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UCRL-CONF-222376

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June 23, 2006

13th International Detonation Symposium
Norfolk, VA, United States
July 23, 2006 through July 28, 2006

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Abstract. The Ignition and Growth reactive flow model for shock initiation and detonation of solid explosives based on triaminotirnitrobenzene (TATB) is applied to three-dimensional detonation wave propagation. The most comprehensive set of three-dimensional detonation wave propagation data is that measured using the trapezoidal prism test. In this test, a PBX 9501 (95% HMX, 2.5% Estane, and 2.5% BDNPA/F) line detonator initiates a detonation wave along the trapezoidal face of a PBX 9502 (95% TATB and 5% Kel-F binder) prism. The failure thickness, which has been shown experimentally to be roughly half of the failure diameter of a long cylindrical charge, is measured after 50 mm of detonation wave propagation by impact with an aluminum witness plate. The effects of confinement impedance on the PBX 9502 failure thickness have been measured using air (unconfined), water, PMMA, magnesium, aluminum, lead, and copper placed in contact with the rectangular faces of the prism parallel to the direction of detonation propagation. These prism test results are modeled using the two-dimensional PBX 9502 Ignition and Growth model parameters determined by calculating failure diameter and tested on recent corner turning experiments. Good agreement between experimentally measured and calculated prism failure thicknesses for unconfined and confined PBX 9502 is reported.

INTRODUCTION

Triaminotrinitrobenzene (TATB) - based solid explosives are widely used due to their excellent safety characteristics. Three high density versions are: LX-17 (92.5% TATB/7.5% KelF); PBX 9502 (95% TATB/5% KelF); and EDC-35 (95% TATB/5% KelF). These explosives exhibit 2 to 3 mm reaction zone lengths and many non-ideal propagation properties when detonating.[1] The Ignition & Growth reactive flow model has been applied to a great deal of experimental data on TATB detonation waves in order to predict this non-ideal behavior in geometries that can not be tested. Numerous one-dimensional embedded gauge and laser interferometer experiments on detonating LX-17 and PBX 9502 have created an excellent database for reactive flow modeling.[2] Various two-dimensional experiments have shed considerable light on the detonation versus charge diameter, failure diameter, and wave curvature properties of detonating TATB.[3] The three-dimensional trapezoidal prism failure test[4] has also provided an excellent text cases for TATB reactive flow modeling. In this paper, a recent two-dimensional corner turning experiment, commonly called the "hockey puck," for PBX 9502 is modeled to confirm the Ignition and Growth parameters obtained from one-dimensional experiments, failure diameter rate sticks, and diverging flow experiments. The PBX 9502 model is then applied to unconfined and confined trapezoidal prism test data with good success.

THE IGNITION & GROWTH MODEL

The Ignition and Growth reactive flow model of shock initiation and detonation of solid explosives has been used to solve many 1D, 2D, and 3D explosive and propellant safety and performance problems.[5-11] The model uses two Jones-Wilkins-Lee (JWL) equations of state, one for the unreacted explosive and one for its reaction products, in the temperature dependent form:

$$p = A\, e^{-R_1 V} + B\, e^{-R_2 V} + \omega C_V T/V \qquad (1)$$

where p is pressure in Megabars, V is relative volume, T is temperature, ω is the Gruneisen coefficient, C_V is the average heat capacity, and A, B, R_1, and R_2 are constants. The reaction rate law for the conversion of explosive to products is:

$$dF/dt = \underset{(0<F<F_{igmax})}{I(1-F)^b(\rho/\rho_o-1-a)^x} + \underset{(0<F<F_{G1max})}{G_1(1-F)^c F^d p^y}$$

$$+ \underset{(F_{G2min}<F<1)}{G_2(1-F)^e F^g p^z} \qquad (2)$$

where F is the fraction reacted, t is time, ρ is the current density, ρ_o is the initial density, and I, G_1, G_2, a, b, c, d, e, g, x, y, and z are constants. The mixture equations assume pressure and temperature equilibration between the unreacted explosive and its reaction products.

