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J. E. Reaugh, J. P. Curtis, M. A. Maheswaran

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Modelling of Deflagration to Detonation Transition in Porous PETN of Density 1.4 g/cc with HERMES

John E. Reaugh[1, a)] John P. Curtis[2, 3)] and Mary-Ann Maheswaran[2)]

[1]*Lawrence Livermore National Laboratory, PO Box 808, Livermore, CA 94501, USA*
[2]*Atomic Weapons Establishment, Reading, Berkshire RG7 4PR, UK*
[3]*Department of Mathematics, University College London, Gower Street, London, WC1E 6BT, UK*

[a)]Corresponding author: jreaugh@llnl.gov

Abstract. The modelling of Deflagration to Detonation Transition in explosives is a severe challenge for reactive burn models because of the complexity of the physics; there is mechanical and thermal interaction of the gaseous burn products with the burning porous matrix, with resulting compaction, shock formation and subsequent detonation. Experiments on the explosive PETN show a strong dependence of run distance to detonation on porosity. The minimum run distance appears to occur when the density is approximately 1.4 g / cc. Recent research on the High Explosive Response to Mechanical Stimulus (HERMES) model for High Explosive Violent Reaction has included the development of a model for PETN at 1.4 g / cc., which allows the prediction of the run distance in the experiments for PETN at this density. Detonation and retonation waves as seen in the experiment are evident. The HERMES simulations are analyzed to help illuminate the physics occurring in the experiments.

INTRODUCTION

The HERMES model (High Explosive Response to MEchanical Stimulus) [1, 2] was originally developed to describe the behavior of solid explosives and propellants in both laboratory experiments and in postulated accidents that result in ignition and burning but not prompt detonations. We have embedded the model in the computer simulation programs LS-DYNA [3] and ALE3D [4], and performed simulations of several different explosives and propellants in various experimental test vehicles. Those low-velocity impact tests that ignited resulted in more-or-less violent reactions that never detonated [1].

HERMES comprises a constitutive description of flow stress as a function of strain, strain-rate, pressure, ambient temperature, and porosity. Surface area and porosity increase with shear deformation, and porosity decreases with compaction. It includes an ignition criterion, the subsonic propagation of an ignition front through damaged material, and the build-up of gas products (and as a result, pressure) as the burn progresses. In this way it describes deformation, ignition, and post-ignition behaviour in the framework of multi-species but single velocity treatment that enforces pressure but not temperature equilibrium between reactant and product. We also wished to simulate the transition from deflagration to detonation (DDT). To this end, we incorporated in HERMES a subset of the CREST [5] detonation model, which we refer to as CREST-lite. We chose CREST, rather than a pressure-based ignition and growth model [6], because CREST intrinsically distinguishes a shock pressure from an adiabatic rise in pressure, both of which occur during DDT. In HERMES, the mass fraction of reactant converted to product increases from deflagration and detonation simultaneously. The equation of state of the gas products is a table of pressure and specific internal energy as a function of mass density and temperature calculated with Cheetah [7], a thermochemical equilibrium computer program. We applied this capability to assess the effect of explosive properties on DDT for moulding powder beads of an HMX-based explosive [8].

There have been several experimental papers published on DDT in PETN powder. One of the most prominent of these is that of a series of experiments at Cambridge University by Luebcke *et al.* [9]. In their experiments, the PETN was contained in a tube drilled into a steel confinement, 45 mm long, with 25 mm square cross-section and clamped at both ends. The explosive was ignited at the base of the tube. They demonstrated DDT in PETN of density approximately 1.4 g/cc (porosity 21.3%) among other starting densities. For this density, they observed a transition distance of 21 ± 4 mm, near the experimental minimum of 17 ± 4mm. They observed both a forward travelling detonation wave and a retonation wave that travelled more slowly. This was also observed in [8] and in our simulations reported here.

Shock to detonation experiments for PETN at density 1.4 g/cc [10] were fitted to the CREST-lite model in HERMES illustrated in Fig. 1. This model was then used in computer simulations of the DDT experimental geometry. Other mechanical properties were not available for PETN powder, so we used our best judgement to estimate them.

MODEL CALCULATIONS

The confinement with square cross-section was modelled as an axisymmetric tube, and the clamped ends by rigid boundaries. Test calculations with the tube outer diameter taken to be the width of the cross-section (minimum confinement) and to give the same area of confinement showed the same transition location. The ignition volume was taken to be a disk with the full inside diameter (5 mm) and 0.5 mm thick, which corresponds to the ignition of a 2-3 grain-thickness layer of the PETN powder reported to comprise 180 μm grains, although the particle size distribution was not stated. The mesh size used for these simulations was 0.1 mm squares. A test calculation with 0.05 mm mesh size gave the same detonation transition distance. For all calculations, we used ALE3D version 4.29.38 with HERMES version 88b.

