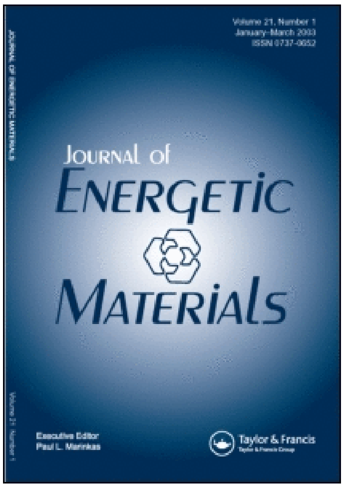

Journal of Energetic Materials
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713770432

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To cite this Article Cowperthwaite, M.(1983) 'Some aspects of nonideal detonation in composite explosives', Journal of Energetic Materials, 1: 2, 141 — 175

To link to this Article: DOI: 10.1080/07370658308010630

URL: http://dx.doi.org/10.1080/07370658308010630

SOME ASPECTS OF NONIDEAL DETONATION IN COMPOSITE EXPLOSIVES*

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ABSTRACT

A theoretical treatment is formulated for steady-state planar detonation waves in composite explosives such as Amatex 20. This treatment provides a more definitve and realistic description of detonation in such explosives, and extends the classical Zeldovich-von Neumann-Doering model of ideal detonation into a propotype model for nonideal detonation. Incomplete decomposition of the slowest reacting component, and incomplete attainment of chemical equilibrium among the detonation products from the different explosive components were assumed to be the kinetic processes responsible for nonideal behavior. The constitutive relationship for the shocked reacting explosive was constructed with different equations of state for the explosives and their products and enough reaction coordinates to account for this type of nonideality. Detonation parameters and Lagrange particle velocity histories were calculated for nonideal detonation waves in an explosive modeling Amatex 20.

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*This work was performed for the U.S. Army Research Office under Contract DAAG29-80-0076.

Journal of Energetic Materials Vol. 1, 127-132

Published in 1983 by Dowden, Brodman & Devine, Inc.

INTRODUCTION

The theoretical work in this paper was performed to provide a more definitive and realistic treatment of detonation in composite explosives such as Amatex 20. We accordingly addressed the problem of steady-state planar detonation in a composite explosive X fabricated from three explosive components, X_1, X_2, and X_3 considered respectively to be like RDX, TNT, and ammonium nitrate (AN). It was necessary in approaching this problem to identify and model rate processes that influence the detonation process and give rise to nonideal detonation. The limiting rate processes considered in the present treatment are chemical reactions that do not proceed to completion in the steady-state reaction zone. Nonideal behavior arises in this case because not all the available chemical energy is used to support the propagation of the detonation wave. A constitutive relationship for shocked reacting explosive was constructed with different equations of state for the explosives and their products and enough reaction coordinates to account for this type of nonideality. This constitutive relationship was combined with the equations governing the reaction zone in a steady-state planar detonation to obtain the equations governing detonation in our composite explosive. These equations demonstrate the dependence of the detonation process on the incompleteness of reactions and on the equation of state of the condensed explosive. The expression relating the particle velocity and the reaction coordinates in a steady-state reaction zone was also derived. This expression was combined with model reaction rate expressions to generate Lagrange particle velocity histories and investigate their dependence on the relative rates of the exothermic reactions.

THEORETICAL TREATMENT

Our theoretical treatment is based on the assumption that planar one-dimensional detonation in our composite explosive can be treated as a Zeldovich-von Neumann-Doering[1-3] (ZND) wave. In this case, states in a steady-state detonation are governed by the Rankine-Hugoniot (RH) jump conditions[4] expressing the balance of mass, momentum, and energy in a steady-state flow. The flow becomes sonic at the Chapman-Jouguet (CJ) point where the global energy release rate (GERR) becomes zero, and when all the reactions contributing to the (GERR) are exothermic, the CJ point is at the end of the reaction zone. Exothermic reactions considered to contribute to the GERR are:

- The global decompositions of the explosive components X_1, X_2, and X_3 into their detonation products in local chemical equilibrium.
- Reactions among the different detonation products of X_1, X_2, and X_3 as they mix and react to approach global chemical equilibrium.

We accordingly define the terms "ideal" and "nonideal" detonation used in this paper as follows.

A steady-state ZND wave is said to be ideal when all the global decomposition reactions of the explosive components proceed to completion and the products of these reactions attain global chemical equilibrium. Otherwise it is said to be nonideal. This definition leads us to assume that the two major factors responsible for nonideal behavior of our composite explosive are:

(1) The incomplete decomposition of a slower reacting explosive component such as AN.

(2) The unattainment of chemical equilibrium among the detonation products from different explosive components.

We envisage the first factor to be important when the decomposition of the slowest reacting component is not self-propagating and terminates when the decomposition of the faster reacting components has gone to completion. We envisage the second factor to be important when the time scale for the detonation products to mix and react exceeds the time scales for the decomposition reactions. The constitutive relationship for reacting composite explosive used in a treatment of nonideal detonation must include enough reaction coordinates to account for nonideality arising from factors (1) and (2). With X_1, X_2, and X_3 considered, respectively, to be like RDX, TNT, and AN, it was necessary to construct a constitutive relationship for the reacting explosive with four reaction coordinates, λ_1, λ_2, λ_3, and λ_4. The first three coordinates account respectively for the global decompositions of X_1, X_2, and X_3, and the fourth accounts for the recombination of the oxygen produced by X_3 and the carbon produced by X_1 and X_2. We now introduce the governing equations and formulate our treatment of nonideal detonation.

Governing Equations

Flow Equations

We first introduce the notation used to describe our one-dimensional flow. Time is denoted by t, Lagrange distance by h, specific volume by v, particle velocity by u, pressure by p, sound speed by c, and specific energy by e; the subscript x denotes explosive, and the superscript o denotes the constant state ahead of the wave. Neglecting the initial pressure, the flow in our steady-state ZND wave is governed by the RH jump conditions written as

$$vD = v_x^o\,(D - u) \tag{1}$$

$$p = Du/v_x^o = (D - u)u/v \tag{2}$$

$$e - e_x^o = \frac{1}{2}\,p\left(v_x^o - v\right) = \frac{1}{2}\,u^2 \tag{3}$$

where D denotes the propagation velocity. We use H as a subscript or as a superscript to denote the shocked state at the wave front, and we use CJ as a subscript to denote the CJ point. Then the equations for the shocked state are obtained by setting $v = v_x^H$, $u = u_H$, $p = p_H$, and $e = e_x^H$ in Eqs. (1)-(3), and the equations for the CJ state are obtained by writing the CJ condition as

$$D - u_{CJ} = c_{CJ} \tag{4}$$

and setting $v = v_{CJ}$, $u = u_{CJ}$, $p = p_{CJ}$, and $e = e_{CJ}$ in Eqs. (1)-(3). The adiabatic inviscid flow in the wave behind the shock is governed by the following expressions for the laws of conservation of mass, momentum, and energy:

$$\frac{\partial v}{\partial t} = v_x^o \frac{\partial u}{\partial h} = - D \frac{\partial v}{\partial h} \tag{5}$$

$$\frac{\partial u}{\partial t} = - v_x^o \frac{\partial p}{\partial h} = - D \frac{\partial u}{\partial h} \tag{6}$$

$$\frac{\partial e}{\partial t} = - p \frac{\partial v}{\partial t} \tag{7}$$

The flow and chemistry in our ZND wave are coupled by the constitutive relationship relating e and the reaction coordinates λ_1, λ_2, λ_3, and λ_4.

