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Paper Number 105

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A NUMERICAL INVESTIGATION OF SELF-PROPAGATING TWO-PHASE DETONATION

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1. Introduction

Considerable research has been conducted during the past three decades addressing the evolution of detonation in granulated energetic material. This research has largely been motivated by concerns over the accidental detonation of damaged high explosives or propellants in response to weak mechanical shock or thermal insult (Asay and Hantel 1991). Here, damaged material refers to cast solid material which has been inadvertently fractured; thus, local granulated regions exist within the material.

A number of two-phase continuum models have been formulated for analyzing deflagration-to-detonation transition (DDT) in granulated explosives (Butler and Krier 1986; Baer and Nunziato 1986; Powers *et al.* 1990). Numerical simulations based on these two-phase models have been modestly successful in predicting most experimentally observed features of DDT including 1) the formation and propagation of a lead compaction wave, 2) the initiation and subsequent acceleration of a burn front in the compacted material, and 3) the final transition to detonation. However, little emphasis has been given to an analysis of fully-developed detonation structure. Moreover, many DDT simulations are performed using coarse computational grids which are incapable of resolving fine-scale detonation structure. As such, fully-developed detonation structures predicted by two-phase DDT simulations are not well-characterized.

The primary objective of this study is to predict and analyze two-phase detonation structures by numerically simulating DDT whereby combustion is induced by weak, planar mechanical shock due to low velocity piston impact (~ 100 m/s), and to compare the predicted, fully-resolved structures with results given by a steady-state detonation analysis. A secondary objective of this work is to classify new steady detonation structures. To this end, we use a variant of the model formulated by Powers *et al.* (1990a). The steady analysis is a minor extension of the work performed by Powers *et al.* (1990b). The unsteady analysis is an extension of the work performed by Gonthier and Powers (1996).

2. Mathematical model

The model assumes the existence of compressible reactive solid particles and a compressible inert gas. Mass, momentum, and energy exchange between the gas and solid are modeled, as is dynamic compaction of the granular bed due to a mechanical stress imbalance. Diffusive transport mechanisms within each phase are ignored. Also, the effects of lateral boundaries on the two-phase flow are not considered; as such, the flow is assumed one-dimensional (in a macroscopic sense). The dimensional model equations are given by the following:

$$\frac{\partial}{\partial \hat{t}} [\hat{\rho}_1 \phi_1] + \frac{\partial}{\partial \hat{x}} [\hat{\rho}_1 \phi_1 \hat{u}_1] = \left(\frac{3}{\hat{r}}\right) \hat{\rho}_2 \phi_2 \hat{a} \hat{P}_1^m H(I - I_{ig}), \quad (1)$$

$$\frac{\partial}{\partial \hat{t}} [\hat{\rho}_1 \phi_1 \hat{u}_1] + \frac{\partial}{\partial \hat{x}} \left[\hat{\rho}_1 \phi_1 \hat{u}_1^2 + \hat{P}_1 \phi_1 \right] = \hat{u}_2 \left(\frac{3}{\hat{r}}\right) \hat{\rho}_2 \phi_2 \hat{a} \hat{P}_1^m H(I - I_{ig}) + \hat{\beta} \frac{\phi_1 \phi_2}{r} (\hat{u}_2 - \hat{u}_1), \quad (2)$$

$$\begin{aligned} \frac{\partial}{\partial \hat{t}} \left[\hat{\rho}_1 \phi_1 \left(\hat{e}_1 + \frac{\hat{u}_1^2}{2} \right) \right] + \frac{\partial}{\partial \hat{x}} \left[\hat{\rho}_1 \phi_1 \hat{u}_1 \left(\hat{e}_1 + \frac{\hat{u}_1^2}{2} + \frac{\hat{P}_1}{\hat{\rho}_1} \right) \right] \\ = \left(\hat{e}_2 + \frac{\hat{u}_2^2}{2} \right) \left(\frac{3}{\hat{r}}\right) \hat{\rho}_2 \phi_2 \hat{a} \hat{P}_1^m H(I - I_{ig}) + \hat{\beta} \frac{\phi_1 \phi_2}{\hat{r}} \hat{u}_2 (\hat{u}_2 - \hat{u}_1) + \hat{h} \frac{\phi_1 \phi_2}{\hat{r}^{1/3}} (\hat{T}_2 - \hat{T}_1), \end{aligned} \quad (3)$$

$$\frac{\partial}{\partial \hat{t}} [\hat{\rho}_2 \phi_2] + \frac{\partial}{\partial \hat{x}} [\hat{\rho}_2 \phi_2 \hat{u}_2] = - \left(\frac{3}{\hat{r}} \right) \hat{\rho}_2 \phi_2 \hat{a} \hat{P}_1^m H(I - I_{ig}), \quad (4)$$

