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THREE-DIMENSIONAL SHOCK-CHANGE RELATIONS FOR REACTIVE FLUIDS

by

R. L. Rabie and Jerry Wackerle

ABSTRACT

The equations of motion governing reactive fluid flow, together with the Rankine-Hugoniot jump conditions and thermodynamic considerations, are used to develop one- and three-dimensional shock-change relations for shock waves propagating in reactive fluids. The relations are derived in Cartesian space coordinates, assuming a uniform, motionless state ahead of the shock. In three dimensions, parameterization of the shock surface in terms of two independent curvilinear surface coordinates and the use of some results from the theory of surfaces are required, but the shock-change relation obtained depends on the surface configuration only through the mean curvature. One form of shock-change relation, both in three dimensions and in its one-dimensional specialization, is developed without recourse to the jump conditions. These conditions and thermodynamic considerations are then used to cast the relations in terms of different state variables and to show the relative effects on the shock change of reaction in, and immediately behind, the shock front. Simplifications are indicated for evaluating thermodynamic derivatives and applying shock-change relations with common equation-of-state assumptions.

I. INTRODUCTION

The shock-change relation in one or more dimensions provides a tool for analyzing a shock wave without having to examine the entire associated flow field. This simplification has obvious merit. Most work in the area of shock change has dealt with one-dimensional systems, and both inert and reactive systems have been treated.[1-9] Such one-dimensional shock-change relations have a large area of application but become inadequate when the shock surface is no longer planar, cylindrical, or spherical. For problems involving arbitrary shock-surface configurations in reactive fluids, one requires three-dimensional shock-change relations that include the geometry of the shock surface. Such relations have been obtained by other workers,[10-13] but much of their work is in coordinate systems and notation unfamiliar to many shock-wave researchers and does not provide full descriptions of the derivations. Here, we employ thermodynamics and notation that we consider more standard in the field, and obtain relations that are more readily comprehended by inspection.

In Sec. II we present a brief development of a one-dimensional shock-change relation to motivate the three-dimensional derivation that follows in Sec. III. The derivations in these two sections are done without recourse to the Hugoniot relations, and the equivalents of one- and three-dimensional relations are not reduced to expressions of the shock change in a single state variable. That is done in Sec. IV, where we present thermodynamic considerations that allow shock-change relations to be recast in terms of different thermodynamic variables and forms indicating the relative effects of reaction within and immediately behind the front. In Sec. V we describe the application of shock-change relations with simplifying assumptions and a commonly used equation-of-state representation.

II. ONE-DIMENSIONAL SHOCK-CHANGE RELATION FOR A REACTIVE FLUID

A familiarity with one-dimensional, reactive-flow, shock-change relations helps in two ways in the development of a three-dimensional relation: (1) the general course of the derivation is similar in both cases and (2) the resulting expressions have a term-by-term correspondence. Therefore, as an introduction to shock-change relations, we give a brief derivation of the one-dimensional case. The goal of a shock-change analysis is to find a set of relations giving the evolution of the shock state in terms of a minimum amount of information about the flow that immediately follows the shock and about the geometrical properties of the shock surface.

In a mixed form, the equations of conservation of mass and momentum for inviscid, nonconducting, reactive flow are

$$\dot{v} = v\,(\frac{\partial u}{\partial x}) + mv\,\frac{u}{x} \qquad (1)$$

and

$$\rho\dot{u} = -\left(\frac{\partial p}{\partial x}\right)_t \quad \text{or} \quad \dot{u} = -v\left(\frac{\partial p}{\partial x}\right)_t \quad . \tag{2}$$

In the above equations v is the specific volume (the reciprocal of the density ρ), u is the particle velocity, p is the pressure, and m is the coordinate system parameter, that is, m = 0, 1, 2 as the geometry is planar, cylindrical, or spherical. The coordinates are mixed in that the superposed dot represents the material or convective derivative, that is,

$$\dot{f} = \left(\frac{\partial f}{\partial t}\right)_x + u\left(\frac{\partial f}{\partial x}\right)_t \quad , \tag{3}$$

while the derivative $\partial/\partial x$ is an Eulerian derivative. The conservation of energy for an adiabatic system takes the form

$$\dot{e} = -p\dot{v} \quad , \tag{4}$$

and the reaction rate is

$$\dot{\lambda} = r(p,v,\lambda) \quad , \tag{5}$$

where e is the specific internal energy and λ is the reaction progress variable.

In addition, a complete equation of state must be obtained for the material, properly defining the energy and pressure

$$e = \hat{e}(s,v,\lambda)$$

and

$$p = \hat{p}(s,v,\lambda) \quad .$$

Further, the second relation must be invertible to give the specific entropy, s, so that the energy may be written

$$e = \hat{e}[s(\hat{p},v,\lambda),\, v,\lambda] = e(p,v,\lambda) \quad . \tag{6}$$

It is the second form of Eq. (6) that will be most useful throughout this report, with the more complete $\hat{e}$ and $\hat{p}$ specification needed only to insure thermodynamic consistency.