Equations for the Explosives

Following the papers by Kamlet et al.,[5-7] we write the molecular formulas of our explosive components X_1, X_2, and X_3, respectively, as $C_{a_i} H_{b_i} N_{c_i} O_{d_i}$ with i = 1, 2, and $H_{b_3} N_{c_3} O_{d_3}$. We also assumed that the decompositions of X_1 and X_2 satisfy the H_2O - CO_2 arbitrary equilibrium condition. The H_2O - CO_2 arbitrary represents N_2, H_2O, and CO_2 as being the only important detonation products, with H_2O having priority in formation over CO_2. We accordingly write the decomposition of X_i, with i = 1, 2, as

$$\begin{aligned} C_{a_i} H_{b_i} N_{c_i} O_{d_i} \rightarrow & \frac{c_i}{2} N_2 + \frac{b_i}{2} H_2O \\ & + \left(\frac{d_i}{2} - \frac{b_i}{4}\right) CO_2 + \left(a_i - \frac{d_i}{2} + \frac{b_i}{4}\right) C \end{aligned} \tag{8}$$

Extending the notion, we assume that the decomposition of X_3 satisfies the H_2O - O_2 arbitrary so that N_2, H_2O, and O_2 are the only detonation products, with H_2O having priority in formation over O_2. We accordingly write the decomposition of X_3 as

$$H_{b_3} N_{c_3} O_{d_3} \rightarrow \frac{c_3}{2} N_2 + \frac{b_3}{2} H_2O + \left(\frac{d_3}{2} - \frac{b_3}{4}\right) O_2 \tag{9}$$

The reaction coordinates λ_1, λ_2, and λ_3 are used to describe the decompositions specified by Eqs. (8) and (9), and the reaction coordinate λ_4 is used to describe the reaction

$$\left(\frac{d_3}{2} - \frac{b_3}{4}\right) O_2 + \left(\frac{d_3}{2} - \frac{b_3}{4}\right) C = \left(\frac{d_3}{2} - \frac{b_3}{4}\right) CO_2 \tag{10}$$

with

$$(d_{3/2} - b_{3/4}) \leq \sum_{i=1}^{2} (a_i - d_{i/2} + b_i/4)$$

that may occur among the decomposition products of X_1, X_2, and X_3. Because of the H_2O - CO_2 and H_2O - O_2 arbitrary assumptions, only one reaction is needed to account for subsequent reactions among detonation products. With the standard heat of formation of a species S_j denoted by $(\Delta H_f^o)_{S_j}$, the standard heats, Q_i, liberated in our exothermic reactions Eqs. (8)-(10) are given by the equations

$$Q_i = - (b_i/2)(\Delta H_f^o)_{H_2O} - (d_i/2 - b_i/4)(\Delta H_f^o)_{CO_2} + (\Delta H_f^o)_{X_i} \tag{11}$$

with i = 1, 2

$$Q_3 = - (b_3/2)(\Delta H_f^o)_{H_2O} + (\Delta H_f^o)_{X_3} \tag{12}$$

$$Q_4 = - (d_3/2 - b_3/4)(\Delta H_f^o)_{CO_2} \tag{13}$$

where $(\Delta H_f^o)_{H_2O}$ = -57.8 kcal/mole and $(\Delta H_f^o)_{CO_2}$ = -94 kcal/mole. We now introduce the notation used to describe our explosive mixture and its reaction products. We let the subscript p denote detonation products, let M_{S_j} denote the molecular weight of a product species S_j, and we let $v^o_{x_i}$, $e^o_{x_i}$, N_i, and α_i denote the initial specific volume, the initial specific internal energy, the number of moles, and the mass fraction of the explosive X_i in our composite explosive X. Then N_i and α_i are related by the equation

$$N_i = \alpha_i / M_{x_i} \qquad i = 1, \ . \ . \ . \ 3 \tag{14}$$

With $\sum_{i=1}^{3} N_i M_{x_i} = 1$. We assume that the mixture of explosives is ideal and write the following equations for its specific volume, specific internal energy, and specific heat of formation:

$$v^o_x = \sum_{i=1}^{3} \alpha_i \, v^o_{x_i} \tag{15}$$

$$e^o_x = \sum_{i=1}^{3} \alpha_i \, e^o_{x_i} \tag{16}$$

$$(\Delta h^o_f)_x = \sum_{i=1}^{3} \alpha_i \, (\Delta h^o_f)_{x_i} \tag{17}$$

where $(\Delta h^o_f)_{S_j} = (\Delta H^o_f)_{S_j} / M_{S_j}$. If we assume that the initial pressure is zero, Eqs. (16) and (17) are identical because $(\Delta h^o_f)_{x_i} = e^o_{x_i}$. We let $\beta^i_{S_j}$ denote the mass fraction of a decomposition product, S_j, of X_i when X_i has decomposed completely. Then under the H_2O - CO_2 and H_2O - O_2 arbitrary assumptions it follows from Eqs. (8) and (9) that

$$\beta^i_{N_2} + \beta^i_{H_2O} + \beta^i_{CO_2} + \beta^i_C = 1 \qquad i = 1, \ 2 \tag{18}$$

and

$$\beta^{i}_{N_2} + \beta^{3}_{H_2O} + \beta^{3}_{O_2} = 1 \qquad (19)$$

where

$$\beta^{i}_{N_2} = c_i M_{N_2} / 2M_{x_i} \qquad i = 1,\ 2,\ 3$$

$$\beta^{i}_{H_2O} = b_i M_{H_2O} / 2M_{x_i} \qquad i = 1,\ 2,\ 3;$$

$$\beta^{i}_{CO_2} = (d_i - b_i/2)\ M_{CO_2} / 2M_{x_i} \qquad i = 1,\ 2;$$

$$\beta^{i}_{C} = \left[2a_i - (d_i - b_i/2) \right] M_C / 2M_{x_i} \qquad i = 1,\ 2;$$

$$\beta^{3}_{O_2} = (d_3 - b_3/2)\ M_{O_2} / 2M_{x_3}$$

We can then write the standard heats $\hat{q}_1$, $\hat{q}_2$, and $\hat{q}_3$ librated by the decomposition of 1 gram of X_1, X_2, and X_3 as

$$\hat{q}_i = -\beta^{i}_{H_2O}\ (\Delta h^{o}_{f})_{H_2O} - \beta^{i}_{CO_2}\ (\Delta h^{o}_{f})_{CO_2} + (\Delta h^{o}_{f})_{x_i} \qquad i = 1,\ 2 \qquad (20)$$

$$\hat{q}_3 = -\beta^{3}_{H_2O}\ (\Delta h^{o}_{f})_{H_2O} + (\Delta h^{o}_{f})_{x_3} \qquad (21)$$

and the standard heat $\hat{q}_d$ librated by the decomposition of X_1, X_2, and X_3 in 1 gram of X as

$$\hat{q}_d = \sum_{i=1}^{3} \alpha_i\ \hat{q}_i \qquad (22)$$

We now consider the reaction among the detonation products, Eq. (10), and write the standard heat of this reaction for 1 gram of X_3 as

$$\hat{q}_4 = -\beta^4_{CO_2} (\Delta h^o_f)_{CO_2} \qquad (23)$$

where $\beta^4_{CO_2} = (d_3/2 - b_3/4)\, M_{CO_2}/M_{x_3}$. Thus, when all the exothermic reactions proceed to completion in our composite explosive, we can write the standard heat of these reactions for 1 gram of X as

$$\hat{q} = \sum_{i=1}^{3} q_i + q_4 \qquad (24)$$

where $q_1 = \alpha_1\hat{q}_1$, $q_2 = \alpha_2\hat{q}_2$, $q_3 = \alpha_3\hat{q}_3$, and $q_4 = \alpha_3\hat{q}_4$.

Constitutive Relationship for Reacting Composite Explosive

Our constitutive relationship for reacting composite explosive is an extension of the constitutive relationship formulated previously[8] for an explosive with one global decomposition reaction. We treat the explosive components and their reaction products as a mixture of phases that attains mechanical but not thermal equilibrium. It is also assumed that no appreciable amount of heat is transferred into the composite explosive as the decomposition reactions propagate and consume the explosive components. In this case, the explosive components are compressed or released isentropically as the reactions proceed, and the pressure increases or decreases along a particle path.

We assume for convenience that the explosives and their products are polytropic materials, and we assume for tractability that the polytroptic indices of the explosive components are equal, i.e., $K_{x_1} = K_{x_2} = K_{x_3} = K_x$, and that the polytropic index of carbon is the same as that of the other reaction products, i. e., $K_C = K_p$. In contrast to classical treatments of detonation, however, we do not assume that $K_x = K_p = K$ so that we can investigate the influence of the equation of state of the condensed explosive on the detonation process.

