Critical Ignition Transients in Condensed Explosives

D. Scott Stewart[1], Sunhee Yoo[1], David E. Lambert[2]

[1]Department of Mechanical Science and Engineering,
University of Illinois at Urbana-Champaign, Urbana, Illinois, 61801, USA

[2]Air Force Research Laboratory,
Munitions Directorate, Eglin Air Force Base, Florida, USA

1 Introduction

A recent paper [1] describes a “passover” experiment that 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 found to be in excellent agreement and this indicates 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 with its speed determined by its total shock curvature (D-kappa). The theory of detonation shock dynamics and its applications to explosive systems is reviewed by Bdzil and Stewart in the most recent issue of *Annual Reviews of Fluid Mechanics* [4].

A central question 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 (D-kappa) simulation, as a precursor to a program burn simulation? Given a well-characterized initiation source, such as a detonator, 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 the higher-order theories of detonation shock dynamics, that have been addressed in [5], [6], and [7].

2 Initiation of detonation from a constant volume explosion and a high pressure hot spot

To test the transient response of our models for PBX-9501, 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, with the detonation speed around 4.5 mm/micro sec. 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.

Note that the D-kappa relation determined from DSD theory can be a plotted as a *D-r* relation, where for a spherical system $\kappa = 2/r$. Only the top branch of the D-kappa (D-r relation) is shown, up to the turning point, in

Correspondence to : dss@uiuc.edu

Figure 1. For the "constant volume explosion" hot spot, 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. 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 order to more accurately model the initiation of explosive by means of an embedded detonator, or a detonator in contact with the explosive, we devised a model of a high-pressure hot spot. In this case we chose an initial shock speed for the expanding products in the hot spot (such as 11 mm/ μsecμ(say), well above the Chapman-Jouguet detonation velocity), and the pressure and the density in the hot spot to be that of the shock state on the reactants Hugoniot. For the velocity distribution in the high-pressure hot spot, we took the radial velocity to be the shock state velocity for the outer half of the hot spot, and decreased the velocity linearly from the constant value at the half radius to zero velocity at the origin of the spot. The intent of this model is to mimic the blast wave energy transfer of a detonator.

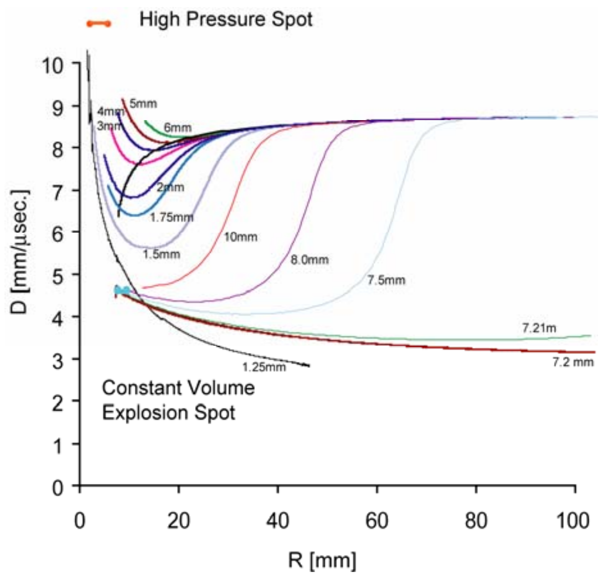

Figure 1. The simulated D_n-R response for PBX-9501, initiated from various hot-spot radii, both spherical low pressure and high pressure

We carried out an extensive set of simulations for the model of PBX-9501 found in reference [1], for a spherical hot spots, for both constant volume thermal explosion (low pressure) and the high-pressure shock state models of hot spots. The results for the high pressure hot spot differed somewhat in that the initial transient was noisy, since there is shock reverberation that occurs (not unlike what likely occurs in a detonator initiation) between the hot spot products interface and the adjacent explosive until pressure equilibration occurs. Some jumps in the lead shock velocity were observed as the blast decayed and the initiating shock from the high-pressure spot transferred into the explosive. But after about a radius or two the solution became smooth with a well-defined transient.

Unlike the constant volume hot spot simulation, where a more or less smooth acceleration was observed, the high pressure hot spot simulations showed, as expected a rapid shock deceleration associated with the blast, followed by a reacceleration as the explosive started to burn.

The set of simulations varied the hot spot size, which represents a variation of the blast energy in the initiating hot spot with the cube of the hot spot radius or approximately linear in the hot spot volume. The composite record of all simulations for PBX-9501 (both low and high pressure hot spots) are shown in Fig. 1. A striking observation is that failure is clearly observed for both high and low-pressure spots, for critical spot radii. The simulations strongly indicate that the explosive is obeying or very nearly controlled by a reduced dynamical system that we have previously described by asymptotic analysis of detonation with trailing sonic locus, [7]. This strongly suggests critical behaviors can be calculated in a systematic theory similar to that proposed and worked out in [7]. If so this has interesting implications for detonator design.

