CHARACTERIZATION OF INITIATION AND DETONATION BY LAGRANGE GAGE TECHNIQUES

UCRL---15482

DE83 001129

Final Report

January 1982

By: M. Cowperthwaite

Prepared for:

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Attention: V. M. Churchill, L-446
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LLNL Subcontract 9371209

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Approved by:

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ABSTRACT

The theoretical work in this report is concerned with a reactive flow Lagrange analysis (RFLA) for shocked explosives that was formulated and developed at SRI International and Lawrence Livermore National Laboratory (LLNL). This RFLA takes a set of Lagrange particle velocity and pressure histories recorded in shocked explosive as input and calculates the flow fields in the explosive and its global rate of decomposition. A similarity solution modeling a type of initiation observed in PBX9404 and incorporating a realistic description of shocked explosive was constructed to provide a means of testing the computational procedures used in the RFLA. These procedures and the RFLA were validated in test calculations performed with the similarity solution at LLNL.

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ACKNOWLEDGMENTS

We are grateful to the personnel at LLL and SRI who have contributed to this program. At LLL, we thank in particular Dr. H. C. Vantine, Mr. L. M. Erickson, Mr. R. R. Ramsberger, and the consultants to LLNL at Kansas State University, Drs. R. S. Lee and W. D. Curtis. At SRI, we thank Mr. J. T. Rosenberg and also Mrs. B. Y. Lew for performing the numerical calculations.

FIGURES

I SUMMARY

The long-range objective of this research is to develop the basic understanding of detonation that is essential for the improved control and effective use of explosives in military applications. Lagrange gage studies of the initiation and propagation of detonation were undertaken jointly by SRI and LLNL to provide the information required for such an understanding of explosives. In these studies, the experimental work was performed at Lawrence Livermore National Laboratory, and the majority of the theoretical work was performed at SRI International.

The experimental studies performed at LLNL during the present program have resulted in the development of particle velocity and stress gages for recording Lagrange histories in the shocked explosive environment. These Lagrange histories provide the information to:

- Establish the hydrodynamic phenomenology of the shock initiation process.
- Validate reactive hydrodynamic codes.
- Calculate the global reaction rate of the shocked explosive.

The theoretical studies performed at SRI and LLNL during the present program have resulted in:

- The formulation of a constitutive relationship for shocked reacting explosive.
- The incorporation of a realistic description of shocked reacting explosive into a similarity solution modeling a type of initiating flow observed in shocked PBX9404.
- The development and validation of a RFLA for calculating global decomposition rates of shocked explosives from a series of particle velocity histories and a pressure history.

Formulation of this constitutive relationship and validation of this RFLA were presented in papers (1,2) at the Seventh Symposium (International) on Detonation held June 16-19, 1981 at the United States Naval Academy, Annapolis, Maryland.

II THEORETICAL WORK

A. Introduction

In the theoretical work performed at SRI under the current contract, a realistic description of shocked reacting explosive was incorporated into a similarity solution modeling a type of initiating flow observed in shocked PBX9404. A realistic description of the explosive was obtained by incorporating a Mie Gruneisen equation of state for the solid, and a polytropic equation of state for the reaction products into the constitutive relationship for shocked explosive developed earlier in the program (1). For the purposes of the similarity solution, the decomposition reaction was assumed to produce reaction products with a fixed relative composition along a particle path and also was assumed to proceed to completion. The constitutive relationship and model similarity solution were used in calculations at LLNL (2) to test the validity of our RFLA for calculating the flow fields and reaction rates in a shocked explosive from a set of particle velocity histories and a pressure history.

Such model solutions to the flow equations are convenient for testing procedures used to calculate flow and thermodynamic variables in a RFLA. They provide a means for determining the best methods for estimating flow derivatives from Lagrange histories recorded in the type of flow modeled by the solution. The accuracy of schemes of estimating the flow derivatives needed to integrate the flow equations, and the accuracy of the methods used to calculate the reaction rate are tested as follows.

Lagrange analyses are first performed with a set of flow histories generated from the solution, and then the flow variables and reaction rates calculated in these analyses are compared with those given by the solution. We first present the model similarity solution and then the constitutive relationship that was incorporated into it.

B. Construction of the Similarity Solution

The similarity solution was constructed using differential geometry and Lie-group-theory. The procedure used before to construct a model similarity solution (3) was extended by removing the constraint that the constitutive relationship of the shocked reacting explosive be invariant under the Lie group G admitted by the flow equations and the Rankine-Hugoniot (RH) jump conditions. The removal of this constraint on the constitutive relationship allows a realistic description of the explosive to be incorporated into the similarity solution. We now present the similarity solution. The details of this construction will not be presented however, because they will be given in another paper.

Our similarity solution is based on the assumptions that the shock is a nonreactive discontinuity and that the one-dimensional flow induced by the shock is adiabatic and inviscid. To describe this type of flow we let t, h, D, u, v, p, e, and λ denote time, Lagrange distance, shock velocity, particle velocity, specific volume, pressure, specific internal energy and the fraction of unreacted explosive. We also use the superscript o to denote the initial unshocked condition, and the subscript i to denote the initial shocked condition. In this case, the equations expressing the conservation of mass, momentum, and energy in the one-dimensional flow behind the shock can be written as

$$\frac{\partial v}{\partial t} = v^o \frac{\partial u}{\partial h} \tag{1}$$

$$\frac{\partial u}{\partial t} = - v^o \frac{\partial p}{\partial h} \tag{2}$$

$$\frac{\partial e}{\partial t} = - p \frac{\partial v}{\partial t} \tag{3}$$

and the RH jump conditions as

$$v^o D = v(D - u) \tag{4}$$

$$u^2 = p(v^o - v) \tag{5}$$

$$e - e^o = \frac{p}{2}(v^o - v) \tag{6}$$

Our similarity solution was constructed in terms of invariants of the infinitesimal generator of the Lie group admitted by Eq. (1) through (6). It can be written in terms of the similarity parameter

$$\eta = \frac{(1 - t/\alpha)}{(1 - h/\beta)^{a/b}} \tag{7}$$

as

$$u = u_i U(\eta)/(1 - h/\beta)^{c/b} \tag{8}$$

$$v - v^o = (v_i - v^o)V(\eta)/(1 - h/\beta)^{\delta/b} \tag{9}$$

$$p = p_i P(\eta)/(1 - h/\beta)^{\varepsilon/b} \tag{10}$$

$$e - e^o = (e_i - e^o)E(\eta)/(1 - h/\beta)^{f/b} \tag{11}$$

where α denotes a characteristic time, β denotes a characteristic distance, a, b, c, δ, ε, and f are group parameters, and the functions $U(\eta)$, $V(\eta)$, $P(\eta)$, and $E(\eta)$ are related by the flow equations (1) through (3). Equations (7) through (11) are written so that $\eta = 1$ and $V(1) = U(1) = P(1) = E(1)$ along the shock path.

We now derive equations for the shocked state, denoted by the subscript H, and use the RH jump conditions to derive relationships among the group parameters. The equation for the shock trajectory is obtained as

$$(1 - h/\beta) = (1 - t/\alpha)^{b/a} \tag{12}$$

by setting $\eta = 1$ in Eq. (7), and the equations for the shocked state as

$$u_H = \frac{u_i}{(1 - h/\beta)^{c/b}} \tag{13}$$

$$v_H - v^o = \frac{(v_i - v^o)}{(1 - h/\beta)^{\delta/b}} \tag{14}$$

$$p_H = \frac{p_i}{(1 - h/\beta)^{\varepsilon/b}} \tag{15}$$

$$e_H - e^o = \frac{(e_i - e^o)}{(1 - h/\beta)^{f/b}} \tag{16}$$

by setting $u = u_H$ and $U(\eta) = 1$, $v = v_H$ and $V(\eta) = 1$, $p = p_H$ and $P(\eta) = 1$, and $e = e_H$ and $E(\eta) = 1$, respectively, in Eqs. (8), (9), (10), and (11).

