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CHARACTERIZATION OF INITIATION AND DETONATION BY LAGRANGE GAGE TECHNIQUES

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ABSTRACT

This report presents theoretical aspects of Lagrange analyses used in Lagrange gage studies of explosives, nonideal detonation, and overdriven detonation. The work on reactive flow Lagrange analysis (RFLA) was concerned with Lagrange particle velocity histories that exhibit double maxima similar to those recorded in RX26 and PBX9404. Conditions for particle velocity histories to exhibit extrema were formulated in terms of envelopes formed by Lagrange pressure histories to show that the second maximum in the particle velocity is not directly associated with the chemical energy release rate. It is therefore not necessary to incorporate the second maximum in particle velocity into RFLA calculations of the energy release rates in RX26 and PBX9404. Lagrange analysis of the flow produced by the expansion of a detonation wave at a free surface was proposed to extend the determination of the release adiabat of detonation products from the Chapman-Jouguet (CJ) state to zero pressure. A solution for the expansion of a Taylor wave at a free surface was constructed to guide such determinations.

Solutions were constructed for steady-state nonideal detonation waves propagating in polytropic explosive with two reacting components. Particular attention was given to the case when one of the reactions is exothermic and the other is endothermic. The equation relating the detonation velocity, the particle velocity, and the reaction coordinates were combined with simplified reaction rate expressions to identify the CJ point as a saddle and to show that the flow in such a nonideal detonation is determined by the rear-boundary particle velocity condition.

Overdriven detonation was treated both as a reactive discontinuity and as a Zeldovich-von Neumann-Doering (ZND) wave. The Rankine-Hugoniot (RH) jump conditions were used to calculate the first and second derivatives on the detonation velocity versus particle velocity Hugoniot at the CJ point. Methods of differential geometry were used to determine the conditions that allow the flow equations and RH boundary conditions to admit similarity solutions for overdriven detonation waves. This geometric approach led to the following conclusions:

(1) The equations governing a reactive discontinuity with polytropic detonation products do not admit a similarity solution for nonsteady overdriven detonation waves.

(2) The equations governing a spherical (ZND) wave do not in general admit a self-similar flow.

(3) Under the strong shock condition, the equations governing a spherical ZND wave admit a similarity solution when the explosive and its products are treated as polytropic materials with the same index.

CONTENTS

I INTRODUCTION

The long range objective of this research program is to develop a more basic understanding and a more realistic description of the initiation and propagation of detonation. Explosives were studied jointly by Lawrence Livermore National Laboratory (LLNL) and SRI International to obtain some of the information required to attain this objective.

The technical work performed at SRI was concerned with theoretical aspects of the following topics:

- Lagrange analysis
- Nonideal detonation
- Overdriven detonation

Details of this theoretical work are presented in the remainder of this report.

II LAGRANGE ANALYSIS

Particle-Velocity Histories Exhibiting Double Maxima

Particle velocity histories exhibiting double maxima were recorded in multiple Lagrange gage studies of the shock initiation process in RX26 and PBX9404 performed at LLNL. The work to understand the significance of multiple extrema in particle velocity records was undertaken because difficulties were encountered in performing reactive flow Lagrange analyses (RFLA) with these records exhibiting double maxima. The reality of such flow features and their relationship to the global energy release rate were established to determine the consequences of omitting the second maximum in particle velocity from the RFLA.

The conditions needed for Lagrange particle velocity histories to exhibit maxima and minima were formulated in terms of envelopes formed by Lagrange pressure (p) histories. Recall[1] that an envelope E formed by intersection points of a family of curves C, described by the equation $f(x,y,\alpha) = 0$ with α a parameter, is determined by the equations $f(x,y,\alpha) = 0$ and $\partial f/\partial\alpha = 0$. E is tangent to C and its equation $y = y_e(x)$ can be obtained by eliminating α between $f(x,y,\alpha) = 0$ and $\partial f/\partial\alpha = 0$. It is convenient to consider the Lagrange pressure histories as a family of curves parametrized by the Lagrange coordinate h and describe this family as $f(t,p,h) = p - p(t,h) = 0$, where t denotes the time. The condition needed for the pressure histories to form an envelope is thus $\partial p/\partial h = 0$.