3 Higher Order DSD-theory with shock acceleration effects

For an ideal equation of state, Kasimov and Stewart, [7] 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 [7] gave a similar development for general equation of state. Further Kasimov and Stewart [7] showed that for states defined by blast waves, generated by explosives in Hydrogen Oxygen mixtures they could predict critical energies in agreement with experiment and define an ignition seperatrix.

Figure 2. shows the results of solving equation (2) for a model fit to a stoichiometric hydrogen-oxygen explosive. In this case the D-kappa curve has a turning point. The solutions found by solving (2) have the same qualitative character as those found by simulation, albeit the reversal of (change of sign) of shock acceleration is exactly at the crossing of the D-kappa curve, according to (2), whereas in our simulations of PBX-9501 that reversal is shifted slightly. That is not unexpected as (2) is the result of asymptotic approximation of the physical system. The general theory outlined by Kasimov is being applied to derive the result corresponding to equation (2) and will be reported on shortly.

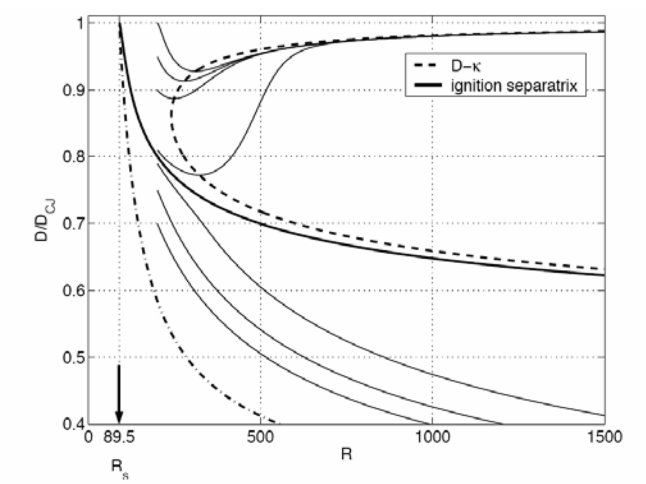

Figure 2. Solution to equation (2), from reference [7] for a model of stoichiometric hydrogen-oxygen. The dashed dot line to the left is the D-R curve from the reactive blast wave solution that defines a critical energy and radius.

4 Conclusions

By means of an example, as applied to a model of HMX-based PBX-9501, 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. Critical behavior and energies can be calculated.

The quantitative predictions of the simulations are sensitive to the calibration of the models, particularly to the reaction rate. Therefore the lack of experimental data for large values of curvature (other than the data taken by Hull,

[8] whose measurements were for overdriven and near-CJ detonation) is an issue, and incorporation of near data may result in some changes to the quantitative predictions. Future work will give a detailed estimate of the output from detonators and comparisons with planned new experiments.

5 Acknowledgements

This work was supported by the US Air Force Research Laboratory, Munitions Directorate F08630-00-1-0002, and the Air Force Office of Scientific Research, Mathematics FA9550-06-1-0044. D. S. Stewart has also been supported by Los Alamos National Laboratory, DOE/LANL 3223501019Z. Special thanks to Dr. Bradley Wescott. A earlier version of this paper will appear in the Proceedings of the 13th International Detonation Symposium, (Norfolk, VA, 2006).

References

[1] Lambert, D. E., Stewart, D. Scott and Yoo, S. and Wescott , B. L., "Experimental Validation of Detonation Shock Dynamics in Condensed Explosives*.* *Journal of Fluid Mechanics,* Vol. 546, pp.227-253 (2006)

[2] Stewart, D. S., Yoo, S. and Wescott, B. L., "High-order Numerical Simulation and Modeling of the Interaction of Energetic and Inert Materials," Combustion Theory and Modeling, Vol. 11, No. 2, , 305-332, (2007)

[3] Bdzil, J. B. and Stewart, D. S.. "The Dynamics of Detonation in Explosive Systems", *Annu. Rev. Fluid Mech.* 39:263-92 (2007)

[4] Wescott, B. L., D. S. Stewart, and W. C. Davis, "Equation of State and Reaction Rate for Condensed-Phase Explosives," *Journal of Applied Physics*, **98**, 053514 (2005)

[5] Yao J, Stewart D S. 1996. On the Dynamics of Multi-dimensional Detonation. J. Fluid Mech. 309:225-275.

[6] Aslam TD, Bdzil JB, Hill LG. 1998. Extensions to DSD theory: Analysis of PBX-9502 rate stick data. Eleventh (Int.) Symp. on Detonation. 21-29

[7] Kasimov, A. and D. S. Stewart D. S., "Asymptotic theory of evolution and failure of self-sustained detonation," *Journal of Fluid Mechanics,* 525, 161-192, ***(***2005)*.*

[8] Kasimov, A. Theory of instability and nonlinear evolution of self-sustained detonation waves, PhD. thesis, Theoretical and Applied Mechanics, University of Illinois, (2004)

[9] Hull, L.M. (1997) Detonation Propagation and Mach Stem Formation in PBX-N9. *LA-UR-97-3827*.