Denoting partial derivatives by subscripts, e.g., $\partial e/\partial v = e_v$, one obtains from Eqs. (4) and (6)

$$- p\dot{v} = e_p \dot{p} + e_v \dot{v} + e_\lambda \dot{\lambda}$$

or

$$\dot{p} + \frac{[e_v + p]}{e_p} \dot{v} = - \left(\frac{e_\lambda}{e_p}\right) \dot{\lambda} = \eta\dot{\lambda} \quad . \tag{7}$$

The factor $(e_v + p)/e_p$ can be evaluated from the above equation-of-state assumptions by observing that

$$e_v = \hat{e}_v - e_p\hat{p}_v$$

and that, from thermodynamics,

$$\hat{e}_v = - \hat{p} = - p$$

so that

$$\frac{[e_v + p]}{e_p} = - \hat{p}_v = \rho^2 \hat{p}_\rho = \rho^2 c^2 \quad , \tag{8}$$

where c is the frozen (λ = constant) Eulerian sound speed. We also note that the parameter η in Eq. (7) is related to the standard "thermicity" coefficient σ, by

$$\eta = \rho c^2 \sigma \tag{9}$$

so that an alternative statement of Eq. (7) is

$$\dot{p}/\rho c^2 + \dot{v}/v = \sigma\dot{\lambda} \quad . \tag{7'}$$

Equation (7) is often termed the master equation or Wood-Kirkwood relation.[14] It or its equivalent is derived in several of the cited references. Note that it applies without change in three dimensions.

The relations above hold throughout the flow, but we now wish to focus attention on the shock itself. We use no subscript for the state behind the shock and subscript 0 for the state ahead. The unshocked state is taken to be uniform and motionless. Thus $u_0 = 0$ and we have, for example,

$$\frac{\partial(p - p_0)}{\partial x} = \frac{\partial p}{\partial x} - \frac{\partial p_0}{\partial x} = \frac{\partial p}{\partial x} .$$

With these conditions, the time rate of change of any flow variable f evaluated along the shock locus is given by

$$\frac{\delta f}{\delta t} = \frac{\partial f}{\partial t} + \frac{dx}{dt}\bigg|_S \frac{\partial f}{\partial x} . \tag{10}$$

The quantity $\frac{dx}{dt}\Big|_S$ is the shock velocity U so that Eq. (10) is just

$$\frac{\delta f}{\delta t} = \frac{\partial f}{\partial t} + U \frac{\partial f}{\partial x} . \tag{11}$$

Using Eq. (3) one gets an alternate form for Eq. (11),

$$\frac{\delta f}{\delta t} = \dot{f} + (U - u) \left(\frac{\partial f}{\partial x}\right) . \tag{12}$$

The shock-change equation is readily derived by applying the kinematic relation, Eq. (12), to the pressure and particle velocity, and using mass and momentum conservation and the master equation to select and reduce the number of quantities that must be evaluated behind the shock. Defining the quantity

$$\mathcal{U} = (U - u)$$

one can write

$$\frac{\delta p}{\delta t} = \dot{p} + \mathcal{U}\left(\frac{\partial p}{\partial x}\right) \tag{13}$$

and

$$\frac{\delta u}{\delta t} = \dot{u} + \mathcal{U}\left(\frac{\partial u}{\partial x}\right) . \tag{14}$$

Eliminating $\dot{u}$ from Eq. (14) and using Eq. (2) gives

$$\frac{\delta u}{\delta t} = - v\left(\frac{\partial p}{\partial x}\right) + \mathcal{U}\left(\frac{\partial u}{\partial x}\right) .$$

The term $(\frac{\partial u}{\partial x})$ is eliminated from the above by using Eq. (1) to get

$$\frac{\delta u}{\delta t} = - v(\frac{\partial p}{\partial x}) + \mathcal{U}[\frac{\dot{v}}{v} - \frac{mu}{x}] \quad .$$

In the last expression, $(\frac{\partial p}{\partial x})$ is removed by using Eq. (13), and results in

$$\mathcal{U}\,\frac{\delta u}{\delta t} = - v[\frac{\partial p}{\partial t} - \dot{p}] + \mathcal{U}^2[\frac{\dot{v}}{v} - \frac{mu}{x}] \quad .$$

The master equation is now invoked to remove $\dot{v}$ and, after minor rearrangement, this manipulation gives

$$\frac{\delta p}{\delta t} + \rho\mathcal{U}\,\frac{\delta u}{\delta t} = (1 - \mu)\dot{p} + \mu\eta\dot{\lambda} - \rho\mathcal{U}^2(\frac{mu}{x}) \quad , \tag{15}$$

where

$$\mu = \frac{\mathcal{U}^2}{c^2}$$

is the square of the frozen (λ = constant) Mach number.

Equation (15) is the essential one-dimensional result, cast in terms of $\dot{p}$, $\dot{\lambda}$, and a term in the curvature of the shock surface, and includes shock-change terms in both the pressure and particle velocity. Reductions to relations for the shock change of a single variable will be deferred until the three-dimensional equation corresponding to Eq. (15) is derived.

