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CREST modelling of PBX 9502 corner turning experiments at different initial temperatures

N J Whitworth
AWE, Aldermaston, Reading, RG7 4PR, UK
E-mail: nick.whitworth@awe.co.uk

Abstract. Corner turning is an important problem in regard to detonation wave propagation in TATB-based explosives. Experimentally, a sudden change in the direction of the propagating wave, such as turning a sharp corner, can result in dead-zones being left behind in the corner turn region, with the observed behaviour being particularly sensitive to the initial temperature of the explosive. In this paper, the entropy-dependent CREST reactive burn model is used to simulate corner turning experiments on the TATB-based explosive PBX 9502. Calculated results of double cylinder tests at three different initial temperatures (-54°C, ∼23°C, and 75°C), and a “hockey puck” experiment at ambient temperature, are compared to the corresponding test measurements. The results show that the model is able to: (i) calculate persistent dead-zones in PBX 9502 without recourse to any shock desensitisation treatment, and (ii) predict changes in corner turning behaviour with initial temperature using one set of coefficients.

1. Introduction
Triaminotriinitrobenzene (TATB)-based explosives have relatively long detonation reaction zone lengths (~2 mm) [1]. As a result, their propagating detonation waves can weaken markedly when attempting to spread out upon meeting an abrupt change in geometry. This leads to sustained unreacted and/or partially reacted pockets of explosive (“dead-zones”) being left behind when their detonation waves attempt to turn 90° corners [2-6], with the initial temperature of the explosive having a significant effect on the observed corner turning behaviour [6].

CREST [7] is a reactive burn model that uses entropy-dependent reaction rates to simulate explosive behaviour, and which has previously shown promise in predicting changes in explosive response with initial temperature using one set of coefficients [8, 9]. In this paper, to further assess the ability of CREST to predict explosive phenomena at different starting temperatures, the model is applied to detonation corner turning data on the TATB-based explosive PBX 9502. Two different geometries, both due to Lawrence Livermore National Laboratory, are considered: (i) a double cylinder test conducted at three different initial temperatures (-54°C, ~23°C, and 75°C) [6], and (ii) a hockey puck experiment at ambient temperature [4].

2. PBX 9502 Corner Turning Experiments
The double cylinder test is shown in figure 1. An RP-1 detonator initiates a 6.35 mm radius, 63.5 mm long, cylinder of the HMX-based explosive LX-14 which is in contact with a large test cylinder of radius 25.4 mm and maximum length 50.8 mm. A steel washer 6.35 mm thick is placed up against the left-hand surface of the PBX 9502. Shorting pins are positioned along
the outer surface of the larger diameter cylinder to record wave breakout times, while the axis pin provides information on the straight-ahead detonation wave propagation. All times are referenced to the corner turn pin in figure 1. Using this test, the corner turning behaviour in PBX 9502 has been studied at three different initial temperatures (-54°C, ~23°C, and 75°C), with the experimental data showing a significant effect due to starting temperature [5].

The hockey puck test is shown in figure 2. It consists of a 44.45 mm radius test cylinder, initiated by a 19.05 mm radius ultrafine TATB (UF-TATB) booster of density 1.80 g/cm³, which is itself lit by a hemispherical detonator of outer radius 6.65 mm. The detonator is made of two layers; an inner layer of 0.93 g/cm³ PETN with a 3.8 mm radius, and an outer layer of the RDX-based explosive PBX 9407. Both the booster and detonator are sunk 15 mm into the main charge with an air-well above them. To record wave breakout times, shorting pins are placed along both the left-hand edge and outer surface of the test cylinder. Again, all times are referenced to the corner-turn pin. Data on PBX 9502 in the hockey puck test is available at ambient temperature only [4].

**Figure 1.** Schematic of the double cylinder corner turning experiment. The bottom line is an axis of symmetry.

**Figure 2.** Schematic of the hockey puck geometry. The bottom line is an axis of symmetry.

3. Numerical Simulations
The CREST reactive burn model [7] utilises an entropy-dependent reaction rate, which is coupled to both a finite strain form of equation of state (EoS) for the non-reacted explosive and a JWL EoS for the reaction products. The entropy is calculated from the non-reacted EoS which, in conjunction with the Snowplough model for porous compaction, allows the reaction rate to adjust to account for changes in initial temperature [8] and initial porosity [10].

