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TITLE MODELING TWO-DIMENSIONAL DETONATIONS WITH DETONATION SHOCK DYNAMICS

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MODELING TWO-DIMENSIONAL DETONATIONS WITH DETONATION SHOCK DYNAMICS *

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Abstract

In any explosive device, the chemical reaction of the explosive takes place in a thin zone just behind the shock front. The finite size of the reaction zone is responsible for: the pressure generated by the explosive being less near the boundaries, for the detonation velocity being lower near a boundary than away from it, and for the detonation velocity being lower for a divergent wave than for a plane wave.

In computer models that are used for engineering design calculations, the simplest treatment of the explosive reaction zone is to ignore it completely. Most explosive modeling is still done this way. The neglected effects are small when the reaction zone is very much smaller than the explosive's physical dimensions. When the ratio of the explosive's detonation reaction-zone length to a representative system dimension is of the order of 1/100, neglecting the reaction zone is not adequate.

An obvious solution is to model the reaction zone in full detail. At present, there is not sufficient computer power to do so economically. Recently we have developed an alternative to this standard approach. By transforming the governing equations to the proper intrinsic-coordinate frame, we have simplified the analysis of the two-dimensional reaction-zone problem. When the radius of curvature of the detonation shock is large compared to the reaction-zone length, the calculation of the two-dimensional reaction zone can be reduced to a sequence of one-dimensional problems.

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INTRODUCTION:

Describing the propagation of detonation in complex multi-dimensional explosive geometries is an important and ongoing problem in the design process for explosively driven devices. In order for the design of the explosive system to be successful, two requirements need to be met. First, the detonation of the explosive system must be relatively insensitive to variations in the initial conditions (e.g., to changes in the temperature and variations in the initiation system). At the same time, the explosive system must be safe from accidental initiation of detonation. The ratio of the explosive's detonation reaction-zone length to a representative system dimension is the parameter that controls these properties. The desirable ratio is of the order of 1/100. Problems of accidental initiation are minimized, yet at the same time the detonation is relatively insensitive to initial conditions. For most explosive geometries, this ratio is small enough so that the integrated momentum through the reaction zone is small in comparison to that in the broad region where the reaction products expand and do work on their surroundings. Thus the reaction zone has little direct influence on the process of driving inert materials that are in contact with it. However, the indirect influences of the reaction zone on the calculation can be much more important. When the ratio parameter is 1/100, a significant fraction of the explosive charge experiences such things as both reduced detonation pressure and velocity near boundaries, as well as a slower detonation velocity for a divergent detonation than for a plane one. These, in turn, lead to large errors in zeroth-order effects such as the time of detonation arrival and the two-dimensional detonation wave shape. From the point of view of the designer, this is a difficult computational regime. Not only does he need to resolve the broad region where the reaction products expand and do work on their surroundings, but he must also resolve the thin reaction zone.

Because of the disparate lengths of the reaction zone and release wave, most of the explosive design codes in use today employ some variant of the constant detonation velocity "Huygens" construction to propagate the detonation wave. This method for propagating the detonation only works well for explosives for which the reaction zone can be ignored (i.e., the ratio parameter is less than 1/1000). Ad hoc "fixes" of this simple model have been used to model systems for which the ratio parameter is larger than 1/1000. One example of such a "fix" includes a lower detonation velocity near the edge of the explosive than in the center. These have met with only limited success.

With all of its shortcomings, the simple "Huygens" method has one real advantage, computational speed. Since the reaction zone does not need to be modeled when this method is employed, design calculations can be done in a short enough time to allow many design iterations to be tried. This is an important feature that design codes need to have.

In order to improve on this simple method, constitutive information must be available about the explosive's reaction zone. This can be either explicit or implicit information. When explicit information is available, one can in principle follow the standard approach and do multi-dimensional simulations that resolve both the reaction zone and the explosive products region. This information is usually supplied in the form of the shock Hugoniot of the "unreacted" explosive, an equation of state (eos) of the explosive products, and a compatible energy-release rate calibrated to one-dimensional experiments.

To be useful, a numerical simulation of the reaction zone must be able to resolve all of the important features of the flow. Fickett [1] has shown that when the standard 1D Lagrangian-mesh artificial-viscosity methods are used, roughly 20 computational cells are needed in the reaction zone to get 10% accuracy. This translates into many tens of thousands of computational cells for a typical 2D numerical calculation. Even with today's supercomputers, such calculations take tens of hours of computation time; they are not practical for routine design calculations. When one reduces the number of cells in the calculation in order to get sensible computation times, the accuracy of the calculations suffers.

In large measure, the inordinately large computation time is a result of the lack of sophistication of the standard method. The uniform fine mesh that's needed to achieve reasonable resolution in the reaction zone, is excessively fine for the release-wave calculation. Today researchers are developing a variety of improved methods that include such features as: (1) multi-grid techniques that employ moving fine zoning near shocks [2], (2) schemes based on the method of characteristics such as CIR and Godunov [2,3] and (3) shock-tracking methods [4]. To date, however, none of these methods has reached the point of maturity where they could replace the standard method for routine detonation calculations.