This three-term rate law describes the three stages of reaction generally observed in shock initiation and detonation of heterogeneous solid explosives. One set of parameters can be normalized to experimental shock initiation and some detonation data, such as failure diameter. However, to model the nanosecond time resolved detonation reaction zone structure, a separate set of parameters is required. Shock initiation and detonation propagation are driven by different fundamental reaction rate controlling processes.[5,12] For detailed detonation modeling, the first term of Eq. (2) represents the ignition of the explosive as it is compressed by the leading shock wave creating heated areas (hot spots) as the voids in the material collapse. The fraction of explosive ignited is equal to the original void volume.[5] The second reaction models the rapid formation of the major reaction product gases (CO_2, N_2, H_2O, CO, etc.) in highly vibrationally excited states[12] and their subsequent expansion and equilibration. The third term is used to describe the relatively slow diffusion controlled formation of the solid carbon particles in the form of diamond, graphite, or amorphous carbon. For TATB-based explosives, the last 20% of the energy release is assumed to be due to solid carbon formation.[13,14] Table 1 lists the Ignition and Gorwth coefficients used for PBX 9502 in this paper. The mesh sizes used in these calculations are 4 or more zones per mm, which produce converged results. Convergence and pressure equilibration are required for all reactive flow modeling applications.

PBX 9502 HOCKEY PUCK MODELING

Two-dimensional corner turning experiments called "hockey pucks" have furnished arrival time at charge boundary and "dead zone" data for TATB-based explosives.[15] Tarver[16] showed that the LX-17 Ignition and Growth detonation model yielded excellent agreement with the experimental arrival times for both the initial diverging section of the detonation wave and the section that turned a ninety degree corner leaving a region of unreacted or partially reacted explosive. Recently the same corner turning test was done using PBX 9502.[17] Figure 1 shows the experimental and calculated arrival times for PBX 9502 using the distances defined as in Ref. 15. Since the ultrafine TATB boosters used in the hockey puck experiments impart some of the diverging flow, the Ignition and Growth parameters listed in Table 1 must be used to model detonating ultrafine TATB. Excellent agreement is obtained in Fig. 1, within the 0.2 μs timing variations observed in several LX-17 shots.[17]

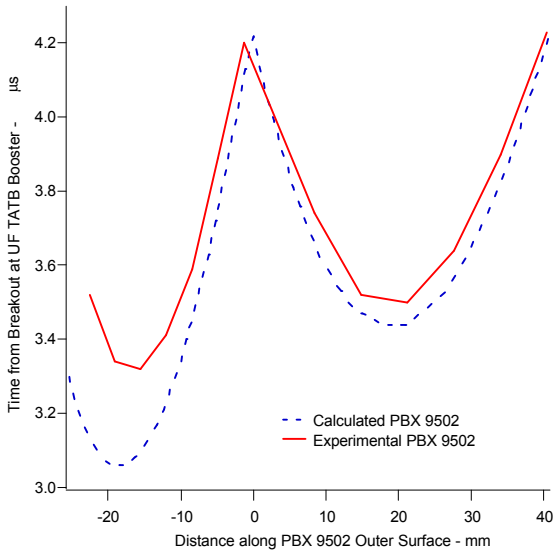

FIGURE 1. EXPERIMENTAL AND CALCULATED ARRIVAL TIMES AT THE OUTER SURFACE OF A PBX 9502 HOCKEY PUCK DIVERGING DETONATION SHOT

The trapezoidal prism test for detonation failure developed by Ramsay[4] is an excellent three-dimensional test of the PBX 9502 reactive flow parameters. As shown in Fig. 2, a detonation wave is initiated with a 150 mm long line-wave generator. This detonation wave travels into a 12 x 12 x 150 mm booster of PBX 9501 (95wt% HMX/ 5%estane-plasticizer binder) and then into a 150 mm long, 50 mm wide wedge of PBX 9502 with a 2˚ taper. The base of the wedge is 8 mm thick and the toe 2 mm thick for most shots. The thickness at the point of detonation failure is measured from the dent formed in a dural aluminum witness plate. An experiment using two PBX 9502 prisms edge-to-edge provided a total run distance of 100 mm and showed that the prism failure thickness is very close to 1/2 of the cylindrical rate stick failure diameter. Various inert materials were used to confine the PBX 9502 prisms and reduce the failure thicknesses according to their impedances.[4] Asay and McAfee[18] also used the prism test to estimate the failure diameter of PBX 9502 heated to 170˚C and 250˚C.