Numerical simulations of the two corner turning geometries were performed using a 2D Eulerian hydrocode incorporating CREST. Unless stated otherwise, a uniform mesh of 20 zones/mm was used in the simulations. Massless Lagrangian marker particles were placed along the relevant surfaces of the test cylinders to record the time of arrival of the shock/detonation wave at positions corresponding to the experimental pin locations.

A CREST model for PBX 9502 has previously been published at this conference [10]. More recently, our model for PBX 9502 has been improved. The updated model has improved EoS for both the unreacted explosive and the detonation products, and a revised reaction rate whose coefficients have been calibrated to shock initiation and detonation size effect data, all at ambient temperature. The updated model has been used in the simulations described below. Due to its complexity, there was not room in this paper to include the details of our improved model, but a journal paper containing this information will be published in the near future.
3.1. Double Cylinder Tests

In simulations of the double cylinder tests, the LX-14 donor charge was modelled via programmed burn using a JWL EoS [11]. The material model for the steel washer was taken from [12], while the PBX 9502 region was modelled using CREST. To model experiments at different initial temperatures, the initial state of the explosive needs to allow for the density and specific internal energy at the appropriate starting temperature. The internal energy comes from an iterative procedure that ensures that the initial conditions are consistent with CREST’s non-reactive EoS [13]. The initial density is estimated from thermal expansion data on the relevant explosive. No changes are required to the reference EoS or reaction rate coefficients.

The initial densities for PBX 9502 at the temperature extremes were estimated using the relationship in [14]. Values of the volumetric coefficient of thermal expansion for PBX 9502 due to Hill et al. [15] were used. Assuming the initial density of PBX 9502 at ambient temperature (23°C) is 1.890 g/cm³, this gives values of 1.911 g/cm³ at -54°C and 1.865 g/cm³ at 75°C. The densities of the LX-14 donor charge and steel washer were not corrected for thermal expansion. The experimental and calculated breakout times at the various initial temperatures are compared in figure 3. The experiments conducted at ambient and 75°C used 25.4 mm long PBX 9502 cylinders, while in the cold shot the test cylinder was 50.8 mm long. It is seen that CREST correctly predicts the observed trend in corner turning behaviour with initial temperature, with the delay in breakout times with decreasing temperature well represented. The straight-ahead detonation propagation is well matched to experiment at the various starting temperatures with the calculated arrival times all agreeing to within ±0.1 µs of experiment.

![Figure 3. Comparison of experimental and calculated breakout times from double cylinder corner turning tests at -54°C (blue), ~23°C (black), and 75°C (red).](image)

The experimental data shows that the detonation wave turns the 90° corner more readily with increasing temperature due to the earlier breakout times. This is reproduced in figures 4 and 5 which show, respectively, density and burn fraction colour plots from the simulations at the three different initial temperatures. The burn fraction colour scale runs from 0 (unburnt) to 1 (fully reacted). The figures illustrate the difference in corner turning behaviour with starting temperature, with the size (volume) of the dead-zone increasing with decreasing temperature. In particular, the plots show the presence of a large dead-zone when PBX 9502 is cooled to -54°C, with the distance from the steel washer at which first detonation breakout occurs being ~30 mm. This is significantly in excess of the corresponding distances at ambient and 75°C.

In performing corner turning reactive flow simulations, fine zoning is usually required to achieve mesh converged results. As an example of the effect of numerical resolution on the CREST simulated results, figure 6 shows the effect of mesh size on the breakout behaviour.
Figure 4. Density colour plots at times corresponding approximately to where first detonation wave breakout occurs along the outer surface of the cylinder; -54°C (top), ambient (middle), and 75°C (bottom).

Figure 5. Burn fraction colour plots at times corresponding approximately to where first detonation wave breakout occurs along the outer surface of the cylinder; -54°C (top), ambient (middle), and 75°C (bottom).