The central issue in improved 2D calculations of detonation is a high-accuracy calculation of the reaction-zone structure, and a relatively coarse grid calculation of the following products release wave. One way of getting a high-accuracy calculation of the reaction-zone structure, is to do it analytically. This alternative brings with it not only the direct computational benefit, but it also brings the advantage of a theoretical understanding of the two-dimensional detonation process. With such an understanding, we could make a fast high-resolution wave-tracking code that solves the reaction-zone flow analytically and the release wave with a coarse grid numerical simulation. This increased knowledge also brings with it the insights that lead to the improvements that are necessary if some of the more sophisticated computational methods mentioned above are to become practical tools.

An analytical solution of the general two-dimensional time-dependent detonation problem is not within reach. However, in many applications of explosives, one observes that the radius of curvature of the detonation shock is large in comparison with the reaction-zone length. Recently we have developed an alternative to the standard numerical approach that's based on the large radius of curvature limit. By transforming the governing equations to the proper intrinsic-coordinate frame, we have simplified the analysis of the two-dimensional reaction zone problem, and reduced it to a sequence of one-dimensional problems. The coordinate frame of choice is one in which the spatial coordinate axes are everywhere locally parallel and perpendicular to the shock. The governing equations consist of a kinematic equation that describes the progress of disturbances moving along the shock, and equations for the reaction-zone dynamics that describe the quasi-steady flow normal to the shock and through the reaction zone. We call this method DETONATION SHOCK DYNAMICS (DSD).

We have divided this paper into four sections. In section II, we give an overview of the theoretical model. This section is divided into three subsections. In Shock Kinematics, we briefly describe our coordinate system and the kinematics of the detonation shock. The subsection entitled Boundary Conditions, is devoted to a discussion of the boundary conditions that are applied at the edges of the explosive. In Reaction-Zone Dynamics, the Euler equations are transformed to the intrinsic-coordinate frame, and the analysis that leads to the quasi-steady description is briefly reviewed. In section III, we demonstrate how our theory can be used to study a representative explosive design problem. In section IV, we summarize our results.

OVERVIEW OF THE THEORY:

The thrust behind our theory is the concept that the response of the detonation shock is local, and is governed by its current local configuration. Philosophically, it is an extension of Whitham's geometrical shock dynamics to detonation [5]. Our theory is a uniform perturbation theory, that is based on the notion that the radius of curvature of the shock is large when compared to the reaction-zone length. It is a nonlinear theory that can be used to describe arbitrarily large departures of the detonation shock shape from the plane one-dimensional state. From the results of our theoretical calculations, the following picture has emerged. In many situations, the dynamics of the detonation reaction zone is decoupled from the evolution of the large following rarefaction wave, and is controlled by the flow near the shock. As a result, we have found that the important waves in the reaction zone, either rarefactions or compressions, are transverse waves. Our theory describes how these two-dimensional waves are generated (e.g., near an explosive edge) and move laterally through the reaction zone (see Figure 1). There are three components to the theory: (1) a kinematic condition for the shock surface, (2) conditions to be satisfied at the boundaries of the explosive and (3) the flow dynamics in the direction normal to the shock (i.e., through the reaction zone). We will briefly describe each of these.

Our theory is based on the time-dependent, two-dimensional reactive Euler equations. As a consequence, the detonation shock (shock) is a surface of discontinuity. Since we wish to treat detonation-wave evolution in complicated two-dimensional geometries, we have developed our theory in a problem determined intrinsic-coordinate system (see Figure 2). It is a shock-centered frame that moves with the local normal detonation-shock velocity (D_n). The space variables are the distances ξ and η locally parallel and perpendicular to the shock.

Shock Kinematics

The principal object of the theory is to calculate the shock shape as a function of time. The intrinsic representation of a curve, such as the shock, is in terms of its curvature (κ) as a function of arc length along the shock (ξ) and time (t). In this coordinate system, the shock shape is described by the shock angle (ϕ) as a function of ξ and t. In terms of these variables, the shock curvature is $\kappa \equiv \phi_{,\xi}$, where the $_{,\xi}$ indicates a partial derivative with respect to arc length. The laboratory coordinates for the shock are returned by

$$z_o^l = z_e^l - \int_0^{\xi} \sin(\phi)\,d\xi \;, \quad r_o^l = r_e^l + \int_0^{\xi} \cos(\phi)\,d\xi \;, \qquad (1)$$

where z_e^l and r_e^l are the coordinates of the edge. Typically we are most interested in describing the changes in the shock shape that are the result of the interaction that occurs between the shock and an explosive edge. For such problems, having the zero of arc length coincide with the edge is the most convenient origin to use for ξ . Figure 3 shows a schematic representation of the shock including the independent variable (ξ) and the definition of the dependent variables D_n and ϕ . The cartesian unit vectors are $\hat{e}_z$ and $\hat{e}_r$.

The geometric compatibility conditions for a moving two-dimensional surface are given in Whitham [5]

$$\phi_{,\alpha} = -\frac{1}{A} D_{n,\beta} \tag{2}$$

and

$$\phi_{,\beta} = \frac{1}{D_n} A_{,\alpha} \quad . \tag{3}$$

The variable α is equivalent to time, and labels a particular shock surface. The constant β rays are orthogonal to the shock and are its propagators. The streamtube area is A , where at fixed α

$$d\xi = A\, d\beta \tag{4}$$

(i.e., the area between two adjacent constant β rays).