We accordingly write the (e-p-v) relationships for the explosive components and their reaction products as

$$e_{x_i} = (\Delta h_f^o)_{x_i} + \frac{pv_{x_i}}{(K_x - 1)} \qquad i = 1,\ 2,\ 3 \tag{25}$$

$$e_p = (\Delta h_f^o)_p + \frac{pv_p}{(K_p - 1)} \tag{26}$$

We denote the specific entropy by s and write the mixture rules for the reacting explosive mixture as

$$e = \Sigma e_x + \bar{e}_p \tag{27}$$

$$v = \Sigma v_x + \bar{v}_p \tag{28}$$

$$s = \Sigma s_x + \bar{s}_p \tag{29}$$

with

$$\Sigma v_x = \sum_{i=1}^{3} \alpha_i(1 - \lambda_i)\ v_{x_i}$$

$$\Sigma s_x = \sum_{i=1}^{3} \alpha_i(1 - \lambda_i)\ s_{x_i}$$

$$\Sigma e_x = (\Delta h_f^o)_x - \sum_{i=1}^{3} \lambda_i\alpha_i(\Delta h_f^o)_{x_i} + \frac{p\Sigma v_x}{K_x - 1} \tag{30}$$

and

$$\bar{e}_p = \sum_{i=1}^{2} \lambda_i\alpha_i\beta^i_{H_2O}(\Delta h_f^o)_{H_2O} + \sum_{i=1}^{2} \lambda_i\alpha_i\beta^i_{CO_2}(\Delta h_f^o)_{CO_2}$$

$$+ \lambda_3\alpha_3\beta^3_{H_2O}(\Delta h_f^o)_{H_2O} + \lambda_3\lambda_4\alpha_3\beta^4_{CO_2}(\Delta h_f^o)_{CO_2} + \frac{p\bar{v}_p}{(K_p - 1)} \tag{31}$$

The combination of Eqs. (27), (30), and (31) after some manipulation gives the constitutive relationship for our reacting mixture as

$$e = (\Delta h_f^o)_x - \sum_{i=1}^{3} \lambda_i q_i - \lambda_4 \lambda_3 q_4 + \frac{pv}{K_p - 1} - \frac{K_{xp} p \Sigma v_x}{K_p - 1} \qquad (32)$$

with $q_i = \alpha_i \hat{q}_i$, $q_4 = \alpha_3 \hat{q}_4$, and $K_{xp} = (K_x - K_p)/(K_x - 1)$. The (e-p-v) relationship for our composite polytropic explosive is obtained from Eq. (32) by setting $\lambda_1 = \lambda_2 = \lambda_3 = 1$, $v = v_p$, and $e = e_p$. The classical (e-p-v-λ_i) equation of state for a polytropic reacting explosive mixture is obtained from Eq. (32) by setting $K_x = K_p = K$.

We now define the sound speed in our reacting mixture by the equation

$$c^2 = Kpv = -v^2 \left(\frac{\partial p}{\partial v}\right)_{s,\lambda_i} \qquad (33)$$

and we then use Eqs. (28) and (29) to express Eq. (33) in a more convenient form. Differentiating Eq. (29) at constant s and λ_i leads to the equation

$$d\Sigma s_x + d\bar{s}_p = 0 \qquad (34)$$

and it follows that $d\bar{s}_p = 0$ because $ds_{x_i} = 0$, $i = 1, 2, 3$ by assumption. Differenting Eq. (28) partially with respect to p at constant s and λ_i and taking account of these entropy conditions gives the equation

$$\left(\frac{\partial v}{\partial p}\right)_{s,\lambda_i} = \sum_{i=1}^{3} \alpha_i (1 - \lambda_i) \left(\frac{\partial v_{x_i}}{\partial p}\right)_{s_{x_i}} + \left(\frac{\partial \bar{v}_p}{\partial p}\right)_{\bar{s}_p,\lambda_i} \qquad (35)$$

which for our polytropic materials can be written after some manipulation as

$$\left(\frac{\partial p}{\partial v}\right)_{s,\lambda_i} = - \frac{K_p p}{\left(v - \bar{K}_{xp} \Sigma v_x\right)} \tag{36}$$

with $\bar{K}_{xp} = (K_x - K_p)/K_x$. The combination of Eqs. (33) and (36) gives the following equation for K

$$K = \frac{K_p v}{\left(v - \bar{K}_{xp} \Sigma v_x\right)} \tag{37}$$

which reduces to $K = K_x$ when $\lambda_1 = \lambda_2 = \lambda_3 = 0$ and $v = v_x$, and to $K = K_p$ when $\lambda_1 = \lambda_2 = \lambda_3 = 1$. The assumption that an explosive component is released down its own isentrope allows us to express the Σv_x term in terms of pressure in a ZND wave. Because the explosive components are polytropic, their specific volumes can be written as

$$v_{x_i} = v_x^o \frac{(K_x - 1)}{(K_x + 1)} \delta_i \left(\frac{p_H}{p}\right)^{1/K_x} \tag{38}$$

where $\delta_i = v^o_{x_i}/v^o_x$. Thus the equation for Σv_x in our ZND wave can be written in terms of pressure as

$$\Sigma v_x = v_x^o \frac{(K_x - 1)}{(K_x + 1)} \left(\frac{p_H}{p}\right)^{1/K_x} \sum_{i=1}^{3} \bar{\alpha}_i (1 - \lambda_i) \tag{39}$$

where $\bar{\alpha}_i = \alpha_i \, v^o_{x_i}/v^o_x$ and $\sum_{i=1}^{3} \bar{\alpha}_i = 1$.

Nonideal Steady-State Detonation Waves

The constitutive relationship can now be combined with the Rankine-Hugoniot jump conditions and the Chapman-Jouguet conditions to generate the equations governing the CJ state in our nonideal ZND wave and to generate the equation governing particle velocity in the steady-state reaction zone.

Chapman-Jouguet Conditions

We set $(\lambda_i)_{CJ} = \hat{\lambda}_i$ at the CJ point in our steady-state ZND wave. Then we can represent ideal detonation by the set $\{\hat{\lambda}_1 = 1, \hat{\lambda}_2 = 1, \hat{\lambda}_3 = 1, \hat{\lambda}_4 = 1\}$ and nonideal detonation by the set $\{\hat{\lambda}_1, \hat{\lambda}_2, \hat{\lambda}_3, \hat{\lambda}_4\}$ with any one of the reaction coordinates satisfying the condition $\hat{\lambda}_i < 1$. In the present case, we assume that the RDX-like component X_1 and the TNT-like component X_2 decompose completely, and represent our nonideal detonation by the set $\{\hat{\lambda}_1 = 1, \hat{\lambda}_2 = 1, \hat{\lambda}_3 < 1, \hat{\lambda}_4 < 1\}$. We are therefore going to consider incomplete decomposition of the AN-like component and incomplete reaction among the carbon from X_1 and X_2 and the oxygen from X_3.

We first combine Eq. (2), (4), and (33) to obtain the following relationship between sound speed and particle velocity at the CJ point:

$$c_{CJ} = \hat{K}\, u_{CJ} \tag{40}$$

where

$$\hat{K} = \frac{K_p}{\left(1 - \bar{K}_{xp} \Sigma \hat{v}_x / v_{CJ}\right)} \tag{41}$$

with $\Sigma \hat{v}_x = \alpha_3 (1 - \hat{\lambda}_3)(v_{x_3})_{CJ}$. Combining Eq. (40) with Eqs. (4) and (1) then gives the equations

$$u_{CJ} = \frac{D}{\hat{K} + 1} \tag{42}$$

$$c_{CJ} = \frac{\hat{K}\, D}{\hat{K} + 1} \tag{43}$$

and

$$v_{CJ} = \frac{\hat{K}}{\hat{K} + 1}\, v_x^o \tag{44}$$

The equation

$$\left[\left(\frac{\partial p}{\partial v}\right)_{s,\lambda_i}\right]_{CJ} = \frac{p_{CJ}}{v_x^o - v_{CJ}} \tag{45}$$

expressing the tangency condition of the isentrope and the Rayleigh line at the CJ point is then used to obtain the following equations for the specific volume at the CJ point:

$$\frac{v_{CJ}}{v_x^o} = \frac{K_p}{K_p + 1} + \frac{\bar{K}_{xp}}{K_p + 1} \frac{\Sigma \hat{v}_x}{v_x^o} \tag{46}$$

$$1 - \frac{v_{CJ}}{v_x^o} = \frac{\left(1 - \bar{K}_{xp} \Sigma \hat{v}_x / v_x^o\right)}{K_p + 1} \tag{47}$$

The combination of Eqs. (44) and (47) then gives the following equation relating the polytropic indices at the CJ point:

$$\hat{K} + 1 = \frac{K_p + 1}{1 - \bar{K}_{xp} \Sigma \hat{v}_x / v_x^o} \tag{48}$$

The equation relating the CJ pressure and the shock pressure at the front of our ZND wave is obtained as

$$\frac{p_{CJ}}{p_H} = \frac{K_x + 1}{2(K_p + 1)} \left(1 - \bar{K}_{xp} \Sigma \hat{v}_x / v_x^o\right) \tag{49}$$

by combining Eq. (47), the strong shock condition

$$1 - \frac{v_H}{v_x^o} = \frac{2}{K_x + 1} \tag{50}$$

and the folowing equation expressing the balance of mass and momentum in a steady-state wave

$$\frac{p_{CJ}}{p_H} = \frac{\left(1 - v_{CJ}/v_x^0\right)}{\left(1 - v_H/v_x^o\right)} \tag{51}$$

The equation for the detonation velocity is obtained by combining the RH jump conditions, the constitutive relationship Eq. (32), and the CJ condition. It is convenient to set

$$\sum_{i=1}^{3} \lambda_i q_i + \lambda_3 \lambda_4 q_4 = Q \tag{52}$$

and combine Eqs. (2), (3), and (32) to obtain the following equation for the particle velocity:

$$u^2 - \frac{2Du}{K_p + 1}\left(1 - K_{xp}\Sigma v/v_x^o\right) = -\frac{2(K_p - 1)}{K_p + 1}Q \tag{53}$$

