugoniot. For each $m^2 > \rho_0^2 c_{W0}^2$ system (4.9) determines a unique solution $(v_*, P_*, \varkappa_*)$. For example, for the mixture where each component can be described by the stiffened gas equation of state, the mixture Hugoniot is given by (4.8). The corresponding volume fractions and specific volumes of each component v_{i*} are determined by

$$\alpha_{i*} = \frac{y_i v_{i*}}{v_*}, \quad v_{i*} = \frac{v_{i0}\left(\dfrac{P_*}{2} + \dfrac{\gamma_i p_{\infty,i}}{\gamma_i - 1}\right)}{\dfrac{P_*(\gamma_i + 1)}{2(\gamma_i - 1)} + \dfrac{\gamma_i p_{\infty,i}}{\gamma_i - 1} - \dfrac{\Gamma - \gamma_i}{\gamma_i - 1} \varkappa v_*^{-\Gamma}}.$$

5. Relaxation process

Once the state denoted by an asterisk is determined, we need to find the final relaxed state in which the turbulent entropy is zero. In most mixtures of materials thermal relaxation occurs much more slower than pressure and velocity relaxation. We will formulate this assumption mathematically.

Let us introduce the entropy concentrations (Resnyansky & Bourne 2004):

$$\chi_i = \frac{y_i \eta_i}{\eta}, \quad i = 1, 2.$$

We will consider one of the entropy concentrations (for example, χ_2) and the mixture entropy η as new variables instead of the phase entropies η_i. We take the evolution equation for the entropy concentrations χ_i in the form

$$\frac{\mathrm{d}\chi_i}{\mathrm{d}t} = \dot{\chi}_i, \quad \dot{\chi}_1 = -\dot{\chi}_2. \tag{5.1}$$

Here $\dot{\chi}_i$ are unknown production terms to be determined. Equation (3.2) can be rewritten in terms of the entropy concentrations:

$$\left(\sum_{i=1}^{2} \chi_i \theta_i\right) \frac{\mathrm{d}\eta}{\mathrm{d}t} = -\eta \dot{\chi}_2 (\theta_2 - \theta_1) + \rho^{\Gamma-1} \frac{\varkappa}{\tau_{rel}},$$

where $\varkappa \geqslant 0$. To satisfy the entropy inequality, we need to assume that $\dot{\chi}_2$ is proportional to the difference of temperatures:

$$\dot{\chi}_2 = \lambda (\theta_1 - \theta_2), \quad \lambda > 0.$$

So, $\dot{\chi}_2$ characterizes the heat exchange between components. The entropy inequality will be

$$\left(\sum_{i=1}^{2} \chi_i \theta_i\right) \frac{\mathrm{d}\eta}{\mathrm{d}t} = \lambda \eta (\theta_2 - \theta_1)^2 + \rho^{\Gamma-1} \frac{\varkappa}{\tau_{rel}} \geqslant 0.$$

In most mixtures of materials, thermal equilibrium is reached much slower than mechanical equilibrium (Krueger & Vreeland 1991; Kapila *et al.* 2001). This means that heat exchange between components is negligible. Hence, a reasonable approximation in the relaxation zone is that $\dot{\chi}_2 = 0$, i.e. the entropy concentrations χ_i satisfy the equation

$$\frac{\partial \chi_i}{\partial t} + \boldsymbol{u} \cdot \nabla \chi_i = 0. \tag{5.2}$$

Equation (5.2) means that the entropy of each phase increases during the relaxation process is due only to the turbulence relaxation and is independent of the temperature difference. Finally, with the assumption $\dot{\chi}_i = 0$, $i = 1, 2$, in the stationary relaxation zone we have

$$\frac{y_i \eta_i}{\eta} = \chi_i = \chi_{i*} = \frac{y_i \eta_{i*}}{\eta_*}. \tag{5.3}$$

When the mixture entropy increases, the entropy of each phase increases according to

$$\eta_i = \frac{\chi_{i*}}{y_i} \eta.$$

Relation (5.3) is equivalent to

$$\frac{\eta_1}{\eta_2} = \frac{\eta_{1*}}{\eta_{2*}}. \tag{5.4}$$

To determine the equilibrium mixture parameters, it is now sufficient to use the conservation of the mass, the momentum and the energy in the turbulence-free state ($\varkappa = 0$), supplemented by (5.4). We remark that it is possible to rigorously prove the existence of shock fronts by using the mixture entropy as the Lyapunov function.

