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SHARP SHOCK MODEL FOR PROPAGATING DETONATION WAVES

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Recent analyses of the reactive Euler equations have led to an understanding of the effect of curvature on an underdriven detonation wave. This advance can be incorporated into an improved sharp shock model for propagating detonation waves in hydrodynamic calculations. We illustrate the model with two simple examples: time dependent propagation of a diverging detonation wave in 1-D, and the steady 2-D propagation of a detonation wave in a rate stick. Incorporating this model into a 2-D front tracking code is discussed.

1. INTRODUCTION

In numerical simulations of most explosive applications it is impractical to resolve the reaction zone of a detonation wave. A sharp shock model or programmed burn, in which an underdriven detonation is simply propagated with the CJ detonation velocity, is often used. This simple model is useful but neglects an important property of detonation waves. Namely, the velocity of a diverging detonation wave and the pressure behind the front are lower than the corresponding values for a planar CJ detonation wave.

Recent analyses[1-7] of the reactive Euler equations have led to an understanding of the correction terms for the wave speed and state variables behind the wave caused by the curvature of the detonation front. These advances may be incorporated into an improved sharp shock model which accounts for front curvature when propagating a detonation wave. That self sustaining underdriven detonation waves decouple from the flow behind is the basis for programmed burn and the improved model, detonation shock dynamics.[7] The sharp shock model is well suited to a front tracking code since it explicitly takes into account the discontinuity of the variables across a wave. Front tracking has the advantage that it can account for waves from behind catching up to and strengthening the detonation wave. This occurs in the overdriven case and is important for converging detonation waves.

2. THE THEORY OF DIVERGING DETONATIONS

An asymptotic analysis of a diverging detonation wave[1-4] in an explosive described by the reactive Euler equations,[8] shows that when the reaction zone length is small compared to the radius of curvature of the front, then to leading order the reaction zone is quasi-steady and may be modeled by a system of ODEs. The flow in the reaction zone of an underdriven detonation wave is transonic. The profile of the reaction zone is determined by the trajectory of the ODEs through a critical saddle point.[1,8,9] This is the natural analog of a planar CJ detonation to diverging geometry. In particular, this analysis determines the detonation velocity $D(\kappa)$ and the state variables at the end of the reaction zone as a function of the mean curvature of the detonation front κ.

For a reaction rate of the form

$$R = \begin{cases} (1-\lambda)^{\nu} f(\text{state variables}) & , \quad T > T_c \\ 0 & , \quad T < T_c \end{cases} \qquad (1)$$

where λ is the reaction progress variable with $\lambda = 0$ corresponding to reactants and $\lambda = 1$ to reaction products, T is the temperature with T_c the temperature below which the reaction rate is taken to be 0, and ν is the order of the reaction, the leading order curvature correction to the detonation velocity has the form

$$D(\kappa) = \begin{cases} D_{CJ} - \alpha_1 \kappa + \text{higher order terms} & \nu < 1 \\ D_{CJ} - \alpha_2 \kappa + \alpha_3 \kappa \ln \kappa + O(\kappa) & \nu = 1 \\ D_{CJ} - \alpha_4 \kappa^{1/\nu} + O(\kappa) & \nu > 1 \end{cases} \qquad (2)$$

where D_{CJ} is the planar CJ detonation velocity, and the α_i's are constants. Parts of these results were found independently by Jones[1,2] Stewart and Bdzil[4] and Damamme.[5] The leading order corrections to pressure, velocity, and density are found to have the same form as the detonation wave speed correction.

For a general equation of state (EOS) and rate law, the system of ODEs has to be solved numerically by way of a shooting algorithm. When κ is sufficiently small at the critical point $\lambda \approx 1$ and the end of the reaction zone may be approximated by the sonic point. Other numerical calculations with this system of ODEs show that above a critical curvature $\kappa > \kappa_*$ there is no trajectory passing through the critical sonic point. This corresponds to the failure of a steady detonation wave to propagate, see ref. 9.

3. APPLICATIONS OF SHARP SHOCK MODEL

In the sharp shock model the reaction zone is not resolved and the detonation wave is treated as a discontinuity. The theory in sec. 2 in effect determines the jump conditions for an underdriven diverging detonation wave. We have applied the sharp shock model to two examples. In the first example a spherically expanding detonation wave is calculated using the Random Choice Method (RCM).[11-13] This illustrates how numerical methods which use Riemann solvers for flows with shocks may be adapted for detonation waves using the wave curve determined from the theory of the previous section. In the second example the steady state detonation wave in a rate stick experiment is calculated by solving an ODE. This illustrates how a 2-D detonation wave is propagated using the wave speed at each point from the local curvature of the front. The procedures in these examples form the basis for incorporating the sharp shock model in a time dependent 2-D numerical algorithm such as front tracking.