For the problems of interest in condensed phase detonation, the shock is seldom normal to the explosive boundary. As a result, the coordinate β is not a convenient independent variable since boundary conditions must be applied at the edge. Changing independent variables from (α, β) to (t, ξ), we have

$$d\xi = A\, d\beta + B\, d\alpha \tag{5}$$

and

$$dt = d\alpha , \tag{6}$$

where the coefficient B describes the change in arc length with time along a constant β ray. Performing this transformation, the surface kinematics [i.e., Eq. (2)] takes on the form of a one-dimensional wave equation along the shock with $\mathcal{B}$ being the wave velocity and $D_{n,\xi}$ is a Burgers Equation-like transport term

$$\phi_{,t} + \mathcal{B}\phi_{,\xi} = -D_{n,\xi} \quad . \qquad (7)$$

The coefficient $\mathcal{B}$ is obtained by requiring that the transformation [Eqs. (5) and (6)] is solvable, from which it follows that

$$A_{,\alpha} = \mathcal{B}_{,\beta} \quad . \qquad (8)$$

From Eqs. (3) and (8) it follows that

$$\mathcal{B} = \int_0^{\xi} \phi_{,\xi} D_n \, d\xi + \mathcal{B}_o(t) \; . \qquad (9)$$

The function $\mathcal{B}_o(t)$ is the amount of shock arc length which crosses the β = constant ray that intercepts the edge and is given by

$$\mathcal{B}_o(t) = D_{ne} \tan(\tilde{\phi}_e) \; . \qquad (10)$$

This intrinsic form of the shock-surface kinematics is fundamental to any shock-tracking method that seeks to describe the evolution of shocks of <u>arbitrary shape</u> in a <u>uniform manner</u>. Clearly, Eqs. (7) and (9) are simply a constraint between D_n and $\mathcal{K} = \phi_{,\xi}$. However, if a second relation between D_n and $\mathcal{K}$ can be obtained, then Eq. (7) becomes a <u>partial-differential equation for the shock surface</u>. It is important to note that Eq. (7) is a "one-dimensional" condition, whose independent variables are the arc length (ξ) [the distance coordinate] and time (t). Further, if we then prescribe the initial shape (ϕ) of the surface, as well as some boundary condition at the intersection of the detonation shock and the explosive boundary, then Eq. (7) can be solved to get the two-dimensional shock locus at any subsequent time.

Boundary Conditions

For the problems we consider in this brief review paper, we do not need to study the complex flow or the detailed boundary conditions that apply in the vicinity of the explosive boundary. It will be sufficient to consider only the condition, if any, that must be applied at the locus generated by the intersection of the detonation shock and the edge. We consider only an explosive/vacuum interface.

At such an interface, the flow experiences a singularity. In the explosive, the pressure just behind the detonation shock is near the Chapman-Jouguet (cJ) pressure; just outside the explosive, the pressure is at or near zero. In order for the flow to execute such a transition, a singularity of Prandtl-Meyer (PM)-type must be imbedded in the flow at the intersection of the shock and the edge. Since locally the flow at this point is quasi steady, it can only be either a sonic or a supersonic flow (as seen by an observer riding along the edge/shock intersection locus). We will discuss the consequences that result from having flows of these two types.

Along the edge/shock locus, the sonic parameter is a function of the normal detonation velocity along the edge, D_{n_e}, and the shock interface angle, $\tilde{\phi}_e$. For a polytropic eos, with γ the polytropic exponent, the expression is

$$C^2 - |U|^2 = D_{ne}^2 \left\{ \frac{\gamma}{\gamma+1}\sqrt{1-\frac{D_{n*}^2}{D_{ne}^2}} - \frac{1}{\gamma+1}\left(1-\frac{D_{n*}^2}{D_{ne}^2}\right) - \tan^2(\tilde{\phi}_e)\right\}, \quad (11)$$

where C is the sound speed, $|U|$ is the magnitude of the particle velocity in the shock-fixed frame and D_{n*} is the minimum value of D_n for a one-dimensional detonation.

If the flow is supersonic along the locus, then disturbances from the edge can not propagate into the detonation reaction zone. The interface moves faster laterally than do acoustic waves. For this case, no boundary condition is applied, and the interface does not affect the detonation.

As the flow turns subsonic, then D_{ne} and $\tilde{\phi}_e$ must be adjusted so that the sonic condition, $C^2 - |U|^2 = 0$, is maintained. This condition serves as a boundary condition for the flow.

The following rule is used along the edge/shock locus: Monitor the sonic parameter on the locus. If $C^2 - |U|^2 < 0$, the flow is supersonic and no condition is applied. When the flow is either sonic or subsonic, then D_{ne} and $\tilde{\phi}_e$ must be adjusted to satisfy the condition $C^2 - |U|^2 = 0$.