$$\frac{\partial}{\partial \hat{t}} [\hat{\rho}_2 \phi_2 \hat{u}_2] + \frac{\partial}{\partial \hat{x}} [\hat{\rho}_2 \phi_2 \hat{u}_2^2 + \hat{P}_2 \phi_2] = -\hat{u}_2 \left(\frac{3}{\hat{r}} \right) \hat{\rho}_2 \phi_2 \hat{a} \hat{P}_1^m H(I - I_{ig}) - \hat{\beta} \frac{\phi_1 \phi_2}{\hat{r}} (\hat{u}_2 - \hat{u}_1), \quad (5)$$

$$\begin{aligned} & \frac{\partial}{\partial \hat{t}} \left[\hat{\rho}_2 \phi_2 \left(\hat{e}_2 + \frac{\hat{u}_2^2}{2} \right) \right] + \frac{\partial}{\partial \hat{x}} \left[\hat{\rho}_2 \phi_2 \hat{u}_2 \left(\hat{e}_2 + \frac{\hat{u}_2^2}{2} + \frac{\hat{P}_2}{\hat{\rho}_2} \right) \right] \\ & = - \left(\hat{e}_2 + \frac{\hat{u}_2^2}{2} \right) \left(\frac{3}{\hat{r}} \right) \hat{\rho}_2 \phi_2 \hat{a} \hat{P}_1^m H(I - I_{ig}) - \hat{\beta} \frac{\phi_1 \phi_2}{\hat{r}} \hat{u}_2 (\hat{u}_2 - \hat{u}_1) - \hat{h} \frac{\phi_1 \phi_2}{\hat{r}^{1/3}} (\hat{T}_2 - \hat{T}_1), \end{aligned} \quad (6)$$

$$\frac{\partial \phi_2}{\partial \hat{t}} + \hat{u}_2 \frac{\partial \phi_2}{\partial \hat{x}} = \frac{\phi_1 \phi_2}{\hat{\mu}_c} \left(\hat{P}_2 - \hat{P}_1 - \hat{f} \right) - \left(\frac{3}{\hat{r}} \right) \phi_2 \hat{a} \hat{P}_1^m H(I - I_{ig}), \quad (7)$$

$$\frac{\partial \hat{n}}{\partial \hat{t}} + \frac{\partial}{\partial \hat{x}} [\hat{u}_2 \hat{n}] = 0, \quad (8)$$

$$\frac{\partial I}{\partial \hat{t}} + \hat{u}_2 \frac{\partial I}{\partial \hat{x}} = \hat{k}_I (1 - I) \left[\frac{\hat{P}_1 \phi_1 + \hat{P}_2 \phi_2 - \hat{P}_{1o} \phi_{1o} - \hat{P}_{2o} \phi_{2o}}{\hat{P}_{1o} \phi_{1o} + \hat{P}_{2o} \phi_{2o}} \right]^2 \exp \left[- \frac{\hat{T}_I}{\hat{T}_1 \phi_1 + \hat{T}_2 \phi_2} \right]. \quad (9)$$

In these equations, the subscripts “1” and “2” denote quantities associated with the gas and solid, respectively. Quantities labeled with overhats “ $\hat{\bullet}$ ” are dimensional, and quantities labeled with subscript “o” are associated with the ambient state. The independent variables are time \hat{t} and position \hat{x} . Dependent variables are as follows: the phase density $\hat{\rho}_i$ ($i = 1, 2$), defined as the mass of phase i per unit volume occupied by that phase; the phase pressure \hat{P}_i ; the phase temperature \hat{T}_i ; the particle velocity \hat{u}_i , measured with respect to a stationary reference frame; the specific internal energy \hat{e}_i ; the volume fraction ϕ_i , defined as the ratio of the volume occupied by phase i to the total volume ($\phi_1 + \phi_2 = 1$); the radius of the spherical solid particles \hat{r} ; the number of particles per unit volume \hat{n} ($\equiv 3\phi_2/4\pi\hat{r}^3$); the intragranular stress \hat{f} ; and an ignition variable I . In Eqs. (1-9), $H(I - I_{ig})$ is the Heaviside unit step function, and I_{ig} , \hat{a} , m , $\hat{\beta}$, \hat{h} , $\hat{\mu}_c$, \hat{k}_I , and \hat{T}_I are constant parameters. Closure is achieved by specifying thermal [$\hat{P}_i = \hat{P}_i(\hat{\rho}_i, \hat{T}_i)$] and caloric [$\hat{e}_i = \hat{e}_i(\hat{\rho}_i, \hat{T}_i)$] state relations for each phase, and by specifying the functional form for f .