The CJ condition $D = (\hat{K} + 1)u_{CJ}$ then gives the following equation for u_{CJ}:

$$u_{CJ}^2\left[1 - \frac{2(\hat{K} - 1)}{K_p + 1}\left(1 - K_{xp}\Sigma\hat{v}_x/v_x^o\right)\right] = -\frac{2(K_p - 1)}{K_p + 1}\hat{Q} \tag{54}$$

where $\hat{Q} = q_1 + q_2 + \hat{\lambda}_3(q_3 + \hat{\lambda}_4 q_4)$ because of our assumption that $\lambda_1 = \lambda_2 = 1$. Combining Eqs. (54) and (48) gives the following equation

$$u_{CJ}^2\left[\frac{1 - \left(2K_{xp} - \bar{K}_{xp}\right)\Sigma\hat{v}_x/v_x^o}{\left(1 - \bar{K}_{xp}\Sigma\hat{v}_x/v_x^o\right)}\right] = \frac{2(K_p - 1)\hat{Q}}{K_p + 1} \tag{55}$$

which with Eqs. (44) and (48) leads to the following equation for the detonation velocity:

$$D^2 = \frac{2(K_p^2 - 1)\hat{Q}}{(1 - \bar{K}_{xp}\Sigma\hat{v}_x/v_x^o)\,[1 - (2K_{xp} - \bar{K}_{xp})\Sigma\hat{v}_x/v_x^o\,]} \qquad (56)$$

The problem of nonideal detonation in our simple treatment of detonation is that of calculating $\Sigma\,\hat{v}_x/v_x^o$, $\hat{\lambda}_3$, and $\hat{\lambda}_4$. It follows from Eq. (39) that the equation for $\Sigma\,\hat{v}_x/v_x^o$ can be written as

$$\Sigma\,\hat{v}_x/v_x^o = \frac{(K_x - 1)}{K_x + 1}\,\bar{\alpha}_3(1 - \hat{\lambda}_3)\left(\frac{p_H}{p_{CJ}}\right)^{1/K_x} \qquad (57)$$

but models for calculating $\hat{\lambda}_3$ and $\hat{\lambda}_4$ must be formulated or their values must be estimated before detonation parameters can be calculated.

Examination of the equations for the CJ parameters shows that the equations for complete decomposition of X_3 with $\hat{\lambda}_3 = 1$ have the same form as those for polytropic explosive with $K_{xp} = \bar{K}_{xp} = 0$. In this case, the equation for the detonation velocity reduces to

$$D^2 = 2(K_p^2)(\,q_1 + q_2 + q_3 + \hat{\lambda}_4\,q_4) \qquad (58)$$

and the nonideality arises solely from the incompleteness of the reaction among the carbon from X_1 and X_2 and the oxygen from X_3.

Dependence of Particle Velocity on Reaction Coordinates

It is convenient to use Eq. (53) to derive the relationship of the particle velocity and the reaction coordinates in a steady-state ZND wave. We write Eq. (53) to make its left-hand side into a perfect square and then combine this equation with the CJ conditions, Eqs. (42) and (48), to obtain the equation

$$\frac{u}{u_{CJ}} = \frac{(1 - K_{xp}\Sigma v_x/v_x^o)}{(1 - \bar{K}_{xp}\ \Sigma \hat{v}_x/v_x^o)} \left[1 + \left\{1 - \frac{2(K_p^2 - 1)Q}{(1 - K_{xp}\Sigma v_x/v_x^o)^2 D^2}\right\}^{1/2}\right] \tag{59}$$

Equation (56) then allows Eq. (59) to be written as

$$\frac{u}{u_{CJ}} = \frac{(1 - K_{xp}\Sigma v_x/v_x^o)}{(1 - \bar{K}_{xp}\Sigma \hat{v}_x/v_x^o)} \times$$

$$\left(1 + \left\{\frac{1 - [1 - (2K_{xp} - \bar{K}_{xp})\Sigma v_x/v_x^o](1 - \bar{K}_{xp}\Sigma v_x/v_x^o)Q}{(1 - K_{xp}\Sigma v_x/v_x^o)^2\ \hat{Q}}\right\}^{1/2}\right) \tag{60}$$

with

$$\Sigma v_x/v_x^o = \frac{K_x - 1}{K_x + 1}\left(\frac{u_H}{u_{CJ}}\right)^{1/K_x}\left(\frac{u_{CJ}}{u}\right)^{1/K_x} \sum_{i=1}^{3} \bar{\alpha}_i(1 - \lambda_i) \tag{61}$$

from Eq. (39), and with $\lambda_1 = \lambda_2 = 1$, $\lambda_3 = \hat{\lambda}_3$, and $\lambda_4 = \hat{\lambda}_4$ at the CJ point where $Q = \hat{Q}$, $\Sigma v_x = \Sigma \hat{v}_x$, and $u = u_{CJ}$. The equation for the particle velocity in a steady-state ZND wave when X_3 decomposes completely is obtained by setting $\hat{\lambda}_3 = 1$ in Eq. (60) as

$$\frac{u}{u_{CJ}} = (1 - K_{xp}\Sigma v_x/v_x^o)\left[1 + \left\{1 - \frac{Q}{(1 - K_{xp}\Sigma v_x/v_x^o)^2\ \hat{Q}_d}\right\}^{1/2}\right] \tag{62}$$

where $\hat{Q}_d = q_1 + q_2 + q_3 + \hat{\lambda}_4 q_4$. The equation for the particle velocity in a steady-state ZND wave in polytropic explosive is obtained from Eq. (60) by setting $K_{xp} = \bar{K}_{xp} = 0$ and is conveniently written as

$$\frac{u}{u_{CJ}} = 1 + \left[\tilde{\alpha}_1(1 - \lambda_1) + \tilde{\alpha}_2(1 - \lambda_2) + \tilde{\alpha}_3(1 - \lambda_3/\hat{\lambda}_3) + \tilde{\alpha}_4(1 - \lambda_4/\hat{\lambda}_i)\right]^{1/2} \tag{63}$$

where

$$\tilde{\alpha}_1 = q_1/\hat{Q}$$

$$\tilde{\alpha}_2 = q_2/\hat{Q}$$

$$\tilde{\alpha}_3 = \lambda_3 q_3/\hat{Q}$$

$$\tilde{\alpha}_4 = \lambda_4 q_4/\hat{Q}$$

$$\tilde{\alpha}_1 + \tilde{\alpha}_2 + \tilde{\alpha}_3 + \tilde{\alpha}_4 = 1$$

Differentiating Eq. (53) with respect to time along a particle path gives the following equation for the deceleration in a steady-state reaction zone:

$$\frac{\partial u}{\partial t}\left[u - \frac{D(1 - \bar{K}_{xp}\Sigma v_x/v_x^o)}{(K_p + 1)}\right] = -\frac{(K_p - 1)\dot{Q}}{K_p + 1} + \frac{K_{xp}(K_x - 1)}{(K_p + 1)(K_x + 1)}\dot{Q}' \qquad (64)$$

where

$$\dot{Q} = q_1\frac{\partial\lambda_1}{\partial t} + q_2\frac{\partial\lambda_2}{\partial t} + (q_3 + \lambda_4 q_4)\frac{\partial\lambda_3}{\partial t} + \lambda_3 q_4\frac{\partial\lambda_4}{\partial t} \qquad (65)$$

and

$$\dot{Q}' = \left(\frac{u_H}{u}\right)^{1/K_x} Du \sum_{i=1} \bar{\alpha}_i \frac{\partial\lambda_i}{\partial t} \qquad (66)$$

Because $\partial u/\partial t$ is finite, it follows in general from Eqs. (64) and (66) that the rates of all the reactions must be zero, i. e., $\partial\lambda_i/\partial t = 0$ for $i = 1, 2, 3$, and 4, at the sonic point where $u = u_{CJ} = D\left(1 - \bar{K}_{xp}\Sigma\hat{v}_x/v_x^o\right)/\left(K_p + 1\right)$. In other words, the CJ point is located at the end of the steady-state reaction zone of our nonideal detonation wave. The following equation,

$$u_H\left(\frac{\partial u}{\partial t}\right)_H = -\frac{2(K_p - 1)\dot{Q}_H}{K_p + 1} + \frac{K_{xp}(K_x - 1)}{K_p + 1} u_H^2 \sum_{i=1}^{3} \tilde{\alpha}_i \frac{\partial \lambda_i}{\partial t}_H \qquad (67)$$

obtained by setting $u = u_H$ and $\lambda_1 = \lambda_2 = \lambda_3 = \lambda_4 = 0$ in Eq. (64), leads to the conclusion that the particle velocity will increase at the front of the wave when $K_{xp}\ (K_x - 1) \sum_{i=1}^{3} \bar{\alpha}_i\ \partial\lambda_i/\partial t_H > 2\ (K_p - 1)\ (\dot{Q}_H/u_H^2)$. Waves with this property will not, however, be considered in this paper. Equations (60), (62), and (63) can be used to calculate Lagrange particle velocity histories when expressions for the reaction coordinates are known as functions of time. The Lagrange histories can then be examined to investigate the influence of the relative rates of the exothermic reactions on particle velocity. Such calculations will be presented next.