Differentiating Eq. 12 gives the following equations for the shock velocity D

$$D = D_i(1 - t/\alpha)^{b/a-1} = D_i(1 - h/\beta)^{1-a/b} \tag{17}$$

where the initial shock velocity D_i is related to α and β by the equation $D_i = b\beta/a\alpha$. Combining Eqs. (13) and (17) then gives the equation relating shock velocity and shock particle velocity as

$$D = D_i \left(\frac{u_H}{u_i}\right)^{(a-b)/c} \tag{18}$$

and combining Eqs. (14) and (15) gives the corresponding equation for the Hugoniot curve in the (p–v) plane as

$$p_H = \bar{B}(1 - v_H/v^o)^{\varepsilon/\delta} \tag{19}$$

where $\bar{B} = p_i/(1 - v_i/v^o)^{\varepsilon/\delta}$. It follows from Eqs. (18) and (19) that $(a - b)/c$ and ε/b must be related because D and p_H are related by the RH jump conditions. Relationships among the group parameters a, b, c, δ, e, and f are obtained by combining Eqs. (13) through (17) with the RH jump conditions written as

$$(v^o - v_H)\, D = v^o u_H \tag{20}$$

$$v^o p_H = D u_H \tag{21}$$

$$2(e_H - e^o) = p_H(v^o - v_H) \tag{22}$$

Substituting Eqs. (13) through (17) into Eqs. (20) through (22) shows that the following relationships

$$a + \delta = b + c \tag{23}$$

$$a + c = b + \varepsilon \tag{24}$$

$$f = \delta + \varepsilon \tag{25}$$

are imposed on the group parameters by the conservation of mass, momentum, and energy across the shock discontinuity at the wave front. The addition and substraction of Eqs. (23) and (24) gives the equations

$$2(a - b) = \varepsilon - \delta \tag{26}$$

$$2c = \varepsilon + \delta \tag{27}$$

that allows us to write the relationship between shock velocity and particle velocity in terms of ε/δ as

$$\frac{D}{D_i} = \left(\frac{u_H}{u_i}\right)^{(\varepsilon/\delta-1)/(\varepsilon/\delta+1)} \tag{28}$$

The relationships imposed on the functions $U(\eta)$, $V(\eta)$, $P(\eta)$, and $E(\eta)$ by the conservation of mass, momentum, and energy are obtained by combining Eqs. (7) through (11) with the flow equations (1) through (3). Substituting the flow derivatives obtained by differentiating Eqs. (7) through (11) into Eqs. (1) through (3) and taking account of Eqs. (23) through (25) leads to the following differential equations, expressing the conservation of mass, momentum, and energy, that relate U, V, P, and E

$$\frac{dV}{d\eta} = \eta \frac{dU}{d\eta} + \frac{c}{a} U \tag{29}$$

$$\frac{dU}{d\eta} = \eta \frac{dP}{d\eta} + \frac{\varepsilon}{a} P \tag{30}$$

$$\frac{dE}{d\eta} = 2P \frac{dV}{d\eta} \tag{31}$$

It follows from Eqs. (29) through (31) that the specification of U or V or P is sufficient to determinc a particular flow. When U is specified, the integrations of of Eqs. (29) and (30) give respectively V and P, and the integration of Eq. (31) gives E. Similarly, when V is specified, the integrations of Eq. (29) and (30) give respectively U and P, Formal integration of Eqs. (29) through (31) gives the expressions for V, P, and E in terms of U as

$$V = \eta U - (1 - c/a) \int_1^\eta U \, d\eta \tag{35}$$

$$P\eta^{\varepsilon/a} = 1 + \int_1^\eta \eta^{(\varepsilon/a - 1)} \frac{dU}{d\eta} \, d\eta \tag{36}$$

$$E = 1 + 2 \int_1^\eta P \left[\frac{c}{a} U + \eta \frac{dU}{d\eta}\right] d\eta \tag{37}$$

Equations (33) and (34) were used to evaluate the integrals in Eqs. (35) through (37) and determine the functional dependence of V, U, and E on η. The integral $I_1 = \int_1^\eta U \, d\eta$ in Eq. (35) was written as

$$I_1 = \left(\frac{1 - m}{2} U_2\right) (\eta - 1) + \frac{m}{2} \left[\frac{1}{12} (\eta^4 - 1) - \frac{\bar{\eta}}{3} (\eta^3 - 1) + \frac{U_1}{2} (\eta^2 - 1)\right] \tag{38}$$

and the equation for P obtained by integrating Eq. (36) was written as

$$P = A \eta^{-\varepsilon/a} + B\eta^2 - C\eta + F \tag{39}$$

with $A = 1 - B + C - F$, $B = m/2(\varepsilon/a + 2)$, $C = m\bar{\eta}/(\varepsilon/a + 1)$, and $F = mU_1/2(\varepsilon/a)$. Equation (37) was rewritten for convenience as

$$E = 1 + 2(\bar{I}_1 + \bar{I}_2) \tag{40}$$

and the integration of Eq. (31) gives E. When P is specified, the integration of Eq. (30) gives U, the integration of Eq. (29) gives V, and E again follows by integrating Eq. (31).

D. Flow Modeling a Shock Initiation Process

Our model similarity solution for shock initiation is expressed in terms of U because a set of particle velocity histories are measured in the Lagrange gage experiments. In constructing the present solution, an expression for $d^2U/d\eta^2$ was chosen to similate significant features of some particle velocity histories recorded in PBX9404. This expression was integrated to determine the corresponding expressions for $dU/d\eta$ and U, and Eqs. 29 through 31 were integrated to determine expressions for V, P, and E. The solution was based on the equation

$$\frac{d^2U}{d\eta^2} = m(\eta - \bar{\eta}) \qquad (32)$$

because the experimentally determined particle velocity histories exhibit a maximum and a point of inflection. In a particular solution, m is constant, and the point of inflection in the particle velocity occurs along a particle path when $\eta = \bar{\eta}$. The equations for $dU/d\eta$ and U obtained by integrating Eq. (32) were written as

$$\frac{dU}{d\eta} = \frac{m}{2}\,(\eta^2 - 2\eta\,\bar{\eta} + U_1) \qquad (33)$$

and

$$U = 1 + \frac{m}{2}(\frac{1}{3}\,\eta^3 - \bar{\eta}\,\eta^2 + U_1\eta - U_2) \qquad (34)$$

where

$U_1 = 2\bar{\eta}\,\hat{\eta} - \hat{\eta}^2$, $U_2 = (1/3 + U_1 - \bar{\eta})$, and $\hat{\eta}$ locates the maximum in particle velocity along a particle path.

with

$$\bar{I}_1 = \frac{c}{a}\int_1^{\eta} \left(AU\eta^{-\varepsilon/a} + B\eta^2 U - C\eta\, U + FU\right) d\eta \tag{41}$$

and

$$\bar{I}_2 = \int_1^{\eta} \left(A\eta^{1-\varepsilon/a}\frac{dU}{d\eta} + B\eta^3\frac{dU}{d\eta} - C\eta^2\frac{dU}{d\eta} + F\eta\frac{dU}{d\eta}\right) d\eta \tag{42}$$

The identity

$$\eta^n \frac{dU}{d\eta} = d(\eta^n U) - n\eta^{n-1}\, U \tag{43}$$

was used to convert $\bar{I}_2$ into a form similar to $\bar{I}_1$ and the equation for E was rewritten as

$$E - 1 = 2(T_A + T_B - T_C + T_F) \tag{44}$$

with

$$T_A = A\left[\eta^{1-\varepsilon/a}U - 1 - (1 - \varepsilon/a - c/a)\int_1^{\eta} \eta^{-\varepsilon/a}U\, d\eta\right] \tag{45}$$

$$T_B = B\left[\eta^3 U - 1 - (3 - c/a)\int_1^{\eta} \eta^2 U\, d\eta\right] \tag{46}$$

$$T_C = C\left[\eta^2 U - 1 - (2 - c/a)\int_1^{\eta} \eta U\, d\eta\right] \tag{47}$$

$$T_F = F\left[\eta U - 1 - (1 - c/a)\int_1^{\eta} U\, d\eta\right] \tag{48}$$

We then set $I_{n+1} = \int_1^{\eta} \eta^n U \, d\eta$ and used the equation

$$I_{n+1} = \frac{1}{n+1} \left(\frac{1 - mU_2}{2}\right)\left(\eta^{n+1} - 1\right)$$

$$+ \frac{m}{2} \left(\frac{1}{3(n+4)} \left(\eta^{n+4} - 1\right) - \frac{\bar{\eta}}{(n+3)} \left(\eta^{n+3} - 1\right)\right)$$

$$+ \frac{m}{2} \frac{U_1}{(n+2)} \left(\eta^{n+2} - 1\right) \tag{49}$$

with $n = -\varepsilon/a$, $n = 2$, $n = 1$, and $n = 0$, to evaluate respectively the integrals $I_{1-\varepsilon/a}$, I_3, I_2, and I_1 in Eqs. (45), (46), (47), and (48). These equations for E were programmed into a code for making Lagrange plots of the flow variables. They were checked by comparing calculated values of internal energy against values obtained by integrating Eq. (31) numerically.