Figure 6. Effect of mesh size on calculated breakout times from simulations of the ambient temperature double cylinder test.

in the case of the double cylinder test at ambient temperature. Simulations were carried out at resolutions of 10, 20, and 40 zones/mm and, although not quite mesh converged, figure 6 demonstrates that corner turning simulations of PBX 9502 using CREST are adequately resolved at a mesh resolution of 20 zones/mm.
3.2. Hockey Puck

In simulations of the hockey puck geometry, the detonator was represented by a single region of PBX 9407. This was modelled via programmed burn using the JWL EoS parameters from [11]. The UF-TATB booster was modelled using CREST [9], as was the PBX 9502 main charge. For robustness purposes, the air-well was modelled as a low density fluid with a perfect gas EoS, where $\rho_0 = 0.1 \text{ g/cm}^3$ and $\gamma = 1.4$.

The calculated breakout times for the PBX 9502 hockey puck are compared with the corresponding experimental data in figure 7. The breakout times are plotted as a function of angle using the convention illustrated in figure 2, where negative angles signify straight-ahead propagation and positive angles identify the corner turn region. The solid red line is the CREST simulation shifted by 0.1 $\mu$s. This shift, justifiable since it is within the quoted experimental timing errors [4], allows the shape of the breakout curve to be more easily compared to experiment. Overall, CREST gives a good match to the experimental breakout data in both the straight ahead and corner turn regions, with the shape and timing well matched. The earliest calculated breakout time in the corner turn region occurs at $\sim 56^\circ$ in agreement with experiment.

Figure 8 shows a density colour plot from the simulation at a time just as the detonation wave breaks out at the left-hand edge of the hockey puck. A dead-zone forms just above the air-well where the detonation wave has had to turn through the 90° corner. The figure illustrates that, calculationally, the detonation wave has overcome the divergence in the flow as the wave spreads out from the corner by the time it arrives at the left-hand face of the PBX 9502 charge. As a result, the detonation wave is starting to travel back towards the corner turn through the already compressed, but largely unburnt, region of explosive. Further compression of this region sees no significant increase in CREST’s reaction rate resulting in a persistent dead-zone.

![Figure 7](image1.png)

**Figure 7.** Comparison of experimental and calculated breakout times for PBX 9502 hockey puck at ambient temperature.

![Figure 8](image2.png)

**Figure 8.** Density colour plot for PBX 9502 hockey puck at ambient temperature at time corresponding approximately to where first detonation wave breakout occurs in the corner turn region.

4. Discussion

Dead-zones that form in the vicinity of the abrupt expansion in corner turning experiments can be subjected to further shock compression(s) as a result of: (i) the detonation wave overcoming the divergence in the flow and propagating back towards the corner turn region (e.g. figure 8), and (ii) shock reflections from confining materials (e.g. figure 4). However, dead-zones persist
throughout the time frame of experiments, indicating no significant increase in reaction rate when subjected to further shocks. Such a phenomenon is often referred to as “shock desensitisation”.

Widely-used pressure-based reactive burn models require a bolt-on desensitisation treatment to predict the persistent dead-zones that are observed experimentally [16, 17]. Such an extension, which restricts the growth of reaction in multiple shock situations, is required otherwise the dead-zone would be short-lived which is not observed in practice. With CREST, an additional desensitisation criterion is not required; the model is able to give a significantly reduced response to following higher pressure shocks since the change in entropy between the first and subsequent shocks is significantly less than the corresponding change in pressure [18].

Another advantage of CREST is that the initial temperature of the explosive can be accounted for by modifying only the initial specific internal energy and density of the explosive. By its use of the Snowplough porosity model, the non-reacted EoS automatically adjusts the shock entropy allowing CREST to predict changes in behaviour with initial temperature without altering the reference EoS or reaction rate coefficients. In contrast, pressure-based models often have to be re-parameterised for different initial temperatures [11].

Although the fits to the experimental data are not perfect, particularly in the case of the double cylinder tests, the corner turning simulations are sensitive to a number of factors. These include uncertainties in: (i) the unreacted EoS at low pressures where experimental Hugoniot data is relatively sparse, and (ii) initial densities at the temperature extremes since these are not measured at the actual shot temperatures, and the thermal expansion of TATB-based explosives is known to be anisotropic [15]. Absolute timing, shape of the breakout curve, and size of dead-zone are all affected by small changes in the non-reacted EoS and initial density of the explosive.