III. A THREE-DIMENSIONAL SHOCK-CHANGE RELATION FOR A REACTIVE FLUID

As previously mentioned, the derivation of a three-dimensional shock-change relation produces some complications. The difficulties occur because in three dimensions the shock is a surface rather than a point as it is in a single dimension. In three dimensions, we specify the location of the surface in the usual manner[15,16] by the relations

$$x_i = x_i(\xi_1,\xi_2,t) \qquad i = 1,2,3 \quad , \tag{16}$$

where the x_i are the rectangular Cartesian coordinates of the surface and the ξ_α, $\alpha = 1,2$ are curvilinear coordinates along the surface. If n_i are the components of the unit vector $\vec{n}$ normal to S, the shock surface, pointing into the unshocked material and the derivatives $\frac{\partial x_i}{\partial \xi_\alpha}$ are tangent to the surface, the condition

$$n_i \frac{\partial x_i}{\partial \xi_\alpha} = 0 \qquad (17)$$

holds on S. (In Eq. (17) and for all further results a repeated index is summed over the range of the index according to Einstein's summation convention.) The components of the first and second fundamental forms of the surface are defined respectively, as[15,16]

$$g_{\alpha\beta} = \frac{\partial x_i}{\partial \xi_\alpha} \frac{\partial x_i}{\partial \xi_\beta} \qquad \alpha, \beta = 1,2 \qquad (18)$$

and

$$b_{\alpha\beta} = \frac{\partial^2 x_i}{\partial \xi_\alpha \partial \xi_\beta} n_i \qquad \alpha, \beta = 1,2 \ . \qquad (19)$$

Then the mean curvature of the surface is

$$\Omega = \frac{1}{2} g^{\alpha\beta} b_{\alpha\beta} \ , \qquad (20)$$

where the $g^{\alpha\beta}$ are the contravariant components constructed from the covariant components using the identity $g^{\alpha\nu} g_{\beta\nu} = \delta^\alpha_\beta$. It is possible to write Ω as a function of the principal radii of curvature of the surface as well, and this results in

$$\Omega = \frac{1}{2} \left(\frac{1}{R_1} + \frac{1}{R_2}\right) \ ,$$

where R_1 and R_2 are the principal radii of curvature of S at the point in question. In addition, one must make use of the Gauss-Weingarten relation[17]

$$\frac{\partial n_i}{\partial \xi_\alpha} = - g^{\beta\gamma} b_{\beta\alpha} \frac{\partial x_i}{\partial \xi_\gamma} \quad . \tag{21}$$

The shock velocity, or propagation velocity of the surface, is defined as normal to the shock surface, so that

$$\vec{U} = |\vec{U}|\vec{n} = U\vec{n} \tag{22}$$

where $U = |\vec{U}|$ is the normal component. As a result of the lack of motion and the homogeneity in the unshocked state, the particle velocity is normal to the shock surface (the tangential component of the particle velocity is conserved across the shock surface). Thus it follows that

$$\vec{u} = |\vec{u}|\vec{n} = u\vec{n} \quad . \tag{23}$$

With the shock-surface parameters set forth and the shock and particle velocities defined, one can generalize some of the definitions used in the one-dimensional case so that they will apply to the three-dimensional case. If

$$\vec{\mathcal{U}} = (\vec{U} - \vec{u}) = (U - u)\vec{n} = \mathcal{U}\vec{n} \quad , \tag{24}$$

the continuity and momentum relations become, respectively,

$$\dot{v} = v(\nabla\cdot\vec{u}) \tag{25}$$

and

$$\dot{\vec{u}} = -v \; \vec{\nabla} p \quad , \tag{26}$$

where the definition of the material time derivative is now

$$\dot{f} = (\frac{\partial f}{\partial t}) + \vec{u}\cdot\vec{\nabla} f \; . \tag{27}$$

The three-dimensional analog of the one-dimensional kinetic relation, Eq. (12), is

$$\frac{\delta f}{\delta t} = \dot{f} + \vec{\mathcal{U}}\cdot\vec{\nabla} f \quad . \tag{28}$$

This form follows from Eqs. (24) and (27) and the condition that the surface propagates normal to itself;[17] thus the components of the shock velocity are

$$U_i = \frac{dx_i}{dt} \qquad\qquad i = 1,2,3 \quad ,$$

and the change of a scaler function f on the propagating surface is just the directional derivative

$$\frac{\delta f}{\delta t} = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial x_i}\frac{dx_i}{dt} = \frac{\partial f}{\partial t} + \vec{U}\cdot\vec{\nabla} f \quad .$$

A similar result is found in Ref. 15, and termed the "kinematic compatibility condition."

After these preliminaries, the derivation of a three-dimensional shock-change relation follows in much the same manner as that of the one-dimensional case, except that the kinematic relation, Eq. (28), now operates on three components of the particle velocity. The resulting three equations can be written as the vector equation

$$\frac{\delta\vec{u}}{\delta t} = \dot{\vec{u}} + (\vec{\mathcal{U}}\cdot\nabla)\vec{u} \quad , \tag{29}$$

where $(\vec{\mathcal{U}}\cdot\nabla)$ is the operator $\mathcal{U}_j \frac{\partial}{\partial x_j} \equiv \mathcal{U}\, n_j \frac{\partial}{\partial x_j}$. Substitution from the momentum equation, Eq. (26), eliminates $\dot{\vec{u}}$

$$\frac{\delta\vec{u}}{\delta t} = -\, v\, \vec{\nabla} p + (\vec{\mathcal{U}}\cdot\nabla)\ \vec{u} \quad . \tag{30}$$