It follows from the momentum equation, $\rho_0\ \partial u/\partial t = -(\partial p/\partial h)$, where ρ_0 denotes the initial density and u denotes the particle velocity, that extrema in the Lagrange particle velocity histories lie on envelopes formed by the Lagrange pressure histories. It also follows that the particle velocity histories will not exhibit extrema unless the pressure histories at neighboring Lagrange positions intersect.

We now formulate conditions needed for the Lagrange particle velocity to attain a maximum or a minimum on an envelope formed by a set of Lagrange pressure histories. We use the following identities:

$$\frac{dp}{dt} = \frac{\partial p}{\partial t} + \frac{\partial p}{\partial h}\frac{dh}{dt} \tag{1}$$

and

$$\frac{d^2p}{dt^2} = \frac{\partial^2 p}{\partial t^2} + 2\frac{\partial^2 p}{\partial h \partial t}\frac{dh}{dt} + \frac{\partial^2 p}{\partial h^2}\left(\frac{dh}{dt}\right)^2 + \frac{\partial p}{\partial h}\frac{d^2h}{dt^2} \tag{2}$$

Along an envelope E formed by a set of Lagrange pressure-time histories

$$\frac{\partial p}{\partial h} = 0 \tag{3}$$

and

$$\frac{d}{dt}\frac{\partial p}{\partial h} = \frac{\partial^2 p}{\partial t \partial h} + \frac{\partial^2 p}{\partial h^2}\frac{dh_e}{dt} = 0 \tag{4}$$

Combining equations (3) and (4) with equations (1) and (2) leads to the equations

$$\frac{dp_e}{dt} = \frac{dp_e}{dt}\frac{dh_e}{dt} = \frac{\partial p}{\partial t} \tag{5}$$

and

$$\frac{d^2p_e}{dt^2} = \frac{\partial^2 p}{\partial t^2} + \frac{\partial^2 p}{\partial h^2}\frac{dh_e}{dt} \tag{6}$$

It is convenient at this stage to use the momentum equation written as $\rho_o \partial^2 u/\partial t^2 = - \partial^2 p/\partial t \partial h$ and rewrite equations (4) and (6) as

$$\frac{dh_e}{dt} = \rho_o \frac{\partial^2 u/\partial t^2}{\partial^2 p/\partial h^2} \tag{7}$$

and

$$\frac{d^2p_e}{dt^2} = \frac{\partial^2 p}{\partial t^2} - \rho_o \frac{\partial^2 u}{\partial t^2}\frac{dh_e}{dt} \tag{8}$$

In this report we consider only the case when $dh_e/dt > 0$, and the partial derivatives $\partial^2 u/\partial t^2$ and $\partial^2 p/\partial h^2$ are constrained by equation (7) to have the same signs. In this case, $\partial^2 u/\partial t^2 < 0$ when $\partial^2 p/\partial h^2 < 0$, and $\partial^2 u/\partial t^2 > 0$ when $\partial^2 p/\partial h^2 > 0$, and we are led to conclusion C1:

C1: When $dh_e/dt > 0$, either the maxima in the (u-t) and (p-h) profiles or the minima in the (u-t) and (p-h) profiles lie on an envelope formed by a set of (p-t) profiles.