Reaction-Zone Dynamics

Equation (7) is a one-dimensional partial-differential relation that D_n and ϕ must satisfy if they are to describe a two-dimensional shock. If a second relation between D_n and ϕ can be found, we can convert this relation to a partial-differential equation (pde), and in the process reduce the two-dimensional shock tracking problem to a one-dimensional one. For a number of cases, we have found such a second relation between D_n and $\kappa = \phi_{,\xi}$. When it exists, this relation contains all the necessary reaction-zone dynamics; the consequences of the interaction of the chemical-heat release with the flow. To find it, we must solve the time-dependent two-dimensional Euler equations. In order to solve these equations for complex explosive geometries, we must express them in terms of a natural system of coordinates that simplifies their form. In the limit that the radius of curvature of the shock is large compared to the reaction-zone length, the coordinates shown in Figure 2. are particularly convenient. Bertrand curves that are everywhere parallel to the shock are the η constant coordinates; the lines perpendicular to these curves are the constant ξ coordinates. These coordinates are related to the laboratory cartesian frame, by

$$z' = z_o' - \eta \cos\phi \qquad (12)$$

and

$$r' = r_o' - \eta \sin\phi \;, \qquad (13)$$

where z_o' and r_o' are given by Eq. (1). Expressed in these coordinates, the Euler equations are

mass $$\mathcal{L}\rho + \rho(\kappa u_\eta - u_{\eta,\eta} + u_{\xi,\xi}) + \cdots = 0, \qquad (14)$$

η-momentum $$\mathcal{L}u_\eta - \frac{1}{\rho}P_{,\eta} + \cdots = 0, \qquad (15)$$

ξ-momentum $$\mathcal{L}u_\xi + \frac{1}{\rho}P_{,\xi} - D_{n,\xi}u_\eta + \cdots = 0 \qquad (16)$$

and

energy $$\mathcal{L}E - \frac{P}{\rho^2}\mathcal{L}\rho + \cdots = 0 \;. \qquad (17)$$

The chemical rate law is

$$\underline{\text{rate}} \qquad \mathcal{L}\lambda + \cdots = \mathcal{R} . \tag{18}$$

We have displayed only those terms that are necessary to do the leading order theory in the small $\mathcal{K}$-limit. In the above

$$\mathcal{L} \equiv \frac{\partial}{\partial t} + (D_n - \mathcal{U}_\eta)\frac{\partial}{\partial \eta} + B\frac{\partial}{\partial \xi} , \tag{19}$$

ρ is the density, $\mathcal{U}_\eta$ is the η-component of the particle velocity (at leading order $\mathcal{U}_\eta > 0$ and $\mathcal{U}_{\eta,\eta} < 0$), $\mathcal{U}_\xi$ is the ξ-particle velocity ($\mathcal{U}_\xi = 0$ at the shock), $\mathcal{P}$ is the pressure, λ is the degree of reaction ($\lambda = 0$ at the shock), $\mathcal{R}$ is the chemical rate and E is the specific internal energy. The above equations, the standard one-dimensional shock conditions, the kinematics [Eq. (7)] and appropriate initial/boundary conditions completely define the two-dimensional problem that must be solved. Even in the small-$\mathcal{K}$ limit, this is a formidable task.

What we have shown recently is that for certain rate-law forms (i.e., expressions for $\mathcal{R}$), the important large-scale dynamics is quasi steady [6]. We considered relatively long-scale disturbances to the shock

$$\epsilon^2 = O(\mathcal{K}) << 1 , \tag{20}$$

$$D_n = D_{cj} + O(\epsilon^2) \tag{21}$$

and two time regimes:

(1) "fast" dynamics $\quad t_1 = \epsilon t$

changes in $\phi = O(\epsilon^{3/2})$, $\xi_{1/2} = \epsilon^{1/2}\xi$ (22)

and

(2) quasi-steady dynamics $t_2 = \epsilon^2 t$

changes in $\phi = O(\epsilon)$, $\xi_1 = \epsilon\xi$ (23)

and larger.

The "fast" scale problem was necessary to treat the influence of the two-dimensional initial/boundary data, and to describe the hydrodynamic wavehead that separates the reaction zone into parts that are either influenced or uninfluenced by the edge. As the flow evolved, the "fast" scale perturbations became smaller, and the disturbances to the one-dimensional state became larger and quasi steady. This quasi-steady regime was particularly simple; the Euler equations reduced to the steady nozzle equations [a steady cylindrically-symmetric system of ordinary-differential equations (ode)]

$$[(D_n - u_\eta)\rho]_{,\eta} + \rho\kappa u_\eta = 0, \quad (24)$$

etc.

The only parameters in these equations, besides the fixed constitutive parameters, are D_n and κ. That is, the initial/boundary data do not appear in the large change reaction-zone dynamics. In some sense then, the <u>dynamics is universal</u>. The resulting one-dimensional problem is simply the detonation "eigenvalue" problem considered by Wood & Kirkwood [7]. Since the propagation of the detonation shock is decoupled from the product expansion region, the theory is free of ad hoc approximations about the influence of the following flow. At least this is the case for diverging detonation.

The quasi-steady problem defines $D_n(\kappa)$. With κ specified, D_n is determined by solving an eigenvalue problem. In addition to yielding $D_n(\kappa)$, this solution also gives the state at the end of the reaction zone as a function of κ. Thus for an important class of problems, the reaction-zone dynamics is given by $D_n(\kappa)$, and the two-dimensional shock-evolution problem is reduced to a one-dimensional problem.

Two points are worth noting. First, the $D_n(\kappa)$ relation only contains limited constitutive information about the explosive. The constants in this relation are integrals through the reaction zone of this information. Secondly, $D_n(\kappa)$ is independent of initial/boundary data. Therefore, when detailed constitutive information about the reaction zone is not known (the typical situation for condensed phase explosives), $D_n(\kappa)$ can be measured directly via simple steady-state two-dimensional hydrodynamic experiments. Thus we have a way of using simple experiments to calibrate the reaction-zone dynamics. In turn, we can use the calibrated $D_n(\kappa)$ relation to predict detonation wave evolution in complex explosive geometries.