Condition (5.4) is well-defined at the final equilibrium state. In particular, the entropy of each phase can be calculated through the equations of state of individual components. On the other hand, it is difficult, even almost impossible, to distinguish the thermodynamic entropies from the turbulent entropy at the shocked state $*$. Indeed, this state is completely non-equilibrium, and the entropy ratio (5.4) should be calculated in terms of average characteristics of the state $*$. The equations of state of each phase at equilibrium state are

$$p_i + p_{\infty,i} = \exp\left(\frac{\eta_i}{c_i}\right) v_i^{-\gamma_i}, \quad i = 1, 2, \quad p_1 = p_2 = p.$$

	p_∞ (Pa)	γ	ρ_0 (kg/m^3)	α_0
Epoxy	5.3×10^9	2.43	1185	0.59
Spinel	141×10^9	1.62	3622	0.41

TABLE 1. Parameters of the expoxy and spinel components used in the experiments.

Here c_i are specific heats which are assumed to be constant. Hence,

$$\eta_i = c_i \ln\left((p + p_{\infty,i})v_i^{\gamma_i}\right).$$

We define the entropy ratio (5.4) of the non-equilibrium state through the total average pressure P_*:

$$\frac{\eta_{1*}}{\eta_{2*}} = \frac{c_1 \ln\left((P_* + p_{\infty,1})v_{1*}^{\gamma_1}\right)}{c_2 \ln\left((P_* + p_{\infty,2})v_{2*}^{\gamma_2}\right)}.$$

Relation (5.4) can be written as

$$\frac{\ln\left((p + p_{\infty,1})v_1^{\gamma_1}\right)}{\ln\left((p + p_{\infty,2})v_2^{\gamma_2}\right)} = a_* = \frac{\ln\left((P_* + p_{\infty,1})v_{1*}^{\gamma_1}\right)}{\ln\left((P_* + p_{\infty,2})v_{2*}^{\gamma_2}\right)}. \tag{5.5}$$

The parameter a_* does not vary significantly with the shock amplitude. Note that with this approach the relaxed state does not depend on the specific heats.

Relation (5.5) supplemented by the conservation of the mass, the momentum and the energy in the form

$$\rho(u - D) = -\rho_0 D = m = m_* = \rho_*(u_* - D), \quad p + m^2(v - v_0) = 0,$$

$$\sum_{i=1}^{2} y_i \left(\frac{(p + \gamma_i p_{\infty,i})v_i}{\gamma_i - 1} - \frac{\gamma_i p_{\infty,i} v_{i0}}{\gamma_i - 1} + \frac{1}{2}p(v_i - v_{i0})\right) = 0$$

determines the final relaxed state (p, v, α_2).

6. Comparison with experiments

We have chosen an epoxy–spinel mixture, experimentally studied in Marsh (1980) with the parameters of the components as given in table 1. The ratio Δ of the specific turbulent energy k/ρ to the specific mixture internal energy ε at state * is shown in figure 3 as a function of the dimensionless shock velocity D/c_{W0}. The Wood sound speed of the epoxy–spinel mixture at the initial state c_{W0} is 3120 m s^{-1}. The turbulent energy increases very slowly at the beginning and attains the level 0.3–0.4 for shock velocities of the order of 10^4 m s^{-1}. This is in agreement with the numerical experiments of Benson *et al.* (1997) where they recorded a similar level for shock loading of granular materials.

Figure 4 shows the dependence of the shock velocity D on the particle velocity u. The upper thin curve corresponds to the intermediate state * where the turbulent entropy $\varkappa$ is maximal, the lower bold line corresponds to the final equilibrium state, and the symbols correspond to the experiments (Marsh 1980). Assume that the front velocity D is prescribed. We see that the two-velocity effects are extremely important at the first stage of compression: the critical state is far from equilibrium. In the relaxation zone, the particle velocity increases because the turbulent energy is transformed into internal energy resulting in a thermodynamic pressure

