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DETERMINATION OF THE LIGHTING RADIUS FOR APPLICATION OF DETONATION SHOCK DYNAMICS CONSISTENT WITH IGNITION TRANSIENTS IN CONDENSED EXPLOSIVES

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14. ABSTRACT

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Three-dimensional simulation of detonation shock motion in a condensed explosive, modeled with a reactive flow in a moderately complex geometry can require enormous amounts of computer time, since the reaction zone behind the leading shock is extremely thin compared to the overall dimensions of the computational domain. Therefore algorithms such as program burn, pre-compute the detonation shock arrival time, and then essentially use a delta function model to release the heat of detonation into few computations cells near the shock wave. Previous validation efforts that use a program burn algorithm based on detonation shock dynamics (DSD) highlighted the prescription of the initial detonation shock for the simulation, in a manner that is self-consistent with the theory and physical experiment. In this paper we use a combination of theory, direct multi-material simulation and experiment to determine a critical radius for the starting detonation shock shape.

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DETERMINATION OF THE LIGHTING RADIUS FOR APPLICATION OF DETONATION SHOCK DYNAMICS CONSISTENT WITH IGNITION TRANSIENTS IN CONDENSED EXPLOSIVES

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Abstract. Three-dimensional simulation of detonation shock motion in a condensed explosive, modeled with a reactive flow in a moderately complex geometry can require enormous amounts of computer time, since the reaction zone behind the leading shock is extremely thin compared to the overall dimensions of the computational domain. Therefore algorithms such as program burn, pre-compute the detonation shock arrival time, and then essentially use a delta function model to release the heat of detonation into few computations cells near the shock wave. Previous validation efforts that use a program burn algorithm based on detonation shock dynamics (DSD) highlighted the prescription of the initial detonation shock for the simulation, in a manner that is self-consistent with the theory and physical experiment. In this paper we use a combination of theory, direct multi-material simulation and experiment to determine a critical radius for the starting detonation shock shape.

INTRODUCTION

In a recent paper [1], a "passover" experiment was designed with a complex detonation transient. A charge with an embedded lead disk in a right circular cylindrical charge of HMX-based, PBX-9501 was initiated from the bottom. A detailed comparison of the motion of the detonation shock was made between experiment, prediction of the asymptotic theory of detonation shock dynamic (DSD–theory) and a multi-material reactive flow simulation as described in [2]. A new wide-ranging equation of state (EOS) and rate law [3] was used to describe the explosive and was employed in both the theoretical (DSD) calculations and the multi-material simulations. The experiment, theory and simulation were found to be in excellent agreement and showed that for a large class of important detonation flows one can use the DSD model. DSD assumes that the detonation shock propagates along its normal direction, determined by its total shock curvature, to get quantitatively accurate results. One of the central questions that remains is, is there a systematic and self-consistent way to determine the location of the initial detonation shock radius (i.e. the location to "light" the explosive) to start the DSD simulation, as a precursor to a program burn simulation?

Therefore, given a well-characterized initiation source, such as a detonator or in a computational setting a prescribed volume of high pressure products that generates a shock in unreacted explosive, one needs to determine the radius for the starting detonation shock shape that is consistent with the assumptions of detonation shock dynamics (DSD) theory. The same study helps determine the minimum energy and size requirements needed to achieve a stable high-order detonation. We also are able to assess significant effects due to shock acceleration. The inclusion of shock acceleration leads to one of the higher-order theories of detonation shock dynamics, that have been addressed in [4], [5], and [6].

In what follows we briefly describe a representative explosive application that was designed using a PBXN-9 charge with 19 detonators placed in an equilateral triangle pattern array. Figure 1 shows a framing sequence of light captured from the emergence of detonation from the initiation points. The detonations emanating from the initiation points do not initially interact and the flow can be modeled as spherical or axi-symmetric. Later the initiating detonation shocks merge and the flow is fully 3D.