Taking the dot product of this equation with $\vec{\mathcal{U}}$ and using p for f in Eq. (28) allows the elimination of $\vec{\nabla} p$, producing

$$\vec{\mathcal{U}}\cdot\frac{\delta\vec{u}}{\delta t} = -\, v[\frac{\delta p}{\delta t} - \dot{p}] + \vec{\mathcal{U}}\cdot(\vec{\mathcal{U}}\cdot\nabla)\ \vec{u} \quad . \tag{31}$$

The last term in Eq. (31) is to be eliminated from the mass conservation relation, but that equation involves the $\nabla\cdot\vec{u}$ rather than the operation shown (a distinction that doesn't arise in the one-dimensional case). Relating $\vec{\mathcal{U}}\cdot(\vec{\mathcal{U}}\cdot\nabla)\vec{u}$ to $\mathcal{U}^2\nabla\cdot\vec{u}$ gives rise to a term proportional to the mean curvature of the surface. To see this, we form the function

$$F = \vec{\mathcal{U}}\cdot(\vec{\mathcal{U}}\cdot\nabla)\vec{u} - (\vec{\mathcal{U}}\cdot\vec{\mathcal{U}})\nabla\cdot\vec{u} = \mathcal{U}^2 \left[n_i n_j \frac{\partial (un_i)}{\partial x_j} - \frac{\partial (un_j)}{\partial x_j}\right] ,$$

where the replacement of u_i with un_i is allowed because $\vec{u}$ is perpendicular to S.

Further expansion gives

$$F = \mathcal{U}^2\left[n_j \frac{\partial u}{\partial x_j} + n_i n_j u \frac{\partial n_i}{\partial x_j} - n_j \frac{\partial u}{\partial x_j} - u \frac{\partial n_j}{\partial x_j}\right] = \mathcal{U}^2 \left[n_i n_j u \frac{\partial n_i}{\partial x_j} - u \frac{\partial n_j}{\partial x_j}\right] . \quad (32)$$

However, by Eq. (21)

$$\frac{\partial n_i}{\partial x_j} = \frac{\partial n_i}{\partial \xi_\alpha} \frac{\partial \xi_\alpha}{\partial x_j} = - \frac{\partial \xi_\alpha}{\partial x_j} g^{\beta\gamma} b_{\beta\alpha} \frac{\partial x_i}{\partial \xi_\gamma} ,$$

so that by Eq. (17)

$$u\, n_i n_j \frac{\partial n_i}{\partial x_j} = - n_i n_j u\, g^{\beta\gamma} b_{\beta\alpha} \frac{\partial x_i}{\partial \xi_\gamma} \frac{\partial \xi_\alpha}{\partial x_j} = 0 .$$

Also by Eqs. (20) and (21)

$$- u \frac{\partial n_j}{\partial x_j} = u\, g^{\beta\gamma} b_{\beta\alpha} \frac{\partial x_j}{\partial \xi_\gamma} \frac{\partial \xi_\alpha}{\partial x_j} = u\, g^{\beta\gamma} b_{\beta\alpha} \delta^\alpha_\gamma = 2\, u\Omega . \quad (33)$$

It follows from Eq. (33) that

$$\vec{\mathcal{U}}\cdot(\vec{\mathcal{U}}\cdot\nabla)\vec{u} = \mathcal{U}^2\nabla\cdot\vec{u} + 2\, \mathcal{U}^2 u\Omega .$$

From Eq. (25) it follows that

$$\vec{\mathcal{U}}\cdot(\vec{\mathcal{U}}\cdot\nabla)\vec{u} = \mathcal{U}^2\rho\dot{v} + 2\, \mathcal{U}^2 u\Omega .$$

In this last result the master equation is used to remove $\dot{v}$ in terms of $\dot{p}$ and $\dot{\lambda}$, giving

$$\vec{U}\cdot(\vec{U}\cdot\nabla)\vec{u} = U^2\rho[\frac{\eta\dot{\lambda} - \dot{p}}{(\rho c)^2}] + 2\, U^2 u\Omega \quad . \tag{34}$$

When this is substituted into Eq. (31) and some terms are rearranged, the three-dimensional shock-change relation emerges as

$$\frac{\delta p}{\delta t} + \rho\, U\, \frac{\delta u}{\delta t} = (1 - \mu)\dot{p} + \mu\eta\dot{\lambda} + 2\rho U^2 u\Omega$$

or

$$\frac{\delta p}{\delta t} + \rho\, U\, \frac{\delta u}{\delta t} = (1 - \mu)\dot{p} + \rho U^2(2\Omega u + \sigma\dot{\lambda}) \quad . \tag{35}$$

In the above equation, the term including $\vec{U}\cdot\frac{\delta\vec{u}}{\delta t}$ has been replaced with one involving velocity magnitudes according to

$$\vec{U}\cdot\frac{\delta\vec{u}}{\delta t} = Un_i\,\frac{\delta(un_i)}{\delta t} = U\, n_i n_i\, \frac{\delta u}{\delta t} + \frac{U}{2}\, u\, \frac{\delta n_i^2}{\delta t} = U\,\frac{\delta u}{\delta t} \quad .$$

Equation (35) is identical to the one-dimensional result, Eq. (15), except for the curvature term. Realizing that in one dimension u and U are the "normal components" identified by the same symbols above and that m/x is just twice the mean curvature of planar, cylindrical, or spherical surfaces, we recognize that Eq. (15) is the one-dimensional specialization of Eq. (35).