We now derive an equation that allows us to use the (p-t) profiles to distinguish between these maxima and minima. We expand the pressure in a Taylor series from a point on an envelope (t_e, h_e) along the envelope and along the Lagrange coordinate h_e to obtain the equations

$$p_e(t_e + \delta t) = p_e(t_e) + \frac{dp_e}{dt}\,\delta t + \frac{1}{2}\,\frac{d^2 p_e}{dt^2}\,(\delta t)^2 + \ldots \qquad (9)$$

$$p(t_e + \delta t,\ h_e) = p_e(t_e, h_e) + \frac{\partial p}{\partial t}\,\delta t + \frac{1}{2}\left(\frac{\partial^2 p}{\partial t^2}\right)(\delta t)^2 + \ldots \qquad (10)$$

Subtracting equation (10) from equation (9) and making use of the tangency condition equation (5), and equation (8), lead to the equation

$$\Delta p(\delta t) = p_e(t_e + \delta t) - p(t_e + \delta t, h_e) = -\frac{\rho_o}{2}\,\frac{\partial^2 u}{\partial t^2}\,\frac{dh_e}{dt}\,(\delta t)^2 + \ldots \qquad (11)$$

which can be combined with equation (7) to give the equation

$$\Delta p(\delta t) = -\frac{1}{2}\left(\frac{\partial^2 p}{\partial h^2}\right)\left(\frac{dh_e}{dt}\right)^2 (\delta t)^2 + \ldots \qquad (12)$$

It follows from equation (12) that $\Delta p(\delta t) > 0$ when $(\partial^2 p/\partial h^2) < 0$ and that $\Delta p(\delta t) < 0$ when $(\partial^2 p/\partial h^2) > 0$, and we are thus led to conclusion C2:

C2: When $dh_e/dt > 0$, maxima in the (u-t) and (p-h) profiles lie on an envelope formed by a set of (p-t) profiles when the envelope is tangent to the (p-t) profiles from above. Alternatively, minima in the (u-t) and (p-h) profiles lie on an envelope formed by a set of (p-t) profiles when the envelope is tangent to the (p-t) profiles from below.

A set of schematic (p-t) profiles for a reactive shock wave with three envelopes, E_1, E_2, and E_3, is shown in Figure 1 to illustrate C1 and C2. It is clear from Figure 1 that $dh_e/dt > 0$ along E_1, E_2, and E_3, that $dp_e/dt > 0$ along E_1, and that $dp_e/dt < 0$ along E_1 and E_2. Maxima in the (u-t) and (p-h) profiles lie on E_1 and E_3 because $\Delta p(\delta t) > 0$ along these envelopes, but minima in the (u-t) and (p-h) profiles lie on E_2 because $\Delta p(\delta t) < 0$ along this envelope. Thus along a particle path in this region of the flow, the particle velocity rises from the shock particle velocity to a maximum, then falls to a minimum, and then again rises to a maximum. On the (p-t) profile shown as OSPT, for example, the particle velocity rises from the shock front shown as OS, attains a maximum at 1, falls to a minimum at 2, rises to a maximum at 3, and then falls.

We are now in a position to address whether the second maximum in the Lagrange particle velocity histories is explicitly associated with the chemical energy release rate and thus needs to be incorporated into the RFLA. Because the energy release rate becomes zero close to a pressure peak when the pressure starts to fall, we claim that the chemical reaction is not directly responsible for the second maximum in the particle velocity and reach conclusion C3:

C3: There is no need to incorporate the second maximum in Lagrange particle velocity into a RFLA for calculating the global energy release rate in a shocked explosive.

Construction of a Self-Similar Solution for Particle Velocity Gages

Lie-group techniques[2] were used to construct a self-similar solution to a partial differential equation formulated for particle velocity gages by Dr. J. Nutt of LLNL. Methods of differential geometry[3] were used to find the infinitesimal generator of a Lie group