When the expressions for U, P, V, and E are known, the initial shocked state must be specified, and values of the group parameters and the flow parameters m, $\bar{\eta}$, and $\hat{\eta}$ must be assigned before flow fields can be calculated for a particular solution. Values of p_i and D_i and ε/δ were first assigned to ensure that shocked states described by the solution are representative of those attained in a real explosive. These values were based on the linear relationship between shock velocity and shock particle velocity for cast TNT, $D = 2.3 + 2.15\ u_H$, given by Dremin (4). With p_i = 20 kilobars and D_i = 3 mm/μs, the values u_i = 0.414 mm/μs and v_i/v^o = 0.8620 g/cm^3 were calculated from the jump conditions. The ratio $\varepsilon/\delta = 2.7$ was then chosen to ensure that shocked states at the front of the wave match those governed by Dremin's linear relationship in the 20–110 kilobar region. In this case $\bar{B}$ = 4201.04 kilobars in Eq. (19) and the exponent of the shock particle velocity in Eq. (28) $(\varepsilon/\delta - 1)(\varepsilon/\delta + 1)$ = 0.4594. The values $\varepsilon/b = 6/7$ and α = 4μs were then chosen to define the variation of the shocked state with distance. In this case, $\delta/b = 6/18.9$, and Equations (26) and (27) give a/b = 24/18.9 and c/b = 11•1/18.9. The initial condition $D_i = b\beta/a\alpha$ with D_i = 3mm/μs then gives β = 15•24 mm. Another procedure was used at LLNL to chose the group parameters in the similarity solution used to test our RFLA. In this procedure, α, β, D_i, and ε/δ were first specified, then the initial condition was used to calculate a/b, and Eq. (26) and (27) were used to calculate c/b, δ/b, and ε/b.

With the shocked state defined, values of $\bar{\eta}$, $\hat{\eta}$, and m must be assigned to define the flow attained behind the shock. The values of $\bar{\eta}$ and $\hat{\eta}$ must be chosen to satisfy the condition $2\bar{\eta} > 1 + \hat{\eta}$ to ensure that the particle velocity profiles exhibit maxima. In the present case, we set $\bar{\eta} = 0.85$ and $\hat{\eta} = 0.6$. The value of m = 36 was chosen to ensure that a particle is further compressed as it leaves the shocked state and that its path in the (p-v) plane lies to the right of the Hugoniot curve.

D. The Constitutive Relationship for Shocked Reacting Explosives

Our model of shocked explosive is based on the idea that reaction starts in hot spots and then propagates into the bulk of the explosive. The reaction propagates because heat is transferred between the hot reaction products and the explosive, but it is assumed that no appreciable amount of heat is transferred into the bulk of the explosive. The explosive and its reaction products are treated as phases that are governed by their own equations of state and attain mechanical, but not thermal, equilibrium. Under the assumption that no appreciable amount of heat is transferred into the bulk of the explosive, the explosive is compressed and released isentropically as the reaction proceeds, and the pressure increases or decreases along a particle path.

With the notation already introduced, we let the subscripts x and p denote explosive and its products and write the specific internal energy and the specific volume of the reacting explosive as

$$e = \lambda e_p + (1 - \lambda)e_x \qquad (50)$$

$$v = \lambda v_p + (1 - \lambda)v_x \qquad (51)$$

Under the assumption of mechanical equilibrium, $p_x = p_p = p$, we write the equations of state of the explosive and its products as

$$e_x = e_x^o + \tilde{e}_x(p, v_x) \tag{52}$$

$$e_p = \Sigma_1^c \alpha_i (e_p^o)_i + \tilde{e}_p(p, v_p, \alpha_1, \ldots \alpha_c) \tag{53}$$

where $\alpha_1, \ldots \alpha_c$, denote the mass fractions of the reaction products. We assume for the sake of simplicity that the detonation products are polytropic with a constant index k, and that the explosive is a Mie-Gruneisen solid with a constant Gruneisen parameter Γ. In this case,

$$\tilde{e}_p = \frac{pv_p}{(k - 1)} \tag{54}$$

and the equation of state of the solid can be written as

$$\tilde{e}_x = \frac{pv_x}{\Gamma} + g(v_x) \tag{55}$$

The equations for the pressure and energy along the Hugoniot curve, written formally as,

$$p = p_H(v_x) \tag{56}$$

$$\tilde{e}_x = \frac{p_H(v_x)}{2} (v_x^o - v_x) \tag{57}$$

define the function $g(v_x)$ over the region spanned by the Hugoniot curve as

$$g(v_x) = \frac{p_H(v_x)}{\Gamma} \left[\left(\frac{\Gamma + 2}{2}\right) (v_x^o - v_v) - v_x^o \right] \tag{58}$$

and thus allow values of $\tilde{e}_x$ to be calculated over this region.

The elimination of v_p among Eqs. (50) through (54) allows us to write the $\tilde{e} = e(p, v, v_x, \lambda)$ relationship for the reacting explosive as

$$e - e_x^o = -\lambda\left[q(\alpha_1,\ldots\alpha_c) + \tilde{e}_x - \frac{pv_x}{(k-1)}\right] + \tilde{e}_x + \frac{p(v - v_x)}{(k-1)} \tag{59}$$

with $q(\alpha_1,\ldots\alpha_c) = -(\Sigma_1^c\ \alpha_i(e_p^o)_i - \tilde{e}_x^o)$ and e_x given by Eqs. (55) and (58). Equation (59) is used to calculate λ along a particle path with values of e, p, and v supplied by a Lagrange analysis, and values of $v_x(p)$ and $\tilde{e}_x(p)$ calculated along the isentrope passing through the shocked state. It is therefore necessary to calculate the equation for the isentropes of the explosive in the (p - v) plane. The isentropic condition, $d\tilde{e}_x = -pdv_x$, and the differential form of Eq. (55) give the following differential equation for the isentropes

$$v_x dp + (\Gamma + 1)pdv_x = -\Gamma\ dg \tag{60}$$

Equation (60) can be integrated to give

$$pv_x^{\Gamma+1} - p_H\left(v_x^H\right)^{\Gamma+1} = -\Gamma\left[v^\Gamma g\right]_{v_x^H}^{v_x} + \Gamma^2 I \tag{61}$$

where

$$I = \int_{v_x^H}^{v_x} v_x^{\Gamma-1}\ g\ dv_x \tag{62}$$

When the Hugoniot curve of the explosive is known, I can be evaluated, Equation (61) can be used to determine v_x as a function of p along an isentrope, and Eqs. (55) and (58) can be used to calculate the corresponding values of $\tilde{e}_x(p)$.

E. Mie-Gruneisen Equations of State for Condensed Explosive

Mie Gruneisen equations of state of condensed explosives constructed in the present work with different Hugoniot curves will now be presented.

1. Hugoniot Curve Used in Model Similarity Solution

When $D = D_i(u_H/u_i)^{(\varepsilon/\delta-1)(\varepsilon/\delta+1)}$ and p_H can be written as $p_H = \bar{B}(v_x^o - v_x)^n$ with $n = \varepsilon/\delta$, as in the model similarity solution, $g(v_x)$ is given by the equation

$$g(v_x) = \frac{\bar{B}}{\Gamma}\left[\frac{(\Gamma + 2)}{2}(v_x^o - v_x)^{n+1} - v_x^o(v_x^o - v_x)^n\right] \tag{63}$$

and the integral

$$I = \frac{\bar{B}}{\Gamma}\int_{v_x^H}^{v_x} v_x^{\Gamma-1}\left[\frac{(\Gamma + 2)}{2}(v_x^o - v_x)^{n+1} - v_x^o(v_x^o - v_x)^n\right] dv_x \tag{64}$$

must be evaluated to obtain the relationships $v_x(p)$ and $e_x(p)$ along an isentrope. Examining Eq. (64) leads to the conclusion that I can be evaluated in closed form, either when Γ is arbitrary and n is an integer, or when $\Gamma = 1$ and n is arbitrary. The latter case is considered here because a value of $n = 2.7$ gives a good fit to the experimental Hugoniot curve of cast TNT in the 20-150 kbar region. We now evaluate the terms in Eq. (61) when $\Gamma = 1$. The first term on the right-hand side of Eq. (61) is written as

$$\Big[v_x g(v_x)\Big]_{v_x^H}^{v} = -\frac{\bar{B}}{2}\Big[3(v_x^o - v_x)^{n+2} - 5(v_x^o - v_x)^{n+1}$$

$$+ 2(v_x^o)^2(v_x^o - v_x)^n\Big]_{v_x^H}^{v} \tag{65}$$

and the integral is written as

$$I = -\frac{\bar{B}}{2}\left[\frac{3}{(n+2)}\,(v_x^o - v_x)^{n+2} - 2\,\frac{v_x^o}{(n+1)}\,(v_x^o - v_x)^{n+1}\right]_{v_x^H}^{v} \tag{66}$$

The equation for the isentropes can then be written as

$$\left[pv_x^2\right]_{v_x^H}^{v_x} = \frac{\bar{B}}{2}\left[\frac{3(n+1)}{(n+2)}\,(v_x^o - v_x)^{n+2} - \frac{(5n+3)}{(n+1)}\,v_x^o(v_x^o - v_x)^{n+1} + 2(v_x^o)^2(v_x^o - v_x)^n\right]_{v_x^H}^{v} \tag{67}$$

2. Linear $D = a_H + b_H u_H$ Hugoniot Curve

When the explosive is assumed to have a linear D-u_H Hugoniot curve of the form

$$D = a_H + b_H u_H \tag{68}$$

the shock pressure is given by the equation

$$p_H = A_H^2\,\frac{(v_x^o - v_x)}{(B_H v_x^o + v_H)^2} \tag{69}$$

with $A_H = a_H/b_H$ and $B_H = (1-b_H)/b_H$. Combining Eqs. (69) and (58) gives the equation for $g(v_x)$ as

$$g(v_x) = \frac{A_H^2}{2} \times \frac{(v_x^o - v_x)^2}{(B_H v_x^o + v_x)^2} - \frac{A_H^2\, v_x(v_x^o - v_x)}{1\;(B_H v_x^o + v_x)^2} \tag{70}$$