3.1 Spherically Diverging Detonation Wave

It has been shown[10] that RCM used for 1-D fluid dynamics can be adapted for calculations with diverging detonation waves. In RCM the state variables of a fluid are represented as piecewise constant over a grid block. At each time step, the waves between adjacent cells are resolved by solving a Riemann problem. The solution to the Riemann problem is determined from the pair of wave curves with initial states from adjacent cells. This Riemann solution is used in updating the states to the next time step. Source terms due to geometry are taken into account by operator splitting.[14] In this method, shock waves are kept perfectly sharp with no smearing.

The RCM can be used for any discontinuous wave if the wave curve can be specified. The sharp shock model is the specification of a wave curve for a detonation wave; the detonation velocity and the state at the end of the reaction zone. For an underdriven detonation only one point on the wave curve is needed. This is the analog of the planar CJ detonation. However, in diverging geometry the wave curve depends on the radius (front curvature) as well as the initial state.

This method has been used to model an experiment performed by Venable at the Los Alamos PHERMEX facility in which a spherically diverging detonation in Comp-B was radiographed. This provides data for the density profile of the Taylor wave behind the detonation.[15] Calculations of this experiment have been described[10] using wave curves determined by the theory in sec. 2. Each calculation corresponded to a model for the explosive consisting of a HOM EOS and an Arrhenius rate law with a different order of reaction. Because of the exponential tail of the reaction with this rate law, the end of the reaction zone was taken to correspond to the sonic point. The state at the end of the reaction zone as a function of κ was fit to the form shown in equation (2). A comparison of density profiles for numerical experiments and radiographic data are shown in Fig. 1 along with the computed planar result. As θ increases, the shape of the density profile more closely approximates the data.

The uncertainty of the rate and sensitivity of the theory suggests that the wave curve for an underdriven diverging detonation be determined empirically. This is especially important for heterogeneous explosives because hot spots due to inhomogeneities affect the rate law giving rise to large uncertainties.

3.2 Modeling the Rate Stick Experiment

A rate stick is a long cylindrical charge of explosive surrounded by a confining wall. Let r and [illegible]

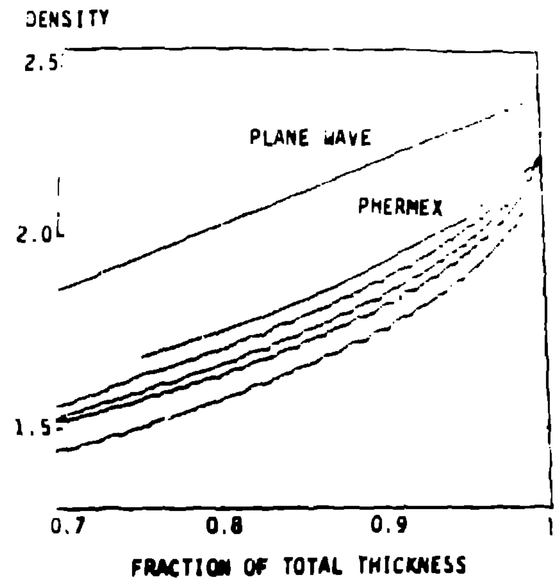

Fig. 1. Calculated and experimental Taylor wave density profiles for the explosive Comp-B. The uppermost curve is the calculated plane wave profile. This is followed by curves representing a spherically expanding Comp-B explosion at a radius of approximately 6.4 cm. The lowest curve is the calculated profile where $\delta = 1/2$ followed by profiles in which $\delta = 1$, $\delta = 2$, and $\delta = 4$, respectively. The curved labelled PHERMEX is the experimental result.

the radial and axial coordinates, and R the charge radius. In steady state the detonation front has the form $Z(r,t) = Z_0(r) + \sigma t$ where σ is the detonation velocity in the axial direction. For a cylindrically symmetric 2-D surface the sum of the principle curvatures is

$$\kappa(r) = -\frac{\partial_r^2 Z + (\partial_r Z/r)[1 + (\partial_r Z)^2]}{[1 + (\partial_r Z)^2]^{3/2}} \tag{3}$$

The axial velocity of a point on the front depends on both the slope $\partial_r Z$ and the local wave speed. This leads to the equation for the shape of the front

$$\sigma = D(\kappa)[1 + (\partial_r Z)^2]^{1/2} \tag{4}$$

Equations (3) and (4) are equivalent to a second order ODE for $Z(r)$. Its solution depends on the boundary condition at the confining wall.