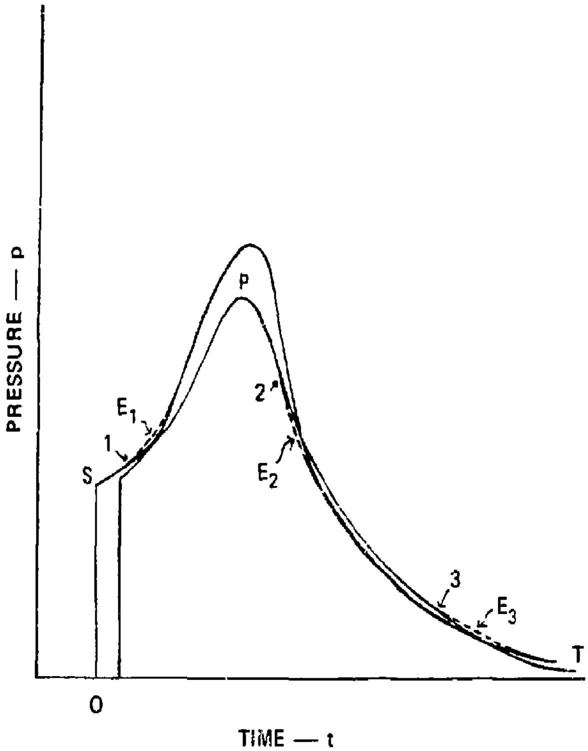

FIGURE 1 A SET OF SCHEMATIC LAGRANGE PRESSURE HISTORIES FORMING THREE ENVELOPES E_1, E_2, AND E_3.

Maxima in the corresponding Lagrange particle velocity histories lie on E_1 and E_3, and their minima lie on E_2.

admitted by the partial differential equation. First integrals of this infinitesimal generator were then used to construct the invariant solution that reduces the partial differential equation into an ordinary differential equation.

Expansion of a Taylor Wave at a Free Surface

Lagrange gage studies of the flow produced by the expansion of a Taylor wave at a free surface in principle provide a means of extending the determination of the release adiabat of the detonation products from the Chapman-Jouguet (CJ) point to zero pressure. The solution for the expansion of the detonation products at a free surface was constructed to guide such Lagrange gage determinations of the release adiabat through the CJ point.

The equations for the particle velocity and pressure in the rarefaction wave reflected into polytropic detonation products with an index K = 3 are presented here, but their derivation is not given. With the notation introduced earlier, we let L and D denote the length of the charge and the detonation velocity, and we let the subscript CJ denote the CJ condition. Then the equations for the particle velocity and pressure in the reflected rarefaction wave can be written as

$$\frac{u_{CJ}}{D} = 1 - \frac{3}{4}\frac{(1 - h/L)^{1/2}(2 - T/t)}{(1 - T/t)^{1/2}} \qquad (13)$$

and

$$\frac{p}{p_{CJ}} = \frac{(T/t)^3 \; (1 - h/L)^{3/2}}{(1 - T/t)^{3/2}} \qquad (14)$$

where T = L/D denotes the time the detonation wave reaches the end of the charge, $h < L$ and $t > T$.

III NONIDEAL DETONATION

We consider a composite explosive with two components capable of reacting, denoted by the subscripts 1 and 2. We denote their mass fractions by α_1 and α_2 and their reaction coordinates by λ_1 and λ_2. For the sake of tractability, we assume that the components and their reaction products are polytropic with the same index K. Our prime concern will be with nonideality that arises because one reaction is exothermic but the other is endothermic. We let v and e denote specific volume and specific internal energy, the subscript o denote the unshocked state, and the superscript x denote the explosive. In this case, the $e = e(p,v,\lambda_1,\lambda_2)$ equation of state of the reacting explosive can be written as

$$e - e_o^x = -\lambda_1 q_1 - \lambda_2 q_2 + \frac{pv}{K-1} \tag{15}$$

where $e_o^x = \alpha_1 (e_o^x)_1 + \alpha_2 (e_o^x)_2$, and q_1 and q_2 are related to the specific heats of reaction Q_1 and Q_2 by the equations $q_1 = \alpha_1 Q_1$ and $q_2 = \alpha_2 Q_2$. It is clear from Eq. (15) that $\lambda_1 = \lambda_2 = 0$ in the unreacted explosive and that $\lambda_1 = \lambda_2 = 1$ when the explosive has fully reacted. We will consider steady-state one-dimensional detonation and denote the detonation velocity by D.