Here again, to obtain an explicit expression for the isentropes we set $\Gamma = 1$, and use Eq. (70) to perform the integration in Eq. (62). In this case, I can be written as

$$I = \frac{3}{2} A_H^2 I_1 - v_x^o A_H I_2 \tag{71}$$

where

$$I_1 = - \left[\frac{(v_x^o - v_x)}{(B_H v_x^o + v_x)} - 2v_x + 2(B_H + 1)\, v_x^o \ln(B_H v_x^o + v_x) \right]_{v_x^H}^{v_x} \tag{72}$$

and

$$I_2 = - \left[\frac{(v_x^o - v_x)}{(B_H v_x^o + v_x)^2} + \ln(B_H v_x^o + v_x) \right]_{v_x^H}^{v_x} \tag{73}$$

The equation for the isentropes can thus be written as

$$p v_x^2 - p_H (v_x^H)^2 = - \left[v_x g \right]_{v_x^H}^{v_x} + I \tag{74}$$

with g given by Eq. (70) and I given by Eq. (71) through (73). Having the equations for calculating $v_x(p)$ and $\tilde{e}_x(p)$ along a particle path, we can now consider the calculation of λ.

F. Calculation of λ in our RFLA

It is clear from Eq. (59) that a value of $q(\alpha_1,\ldots\alpha_c)$ must be known before λ can be calculated in a RFLA. It is also clear that the heat of reaction will vary along a particle path if the relative composition also varies. We bypass this complication, however, by assuming that the relative composition is fixed along a particle path and set $q(\alpha_1,\ldots\alpha_c) = q(h)$ accordingly. We use the superscript ^ to denote quantities evaluated along a particle path, and use H as both a superscript and a subscript to denote quantities evaluated along the shock path. Combining the equation for energy along a particle path

$$\hat{e} - e_x^o = - \int_{v_x^H}^{\hat{v}} p d\hat{v} + \frac{1}{2} p_H (v_x^o - v_x^H) \tag{75}$$

with Eq. (59) gives the following equation for calculating the reaction coordinate along a particle path

$$\hat{\lambda} \left[q(h) + \hat{e}_x - \frac{p\hat{v}_x}{(k-1)} \right] = \hat{e}_x + \frac{p(\hat{v} - \hat{v}_x)}{(k-1)} + \int_{v_x^H}^{\hat{v}} p d\hat{v} - \frac{p_H}{2}(v_x^o - v_x^H) \tag{76}$$

At this stage q(h) must be known before Eq. (64) can be used to calculate $\hat{\lambda}$ from the Lagrange flow variables and from an isentrope of the condensed explosive. Values of q(h) must be compatible with the conditions $0 < \hat{\lambda} \leq 1$ when $\partial\lambda/\partial t = 0$. They were chosen to make $\hat{\lambda} = 1$ when $\partial\lambda/\partial t = 0$, and were calculated by setting $\hat{\lambda} = 1$ in Eq. (76) when the flow satisfied the equation $\hat{v}\, \partial p/\partial t = - k\hat{p}\partial v/\partial t$ expressing the condition that $\partial\lambda/\partial t = 0$.

G. Similarity Solution Modeling a Shock Initiation Process

We are now in a position to calculate the reaction coordinate and the reaction rate in our similarity solution based on the particle velocity tield defined by Eq. (32). For the sakc of simplicity in performing these calculations however, another equation of state was constructed for the explosive to eliminate the iterative process needed to calculate $\hat{v}_x$ as a function of p from Eq. (67) when the explosive is described by the Mie-Gruneisen equation. In this construction an isentropic $(p - v_x)$ relationship was chosen to model the isentropes given by the Mie-Gruneisen equation, and the first law of thermodynamics was integrated using the Hugoniot curve as a boundary condition to obtain an $\tilde{e}_x(p, v_x)$ relationship for the explosive. This isentropic relationship was written as

$$p = p_H \frac{(v_x^f - \hat{v}_x)^r}{(v_x^f - v_x^H)^r} \tag{77}$$

where the superscript f denotes quantities evaluated on the p = 0 isobar, and r is a parameter to be evaluated. The volume v_x^f is a function of p_H and is therefore constant along an isentrope, but it must be calculated for each isentrope. Integrating $d\hat{e}_x = - p d\hat{v}_x$ from the Hugoniot with Eq. (77) gives the equation for the energy along an isentrope as

$$\hat{e}_x - e_x^H = p \frac{(v_x^f - \hat{v}_x)}{(r + 1)} - p_H \frac{(v_x^f - v_x^H)}{(r + 1)} \tag{78}$$

The equation for calculating v_x^f was derived by equating values of e_x^f computed for two different processes. One of these was the dynamic, adiabatic process of shock compression followed by isentropic release, and the other was the static addition of heat at p = 0. The change in energy in the dynamic process was written as

$$e_x^f - e_x^o = e_x^f - e_x^H + e_x^H - e_x^o \tag{79}$$

where $e_x^H - e_x^o = \frac{1}{2} p_H(v_x^o - v_x^H)$ is given by the Hugoniot equation, and where

$$e_x^f - e_x^H = - p_H \frac{(v_x^f - v_x^H)}{(r + 1)} \tag{80}$$

is given by Eq. (78). Combining the equation for $e_x^f - e_x^o$ in the heating process

$$e_x^f - e_x^o = \frac{(c_x^o)}{\Gamma} \rho_x^o (v_x^f - v_x^o) \tag{81}$$

and Eq. (80), after some rearrangement, gives the following equation for calculating v_x^f along an isentrope passing through p_H

$$(v_x^f - v_x^o) \left[\frac{(c_x^o)\ \rho_x^o (r + 1)}{\Gamma\ p_H} + 1 \right] = (v_x^o - v_x^H) \frac{(r - 1)}{2} \tag{82}$$

where c_x^o denotes the sound speed in the unshocked explosive and ρ_x^o denotes its initial density. Equations (77), (78), and (82) provide the values of $v_x = \hat{v}_x(p)$ and $e_x = \hat{\tilde{e}}_x(p)$ for the calculations of $\hat{\lambda}$ with Eq. (76). The agreement between isentropes constructed from Eq. (67) and isentropes constructed from Eq. (77) and (82) shows that these equations provide an excellent model of the Mie Gruneisen solid for calculating λ.

Compatible values of r and ε/δ must be chosen before values of λ can be calculated with our similarity solutions. To satisfy thermodynamic constraints, these parameters must be chosen to make the Hugoniot curve steeper than the isentropes in the $(p - v_x)$ plane. We thus derive an equation for evaluating the ratio of the slope of the Hugoniot to the slope of an isentrope at a point on the Hugoniot. Differentiating Eq. (19) gives the equation for the slope of the Hugoniot curve as

$$\left(\frac{dp}{dv_x}\right)_H = - \frac{(\varepsilon/\delta) p^H}{\left(v_x^o - v_x^H\right)} \tag{83}$$

and differentiating Eq. (77) gives the equation for the slope of an isentrope at a point on the Hugoniot curve as

$$-\left(\left(\frac{\partial p}{\partial v_x}\right)_s\right)_H = \frac{r\ p_H}{(v_x^f - v_x^H)} \tag{84}$$

The ratio of the slopes of the Hugoniot and an isentrope at a point on the Hugoniot can then be written as

$$\left[\frac{dp/dv_x}{(\partial p/\partial v_x)_s}\right]_H = \frac{\varepsilon/\delta}{r}\left[\frac{1 + (v_x^f - v_x^o)}{(v_x^o - v_x^H)}\right] \tag{85}$$

with $(v_x^f - v_x^o)/(v_x^o - v_x^H)$ given by Eq. (82).

For a given value of ε/δ we choose the value of r to make $[(dp/dv_x)/(\partial p/\partial v_x)_s]_H > 1$ at the initial shock pressure because $(v_x^f - v_x^o)/(v_x^o - v_x^H)$ increases along the Hugoniot curve as p_H increases. We set a limit on r at the initial shock pressure by setting $[(dp/dv_x)/(\partial p/\partial v_x)_s]_H = 1$ in Eq. (85) and solving Eq. (85) and (82) for r.

Plots at the Lagrange distances 4.71 mm, 10.12 mm, and 12.75 mm made from the similarity solution with the following set of parameters ($\varepsilon/\delta = 2.7$, $\varepsilon/b = 6/17$, $\alpha = 4\ \mu s$, $m = 28$, $\bar{\eta} = 0.85$, $\hat{\eta} = 0.6$, and $r = 2.75$) are shown in Fig. 1 through 8. Examination of these figures shows that the flow exhibits similar features to those given by the previous similarity solution. Because this type of flows has been discussed already (3) it will receive no further attention in this report.