IV. THERMODYNAMIC CONSIDERATIONS IN FORMING SHOCK-CHANGE RELATIONS

To effect convenient applications of Eq. (35), one must know or assume the $e(p,v,\lambda)$ equation of state, invoke the shock-jump conditions or Hugoniot relations (not yet used in the development), and specify explicitly or implicitly the amount of reaction (change in λ) occurring in the shock process. With these requirements met, thermodynamic considerations allow the casting of shock-change relations in a variety of forms, as are appropriate for different physical problems, measurements, and equation-of-state assumptions.

For a uniform, motionless state ahead of the shock, the Hugoniot relations are

$$\rho_0 U = \rho \mathcal{U} = J \tag{36}$$

$$p - p_0 = \rho_0 U u = J u \tag{37}$$

and

$$e - e_0 = \frac{1}{2}(p + p_0)(v_0 - v) = \frac{1}{2}u^2 + p_0(v_0 - v) \quad . \tag{38}$$

Here the subscript zero denotes the state ahead of the shock, J is the negative of the mass flux, and the velocities are scalar quantities in both the one- and three-dimensional cases, representing normal components in the latter instance. In addition, we note that for any two state variables, F and f,

$$\frac{\delta F}{\delta t} = \left.\frac{dF}{df}\right|_{H} \frac{\delta f}{\delta t} \tag{39}$$

where the subscript H denotes evaluation along the shock Hugoniot.

A common practice is to define the shock Hugoniot by a shock velocity-particle velocity relation, that is:

$$U = U_H(u) \quad . \tag{40}$$

With such a specification and the Hugoniot relations [Eqs. (36)-(38)], the pressure, volume, energy, and velocities immediately behind the shock may be expressed in terms of a single variable. For example, if the specific volume is chosen for this parameterization, Eqs. (36)-(38) and (40) yield $p = p_H(v)$, $e = e_H(v)$, $u = u_H(v)$, and $U = U_H(v)$. Specification of $\lambda_H(v)$ must, however, be done either by a separate additional assumption or by the additional use of a complete $e(p,v,\lambda)$ equation of state.

In recasting Eq. (35), it is convenient to use the particle velocity as the independent variable, denoting differentiation by this variable with a prime, and to define the dimensionless variable

$$\psi = \frac{J}{dp/du|_H} = \frac{\dot{J}}{p'} \quad . \tag{41}$$

With this definition and Eqs. (36), (37), and (39), a pressure form of Eq. (35) may be written:

$$\frac{\delta p}{\delta t} = \frac{(1 - \mu)\dot{p} + \mathcal{U}[2(p - p_0)\Omega + J\sigma\dot{\lambda}]}{(1 + \psi)} \quad . \tag{42}$$

Alternatively, we may eliminate the pressure from Eq. (35). First using Eqs. (28) and (26), we obtain

$$\dot{p} = \frac{\delta p}{\delta t} + \rho\vec{\mathcal{U}}\cdot\dot{\vec{u}} = \frac{\delta p}{\delta t} + J\,\dot{u} \quad . \tag{43}$$

Here the second form follows from

$$n_i\frac{\delta u_i}{\delta t} = \frac{\delta u}{\delta t} = n_i\dot{u}_i + n_i(\vec{\mathcal{U}}\cdot\vec{\nabla}u_i) = n_i\dot{u}_i + \mathcal{U}\,n_in_j\,\frac{\partial u_i}{\partial x_j}$$

$$= n_i\dot{u}_i + \vec{\mathcal{U}}\cdot\vec{\nabla}u - \mathcal{U}u\,n_in_j\,\frac{\partial n_i}{\partial x_j} \quad ;$$

the last term above was shown to vanish (see preceding section) so that by Eq. (20), $n_i\dot{u}_i = \dot{u}$. Equations (37), (39), and (41)-(43) can then be used to give

$$\frac{\delta u}{\delta t} = \frac{(1 - \mu)\dot{u} + \mathcal{U}(2u\Omega + \sigma\dot{\lambda})}{(1 + \mu/\psi)} \quad . \tag{44}$$

To develop a shock-change relation in the specific volume, we introduce a parameter defined in analogy to the square of the Mach number μ, specifically

$$\nu = -\frac{\mathcal{U}^2}{v^2 dp/dv|_H} = -\frac{J^2}{dp/dv|_H} = -\frac{J^2 v'}{p'} \quad . \tag{45}$$

v' can be related to p' by differentiating the Hugoniot relations, Eqs. (36) and (37), and eliminating U', yielding

$$v' = \frac{p' - 2J}{J^2} = \frac{1}{J}\,(1/\psi - 2) \quad . \tag{46}$$

Thus

$$\psi = \frac{1 + \nu}{2} \; , \tag{47}$$

and an alternative form of the shock-change relation in pressure, Eq. (42), is

$$\frac{\delta p}{\delta t} = \frac{(1 - \mu)\dot{p} + \mathcal{U}[2(p - p_0)\Omega + J\sigma\dot{\lambda}]}{(3/2 + \nu/2)} \quad . \tag{48}$$