The equation relating the particle velocity and reaction coordinates is readily obtained by combining Eq. (15) with the Rankine-Hugoniot (RH) conditions, expressing the balance of mass, momentum, and energy in the steady-state wave, written as

$$pv = (D - u)u \tag{16}$$

$$e - e_o^x = \frac{u^2}{2} \tag{17}$$

The combination of Eqs. 15 through 17 to eliminate $(e - e_o^x)$ and pv leads to the equation

$$u^2 - \frac{2uD}{K + 1} = - \frac{2(K - 1)}{(K + 1)} \; (\lambda_1 q_1 + \lambda_2 q_2) \qquad (18)$$

We now introduce the sound speed c with the equation $c^2 = Kpv$, set $\lambda_1 = \hat{\lambda}_1$ and $\lambda_2 = \hat{\lambda}_2$ in the CJ state, and use the CJ condition $u_{CJ} + c_{CJ} = D$ to obtain an expression for the detonation velocity. With these equations, Eq. (16) given the CJ conditions as

$$u_{CJ} = \frac{c_{CJ}}{K} = \frac{D}{K + 1} \qquad (19)$$

and the equation for D follows from Eq. (18) as

$$D^2 = (K + 1)^2 \, u_{CJ}^2 = 2(K^2 - 1) \; (\hat{\lambda}_1 q_1 + \hat{\lambda}_2 q_2) \qquad (20)$$

It is then convenient to combine Eqs. (18) and (20) and write the equation for particle velocity as

$$\frac{u}{u_{CJ}} - 1 = \pm \left[\beta_1(\hat{\lambda}_1 - \lambda_1) + \beta_2(\hat{\lambda}_2 - \lambda_2)\right]^{1/2} \qquad (21)$$

where $\beta_1 = q_1/(\hat{\lambda}_1 q_1 + \hat{\lambda}_2 q_2)$ and $\beta_2 = q_2/(\hat{\lambda}_1 q_1 + \hat{\lambda}_2 q_2)$. Setting $\lambda_1 = \lambda_2 = 0$ in Eq. (21) gives two values for u_f, the particle velocity at the wave front: $u_f = 0$ and $u_f = 2u_{CJ}$. The negative sign in Eq. (21) thus gives the equation for the classical CJ detonation,[4] and the positive sign gives the equation for a Zeldovich-von Neumann-Doering (ZND) wave.[5]

When $q_1 > 0$ and $q_2 > 0$ in our polytropic explosive we use the condition $\hat{\lambda}_1 = \hat{\lambda}_2 = 1$ to define ideal detonation, and the conditions $(\hat{\lambda}_1 = 1, \hat{\lambda}_2 < 1)$, $(\hat{\lambda}_1 < 1, \hat{\lambda}_2 = 1)$, and $(\hat{\lambda}_1 < 1, \hat{\lambda}_2 < 1)$ to define nonideal detonation. In this case the problem of nonideal detonation can be considered as that of calculating the values of $\hat{\lambda}_1$ and $\hat{\lambda}_2$ for incomplete reaction at the CJ point.

We will now consider the case when both reactions go to completion, but one of them is endothermic and assume that $q_1 > 0$ and $q_2 < 0$. Formally, there are three cases to consider, $\partial\lambda_1/\partial t = \partial\lambda_2/\partial t$, $\partial\lambda_1/\partial t > \partial\lambda_2/\partial t$, and $\partial\lambda_2/\partial t < \partial\lambda_1/\partial t$, but we reject the last case on physical grounds. It is convenient to introduce the differential equation governing the flow

$$\left[D - (K + 1)u\right] \frac{\partial u}{\partial t} = (K - 1) \left\{q_1 \frac{\partial\lambda_1}{\partial t} + q_2 \frac{\partial\lambda_2}{\partial t}\right\} \quad (22)$$

when considering the first two cases.

When $\partial\lambda_1/\partial t = \partial\lambda_2/\partial t$, it is clear from Eq. (22) that the detonation wave is equivalent to a wave supported by a single reaction with a reduced heat of reaction $q = q_1 + q_2$. The CJ point lies at the end of the reaction zone, and the equation for the detonation velocity follows from Eq. (20) as $D^2 = 2(K^2 - 1)\,(q_1 + q_2)$.