Direct calculations of $D_n(\kappa)$ performed with the simple polytropic eos, show that the form of the rule is sensitive to the form of the rate law [8]. Calculations were done for two state-independent rates with different depletion forms; square-root depletion

$$\mathcal{R} = \sqrt{1-\lambda} \qquad (25)$$

and simple depletion

$$\mathcal{R} = (1-\lambda) \; . \tag{26}$$

The $D_n(\mathcal{K})$ rule for Eq. (25) is

$$D_n = 1 - \alpha \mathcal{K}' \, , \tag{27}$$

while for Eq. (26) we have

$$D_n = 1 + \beta \mathcal{K} \ln(\mathcal{K}) - \alpha \mathcal{K} \; . \tag{28}$$

The constants α and β are not to be confused with Whitham's curvilinear coordinates. D_{CJ} is set to one. In the next section, we give a brief tutorial that describes how this theory can be applied to explosive engineering design problems.

APPLICATIONS:

The simplest time-dependent problem that can be done is the constant-velocity detonation or "Huygens" construction for a diverging detonation. For convenience we take $D_n = 1$. Equation (7) then becomes the simple nonlinear-wave equation for the shock angle (see Figure 3)

$$\phi_{,t} + (\phi - \phi_e)\phi_{,\xi} = 0 \, , \tag{29}$$

where ϕ_e is the value of ϕ at the edge (i.e., at $\xi = 0$). Equation (29) states that ϕ = constant along the characteristic lines $\xi - (\phi - \phi_e)t$ = constant, that is

$$\phi = \phi_0 \quad \text{along} \quad \xi - (\phi_0 - \phi_e)t = \xi_0 \, . \tag{30}$$

If we consider a flow where the two-dimensional shock is convergent initially, then the initial angle, ϕ_0, is a decreasing function of the initial arc length, ξ_0. Such a flow looks compressive, in the sense that the characteristic lines are convergent. After a finite time, some of the characteristics cross one another and the solution becomes multi-valued. Physically, the rule $D_n = 1$ does not apply to a convergent detonation, so we will not consider this case further.

When the two-dimensional shock is initially divergent, the initial angle is an increasing function of arc length, and the characteristic lines are rarefaction-like. An example of a divergent-wave problem that is often encountered in designs is shown in Figure 4. It is a prototypical example of a diverging detonation that features the diffraction of the detonation (i.e., the "shadow zone" problem). The left-most vertical line is a symmetry plane; the lower horizontal line and the upper circular arc are the edges of the explosive. The wave is initially circular with a radius R_a. Since the wave is perpendicular to the horizontal edge, the flow along that edge/shock locus is sonic, and the edge does not influence the shock evolution. When the expanding wave first reaches the circular boundary, the flow along the upper edge/shock locus is supersonic. It remains supersonic until the detonation reaches the point where the dashed line is tangent to the arc. The region above the dashed line is not in direct line of sight of the initial data; it is a "shadow zone". Diffraction is the process that allows the wave to spread into this region. The solution in this region is determined by the boundary data supplied along the circular edge.

In both regions of the problem, the solution takes a simple form. The great advantage of our formulation over older methods is this simplicity of representation. The calculations shown in Figure 4, are free of reaction-zone effects. We conclude this section by showing how detonation shock dynamics can be used to include the important finite size reaction-zone effects for this example.

We assume that the reaction-zone dynamics is given by Eq.(27)

$$D_n = 1 - \alpha \kappa$$

and introduce the change of variable

$$\phi = \phi_e + \tilde{\phi} , \tag{31}$$

where ϕ_e is the angle that the tangent to the edge makes with the reference direction $\hat{e}_z$. Substituting these into the kinematic equation [i.e., Eq. (7)], yields a "Burgers" equation

$$\tilde{\phi}_{,t} - \frac{R_2 D_{ne}}{R_3 \cos(\tilde{\phi}_e)} + B \tilde{\phi}_{,x} = \frac{\alpha}{R_2} \tilde{\phi}_{,xx} , \quad (32)$$

as the propagator for the shock. The independent variables in Eq. (32) are scaled time (t) and scaled arc length (x). The finite length reaction-zone effects enter this equation as the transport term on the right-hand side. This is similar to the structure of wave-hierarchy problems that arise in one-dimensional wave propagation problems in reactive materials [9]. The second term on the left-hand side represents the diffraction effect. Equation (32) is a one-dimensional parabolic pde. In the quasi-steady limit, the reactivity acts to smooth the shock locus.

Equation (32) was solved numerically for the design problem shown in Figure 4. A mesh was used with one thousand points along the shock. The computation time was one minute on the Cray-1 supercomputer. The results of the wave tracking calculation for a set of parameter values that highlight the finite-length reaction-zone effects are shown in Figure 5.