Equations (1-3) and (4-6) are the mass, momentum, and energy evolution equations for the gas and solid, respectively. Equation (7) is a dynamic compaction equation, Eq. (8) is a particle number evolution equation, and Eq. (9) is an evolution equation for the ignition variable.

3. Numerical method

The non-strictly hyperbolic system of model equations were solved using a new high-resolution upwind numerical method (Gonthier and Powers 1997). The method, which is based on Godunov’s approach, does not require the explicit use of artificial viscosity, can accurately capture shocks with minimal smearing, and can accurately resolve disparate time scales associated with rate-dependent processes. Rather than using the exact solution of the two-phase Riemann problem at each computational cell boundary to advance the solution in time, an approximate solution is used for increased computational efficiency. The method is convergent, and the spatial convergence rate was determined based on comparisons of numerical predictions with known theoretical results for several test problems. Global convergence rates of ~ 1.0 were determined for problems having embedded shocks, and rates of ~ 1.7 were determined for problems having continuous solutions.

4. Results

The numerical simulations predicted most experimentally observed features characteristic of piston-initiated DDT in granular HMX. Experimentally observed time scales, wave speeds, and pressure magnitudes are correctly predicted. Several classes of steady two-phase detonation wave structures were predicted to

evolve: Chapman-Jouguet (*CJ*) and weak detonation structures having a lead shock in the gas and an unshocked solid, *CJ* structures having a lead shock in the solid and an unshocked gas, and *CJ* structures having a shock in both the gas and solid (Gonthier 1996). Which structure evolved was found to depend on the material compaction rate, the interphase drag rate, and the ambient mixture density. The results indicate that the *CJ* wave speed is not the unique wave speed for a self-propagating two-phase detonation. Numerically predicted structures agree well with results given by the strictly steady-state detonation wave analysis.

Shown in Fig. 1 is the predicted gas velocity history (measured relative to a fixed laboratory frame) for the evolution of a two-phase weak detonation having a lead shock in the gas and an unshocked solid. Here, $\hat{\xi}$ is position measured relative to a coordinate system attached to the piston, and $\hat{\tau} = \hat{t}$. Also shown in this figure is the spatial profile at $\hat{\tau} = 120 \mu s$. For this simulation, a virial equation of state was used for the gas and a Tait equation of state was used for the solid. The moving piston (located at $\hat{\xi} = 0 \text{ cm}$) induces the formation of a compaction wave propagating at 402 m/s . Ignition is predicted to occur near the piston surface approximately $135 \mu s$ after piston impact; subsequently, there is predicted a rapid transition to detonation. The resulting detonation is propagating at 6168 m/s . A comparison of the *shocked gas - unshocked solid* weak detonation structure predicted by both the numerical simulation and the steady-state analysis is given in Fig. 2. Good agreement exists between the predicted solutions.

5. Acknowledgments

This study was supported by the NASA Lewis Research Center, Cleveland, Ohio USA, under Contract Number NASA-NCC-325. Partial support for this study was given by the Department of Aerospace and Mechanical Engineering, University of Notre Dame, and the United States Air Force, Wright Laboratories, Eglin Air Force Base, Florida USA.

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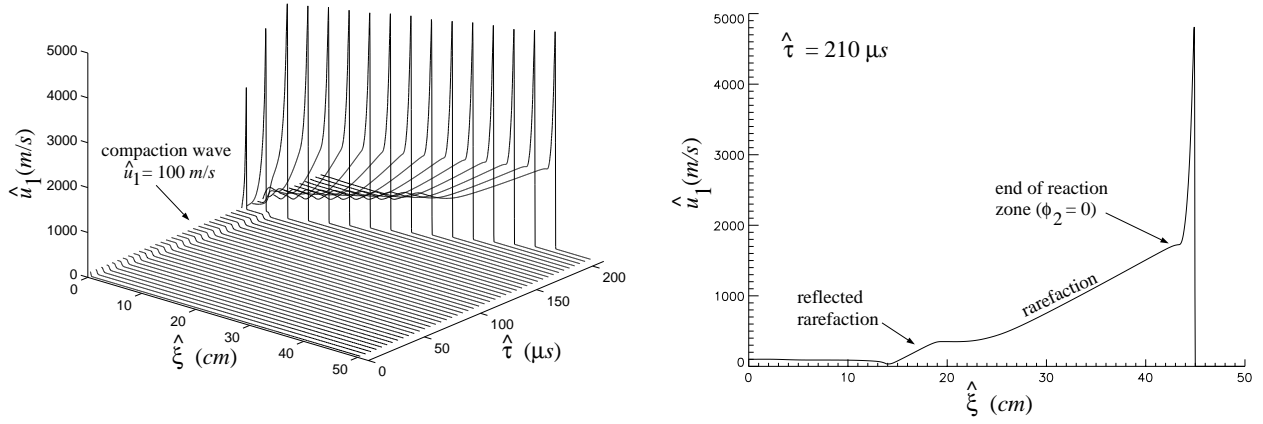


Figure 1: Predicted gas velocity history for the *shocked gas-unshocked solid* weak detonation simulation.