When $\partial\lambda_1/\partial t > \partial\lambda_2/\partial t$, complications arise because the right-hand side of Eq. (22) will become zero when the reactions are proceeding, and the CJ point will lie within the reaction zone. This type of wave with an infinite reaction time has been discussed in some detail by Fickett and Davis.[5] Here we will adopt a different approach and also consider a wave with a finite reaction time τ_R. We assume that the reaction coordinates satisfy the equations

$$(1 - \lambda_1) = \left(1 - \frac{(t - \tau)}{\tau_R}\right)^{n_1} \quad (23)$$

$$(1 - \lambda_2) = \left(1 - \frac{(t - \tau)}{\tau_R}\right)^{n_2} \quad (24)$$

where τ is the Lagrange time and the parameters n_1 and n_2 satisfy the condition $n_1 > n_2$. It follows from Eqs. (23) and 24) that λ_1 and λ_2 are related by the equation

$$\left(1 - \lambda_2\right) = \left(1 - \lambda_1\right)^{n_2/n_1} \quad (25)$$

In our approach, we rewrite Eq. (18) as

$$D = \frac{(K+1)}{2} u + \frac{(K-1)}{u} (\lambda_1 q_1 + \lambda_2 q_2) \qquad (26)$$

and show that the CJ point is a saddle point on the $D = \tilde{D}(u,\lambda_1)$ surface. Differentiating Eq. (26) partially with respect to u and λ gives the equations to determine if the surface has a critical point C as

$$\frac{\partial D}{\partial u} = \frac{(K+1)}{2} - \frac{(K-1)}{u^2} (\lambda_1 q_1 + \lambda_2 q_2) \qquad (27)$$

$$\frac{\partial D}{\partial \lambda_1} = \frac{(K-1)}{u} \left(q_1 + q_2 \frac{\partial \lambda_2}{\partial \lambda_1}\right) \qquad (28)$$

with

$$\frac{\partial \lambda_2}{\partial \lambda_1} = \frac{n_2}{n_1} (1 - \lambda_1)^{\frac{n_2}{n_1} - 1} \qquad (29)$$

It follows from Eqs. (27) and (28) that the surface satisfies the conditions for a critical point $\partial D/\partial u = \partial D/\partial \lambda_1 = 0$, so we denote quantities evaluated at the critical point C by the subscript C. Differentiating Eqs. (27) and (28) gives the equations for the second derivatives required to determine the nature of the critical point C as

$$\frac{\partial^2 D}{\partial u^2} = \frac{2(K-1)}{u^3} (\lambda_1 q_1 + \lambda_2 q_2) \qquad (30)$$

$$\frac{\partial^2 D}{\partial \lambda_1 \partial_u} = -\frac{(K-1)}{u^2} \left(q_1 + q_2 \frac{\partial \lambda_2}{\partial \lambda_1}\right) \qquad (31)$$

$$\frac{\partial^2 D}{\partial \lambda^2} = \frac{(K-1)}{u} q_2 \frac{\partial^2 \lambda_2}{\partial \lambda_1^2} \qquad (32)$$

with

$$\frac{\partial^2 \lambda_2}{\partial \lambda_1^2} = -\frac{n_2}{n_1} \left(\frac{n_2}{n_1} - 1\right) (1 - \lambda_1)^{\frac{n_2}{n_1} - 2} \qquad (33)$$