The important parameters in this calculation are (α/R_2) the ratio of the reaction-zone length parameter to the radius of the booster, and (R_2/R_3) the ratio of the booster to the edge radius. The dashed contours correspond to the standard "Huygens" construction studied in Figure 4. The dotted contours show the cylindrically expanding finite-length reaction-zone wave without any edge effect. The solid contours show the complete DSD calculation, including the edge effects. Although the results shown in the figure speak well for themselves, a few comments are in order. Even in regions of the flow that are not influenced by the edge, the finite-length reaction-zone effects cause the detonation to lag behind the "Huygens" wave. Near the lower edge, the complete DSD calculation is strongly curled back. Along this edge, the phase velocity of the detonation wave is initially low, but as time passes it builds back to that for a cylindrically expanding wave. Along the upper surface, no edge effect is observed until the detonation wave passes into the "shadow zone". After this occurs, the detonation wave is continually undergoing wave diffraction. Since the phase velocity at the edge quickly reaches a steady value that is well below D_{CJ}, the curl back is more pronounced in this region than at the lower edge. The value of this velocity is a function of the radius of the upper explosive/vacuum interface.

SUMMARY:

We have developed a theory for propagating two-dimensional detonation shocks in complex explosive assemblies. The three components of our method are:

(1) shock kinematics [Eq. (7)],

(2) boundary conditions [Eq. (11)] and

(3) reaction-zone dynamics [e.g., Eq. (27)].

In spirit it is the detonation analog of Whitham's inert shock propagation theory, geometrical shock dynamics. It is a rationally derived theory that applies when the radius of curvature of the detonation shock is large compared to the reaction-zone length. A fully nonlinear theory, it describes the large amplitude changes in the two-dimensional detonation shock that occur over long times.

The DSD method that we've developed is a powerful tool that can be used to efficiently model reaction-zone effects in numerical simulations of detonation. Using this method, typical explosive design calculations can be performed with about one minute of supercomputer time. This is to be compared to the tens of hours that are required for a modest resolution full numerical simulation of the problem. In addition to the direct computational benefit, this theory also increases our understanding of time-dependent two-dimensional detonation. For example, this theory defines the relationship between the detonation wave phase velocity and the radius of the explosive edge in the "shadow zone".

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FIGURE CAPTIONS:

Figure (1) A schematic diagram that shows how chemical/mechanical energy are transported laterally through the reaction zone. The kinematic condition is applied along (1), boundary conditions are applied at (2) and the reaction-zone dynamics describes the flow along (3). To leading order, the reaction zone is insulated from rarefactions from the rear.

Figure (2) The intrinsic-coordinate system that was used in the calculation. The shock curvature is $\kappa = \phi_{\xi}$ and

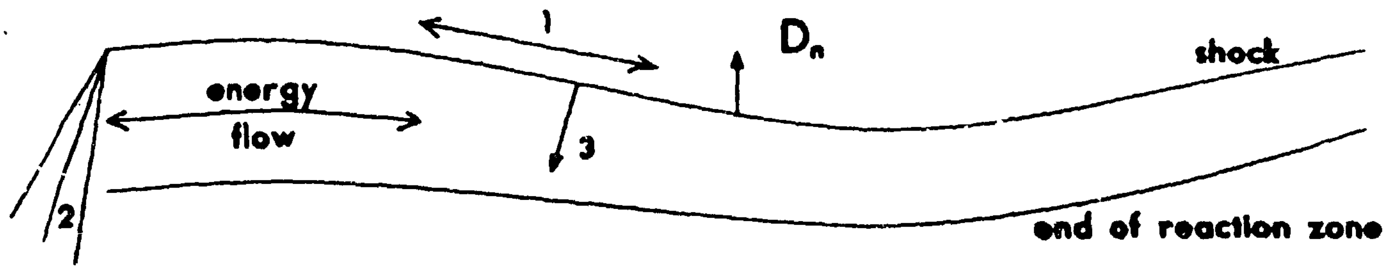
$$z' = z_0' - \eta \cos\phi \;, \quad r' = r_0' - \eta \sin\phi \,.$$

Figure (3) Intrinsic coordinates and shock kinematics. The independent variables are arc length (ξ) and time (t), while the dependent variables are the normal shock velocity (D_n) and the shock normal angle (ϕ). The curves β = constant are normal to the shock, and ϕ_e is the angle between the tangent to the edge and normal to the shock.

Figure (4) A prototypical diverging detonation problem. The wave is propagated with $D_n = 1$, a "Huygens" construction. Below the dashed line, the wave is free of boundary effects and expands as a circle. Above the dashed line, the wave shape is determined by applying the sonic condition along the radius R_a circular edge.

Figure (5) The DSD calculation of the example considered in Figure 4. The reaction-zone dynamics rule was $D_n = 1 - \alpha\kappa$, where the magnitude of α is shown. Three calculations are displayed :

–·–·–·– $D_n = 1$ "Huygens",
– – – – – $D_n = 1 - \alpha\kappa$ circularly expanding wave and
——— the full DSD calculation.