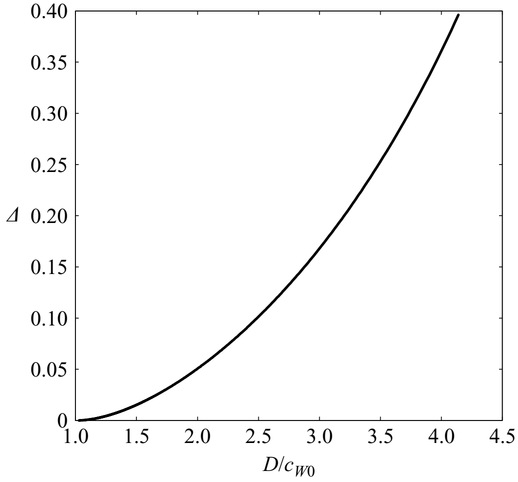

FIGURE 3. Ratio Δ of the specific turbulent energy k/ρ to the specific internal energy ε at point * is shown as a function of the dimensionless shock velocity D/c_{W0}. The Wood sound velocity of the epoxy–spinel mixture at the initial state c_{W0} is $3120\,\mathrm{m\,s^{-1}}$.

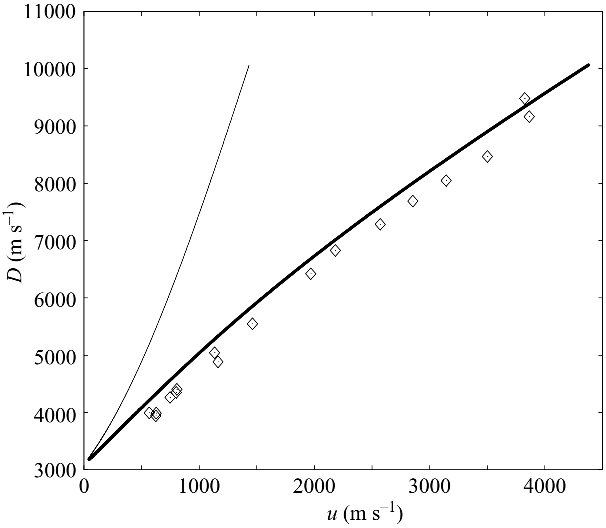

FIGURE 4. Dependence of the shock velocity D on the particle velocity u. The upper thin curve corresponds to the intermediate state * where the turbulent entropy is maximal, the lower bold line corresponds to the final equilibrium state. The symbols correspond to the experiments (Marsh 1980).

increase. The final equilibrium state is in excellent agreement with the experimental data.

We also compared two (D, u) diagrams. One corresponds to the final equilibrium state obtained by the two-stage mechanism proposed in this paper (bold line in figure 5), and the other one corresponds to the approach by Dremin & Karpukhin (1960), McQueen *et al.* (1970), and Alekseev *et al.* (1971) (the dashed line in figure 5). Both approaches agree well with the experimental data. The main difference between them is that the last approach is not able to capture an important 'virtual' parameter

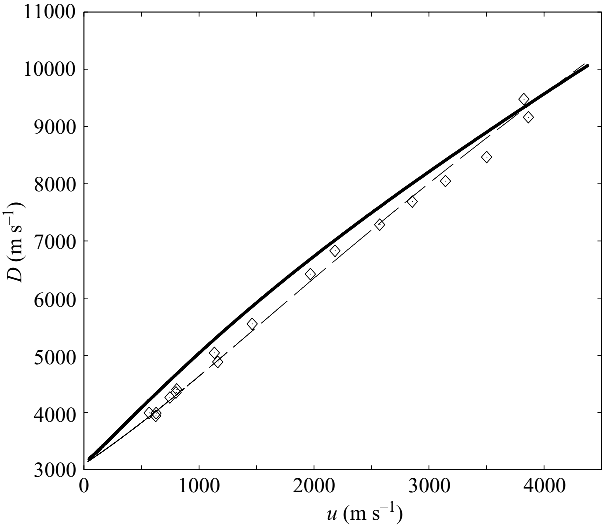

FIGURE 5. Dependence of the shock velocity D on the particle velocity u. The bold line corresponds to the final equilibrium state obtained through a two-step mechanism proposed here. The dashed line corresponds to the approach by Dremin & Karpukhin (1960) who used the Hugoniots of components. The symbols correspond to the experiments (Marsh 1980).

of the shock loading process – the mixture microkinetic energy. Accounting for the microkinetic energy results in an important difference in the partition of the energies between phases.

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