Setting $\partial D/\partial u = \partial D/\partial \lambda = 0$ in Eqs. (27) and (28) shows that the following equations are satisfied at C

$$u_C^2 = \frac{(K - 1)}{(K + 1)} \left[(\lambda_1)_C \, q_1 + (\lambda_2)_C \, q_2 \right] \tag{34}$$

$$\left(\frac{\partial \lambda_2}{\partial \lambda_1}\right)_C = -\frac{q_1}{q_2} \tag{35}$$

and it follows from Eq. (30) that $(\partial^2 D/\partial u^2)_C > 0$ and from Eq. (31) that $(\partial^2 D/\partial \lambda_1 \partial u)_C = 0$. Moreover, because $n_1 > n_2$ and $q_2 < 0$, it follows from Eqs. (32) and (33) that $(\partial^2 D/\partial \lambda_1^2)_C < 0$. Thus the second derivatives satisfy the inequality

$$\left(\frac{\partial^2 D}{\partial \lambda_1 \partial u}\right)_C - \left(\frac{\partial^2 D}{\partial \lambda_1^2}\right)_C \left(\frac{\partial^2 D}{\partial u^2}\right)_C > 0$$

and the critical point C is a saddle point. The combination of Eqs. (26) and (34) leads to the equation

$$D = (K + 1) \, u_C \tag{36}$$

which shows that the sonic condition is satisfied at C and allows us to identify the saddle point with the CJ point in the flow. We accordingly set $(\lambda_1)_C = \hat{\lambda}_1$, $(\lambda_2)_C = \hat{\lambda}_2$, and $u_C = u_{CJ}$. Recalling that the flow is governed by Eq. (21), we can now calculate $\hat{\lambda}_1$, $\hat{\lambda}_2$, and u_{CJ} and thereby obtain a solution for this type of nonideal detonation. The combination of Eqs. (35) and (29) leads to the following equations for $\hat{\lambda}_1$ and $\hat{\lambda}_2$,

$$\hat{\lambda}_1 = 1 - \left(-\frac{n_1 q_1}{n_2 q_2}\right)^{\frac{n_1}{n_2 - n_1}} \tag{37}$$

$$\hat{\lambda}_2 = 1 - \left(-\frac{n_1 q_1}{n_2 q_2}\right)^{\frac{n_2}{n_2 - n_1}} \tag{38}$$

and the corresponding values of u_{CJ} and D follow from Eqs. (34) and (36).

We now consider the significance of identifying the saddle point as the CJ point in the ZND wave. In the ZND wave, the flow before the CJ point where λ_1 and λ_2 satisfy the conditions $0 < \lambda_1 < \hat{\lambda}_1$ and $0 < \lambda_2 < \hat{\lambda}_2$ is governed by Eq. (24) with the positive sign. But because the CJ point is a saddle point, the flow after the CJ point, where λ_1 and λ_2 satisfy the conditions $\hat{\lambda}_1 < \lambda_1 < 1$ and $\hat{\lambda}_2 < \lambda_2 < 1$, can be governed by Eq. (24) with either the positive sign or the negative sign. After the CJ point, the particle velocity decreases in the flow governed by the positive sign, but increases in the flow governed by the negative sign. As discussed by Fickett and Davis,[5] the flow behind the CJ point is determined by the rear-boundary condition because both waves must be supported by a constant velocity piston. Lagrange particle velocity histories were calculated for both types of wave, but they are not presented here.

IV OVERDRIVEN DETONATION

For overdriven detonation, we considered the properties of the detonation velocity-particle velocity (D-u) Hugoniot for detonation products and looked for a similarity solution for overdriven detonation. We discuss the Hugoniot first and then the similarity solution.

Properties of the (D-u) Hugoniot of a Reactive Discontinuity.

We derive equations for the slope and second derivative of the (D-u) Hugoniot at the CJ point. It is convenient to write the RH equations expressing the conservation of mass and momentum across the reactive discontinuity as

$$v = v_o \left(1 - \frac{u}{D}\right) \tag{39}$$

$$p = \rho_o \, Du \tag{40}$$

where $\rho_o = 1/v_o$ denotes the initial density of the explosive. Differentiation of Eqs. (39) and (40) with respect to u leads to the following equations

$$\frac{dv}{du} = -\frac{v_o}{D} + \frac{v_o u}{D^2} \frac{dD}{du} \tag{41}$$

$$\frac{d^2 v}{du^2} = \frac{2v_o}{D^2} \frac{dD}{du} - \frac{2v_o u}{D^3} \left(\frac{dD}{du}\right)^2 + \frac{v_o u}{D^2} \frac{d^2 D}{du^2} \tag{42}$$

$$\frac{dp}{du} = \rho_o D + \rho_o u \frac{dD}{du} \tag{43}$$

$$\frac{d^2 p}{du^2} = 2\rho_o \frac{dD}{du} + \rho_o u \frac{d^2 D}{du^2} \tag{44}$$