The ideal experiment would be a single point initiation characterization into a PBXN-9 charge, but the 19-point experiment was a related and pertinent data set. The multi-point experiment provides redundancy and statistical significance that enables an estimate of the initial starting shock radius.

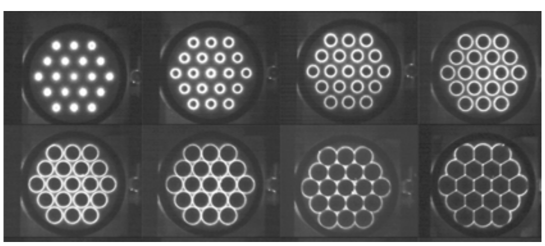

Figure 1. Framing sequence a 19 point array of detonators (order proceeds from top left to bottom right.)

A simple, axi-symmetric simulation is used to estimate the effective DSD lighting radius. The lighting radius is defined to be the minimum radius from an initiation site, such that subsequent shock evolution according to the shock normal velocity, total shock curvature propagation law (a D-kappa relation), is an accurate representation of the detonation shock motion. The properties of the initiation system also determine the lighting radius and in general those details must be considered.

WIDE-RANGING EQUATION OF STATE AND RATE LAW

The simulations use the wide-ranging equation of state and a reaction rate law that is fully described in recent papers [3] and [1], along with the calibration procedures, and the definition of the parameters listed below. Basically one uses: Hugoniot data for unreacted explosive and products, the assumption of a simple mixture of reactants and products and some information about products expansion and some simple thermal properties to calibrate the equation of state. Once the equation of state is fixed, one uses shock-to-initiation data (Pop-plot) and experimentally determines D-kappa data for the explosive to calibrate the rate law. The resulting equation of state and rate law pair is then used to predict behavior over a wide range of states without further calibration.

PBXN-9 is a HMX based explosive used in conventional munitions. It is less sensitive to certain insults, but is still a high performance explosive (92% HMX). Unlike PBX-9502, there is little detonation shock velocity versus curvature data available for PBXN-9, with the exception of overdriven experiments carried out by L. Hull, [7]. Calibration of PBXN-9 was carried out in collaboration with B. L. Wescott.

Products

The wide-ranging equation of state for the products has six (6) adjustable parameters. The constraints that determine the parameters are (quoting from ref. [3]), "…the principal isentrope must pass through the CJ-point determined from experiment. Second, the principal isentrope and Rayleigh line must be tangent at the CJ-state. Third, the total energy from expansion down the isentrope must be the total energy liberated by the explosive. Fourth, adiabatic gamma, γ, at large volume must be the ideal gas value for the products. Fifth, the energy from the expansion down the isentrope must be partitioned down the high pressure part above 0.1 GPa where useful work – driving metal is done and the low-pressure part that accounts for the rest of the chemical energy. Sixth, Gruneisen, Γ, must be adjusted in the high pressure region to describe the Hugoniot curve for the overdriven detonations that are far from the principal isentrope. These six requirements determine the six adjustable parameters."

This calibration process showed good agreement with the JWL EOS expansion data of ref. [8].

Reactants

The reactants EOS is also of the Mie-Gruneisen form with six (6) adjustable parameters. Calibration is made so that the products and reactants Hugoniot curves do no cross at high pressures. Experimental shock velocity (U_s) versus particle velocity (U_p) data of ref. [8] is used and an argument about the reactant temperature on the isentrope is used.

A mixture equation of state combines the reactants and products EOS and assumes pressure and temperature equilibrium conditions.

Reaction Rate Laws

L. Hull, [7] carried out a Mach stem experiment that measured the D-kappa relation for converging detonations as $D_n = 8.56(1-0.7948\ \kappa)$ ($\kappa < 0$), where D_n is measured in mm/μs, and κ is measured in mm^{-1}. At this time no experimentally determined data for $\kappa > 0$ (divergent geometry) is available. Therefore, Hull's experimental correlation from the Mach stem experiments is used to constrain the theoretically determined D-kappa relation. Four data points for shock initiation (PoP-plot data) available from ref. [8] with shock input pressures in the range from 3 to 13 GPa, were used to constrain the rate law.