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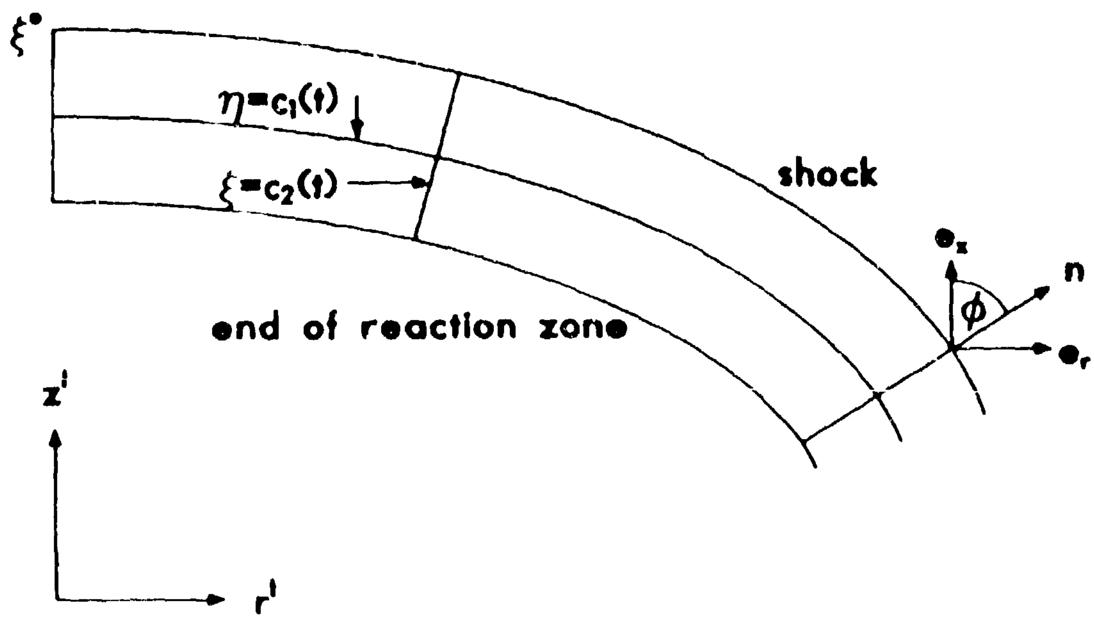

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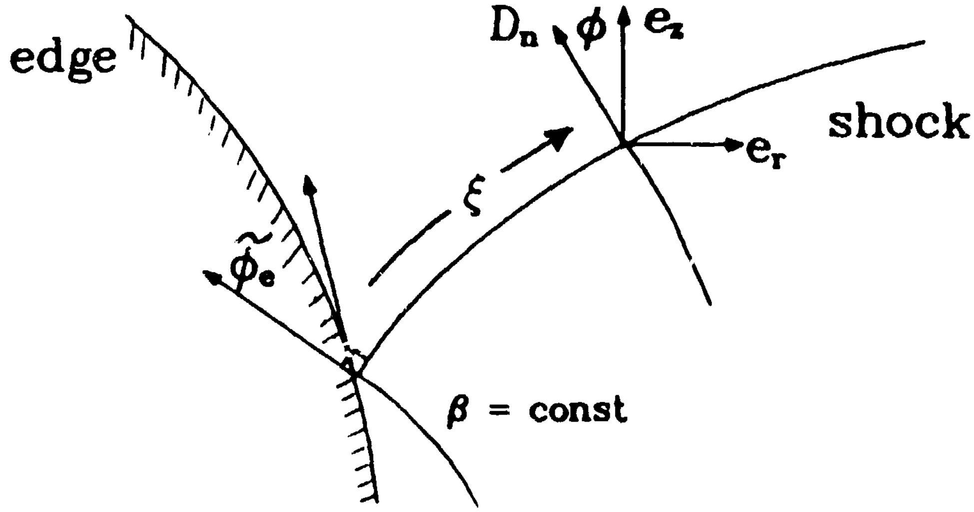