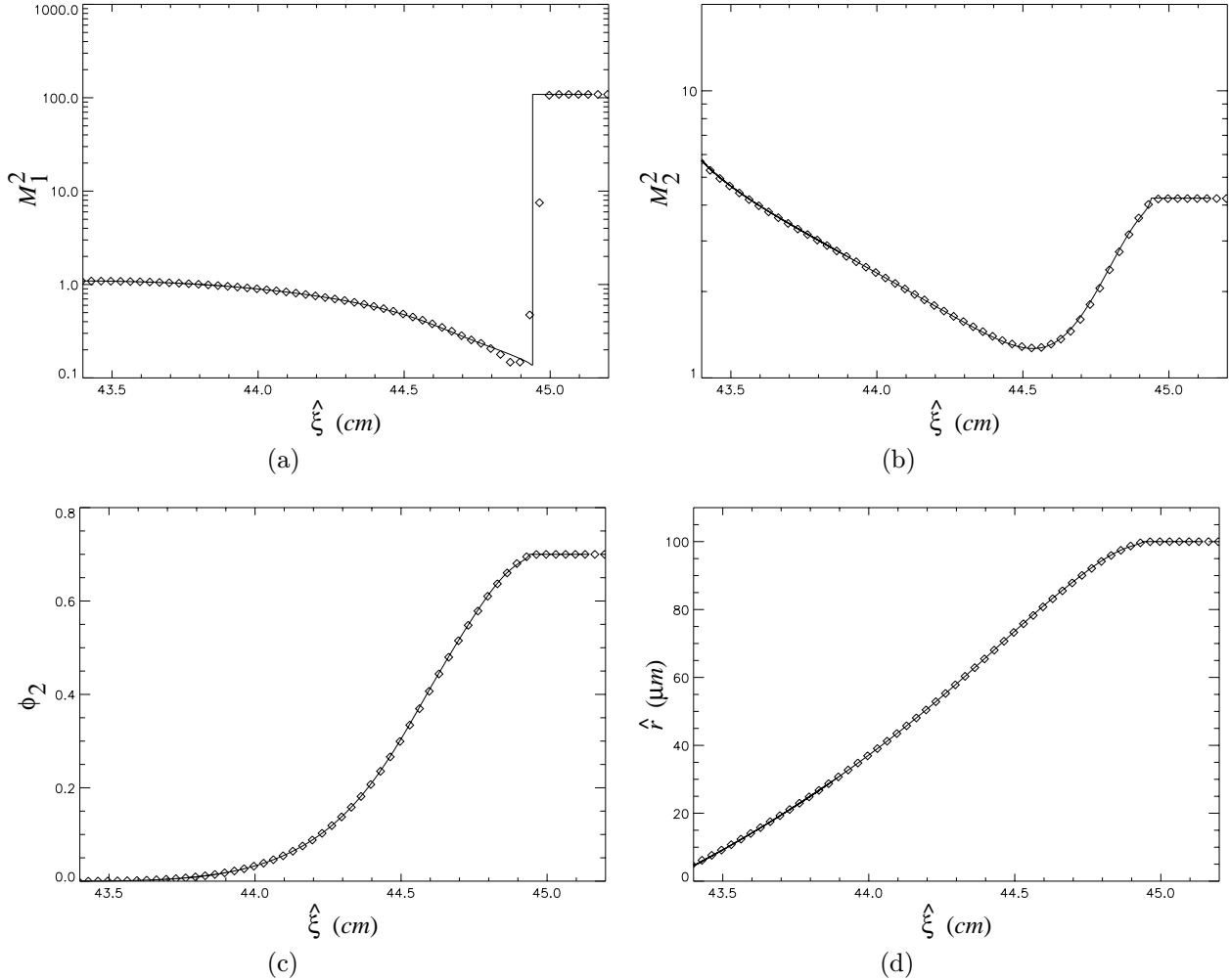


Figure 2: Comparison of the *shocked gas-unshocked solid* weak detonation structure predicted by the numerical simulation and the steady-state analysis: (a,b) gas and solid Mach number squared (relative to the wave); (c) solid volume fraction; and (d) particle radius.