Model Nonideal Detonation Calculations

Properties of the explosive X, its components X_1, X_2, and X_3, and their detonation products were chosen to model Amatex 20. We set v_x^o = 0.6201 cm^3/g so that the initial density ρ_o^x = 1.613 g/cm^3, and we assigned X_1, X_2, and X_3 the values of the parameters shown in Table 1.

We set $\hat{q}_4$ = 587.5 cal/g and q_4 = 235 cal/g according to Eqs. (23) and (24), and set set K_x = 5.34 and K_p = 2.67, so that K_{xp} = 0.6152 and $\bar{K}_{xp}$ = 0.5. In this case, $q_d = \sum_{i=1}^{3}$, q_i = 951.1 cal/g, $\hat{q}_d + q_4$ = 1186.1 cal/g, and when X_1, X_2, and X_3 decompose completely, the detonation velocity D, the shock pressure p_H, the CJ pressure p_{CJ}, and the CJ particle velocity u_{CJ} vary from values of 6.98 mm/µs, 247.7 kbar, 214 kbar, and 1.90 mm/µs to values of 7.80 mm/µs, 309.6 kbar, 267.4 kbar, and 2.12 mm/µs as $\hat{\lambda}_4$ varies from zero to one. We will now calculate detonation parameters when $\hat{\lambda}_1 = \hat{\lambda}_2 = 1$, $\hat{\lambda}_3 < 1$, and $\hat{\lambda}_4 < 1$.

Detonation Parameters

We calculate detonation parameters for a nonideal detonation with $\hat{\lambda}_3 < 1$ and $\hat{\lambda}_4 < 1$. Our calculations are based on the intuitive hypothesis that the slope of the D versus $\hat{\lambda}_3$ curve is postive as $\hat{\lambda}_3$ approaches 1 when $\hat{\lambda}_4$ is a function of λ_3. We accordingly differentiate Eq. (56) and set $dD/d\hat{\lambda}_3 > 0$ when $\hat{\lambda}_3 = 1$ to find conditions to satisfy this hypothesis. For notational simplicity, we set $\bar{K}_{\hat{x}p} = K_1$ and $2K_{xp} - \bar{K}_{xp} = K_2$. Differentiating Eq. (56) with respect to $\hat{\lambda}_3$ then gives the equation

$$\frac{2}{D}\frac{dD}{d\hat{\lambda}_3} = \frac{1}{\hat{Q}}\frac{d\hat{Q}}{d\hat{\lambda}_3} + \frac{d(\Sigma\hat{v}_x/v_x^o)}{d\hat{\lambda}_3}\left[\frac{K_1 + K_2 - 2K_1K_2\Sigma v_x/v_x^o}{(1 - K_1\Sigma\hat{v}_x/v_x^o)(1 - K_2\Sigma\hat{v}_x/v_x^o)}\right] \tag{68}$$

which reduces to

$$\left.\frac{2\ dD}{D\ d\hat{\lambda}_3}\right|_{\hat{\lambda}_3 = 1} = \left.\frac{q_3 + q_4(\hat{\lambda}_4 + d\hat{\lambda}_4/d\hat{\lambda}_3)}{q_1 + q_2 + q_3 + \hat{\lambda}_4 q_4}\right|_{\hat{\lambda}_3 = 1}$$

$$- 2K_{xp}\,\bar{\alpha}_3\,\frac{(K_x - 1)}{(K_x + 1)}\left(\frac{2(K_p + 1)}{(K_x + 1)}\right)^{1/K_x} \tag{69}$$

when $\hat{\lambda}_3 = 1$. We set $\hat{\lambda}_4 = n\ \hat{\lambda}_3$ with $n < 1$ for simplicity so that $(dD/d\ \lambda_3)_{\hat{\lambda}_{3=1}} > 0$ when

$$\frac{q_3 + 2n\ q_4}{q_1 + q_2 + q_3 + n\ q_4} > 2\ K_{xp}\,\bar{\alpha}_3\,\frac{(K_x - 1)}{(K_x + 1)}\left(\frac{2(K_p + 1)}{(K_x + 1)}\right)^{1/K_x} \tag{70}$$

Solving this inequality for n shows that

$$(dD/d\hat{\lambda}_3)_{\hat{\lambda}_3 = 1} > 0$$

Table 1

VALUES OF THE PARAMETERS FOR X_1, X_2, and X_3

X_1	α_i	$v^o_{x_i}$ (cm^3/g)	$\bar{\alpha}_i$	$\hat{q}_1$ (cal/g)	q_1 (cal/g)
X_1	0.2	0.5649	0.1821	1482.4	296.5
X_2	0.4	0.667	0.4302	1282.8	513.1
X_3	0.4	0.6009	0.3877	353.7	141.4

when $n > 0.454$. We are now in a position to calculate detonation parameters for specific values of n and $\hat{\lambda}_3$. We set $n = 0.6$, and use Eqs. (49), (57), (56), (48), (42), (2), and (46) to calculate values of the detonation parameters for specific values of $\hat{\lambda}_3$ as follows. Equations (49) and (57) are solved for a given value of $\hat{\lambda}_3$ to find the corresponding values of (p_H/p_{CJ}) and $\Sigma \hat{v}_x/v_x^o$. Equations (56) and (48) are then used to calcuate the values of D and $\hat{K}$, and equations (42), (2), and (46) are used to calculate the values of u_{CJ}, p_{CJ} and v_{CJ}/v_x^o. Calculated values of the detonation parameters are given in Table 2.

Values of the detonation velocity are given to three figures in Table 2 to show that the detonation velocity has a minimum at $\lambda_3 \approx 0.75$, while the CJ pressure and particle velocity increase monotonically as λ_3 increases from a value of 0.45 to a value of 1. The detonation velocity exhibits a minimum because K decreases monotonically with $\hat{\lambda}_3$ as u_{CJ} increases. This minimum demonstrates the influence of the equations of state of the condensed explosives on the nonideal detonation process in composite explosives.

Lagrange Particle Velocity Histories

It is clear from Eq. (60) that expressions for time variations of the reaction coordinates λ_1, λ_2, λ_3, and λ_4 must be known before we can calculate the Lagrange particle velocity history in the reaction zone of a nonideal steady-state reaction zone. Bearing in mind that the rates of all the exothermic reactions must be zero at the CJ point, we formulated simple expressions for the reaction coordinates to perform such calculations. These expressions are based on the following equation for a reaction that proceeds to completion.

$$(1 - \lambda_i) = \left[1 - \frac{(t - \tau)}{T}\right]^{n_i} \qquad (71)$$

where $n_i > 2$, the Lagrange time τ denotes the time a particle enters the wave, and the overall reaction time T denotes the time it takes a particle to travel from the shock front to the CJ plane. Equation (71)

Table 2

DETONATION PARAMETERS FOR $\hat{\lambda}_3 \leq 1$ AND $\hat{\lambda}_4 = 0.6\ \hat{\lambda}_3$

$\hat{\lambda}_3$	D (mm/μs)	p_{CJ} (kbar)	u_{CJ} (mm/μs)	v_{CJ}/v_x^o	K	p_H/p_{CJ}
0.45	7.505	228.7	1.889	0.7483	2.972	1.253
0.55	7.479	230.6	1.911	0.7444	2.913	1.234
0.65	7.464	233.1	1.936	0.7406	2.856	1.216
0.75	7.459	236.1	1.963	0.7369	2.800	1.199
0.85	7.463	239.8	1.992	0.7331	2.747	1.182
0.95	7.475	243.9	2.023	0.7294	2.695	1.166
1.00	7.484	246.2	2.039	0.7275	2.670	1.158

is written so that $\lambda_i = 0$ at the shock front where $t - \tau = 0$, and $\lambda_i = 1$ at the CJ point where $(t - \tau) = T$. Differentiating Eq. (71) with respect to time along a particle path gives the equation for the reaction rate as

$$\frac{\partial \lambda_i}{\partial t} = \frac{n_i}{T}\left[1 - \left(\frac{t - \tau}{T}\right)\right]^{n_i - 1} = \frac{n_i}{T}(1 - \lambda_i)^{(n_i - 1)/n_i} \qquad (72)$$

and it follows from Eq. (72) that we are restricting our consideration to reactions with negligible activation energies.