A simple depletion law with a pressure dependent rate was assumed of the form

$$r = k\left(\frac{p}{p_{cj}}\right)^N (1-\lambda)^\nu \qquad (1)$$

and the values of the rate law parameters calibrated with Hull's data and the shock initiation data are shown in Table 1.

TABLE 1. Calibrated value of parameters.

***k* (μs^{-1})**	***N***	***ν***
14	2.5	0.7

Once the wide-ranging EOS, and rate law description is specified, one can readily solve the nonlinear Eigen value problem of DSD theory to determine the normal velocity, total shock curvature relation (i.e. the D-kappa curve).

INITIATION OF DETONATION FROM A CONSTANT VOLUME SOURCE

To test the transient response of our model of PBXN-9 we used a finite volume of motionless products of radius $r_{initial}$ at the constant initial volume v_0, with a pressure that is defined by a constant volume thermal explosion. This is the product state that is achieved for detonation of infinite velocity, defined by the intersection of the vertical Rayleigh line with the product Hugoniot, as plotted in a p, v – plane. The initial pressure is approximately 15 GPa. The corresponding run to detonation distance for a similar input shock to PBXN-9 is approximately 2 mm. With this initial state well-defined, we only varied the initial (hot spot) radius $r_{initial}$, and then solved the reactive Euler equations for the model specified above. The lead shock location is recorded along with its velocity and acceleration as a function of time for various initial (hot spot) sizes.

The results of such simulations are shown in Figure 2, which shows the lead shock normal velocity D_n as a function of the lead shock position r. Different initial (hot spot) radii, that define the initiation source, are explicitly labeled for $r_{initial}$ = 4.5 mm, 5.0 mm, 6.0 mm and 7.0 mm. Note that the D-kappa relation determined from DSD theory is also plotted as a *D-r* relation, where for a cylindrical system $\kappa = 1/r$. Only the top branch of the D-kappa (D-r relation) is shown, up to the turning point.

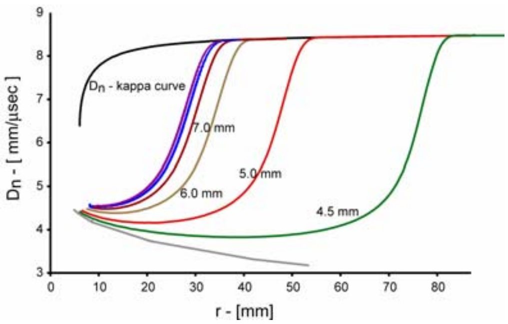

Figure 2. The simulated D_n-r response for PBXN-9, initiated from various hot-spot radii.

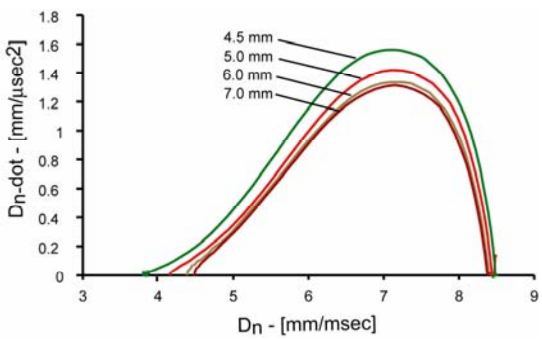

Figure 3. Normal shock acceleration (Dndot) corresponding to Figure 2, versus normal shock velocity.