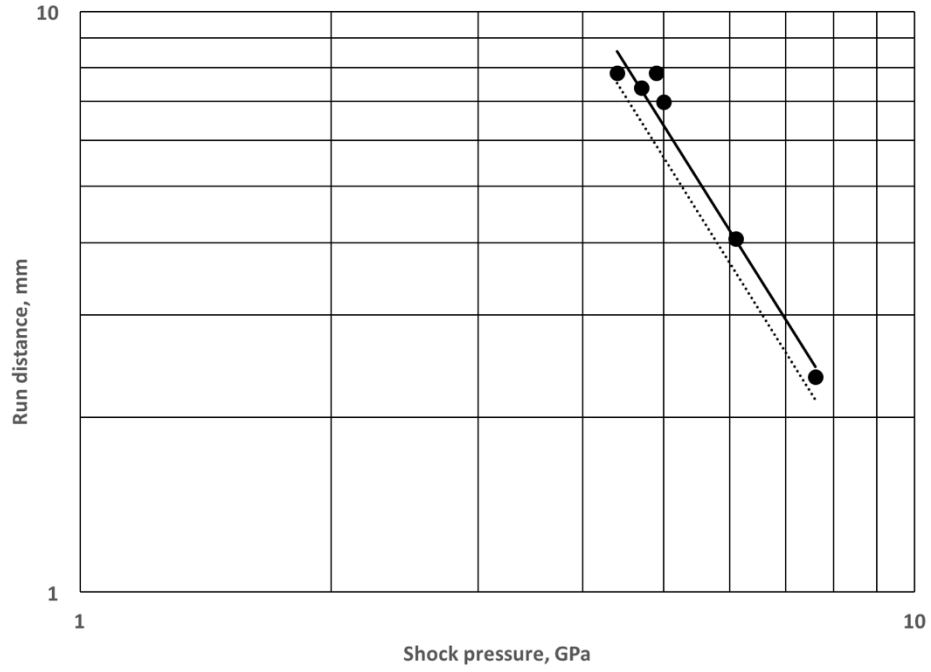

FIGURE 1. Shock to detonation experiments (points) and model results (line) for PETN at density 1.4 g/cc. The shock stress plotted for the experimental points are the results of our calculation for the impact of a 7075 Aluminium plate at the experimental velocity reported. Dashed line represents an alternative fit that bounds the most sensitive experimental results.