5. Conclusions

Overall, within a number of uncertainties, the simulated results using CREST agree well with PBX 9502 corner turning data from two different experimental geometries. In particular, (i) CREST is able to predict the trend in corner turning behaviour with initial temperature using one set of coefficients, and (ii) the model can predict persistent dead-zones in PBX 9502 without recourse to any additional desensitisation treatment.

Improved experimental data that can provide more of a quantitative insight into the internal flow characteristics in detonation corner turning tests is required. Although proton radiography can capture the development of dead-zones within explosives dynamically [3], a number of questions still remain to be answered e.g. to what extent does the “dead” material contribute energy to the flow? Such improved data, when available, will provide a more stringent test of a reactive burn model than the simple time-of-arrival data compared in this paper.

References

[1] Seitz W L, Stacy H L, Engelke R, Tang P K and Wackerle J 1989 Proc. 9th Int. Detonation Symp. (Portland, Oregon) (Office of Naval Research) p657
[2] Cox M and Campbell A W 1981 Proc. 7th Int. Detonation Symp. (Annapolis, Maryland) (Naval Surface Weapons Center) p624
[3] Fern E N, Morris C L, Quintana J P, Pazuchanic P, Stacy H, Zumbro J D, Hogan G and King N 2001 AIP Conf. Proc. 620 p966
[4] Souers P C et al 2006 Dead Zones in LX-17 and PBX 9502 Propell, Explos, Pyrot 31, 89-97
[5] Souers P C, Hernandez A, Cabacungan C, Garza R, Launderbach L, Liao S B and Vitello P 2009 Air Gaps, Size Effect, and Corner Turning in Ambient LX-17 Propell, Explos, Pyrot 34, 32-40
[6] Souers P C, Launderbach L, Garza R, Vitello P and Hare D E 2010 Proc. 14th Int. Detonation Symp. (Coeur d’Alene, Idaho) (Office of Naval Research) p1237
[7] Handley C A 2006 Proc. 13th Int. Detonation Symp. (Norfolk, Virginia) (Office of Naval Research) p864
[8] Whittworth N J and Lambourn B D 2009 AIP Conf. Proc. 1195 p458
[9] Whittworth N J 2011 AIP Conf. Proc. 1426 p213
[10] Handley C A and Lambourn B D 2009 AIP Conf. Proc. 1195 p221
[11] Tarver C M 2012 Modeling Detonation Experiments on Triaminotrinitrobenzene (TATB)-Based Explosives LX-17, PBX 9502, and Ultrafine TATB J. Energ. Mater. 30, 220-251
[12] Tarver C M 2010 Corner Turning and Shock Desensitization Experiments plus Numerical Modeling of Detonation Waves in the Triaminotrinitrobenzene Based Explosive LX-17 J. Phys. Chem. A 114, 2727-2736
[13] Whitworth N J, Handley C A and Lambourn B D 2010 Proc. 14th Int. Detonation Symp. (Coeur d’Alene, Idaho) (Office of Naval Research) p61
[14] Gustavsen R L, Gehr R J, Bucholtz S M, Seitz W L, Sheffield S A, Alcon R R, Robbins D L and Barker B A 2006 Proc. 13th Int. Detonation Symp. (Norfolk, Virginia) (Office of Naval Research) p970
[15] Hill L G, Bdzil J B and Aslam T D 1998 Proc. 11th Int. Detonation Symp. (Snowmass, Colorado) (Office of Naval Research) p1029
[16] de Oliveira G, Kapila A K, Schwendeman D W, Bdzil J B, Henshaw W D and Tarver C M 2006 Proc. 13th Int. Detonation Symp. (Norfolk, Virginia) (Office of Naval Research) p13
[17] Wescott B L, Stewart D S and Davis W C 2006 Proc. 13th Int. Detonation Symp. (Norfolk, Virginia) (Office of Naval Research) p744
[18] James H R and Lambourn B D 2010 Proc. 14th Int. Detonation Symp. (Coeur d’Alene, Idaho) (Office of Naval Research) p1172

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