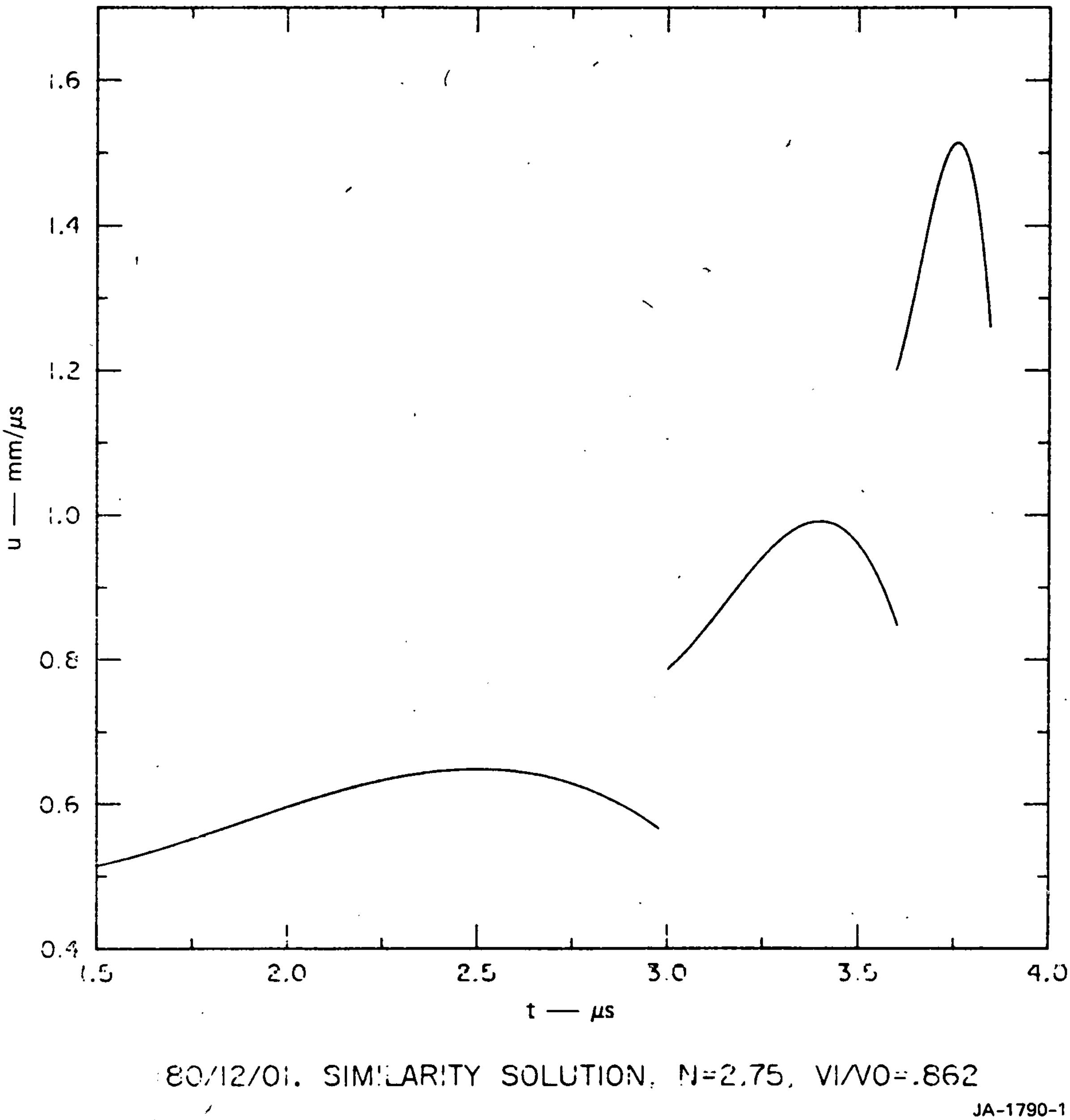
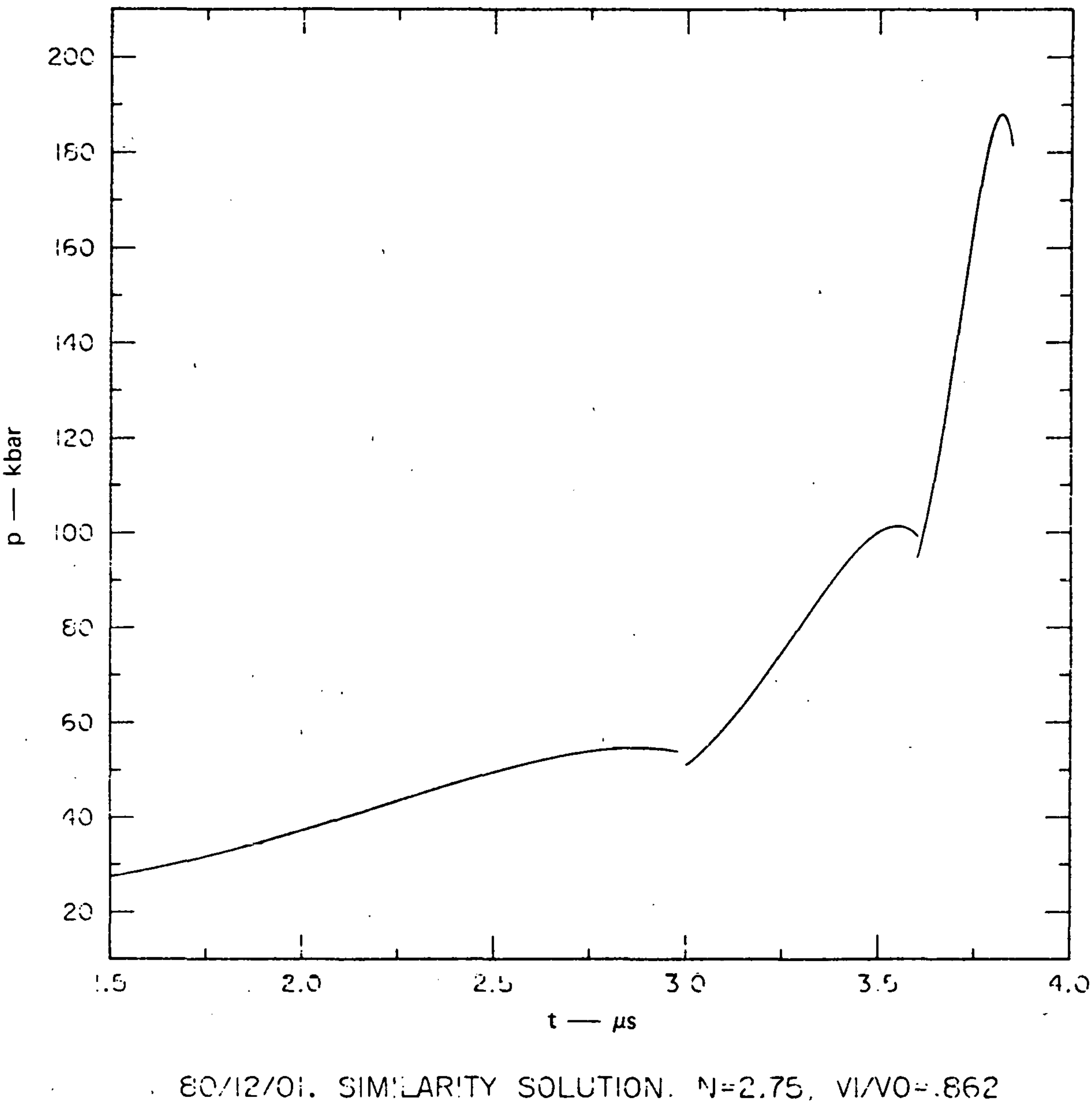
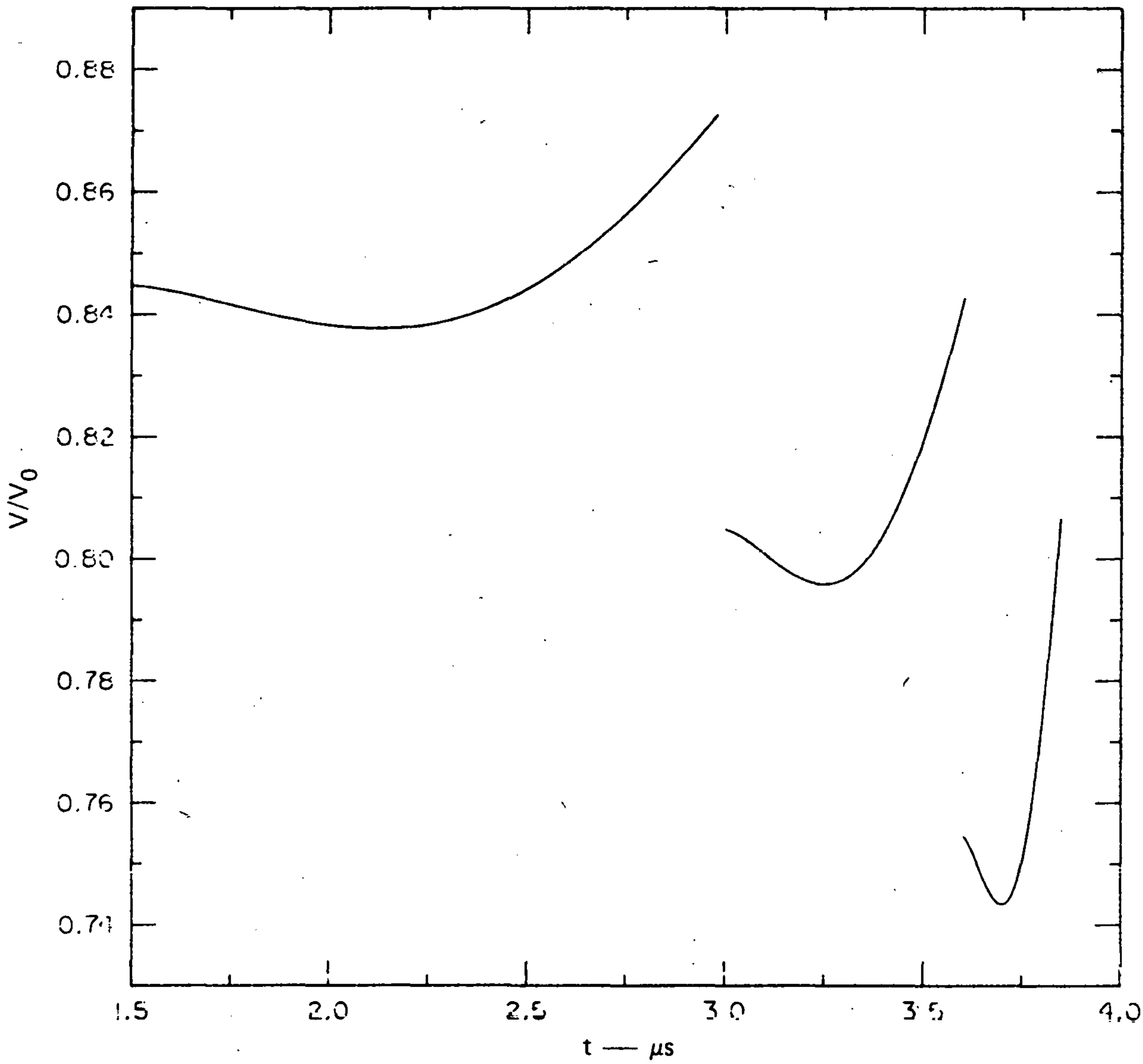