Using this relation, together with the master equation to replace $\dot{p}$ with $\dot{v}$, and Eqs. (36), (37), and (39), we find the change in specific volume to be

$$\frac{\delta v}{\delta t} = \frac{(1/\mu - 1)\dot{v} - 2(v_0 - v)\mathcal{U}\Omega - (v/\mu)\sigma\dot{\lambda}}{(3/2\nu + 1/2)} \quad . \tag{49}$$

A more complicated, but more useful, form is obtained by using Eq. (28) to replace $\dot{v}$ with the normal component of the specific volume gradient

$$\frac{\delta v}{\delta t} = \left[\frac{2\,\mu\nu}{(2\nu - 3\mu - 3\mu\nu)}\right]\left[(1/\mu - 1)\mathcal{U}\vec{n}\cdot\vec{\nabla}v + 2(v_0 - v)\mathcal{U}\Omega + (v/\mu)\dot{\lambda}\right] \quad . \tag{50}$$

None of the above shock-change relations have any explicit reference to the jump in progress variable, λ, in the shock front. This does not mean that reaction in the front does not affect the shock change but means rather that the effect of shock-front reaction is implicitly contained in the Hugoniot specifications, essentially in the parameters ψ or ν. These parameters can be specified by Hugoniots constructed from data or assumption, and these Hugoniots can be either reactive or unreactive, that is, they may or may not involve reaction across the shock front. Although the Hugoniot specification and shock-front reaction have some quantitative effect on the shock-change relations through the evaluation of μ and σ from the equation of state, the stronger effect is in the influence on ψ or ν. It is instructive to examine these effects.

Considering first a Hugoniot specified in terms of particle velocity, the energy jump condition, Eq. (38), and the equation of state can be differentiated by u to give

$$u - p_0 v' = e_p p' + e_v v' + e_\lambda \lambda' \quad . \tag{51}$$

Noting that

$$e_p = 1/\rho\Gamma \quad , \tag{52}$$

where Γ is the Grüneisen ratio, the addition of p to both sides of Eq. (51) and use of Eqs. (7), (8), (37), (41), and (46) yields

$$\frac{\rho\Gamma u}{J}(1 - \psi) = 1 + \frac{(1 - 2\psi)}{\mu} - \frac{\mathcal{U}\psi\sigma\lambda'}{\mu} \; .$$

Defining*

$$\kappa = 1 - \frac{\rho\Gamma u}{J} = 1 - \rho\Gamma(v_0 - v) \tag{53}$$

and rearranging gives

$$1/\psi = \frac{2 - \mu + \mu\kappa + \mathcal{U}\sigma\lambda'}{(1 + \mu\kappa)} = \frac{\beta + \mathcal{U}\sigma\lambda'}{\alpha} \quad , \tag{54}$$

where**

$$\alpha = 1 + \mu\kappa \tag{55}$$

and

$$\beta = 2 - \mu + \mu\kappa \quad . \tag{56}$$

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*This unusual expression of the Grüneisen ratio and compression has in common with our other dimensionless variables the feature of being equal to unity as the shock strength vanishes and of decreasing with increasing shock strength.

**Note that α and β both have values of 2 in the vanishing shock-strength limit and that both decrease with increasing shock strength.

Similarly, differentiating the energy relations by v gives

$$\frac{1}{2}\left[\frac{J^2}{\nu}(v_0 - v) + (p + p_0)\right] = \frac{e_p J^2}{\nu} - e_v - e_\lambda(\partial\lambda/\partial v)_H \tag{57}$$

which, with some manipulation, gives

$$\frac{1}{\nu} = \frac{2 - \mu + \mu\kappa - 2v\sigma(d\lambda/dv)_H}{\mu(1 + \kappa)} = \frac{\beta - 2v\sigma(d\lambda/dv)_H}{(2\alpha - \beta)} \quad . \tag{58}$$

The reaction, if any, in the shock front might be expected to increase with increasing shock strength; that is, $\lambda' > 0$ and $(d\lambda/dv)_H < 0$. In the usual case, κ or $\mu\kappa$ should be >-1 so that the effect of exothermic ($\sigma > 0$) reaction in the shock front is to reduce ψ or ν. The result is a "stiffening" of the shock Hugoniot by reaction, with a corresponding effect of the shock change on the different state variables. Inspection of Eqs. (42) or (48) shows that the reductions in ψ or ν tend to increase the change in shock pressure. Similarly, examination of Eqs. (44) and (49) shows the shock change in particle velocity and specific volume to be reduced by reaction in the front.

Another expression of the effect of shock-front reaction can be obtained by using Eq. (39) to relate λ' or $(d\lambda/dv)_H$ to the change in reaction in the shock front, $\delta\lambda/\delta t$. For example, operating on Eq. (54) gives:

$$\frac{1}{\psi}\frac{\delta u}{\delta t} = \left(\frac{\beta}{\alpha}\right)\frac{\delta u}{\delta t} + \left(\frac{U\sigma}{\alpha}\right)\frac{\delta\lambda}{\delta t} \quad , \tag{59}$$

which when used with Eq. (44) gives

$$\frac{\delta u}{\delta t} = \left[\frac{\alpha}{\alpha + \mu\beta}\right] \left\{(1 - \mu)\,\dot{u} + U\left[2u\Omega + \sigma\left(\dot{\lambda} - \frac{\mu}{\alpha}\frac{\delta\lambda}{\delta t}\right)\right]\right\} \quad . \tag{60}$$