We use Eq. (71) with $i = 1$ and $i = 2$ to model respectively the decomposition of X_1 and X_2. To account for the fact that the faster reacting RDX-like component X_1 my decompose completely within the reaction zone, we introduce a parameter $f > 1$ and modify Eq. (71) by setting

$$1 - \lambda_1 = \left[1 - \frac{f}{f - 1}\left(\frac{t - \tau}{T}\right)\right]^{n_1} \text{ for } 0 < (t - \tau)/T < (f - 1)/f \qquad (73)$$

and

$$\lambda_1 = 1 \text{ for } (t - \tau)/T > (f - 1)/f \qquad (74)$$

In this case, the decomposition of X_1 is complete when $(t - \tau)/T = (f - 1)/f$; when $f = 3$, for example, the X_1 decomposition time is $2T/3$. It is clear that Eq. (73) can be written in the same form as Eq. (71) by scaling the reaction time and setting the new reaction time as $T_1 = (f - 1)\,T/f$.

To model the case when the decomposition of X_3 is not self-propagating, we simply set

$$\frac{\partial \lambda_3}{\partial t} = n_3 \frac{\partial \lambda_2}{\partial t} \qquad (75)$$

with $n_3 < 1$ and $\partial\lambda_2/\partial t$ given by Eq. (72) with $i = 2$, so that the decomposition of X_3 ceases at the end of the reaction zone where it is not being supported by the decomposition of the other more energetic components. Integrating Eq. (75) give the equation

$$\lambda_3 = n_3 \lambda_2 \tag{76}$$

and it follows that λ_3 will have a value of $\hat{\lambda}_3 = n_3$ at the end of the reaction zone where $\hat{\lambda}_2 = 1$.

To model the case when the recombination reaction of the oxygen from X_3 and the carbon from X_1 and X_2 proceeds at a lower rate than the production of the oxygen, we set

$$\frac{\partial\lambda_4}{\partial t} = n_4 \frac{\partial\lambda_3}{\partial t} = n_4 n_3 \frac{\partial\lambda_2}{\partial t} \tag{77}$$

with $n_4 < 1$, so that

$$\lambda_4 = n_4\lambda_3 = n_4 n_3 \lambda_2 \tag{78}$$

and $\hat{\lambda}_4 = n_4\hat{\lambda}_3 = n_4 n_3$ at the end of the reaction zone where $\hat{\lambda}_2 = 1$. Equations (71), (73), (74), (76), and (78) with Eq. (53) rewritten as

$$\left(\frac{u}{u_{CJ}}\right)^2 - A\left(\frac{u}{u_{CJ}}\right)\left(1 - K_{xp}\Sigma v_x/v_x^o\right) = \left(1 - A\left(1 - K_{xp}\Sigma\hat{v}_x/v_x^o\right)\right)\frac{Q}{\hat{Q}} \tag{79}$$

with $A = 2D/(K_p + 1)\, u_{CJ}$, were used to calculate Lagrange particle velocity histories in the reaction zone of nonideal detonation waves with $\hat{\lambda}_3 = 0.8$ and $\hat{\lambda}_4 = 0.6$. In this case, $D = 7.46$ mm/μs, $u_{CJ} = 1.977$ mm/μs, and $u_H/u_{CJ} = 1.190$; the equations for calculating values of λ_3 and λ_4 are obtained as $\lambda_3 = 0.8\ \lambda_2$ and $\lambda_4 = 0.6\ \lambda_3$ by setting $n_3 = 0.8$ and $n_4 = 0.6$ in Eqs. (76) and (78).

A Newton-Raphson method was ued to calculate values of (u/u_{CJ}) from Eq(79) throughout the reaction zone with values of λ_1 and λ_2 calculated from Eqs. (71), (73), and (74). The results of three such calculations, based on the assumption that X_1 decomposes faster than X_2, are shown graphically in Figures 1a-3a and 1b-3b. The profiles in Figures 1a and 1b, 2a and 2b, and 3a and 3b were calculated respectively with the following sets of parameters: $\{n_1 = 3,\ f = 4,\ n_2 = 2\}$. $\{n_1 = 2,\ f = 3,\ n_2 = 2\}$, and $\{n_1 = 3,\ f = 3,\ n_2 = 3\}$.

Differentiaing Eq. (66) partially again with respect to t shows in general that $(\partial u/\partial t)_{CJ} < 0$ when $\left(\partial^2\lambda_2/\partial t^2\right)_{CJ} > 0$, and that $(\partial u/\partial t)_{CJ} = 0$ when $\left(\Phi^2\ \lambda_2/\partial t^2\right)_{CJ} = 0$ when λ_1, λ_3 and λ_4 are governed by Eqs. (73), (75), and (77). Examination of the particle velocity histories shows that these conditions are satisfied because $(\partial u/\partial t)_{CJ} < 0$ in Figures 1a and 2a where $n_2 = 2$ and $(\partial^2\lambda_2/\partial t^2)_{CJ} > 0$, and $(\partial u/\partial t)_{CJ} = 0$ in Figure 3a where $n_2 = 3$ and $(\partial^2\lambda_2/\partial t^2)_{CJ} = 0$. Further examination of Figures 1a-3a show that detailed properties of the Lagrange particle velocity history depend on the equations of state of the explosive and the detonation products as well as the energy release rate. However, the qualitative features of the particle velocity history are governed by the energy release rate, as shown by the observations that (1) the history calculated with $(n_1 = 3,\ n_2 = 2)$ is generally steeper than the history calculated with $(n_1 = 2,\ n_2 = 2)$, and (2) the history calculated with $(n_1 = 3,\ n_2 = 3)$ is generally steeper than the history calculated with $(n_1 = 3,\ n_2 = 2)$.

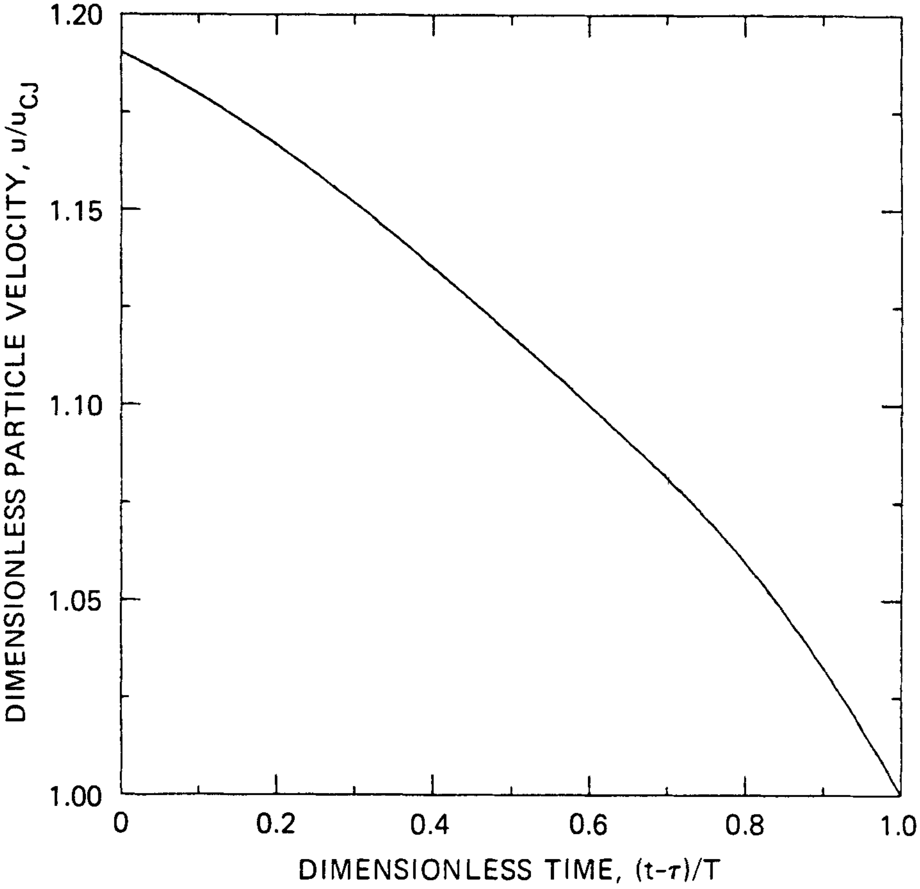

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FIGURE 1a PARTICLE VELOCITY vs TIME IN REACTION ZONE CALCULATED WITH $n_1 = 3$, $f = 4$, AND $n_2 = 2$