FIGURE 1 THREE PARTICLE-VELOCITY-TIME PROFILES FOR A REACTIVE SHOCK (ϵ/δ = 2.7, ϵ/b = 6/7, α = 4μs)



JA-1790-2

FIGURE 2 THREE PRESSURE-TIME PROFILES FOR A REACTIVE SHOCK
(ϵ/δ = 2.7, ϵ/b = 6/7, α = 4μs)

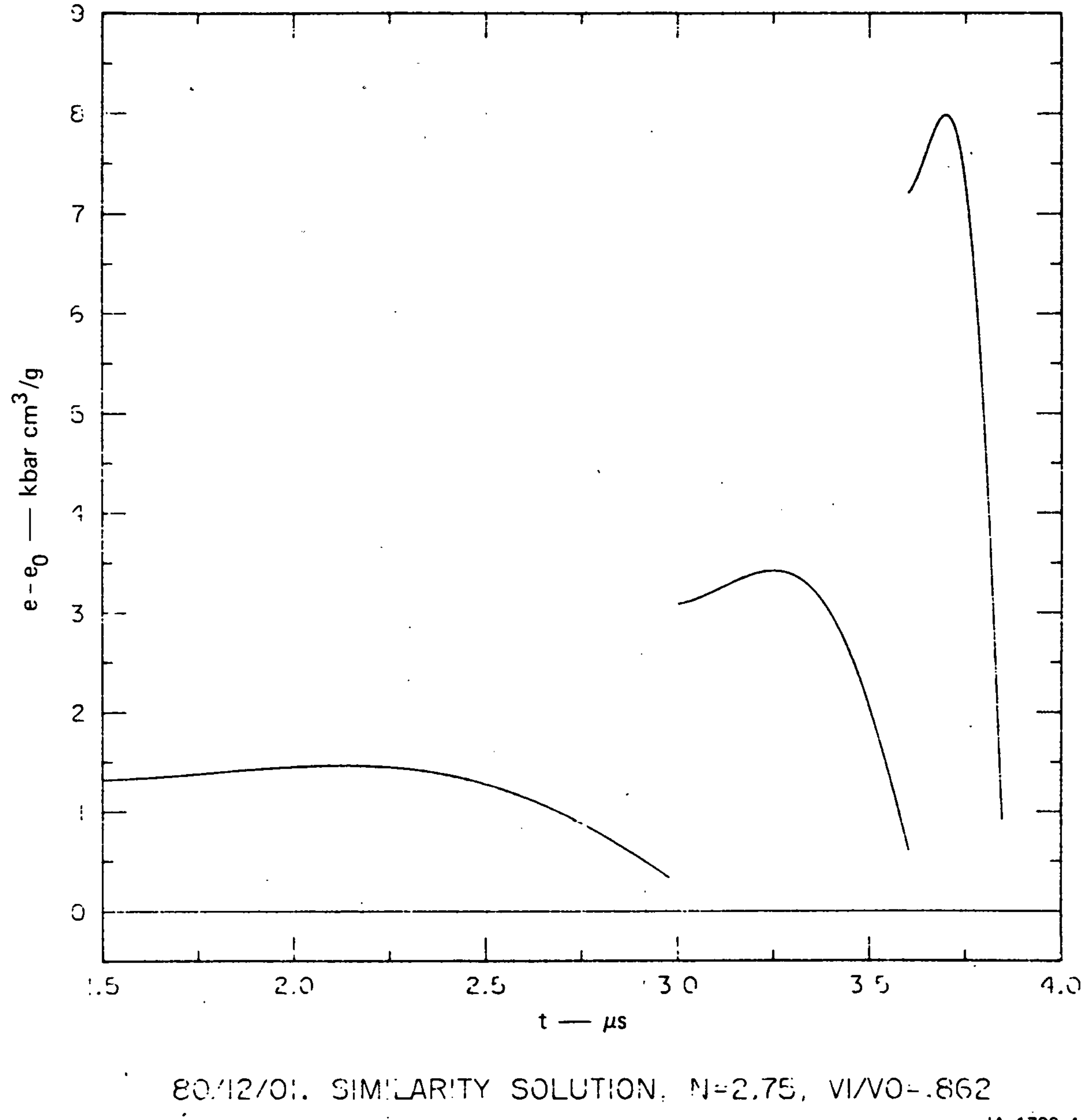


80/12/01. SIMILARITY SOLUTION, N=2.75, VI/V0=.862

JA-1790-3

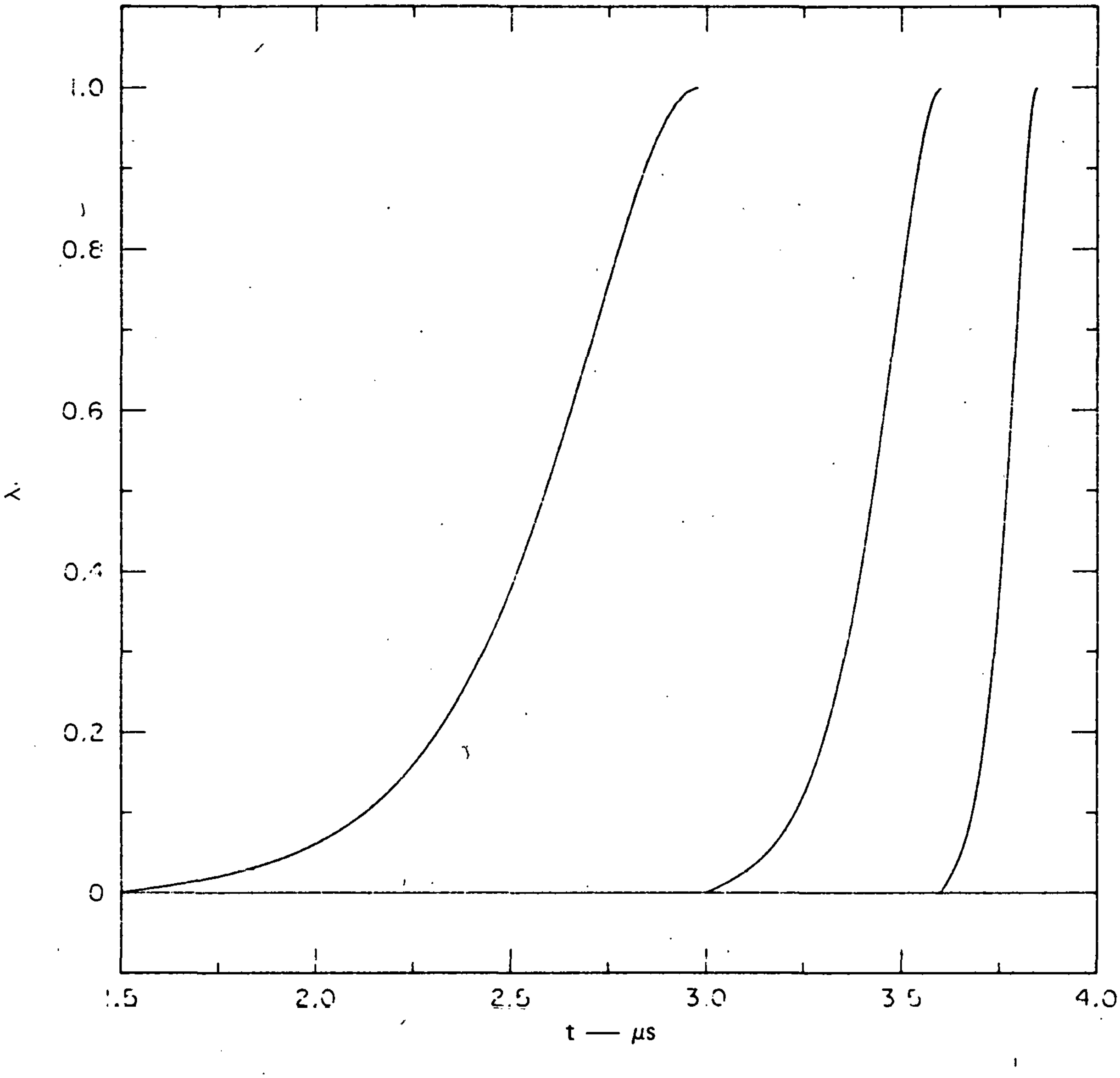
FIGURE 3 THREE RELATIVE SPECIFIC VOLUME-TIME PROFILES FOR A REACTIVE SHOCK