The leading singularity at the boundary is the wave pattern consisting of an incoming shock in the unreacted high explosive (HE) overtaking the HE wall contact and giving rise to an outgoing transmitted shock in the wall. There are two cases to consider, see Fig. 2. In the terminology of front tracking[16] the wave patterns are degenerate diffraction nodes. The strongly confined case corresponds to a transmission node, no reflected wave. The weakly confined case corresponds to an anomalous reflection node, some shock with reflected rarefaction (Prandtl-Meyer fan).[17] The wave pattern is determined by a shock polar analysis, see Fig. 3. The shock polars depend on the wave speed σ, and the shock Hugoniots for the unreacted HE and the wall. The intersection of the shock polars then determines the shock strength and the turning angle θ as a function of σ. Finally, from the mass flow equation through an oblique shock we find

$$\partial_r Z(R) = \text{[illegible]} \tag{5}$$

where m^2 [illegible] $\Delta P/\Delta V$ is the square of the mass flow through the HE shock, ρ_0 is the initial HE density, P [illegible]

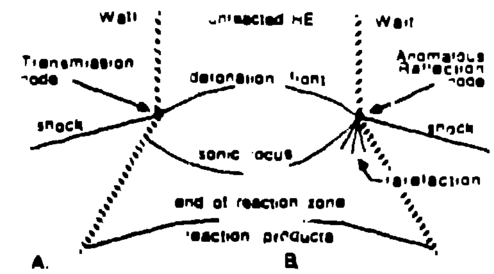

Fig. 2. Sketch of wave patterns at boundary: A. Strongly confined case; B. Weakly confined case.

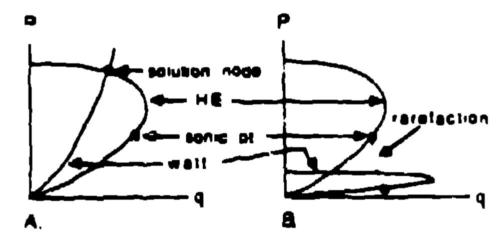

Fig. 3. Sketch of shock polars for degenerate diffraction nodes: A. Transmission node; B. Anomalous reflection node.

is pressure, and V is specific volume. In the weakly confined case the detonation wave is determined by the sonic point on the unreacted HE shock polar.

Because the boundary conditions for the detonation front are the slopes $\partial_r Z(R)$ at the wall from the shock polar analysis and $\partial_r Z(0) = 0$ on the axis, the second order ODE is an eigenvalue problem. Varying R and solving the eigenvalue problem determines the diameter effect, i.e., σ as a function of R. The radius at failure R_f is determined by the condition that $\kappa(-R_f) = \kappa_*$. A solution to the eigenvalue problem for the detonation front does not exist for $R < R_f$.

From experimental rate stick data of the axial detonation velocity and the shape of the detonation front, $D(\kappa)$ and κ_* may be empirically determined using equations (3) and (4) independent of the need for assumptions on the EOS of HE reactants or products, or the reaction rate. Further details of this model for the rate stick experiment are presented elsewhere.[18,19]

4 FRONT TRACKING ALGORITHM

The sharp shock model treats a detonation wave as a discontinuity. Consequently, it is well suited to the front tracking algorithm for gas dynamics.[16,20] Fronts such as shocks and contacts are superimposed on a mesh for the smooth flow using double valued state variables to account for discontinuous waves. The states along the front serve as boundary conditions for the smooth flow within connected interior regions. A front is propagated by solving a Riemann problem to determine the local wave speed at each point. Compared to other numerical algorithms, front tracking yields a higher degree of accuracy for a given mesh resolution.

Front tracking is a general algorithm for problems with discontinuities. The physical information which describes the subgrid structure needed to propagate a discontinuity is found in the wave curve. Reaction zone analysis, which has been performed for an underdriven detonation, determines the wave curve. The new feature is that the wave curve depends on the local curvature as well as the ahead state. In general the reaction zone analysis is also needed for an overdriven detonation wave. This would then allow the front tracking algorithm to be used for both converging and diverging detonation waves. The underlying physical approximation that allows the sharp shock model to be used in front tracking is that the reaction zone is quasi-steady.

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