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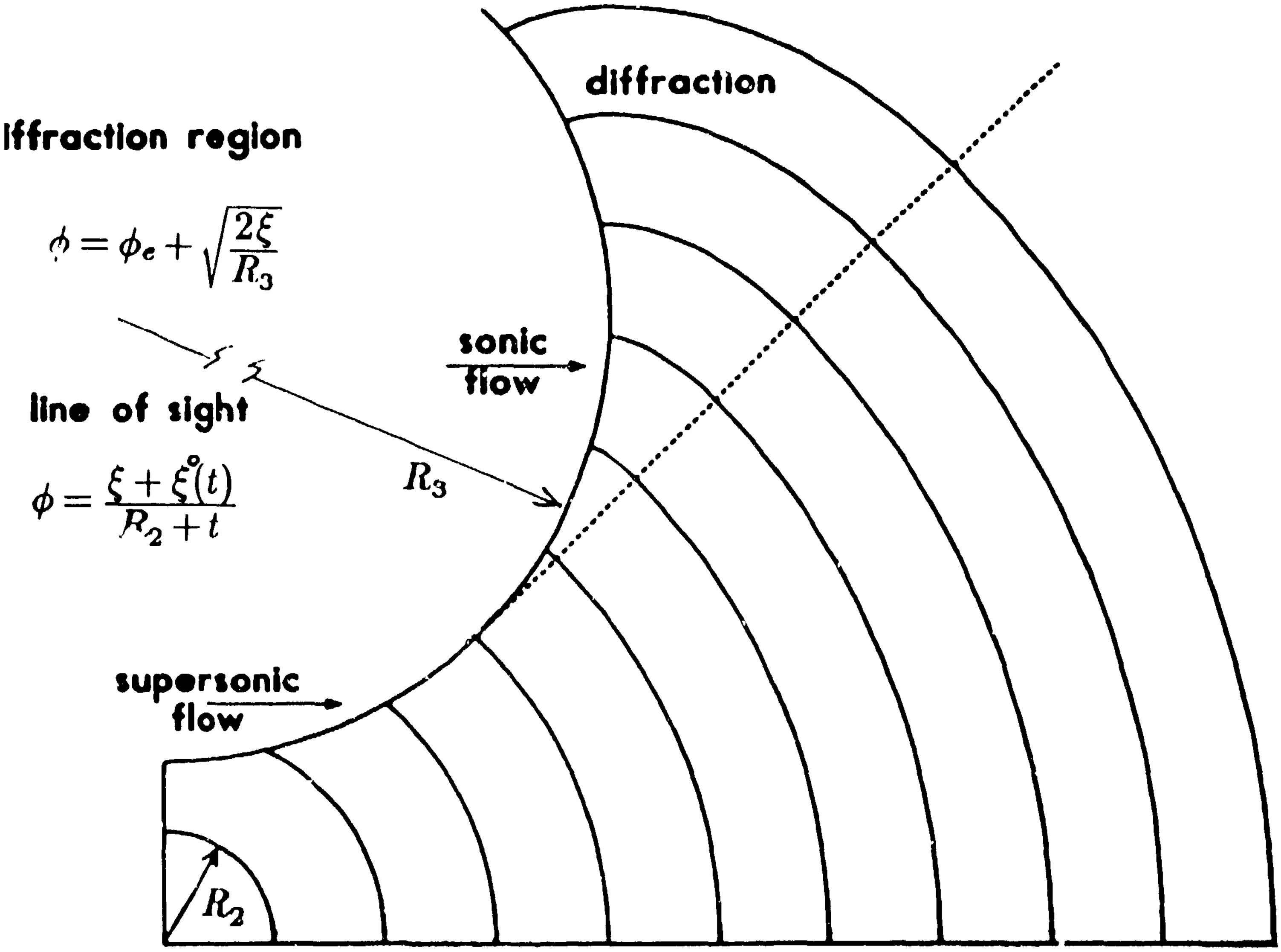

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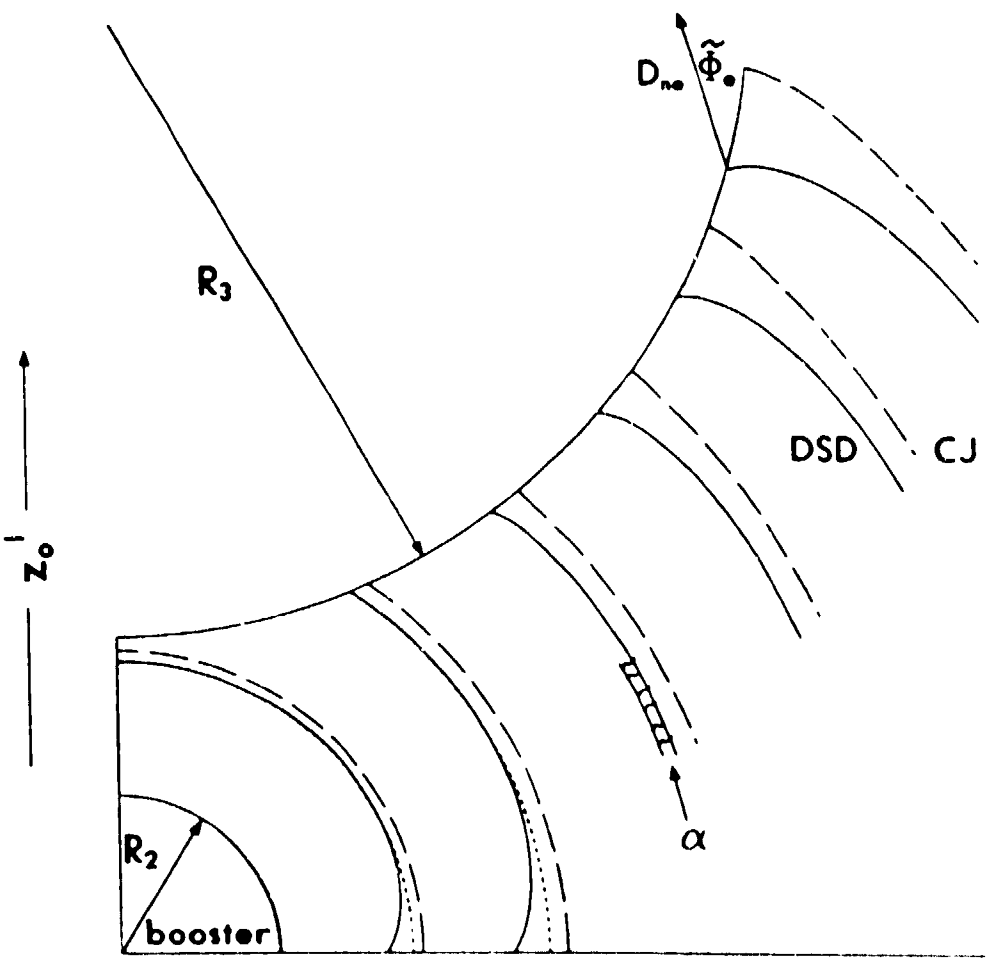

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