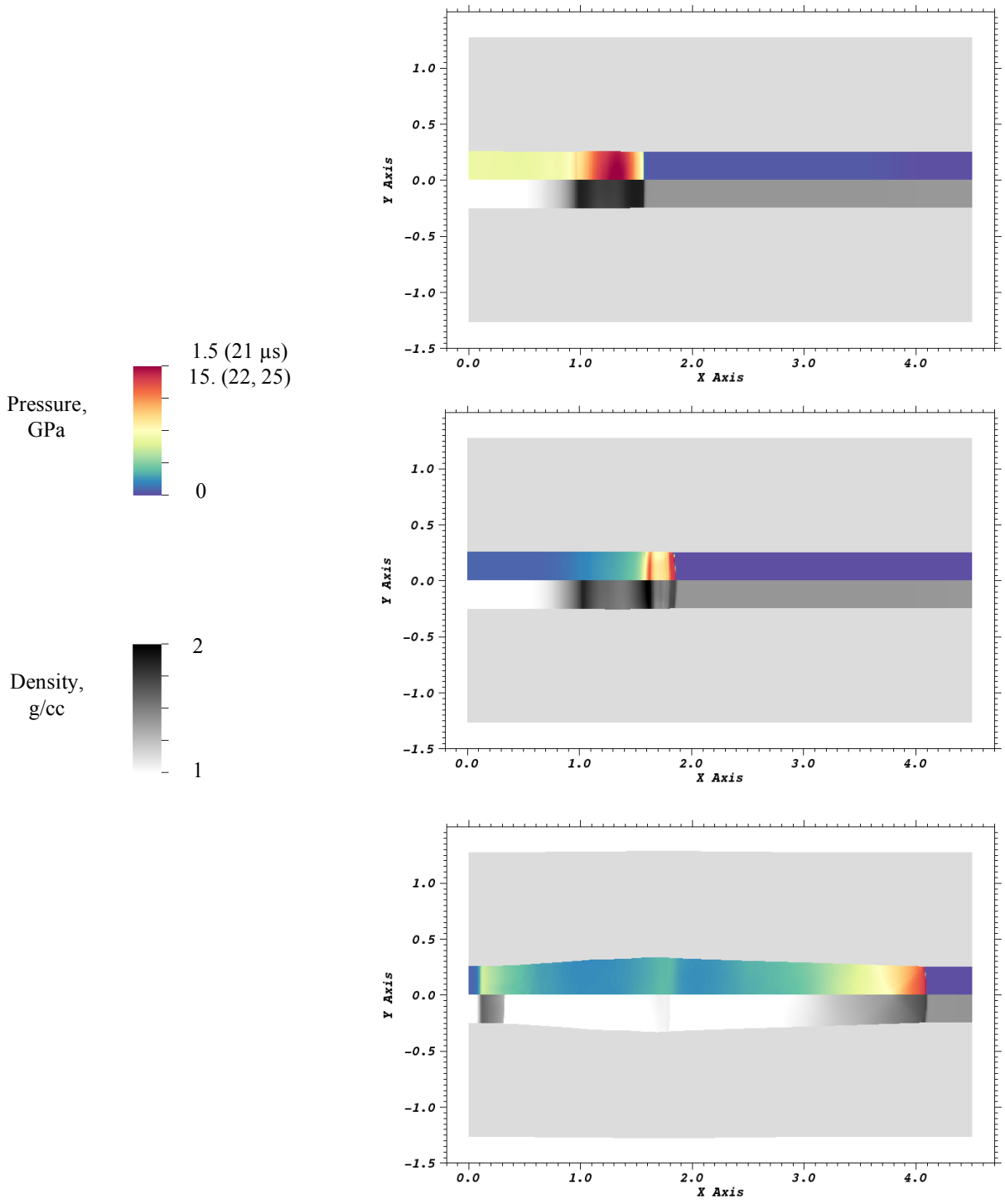

FIGURE 2. Sequence of results 21, 22, and 25 µsec (top to bottom) after ignition on the left. The lower half of each image is a grey-scale of density from 1 g/cc (white) to 2 g/cc (black). The top half of each image is a fringe plot of PETN pressure from 0 (blue) to 1.5 GPa (red) at 21 µsec and to 15 GPa at 22 and 25 µsec. Steel confinement is light grey. Axis dimensions in cm.

We show in Fig. 2 the results of a calculation with parameters chosen to represent nominal values. The top figure is at 21 µsec after ignition of the small volume of powder, just before the transition to detonation. The peak pressure

at 21 μsec is about 1.5 GPa, which is less than 10% of the detonation pressure in density 1.4 g/cc PETN (18 GPa). The pressure increase is caused by the CREST-lite detonation rate-law response to a 0.7 GPa shock in low-density powder. The pressure rise catches up to the front and reinforces the shock pressure, leading to an accelerated reaction rate. The middle figure is at 22 μsec, just after the transition. It is clear that the (right-going) detonation is propagating into essentially undisturbed powder. The (left-going) retonation is propagating into a region of both variable density and variable composition – the powder at the far-left side has burned about 20% of its mass. As a result, the retonation moves generally slower but does not have a constant speed. The last plot at 25 μsec shows the retonation has slowed considerably as it is driving into low-density, partially depleted explosive. The detonation transition distance is taken to be the axial location of the maximum radius of the steel channel, 17 mm.

One of the parameters that has a significant effect on the transition distance is the velocity of the ignition front that streams through the porous bed. The ignition front velocity in thermally damaged explosive, which is much less porous, has been reported as high as 100 m/s [11]. Measurements for porous beds have been even faster [12]. The transition location we calculate has a significant dependence on that value, which has not been measured for PETN. The calculation illustrated in Fig. 2 used an ignition front velocity of 300 m/s. A companion calculation using 100 m/s gives a smaller volume of low-density material at 21 μs, a considerably lower pressure behind the high-density plug, and a shorter length plug. Figure 3 illustrates our calculated transition distance as a function of the ignition front velocity for 180 μm mono-sized spheres, and for a log-normal distribution of spheres with median 180 μm but specific surface area 1.8 times larger than for mono-spheres, 330 cm^2/g vs. 190 cm^2/g. Our treatment of log-normal distributions of particle sizes is discussed in [8].