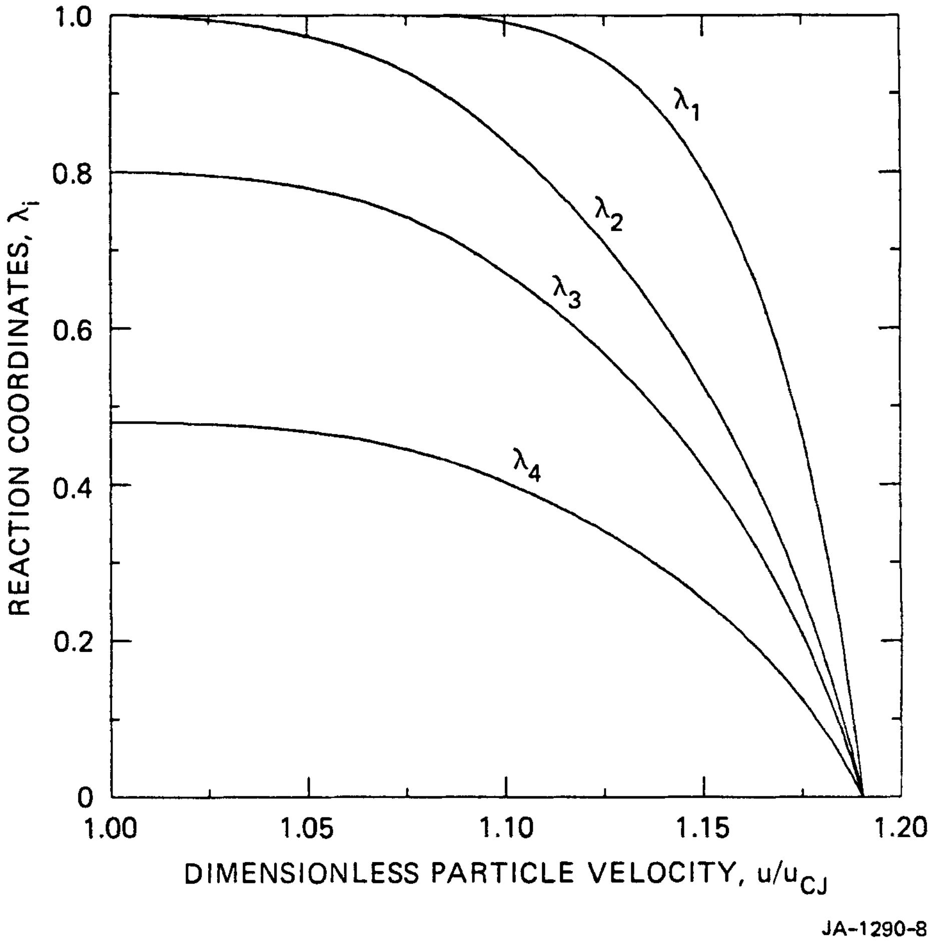

FIGURE 1b REACTION COORDINATES vs PARTICLE VELOCITY IN REACTION ZONE CALCULATED WITH $n_1 = 3$, $f = 4$, AND $n_2 = 2$

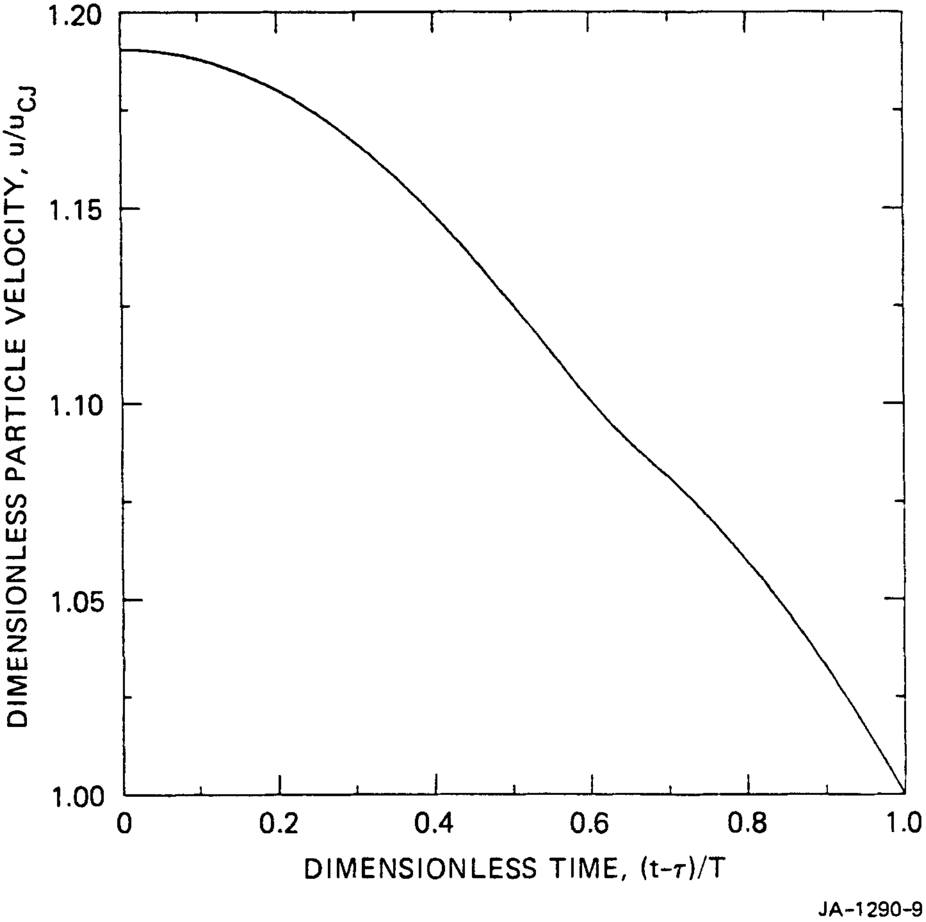

FIGURE 2a PARTICLE VELOCITY vs TIME IN REACTION ZONE CALCULATED WITH $n_1 = 2$, $f = 3$, AND $n_2 = 2$

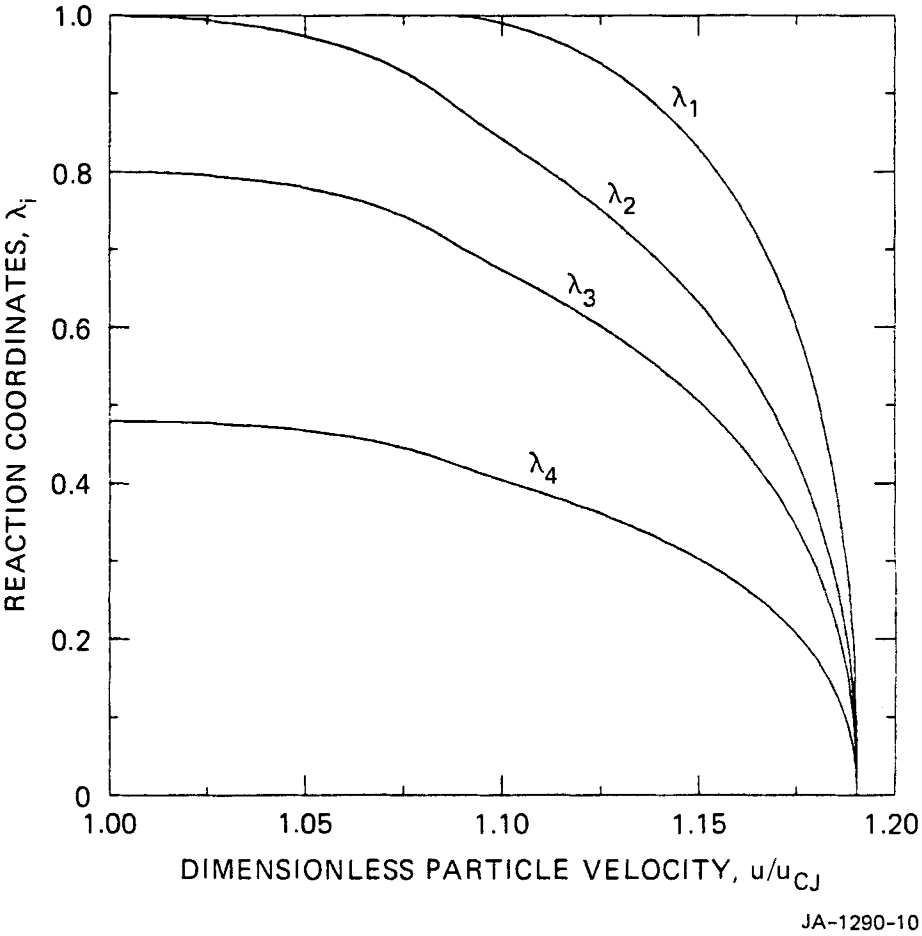

FIGURE 2b REACTION COORDINATES vs PARTICLE VELOCITY IN REACTION ZONE CALCULATED WITH $n_1 = 2$, $f = 3$, AND $n_2 = 2$

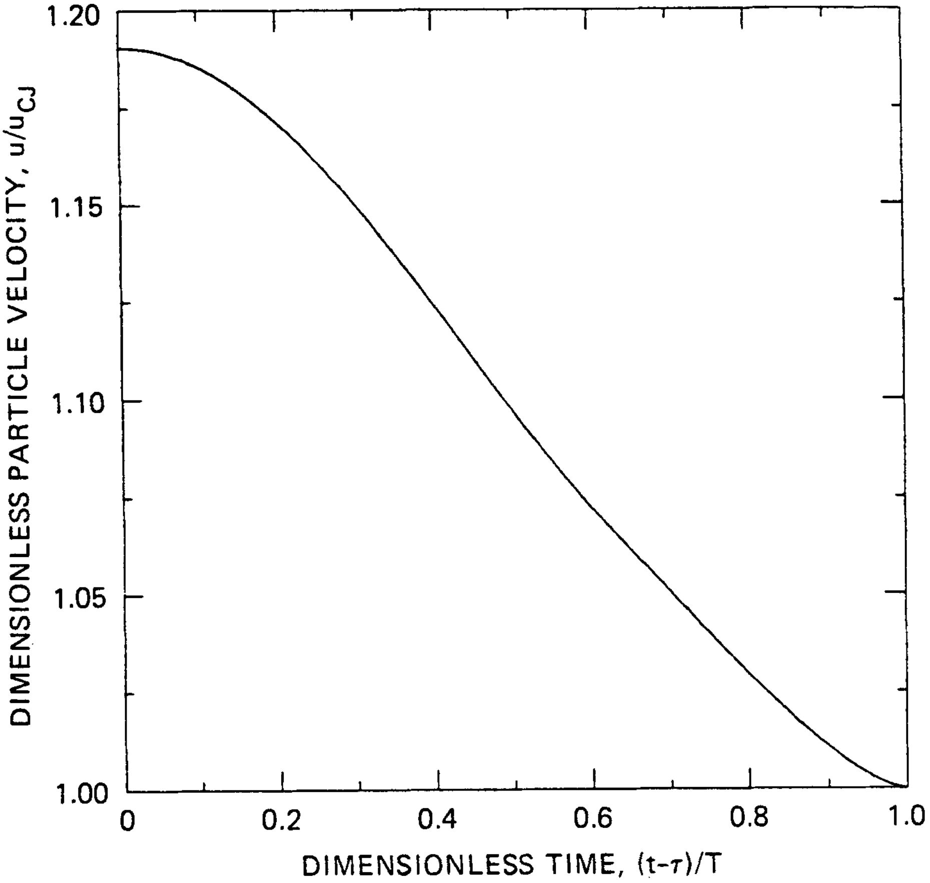

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FIGURE 3a PARTICLE VELOCITY vs TIME IN REACTION ZONE CALCULATED WITH $n_1 = 3$, $f = 3$, AND $n_2 = 3$

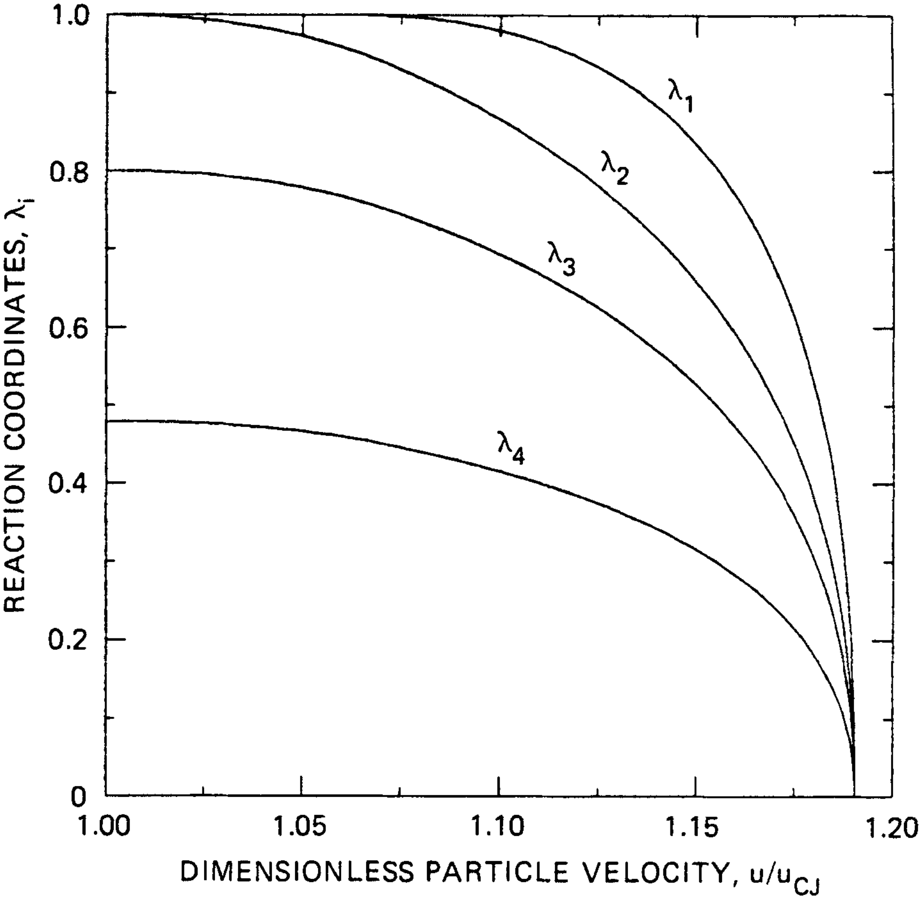

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FIGURE 3b REACTION COORDINATES vs PARTICLE VELOCITY IN REACTION ZONE CALCULATED WITH $n_1 = 3$, $f = 3$, AND $n_2 = 3$

CONCLUSIONS

We have formulated a treatment of steady-state detonation waves in composite explosives. Our formulation extends the classical ZND model for ideal detonation into a prototype model for nonideal detonation. The constititive relationship used to describe shocked reacting explosive is based on the assumption that the explosive and its detonation products are governed by different mechanical equations of state and attain mechanical, but not thermal, equilibrium. The kinetic processes responsible for nonideal behavior are assumed to be incomplete decomposition of the slowest reacting explosive component and the incomplete attainment of chemical equilibrium among the detonation products from the different explosive components.

To make our model applicable to Amatex 20, we considered a composite explosive containing an RDX-like component X_1, a TNT-like component X_2, and an AN-like component X_3. In this case the constitutive relationship must include four reaction coordinates: λ_1, λ_2, and λ_3 describe the decomposition of X_1, X_2, and X_3; λ_4 describes the reaction of the oxygen produced by X_3 and the carbon produced by X_1 and X_2. The reaction coordinates at the end of the reaction zone, $\hat{\lambda}_1$, $\hat{\lambda}_2$, $\hat{\lambda}_3$, and $\hat{\lambda}_4$, satisfy the conditions $\hat{\lambda}_1 = \hat{\lambda}_2 = \hat{\lambda}_3 = \hat{\lambda}_4 = 1$ in an ideal detonation wave, and satisfy the conditions $\hat{\lambda}_1 = \hat{\lambda}_2 = 1$, $\hat{\lambda}_3 < 1$, and $\hat{\lambda}_4 < 1$ in a nonideal detonation wave.