If this relation is used with Eqs. (37), (39), (41), (43), and (59), there results

$$\frac{\delta p}{\delta t} = \left[\frac{\alpha}{\alpha + \beta}\right] \left\{(1 - \mu)\dot{p} + U\left[2(p - p_0)\Omega + J\sigma\left(\dot{\lambda} + \frac{1}{\beta}\frac{\delta\lambda}{\delta t}\right)\right]\right\} \quad . \tag{61}$$

Similarly, applying Eqs. (39) and (58) to the shock-change relations in specific volume, Eqs. (49) and (50), yields

$$\frac{\delta v}{\delta t} = [\frac{2\alpha - \beta}{\alpha + \beta}] \left\{\frac{(1 - \mu)}{\mu} \dot{v} - 2(v_0 - v)\mathcal{U}\Omega - \frac{v}{\mu} \sigma[\dot{\lambda} - \frac{3}{(1 + \kappa)} \frac{\delta\lambda}{\delta t}]\right\} , \tag{62}$$

and in terms of $\vec{\nabla} v$

$$\frac{\delta v}{\delta t} = [\frac{\beta - 2\alpha}{3\alpha - (1 + \kappa)}] \left\{\mathcal{U} \frac{(1 - \mu)}{\mu} \vec{n}\cdot\vec{\nabla} v + 2(v_0 - v)\mathcal{U}\Omega + \frac{v}{\mu} \sigma[\dot{\lambda} - \frac{3}{(1 + \kappa)} \frac{\delta\lambda}{\delta t}]\right\} . \tag{63}$$

With the same conditions of κ or $\mu\kappa > -1$, Eqs. (60)-(63) show the same effects of shock-front reaction ($\delta\lambda/\delta t > 0$) as described earlier. More important, these equations explicitly express how the shock changes are effected by reaction both in the front and immediately behind the front. Experimental determinations may be made of the changes in shock strength, material time derivatives or gradients of state variables, and curvatures; ordinarily direct measurements of the reaction rate or the energy release rate are not possible. When the curvature is provided by experiment (or, more commonly, when planar waves, $\Omega = 0$, are available) and when the shock change and time derivative or gradient behind the front is provided in only a single state variable, relations like Eqs. (60)-(63) and a full equation of state yield only the net reaction rate or energy release in the front and immediately behind it. If, however, such measurements are obtained for two state variables, $\dot{\lambda}$ can be eliminated from the two appropriate shock-change relations, and $\delta\lambda/\delta t$ can be evaluated. Seen another way, such measurements of, for example, pressure and particle velocity, can yield $\delta\lambda/\delta t$ through the combination of Eqs. (39), (41), (43), and (54) without consideration of $\dot{\lambda}$. Again, a known equation of state must be assumed.

Some of the results formulated and points emphasized above are stated in a paper by Chen and Kennedy,[13] who used an order of thermodynamic considerations different from ours. They first used only the flow relations, Hugoniot relations, and equation-of-state characterizations to develop shock-change relations similar to our Eqs. (60) and (63). That was followed by a Hugoniot specification, a determination equivalent to our expression of ν in Eq. (58), and the formulation of a shock-change relation with the shock-front reaction contained in a term involving $(d\lambda/dv)_{\mathcal{H}}$. Reference 13 deals only with shock-change relations in specific volume and particle velocity, and with some labor it can be shown that Eqs. (3.1)-(3.3) of that paper are identical to our Eq. (64) and that their Eqs. (3.5)-(3.7) are the same as our Eq. (60), except in one respect: Ref. 13 states that relative contributions of (in our notation) $\dot{\lambda}$ and $\delta\lambda/\delta t$ are related by a factor $3/(1 + \kappa)$ for both the relations in specific volume and particle velocity, whereas we found that the factor was $\mu/(1 + \mu\kappa)$ in the particle-velocity equation. In re-examining his formulation, Chen[18] found and corrected an error, thereby eliminating the disparity between the two results. For example, in Ref. 13 where the effect of different (unreactive and reactive) Hugoniots for PBX-9404 is discussed, Chen's correction reduces by about a factor of 4 the spread between the upper and lower curves of Fig. 4, Ref. 13, but in no way invalidates Chen's and Kennedy's point regarding the influence of assumed shock-front reaction on determinations of $\dot{\lambda}$.

V. SIMPLIFYING ASSUMPTIONS IN THE APPLICATION OF SHOCK-CHANGE RELATIONS

Our interest in shock-change relations is in their application to practical shock-propagation problems in condensed materials, particularly in predicting complicated shock-initiation and detonation-wave configurations in solid explosives. For such applications, high-speed streak- and framing-camera observations can define shock surfaces, and embedded- (Lagrangian-) gauge measurements of pressure or particle velocity can give the necessary data for use, respectively, in Eqs. (42) or (61) and in Eq. (43) or (60). Flash x-ray observations might be used with the relations in specific volume, such as Eqs. (50) or (63).

Although treating real solids as ideal fluids is a common practice in shock-wave physics, we note that at shock strengths low enough for elastic-plastic effects to be important, or in crystals or other elastically anisotropic materials, the formulations become considerably more complicated; the scalar pressures and specific volumes must be replaced by stress and strain tensors, and the great simplification resulting from having the particle velocity normal to the shock front may no longer be used. For porous materials, even the assumption of a shock discontinuity is questionable. In addition, the equations of state of most materials of interest--especially as related to the reaction coordinate in explosives--are far from being as well defined as is assumed in the development. The approximations suggested below are typical of the extent of information commonly available.