(ϵ/δ - 2.7, ϵ/b = 6/7, α = 4μs)



JA-1790-4

FIGURE 4 THREE SPECIFIC INTERNAL ENERGY-TIME PROFILES FOR A REACTIVE SHOCK
(ϵ/δ = 2.7, ϵ/b = 6/7, α = 4μs)



JA-1790-5

FIGURE 5 THREE REACTION COORDINATE-TIME PROFILES FOR A REACTIVE SHOCK
(ϵ/δ = 2.7, ϵ/b = 6/7, α = 4μs, r = 2.75)

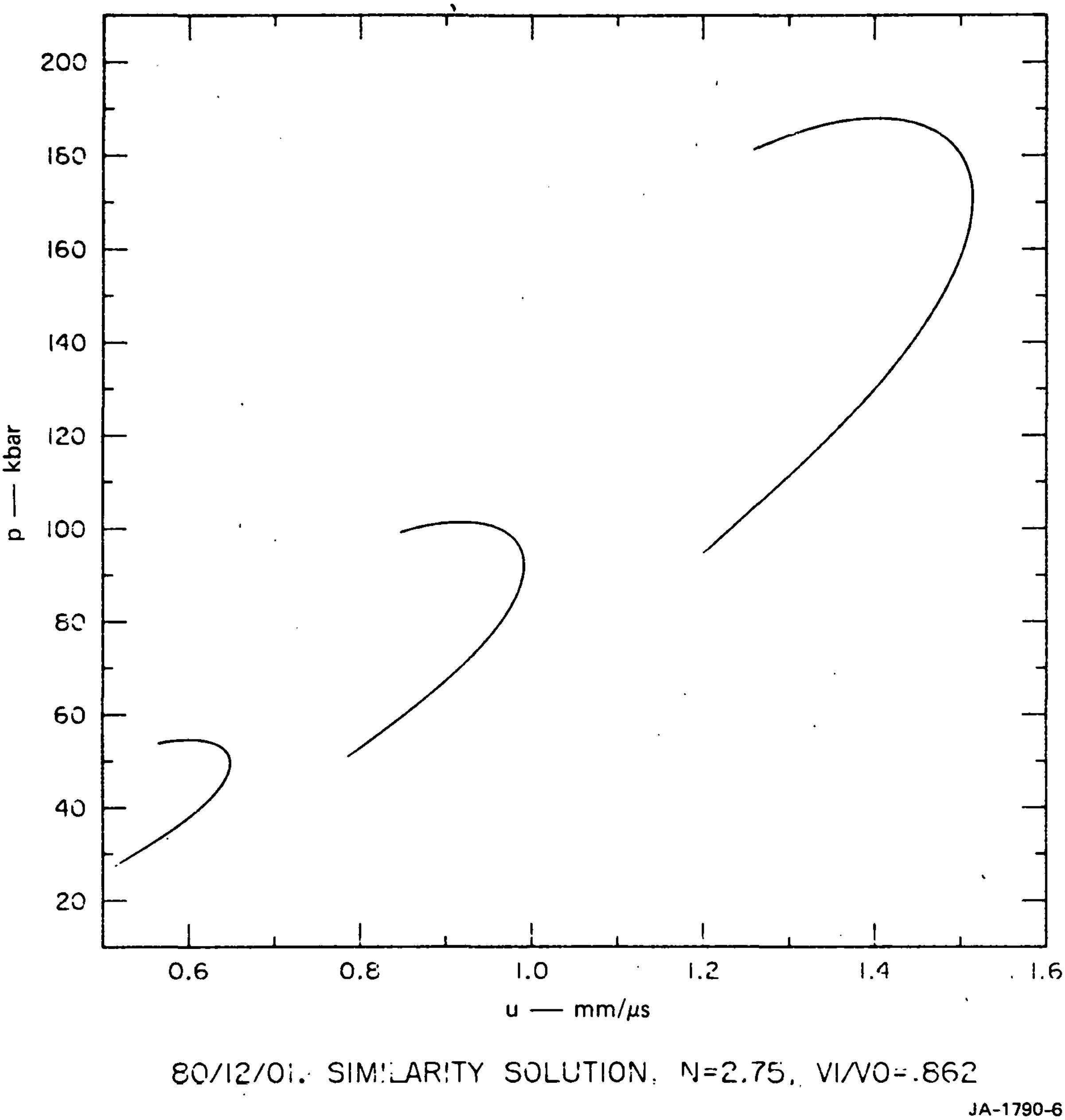


FIGURE 6 THREE LAGRANGE PRESSURE-PARTICLE VELOCITY CURVES FOR A REACTIVE SHOCK

(ϵ/δ = 2.7, ϵ/b = 6/7, α = 4μs)