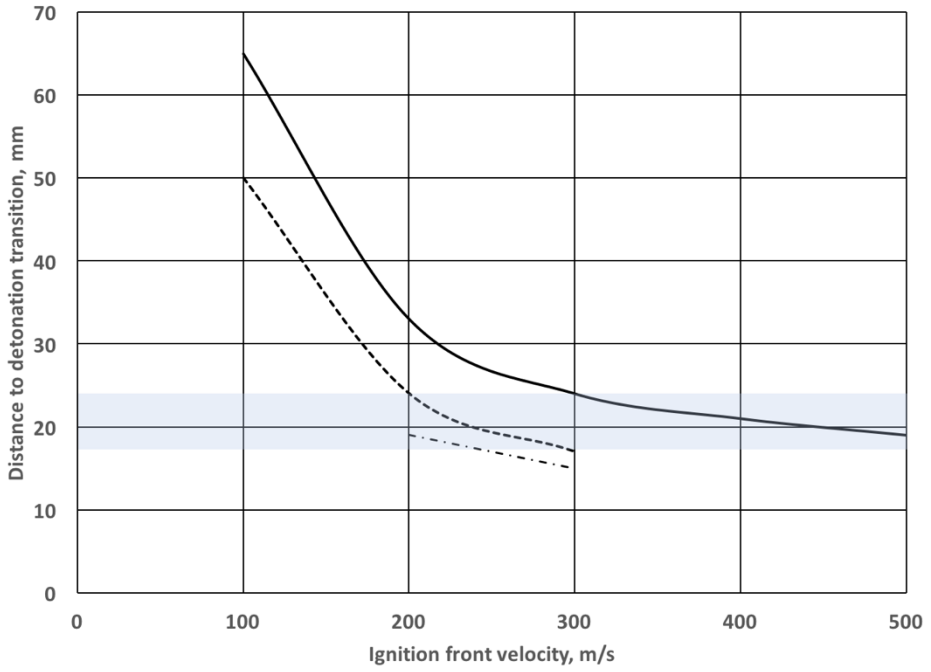

FIGURE 3. Calculated transition distance as a function of ignition front velocity for mono-sized 180 μm spheres (solid) and for a log-normal distribution centered at 180 μm with the half-maximum 51 μm to 630 μm (dashed). The experimental results for 1.4 g/cc PETN are within the colored band around 20 mm. Dash-dot line shows the effect of reducing the crush pressure for squeezing out the porosity from 200 MPa to 50 MPa for the log-normal distribution. Calculations with transitions larger than 40 mm were made with a double-length fixture.

When we used the more shock-sensitive fit to the SDT data (dashed line in Fig. 1) the transition distance was only slightly shorter, less than a 0.5 mm change, which is nearly our granularity in recording the transition distance. The effect of the crush pressure on the transition distance is shown in Fig. 3. The resistance to densification can be measured quasi-statically, but to our knowledge has not been measured for PETN powder. The accuracy of quasi-

static densification applied to the dynamic event in DDT is uncertain. The extreme shock sensitivity of low-density explosive powders makes dynamic measurements difficult.

Finally, we examined the effect of friction between the PETN powder and the steel surface. All the calculations previously discussed were performed with no frictional resistance at the wall. Measurements for the friction coefficient between steel and formulated explosives (high-density plastic bonded explosives) [13] gave a value of approximately 0.4. The measurement has not been made for either PETN formulations or powder. For our calculation using that value, the transition distance decreased from 17 to 16 mm. However, our parameter for ignition from shear localization (which has not been calibrated for PETN) was large enough to be of potential concern. The region of highest ignition parameter was adjacent to the wall, near the base of the high-density plug., The calculated transition distance was about the same, whether or not we permitted ignition to occur there. The location of that ignition site is so close to the location of the ignition front that propagates from the base of the fixture that the burning is not significantly changed.

CONCLUSIONS

We have conducted a parameter study using the HERMES model to calculate DDT of PETN powder in Luebcke's DDT apparatus. By doing so, we highlight the independent measurements (and simulations) needed to validate a model. Many DDT experiments were performed as SDT tests, using a moving piston rather than static ignition to start the test. Measurements and simulations of SDT for the powder morphology and starting density are needed for both kinds of tests. The particle size distribution must be measured. From our calculational results, measuring the ignition front velocity is especially important. The resistance to compaction and compressive strength of the explosive must be measured. If friction is significant, the possibility of shear ignition along the tube wall may be an important consideration especially when light output is used as a diagnostic tool.

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