Clearly, the application of shock-change relations is simplified by the assumption that no reaction occurs in the shock front, that is $\delta\lambda/\delta t = \lambda' = d\lambda/dv)_H = 0$. This assumption, usual in the Zel'dovich-von Neumann-Doering theory of detonation, can be argued on the basis that any reaction requires a finite activation time, whereas the shock is an instantaneous process. Further, in the initiation and detonation studies of condensed explosives--our principal area of interest for shock-change analysis--there is no firm experimental evidence that the assumption is incorrect.

With the shock front assumed unreactive, one need consider only the equation of state of the unreacted material for the evaluation of all of the thermodynamic derivatives used above except for η and σ, but these derivatives with respect to λ still require some assumption of a complete (involving λ) equation of state. If only a determination of energy release rate $\dot{R}$ is desired, the need for a complete equation of state can be avoided by using

$$\dot{R} = e_\lambda \dot{\lambda} = - \frac{\eta}{\rho\Gamma} \dot{\lambda} = \frac{-c^2\sigma\lambda}{\Gamma} \quad . \tag{64}$$

The Mie-Grüneisen form, $\Gamma = \Gamma(v)$, with

$$\rho\Gamma = \rho_0\Gamma_0 \tag{65}$$

and the Hugoniot reference locus specified by

$$U = C + Su \quad , \tag{66}$$

where C and S are constants, is a good approximation for the equations of state of many unreacted solids. With these relations, one finds

$$\kappa = 1 - \Gamma_0(1 - v/v_0) = 1 - \frac{\Gamma_0 u}{U} = \kappa_0 \quad . \tag{67}$$

Use of the Hugoniot relations, appropriate definitions, and Eq. (66) gives

$$\psi = \frac{U}{U + Su} \tag{68}$$

and

$$\nu = \frac{C}{U + Su} \quad . \tag{69}$$

Solving Eqs. (54)-(56) with Eq. (68) and assuming that $\lambda' = 0$ gives

$$\mu = \frac{C}{U + Su\kappa_0} \tag{70}$$

$$\alpha = \frac{U(1 + \kappa_0)}{U + Su\kappa_0} \tag{71}$$

and

$$\beta = \frac{(U + Su)\ (1 + \kappa_0)}{U + Su\kappa_0} \tag{72}$$

Inspection of Eqs. (67) through (72) evidences the weak shock limits and reductions cited in the previous section for the dimensionless parameters. Note that in the strong shock limit, $\kappa \to 1 - \frac{\Gamma_0}{S}$, so that $\Gamma_0/S \geq 2$ would be required for the anomalous condition of $\kappa \leq -1$ discussed earlier. The normal case is $\Gamma_0/S \geq 1$; $\Gamma_0/S \geq 2$ is rare.

Use of the above equations and the Hugoniot relations allows one to write any of the shock-change equations of the previous section in terms of $\dot{R}$, any one state variable (u, p, v) or the shock velocity, and four constants, ρ_0, Γ_0, C, and S. Because the resulting expressions look complicated and provide no further illumination of the shock-change behavior, such formulations are not recorded here.

NOMENCLATURE

b a tensor, the second fundamental form of a surface

c frozen Eulerian sound speed

C constant in the linear shock-particle velocity relation

e specific internal energy

f,F arbitrary functions defined in the flow

g a tensor, the first fundamental form of a surface

J mass flux normal to the shock surface

m coordinate coefficient in one-dimensional flow equations

p hydrostatic pressure

r radius of curvature

R principal radius of curvature

s specific entropy

S coefficient of u in the linear shock-particle velocity relation

$\mathcal{S}$ shock surface

t time

$\vec{u}$ particle velocity

$\vec{U}$ shock velocity

v specific volume

x Cartesian coordinate

Γ Grüneisen's parameter

κ dimensionless variable, $1 - \rho\Gamma(v - v_0)$

λ reaction progress variable

μ square of the Mach number

ξ curvilinear shock-surface coordinate

ρ density $= \frac{1}{v}$

η $\eta = \rho c^2 \sigma$

σ the "thermicity" coefficient, $\frac{1}{\rho c^2} \left(\frac{\partial p}{\partial \lambda}\right)_{e,v}$

Ω the mean curvature of a surface

ν dimensionless variable, $\nu = J^2/(dp/dv)_{H}$

ψ $\psi = J/(dp/du)_{H}$

Sub- and Superscripts

H subscript denoting the Hugoniot curve

i,j,k subscripts denoting any one of the three Cartesian coordinates

0 subscript denoting value of the function in the fiducial state

α,β,γ subscripts denoting one of the two curvilinear shock-surface coordinates

Other Symbols

$\vec{n}$ unit normal vector on the shock surface

$\vec{\mathcal{U}}$ difference in shock and particle velocity $= (\vec{U} - \vec{u})$

∇ differential vector operator del $= \hat{e}_i \frac{\partial}{\partial x_i}$

$\dot{f}$ material derivative of function f

$\frac{\delta f}{\delta t}$ derivative of function f along shock locus

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