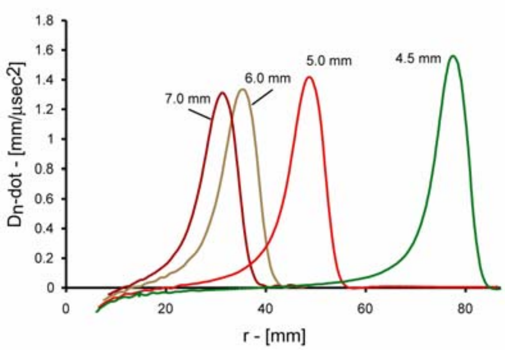

Figure 4. Normal shock acceleration (Dndot) corresponding to Fig. 2, versus the shock position.

A typical transient for this source shows a slight initial deceleration followed by a rapid acceleration then slower acceleration as the quasi-steady detonation, described by the D-kappa relation is attained. Figure 3 shows a plot of the shock acceleration versus the normal detonation velocity realized for various initial hot spot radii, as seen in Figure 2. Figure 4 shows a plot of shock acceleration versus shock position as a function of initial hot spot radii.

The results show clearly that the D-kappa relation (*D-r* relation) is an attractor of the unsteady solution. In these simulations one can clearly demark a radius where the quasi-steady D-kappa response is achieved, and one could consider that to be the “lighting radius”. At a sufficiently large radius one could safely assume that the detonation propagated according to the D-kappa rule. But it is clear that that radius depends strongly on the strength of the initiation source and the subsequent transient. In fact, that is the main point of our article.

Figure 5 shows a plot of the “lighting radius” as a function of the “initial starting (hot spot) radius”. The results strongly suggest that there is a minimum radius of the hot spot such that it is not possible to ignite a detonation (below 4 mm).

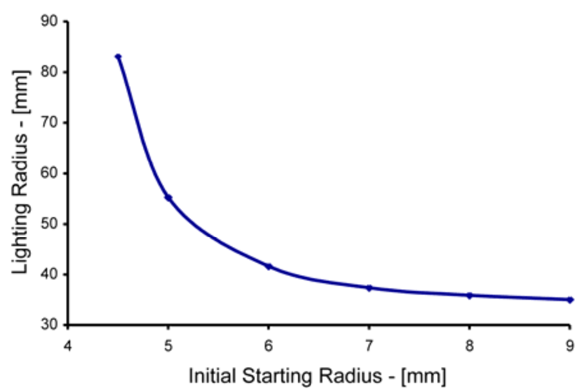

Figure 5. The lighting radius, (above which a DSD, D-kappa propagation rule would hold) as a function of the initial starting radius.

HIGHER ORDER DSD-THEORY WITH SHOCK ACCELERATION EFFECTS

For an ideal equation state, Kasimov and Stewart, [6] with weak curvature asymptotics and slow evolution on the time scale of particle transit through the reaction zone, derived an extended DSD shock evolution equation of the general form

$$\frac{dD_n}{dt} = A(D_n) - \kappa \; B(D_n) \tag{2}$$

where $A(D_n)$ and $B(D_n)$ are functions that have explicit forms defined by the EOS and rate law. In his PhD. thesis, Kasimov [9] gave a similar development for general equation of state. Further Kasimov and Stewart [6] showed that for states defined by blast waves, generated by explosives in Hydrogen Oxygen mixtures that they could predict critical energies and define an ignition seperatrix. The integral curve obtained when plotted in a *D-r* plane looked in a qualitative manner, quite similar to those shown in Fig. 2. In the absence of shock acceleration, the D-kappa curve is obtain directly from (2) by setting the acceleration term equal to zero.

The general theory outlined by Kasimov is being applied to derive the result corresponding to equation (2) and will be reported on shortly.

CONCLUSIONS

By means of an example, as applied to a model of PBXN-9, prescribed by the wide-ranging EOS/rate law, we have shown that significant transients must be considered. Further the lighting radius for the application of DSD must take into account the nature of the initiation; however it seems that this behavior is regular. Future work will give a detailed estimate of the output from detonators and companions with planned new experiments in PBXN-9.

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