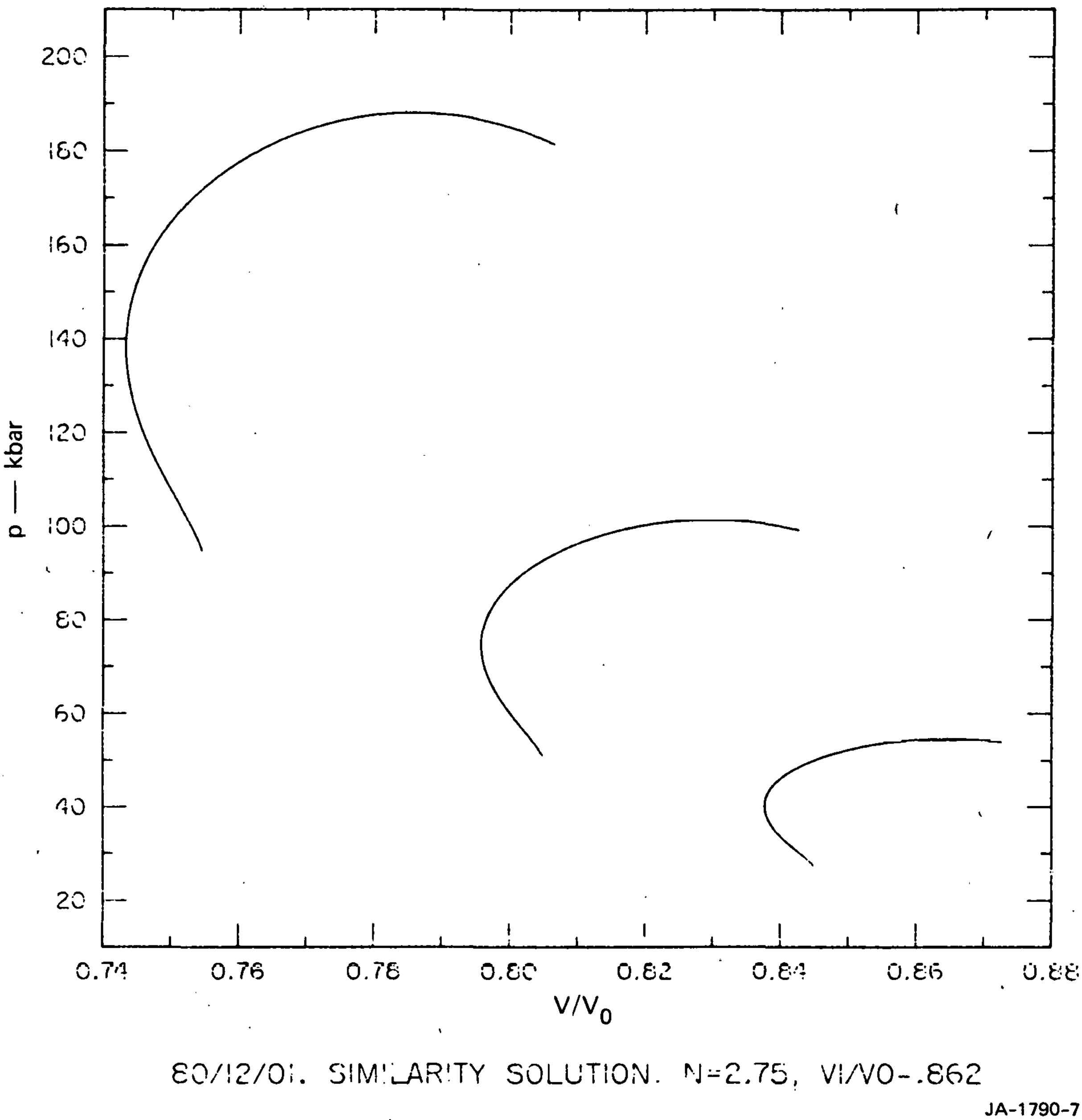
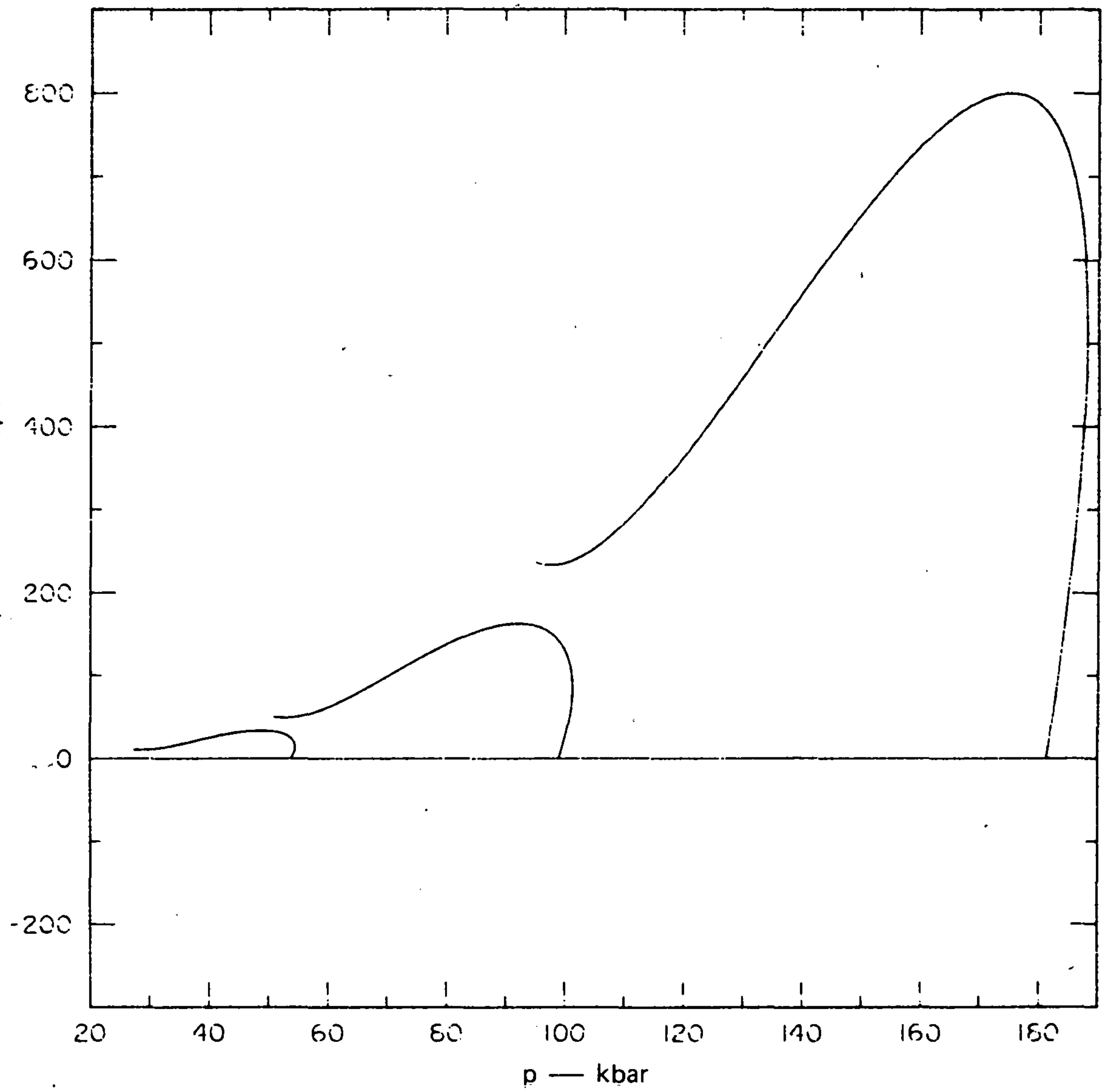


FIGURE 7 THREE LAGRANGE PRESSURE-RELATIVE SPECIFIC VOLUME CURVES FOR A REACTIVE SHOCK
(ϵ/δ = 2.7, ϵ/b = 6/7, α = 4μs)



80/12/01. SIMILARITY SOLUTION. N=2.75, VI/VO=.862

JA-1790-8

FIGURE 8 THREE LAGRANGE VOLUMETRIC CHEMICAL ENERGY RELEASE RATE-PRESSURE CURVES FOR A REACTIVE SHOCK

(ϵ/δ = 2.7, ϵ/b = 6/7, α = 4μs, r = 2.75)

III RESULTS AND CONCLUSIONS

The Lagrange gages and RFLA developed in the present program have put multiple Lagrange gage studies of shocked explosives on a firm foundation. We are now in a position to calculate flow fields and reaction rates in PBX9404, TATB, and RX26 from the Lagrange histories that have already been recorded in these explosives at LLNL. We suggest that these calculations be performed at LLNL as the first step in any work undertaken to continue the Lagrange Gage program. The calculated reaction rates must then be used to formulate rate laws for PBX9404, TATB, and RX26 in terms of the compressed state variables. We suggest that this work be performed at SRI as the second step in the continuation of the program.

It is then necessary to determine if the calculated reaction rates provide an insight into the decomposition of these shocked explosives. Correlation of the reaction rates in RX26 with the reaction rates in PBX9404 and TATB can be taken as evidence that Lagrange gages studies provide the information needed to provide an insight into the decomposition of shocked explosives.

It is also necessary to determine if the calculated rate laws realistically describe explosive decomposition in hydrocodes. This can be done by testing the abilities of the rate laws to predict flow histories in types of flow different from those used in their formulation. Successful predictions in these test calculations can be taken as evidence that the rate laws are realistic and support the continued use of Lagrange gage techniques to determine rate laws in other explosives. But unsuccessful predictions lead to the conclusion that rate laws must be constructed from reaction rates calculated from different types of flow. In this case, the determination of rate laws by Lagrange techniques may not be cost effective because too many experiments are required to make the determinations.

Although Lagrange techniques may not be cost effective for rate law determinations, we recommend continuing Lagrange gage studies of shocked explosives to provide the data required to:

(1) Test constitutive relationships and rate laws used for shocked explosives in hydrocodes.

(2) Extend the domains of the pressure-volume plane over which the mechanical equations of state of detonation products are known.

(3) Quantify and understand the final build-up to detonation in the shock initiation process.

REFERENCES

(1) M. Cowperthwaite, "A Constitutive Model for Calculating Chemical Energy Release Rates from the Flow Fields in Shocked Explosives," The Seventh Symposium (International) on Detonation, Volume I, p 256, United States Naval Academy, Annapolis, Maryland, June 1981.

(2) H. C. Vantine, R. R. Rainsberger, W. D. Curtis, R. S. Lee, M. Cowperthwaite, and J. T. Rosenberg, "The Accuracy of Reaction Rates Inferred from Lagrange Analysis and In-Situ Gage Measurements," The Seventh Symposium (International) on Detonation, Volume II, p 593, United States Naval Academy, Annapolis, Maryland, June 1981.

(3) M. Cowperthwaite, "Model Solutions for the Shock Initiation of Condensed Explosives," Symposium H.D.P., Behavior of Dense Media Under High Dynamic Pressures. Paris, France, August 1978, p 201.

(4) G. I. Kanel and A. N. Dremin, "Decomposition of Cast Trotyl in Shock Waves," Combustion, Explosion, and Shock Waves, 13 (1), 71, 1977.