Equations for the derivatives at the CJ point follow readily by combining Eqs. (41) through (44) with the equation

$$\left(\frac{dp}{du}\right)_{CJ} = \rho_o D_{CJ} \qquad (45)$$

expressing the condition that the Rayleigh line is tangent to the detonation products Hugoniot at the CJ point. Combination of Eqs. (45) and (43) gives the equation

$$\left(\frac{dD}{du}\right)_{CJ} = 0 \qquad (46)$$

and it follows from Eqs. (41), (42), and (44) that

$$\left(\frac{dv}{du}\right)_{CJ} = -\left(\frac{v_o}{D}\right)_{CJ} \qquad (47)$$

$$\left(\frac{d^2v}{du^2}\right)_{CJ} = v_o \left(\frac{u}{D^2}\right)_{CJ} \left(\frac{d^2D}{du^2}\right)_{CJ} \qquad (48)$$

$$\left(\frac{d^2p}{du^2}\right)_{CJ} = \rho_o\, u_{CJ} \left(\frac{d^2D}{du^2}\right)_{CJ} \qquad (49)$$

We now differentiate the identity

$$\frac{dp}{du} = \frac{dp}{dv}\,\frac{dv}{du} \qquad (50)$$

to obtain the following equation

$$\frac{d^2p}{du^2} = \frac{d^2p}{dv^2}\left(\frac{dv}{du}\right)^2 + \frac{dp}{dv}\,\frac{d^2V}{du^2} \qquad (51)$$

for the second derivatives along the Hugoniot curve. The combination of Eq. (51) at the CJ point with the CJ condition written as $(dp/dv)_{CJ} = -(D/v_o)^2_{CJ}$ and Eqs. (47) and (48) leads after some manipulation to the equation

$$\left(\frac{d^2D}{du^2}\right)_{CJ} = \left(\frac{v_o^2}{2(pD)}\right)_{CJ} \left(\frac{d^2p}{dv^2}\right)_{CJ} \qquad (52)$$

relating the second derivation of the (D-u) and (p-v) Hugoniots at the CJ point. Because $(d^2p/dv^2)_{CJ} > 0$ and $(d^2p/du^2)_{CJ} > 0$, it follows from Eqs. (46), (49), and (52) that the (D-u) Hugoniot curve for a reactive discontinuity has a minimum at the CJ point. This being the case, we suggest that (D-u) Hugoniots for detonation products may be conveniently fitted with the following function form:

$$D = D_{CJ} + A\,(u/u_{CJ} - 1)^n \qquad (53)$$

where A and $n > 1$ are parameters to be determined from experimental data.

Similarity Solutions for Overdriven Detonation

In our approach, a similarity solution to a set of governing equations is constructed in terms of a Lie group admitted by the equations. We thus used methods of differential geometry to look for a Lie group admitted by the equations governing overdriven planar and spherical detonation waves. These detonation waves were treated as a nonreactive flow induced by a reactive shock discontinuity or as a ZND wave --a reactive flow induced by a nonreactive shock discontinuity. In either case, we must find a Lie group admitted by the differential flow equations and the RH jump conditions. We summarize the results of our investigation as follows:

- The equations governing a reactive discontinuity with polytropic detonation products do not admit a similarily solution for nonsteady overdriven detonation because the group admitted by the RH jump conditions is not admitted by the energy equation.
- The equation governing a spherical ZND wave do not in general admit a self-similar flow because the group admitted by the RH jump conditions is not admitted by the continuity equation for divergent flow.

- Under the strong shock condition, the equations governing a spherical ZND wave admit a similarity solution when the explosive and its reaction products are treated as polytropic materials with the same index.

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