The constitutive relationship was combined with the Rankine-Hugoniot jump conditions and the CJ sonic condition to obtain the equations for the CJ parameters at the end of the reaction zone in a steady-state nonideal detonation wave. The equation governing particle velocity was combined with the CJ condition, relating particle velocity and detonation velocity in a nonideal detonation wave, to obtain the equation relating the detonation velocity to the chemical energy released in the wave. These equations for nonideal detonation specify the dependence of the detonation parameters on the reaction coordinates and demonstrate that the detonation process is influenced by the equation of state of the explosive. Detonation calculations, using explosive parameters chosen to model Amatex 20, were performed with values of $\hat{\lambda}_3$ in the range $0.45 < \hat{\lambda}_3 < 1$ and $\hat{\lambda}_4 = 0.6\,\hat{\lambda}_3$ to investigate the dependence of nonideal detonation parameters on the degree of incomplete decomposition of the explosive. Simplistic reaction rate functions were also constructed and used to calculate Lagrange particle velocity histories in nonideal detonation waves.

We conclude that the result of our theoretical study is a well-formulated model for steady-state detonation that provides us with a better understanding of nonideal detonation. However, we are still faced with a major problem of formulating a realistic treatment of the decomposition of AN and subsequent reactions along the detonation products. Before the present model of nonideal detonation can be used to calculate realistic nonideal detonation parameters, we must incorporate (1) models for these kinetics processes that predict values of $\hat{\lambda}_3$ and $\hat{\lambda}_4$; and (2) more realistic equations of state.

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