This prism test is truly three-dimensional and must be modeled as such. Three-dimensional meshes of the entire prism were constructed. Table 2 contains the PBX 9501 detonation wave and Jones-Wilkins-Lee (JWL) equation of state parameters used to model the ideal Chapman-Jouguet (C-J) detonation of the booster charge. Table 3 contains the inert Gruneisen equations of state used to model the confining materials.

UCONFINED COMPUTATIONAL RESULTS

3D reactive flow modeling of the unconfined prism test shows that the whole prism face begins to react when initiated by a PBX 9501 donor detonation wave or by an initial pressure boundary condition of 50 GPa is used. The reaction begins to fail almost immediately at the narrow edge of the wedge. This failure of reaction continues until a wedge thickness of approximately 3.2 mm is reached after 2 to 3 cm of propagation. This calculated failure thickness agrees well with the experimental value of 3.5 mm. The calculated PBX 9502 detonation wave appears to be expanding slightly as it approaches the bottom of the prism.

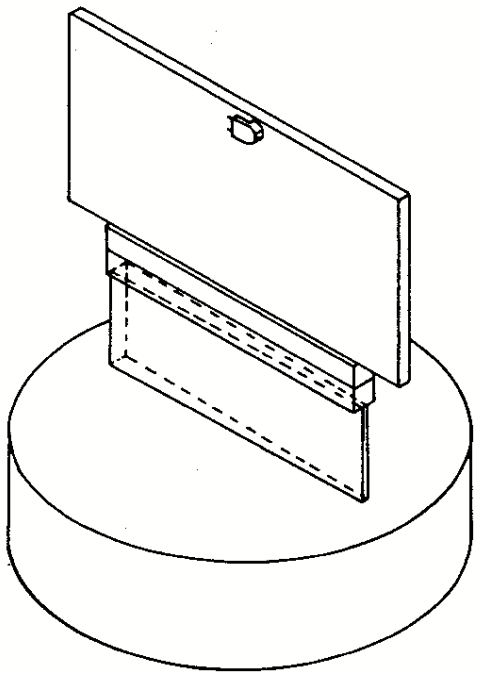

FIGURE 2. UNCONFINED TRAPEZOIDAL PRISM TEST ASSEMBLY

This result also seems to agree with experiment, because Ramsay[4] showed that the PBX 9502 detonation wave was not completely stable after 5 cm of propagation by initiating two prisms edge-to-edge for a total run distance of 100 mm and measuring a slightly larger failure thickness of 4 mm. TATB-based explosives exhibit extremely long run distances to failure in cylindrical charges.[19]

Figure 3 contains particle velocity contours for detonating PBX 9502 taken just before the bottom of the prism is reached. The blue (darker) region shows the unreacted PBX 9502 that failed to react, while the yellow and orange (lighter) regions show a curved lower pressure and velocity region and a nearly flat high pressure, high velocity region, respectively, of the detonation wave front. These regions correspond to the assumed von Neumann spike particle velocity of approximately 2.4 km/s and the assumed Chapman-Jouguet (C-J) particle velocity of approximately 2.1 km/s. The red (brightest) regions of the charge edges represent the

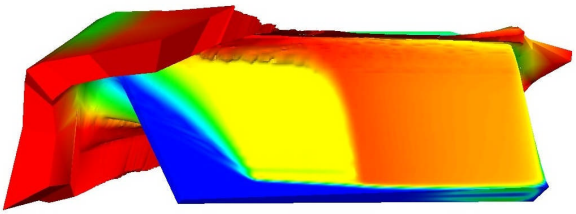

FIGURE 3. PBX 9502 PARTICLE VELOCITY CONTOURS IN AN UNCONFINED PRISM TEST CALCULATION

highest particle velocities of the expanding reaction products exceeding 3 km/s. Thus the unconfined prism test Ignition and Growth calculations simulate quite accurately the experimentally results. 100 mm long prisms will be calculated to determine when and if the detonation wave becomes stable.

CONFINED PRISM CALCULATIONS

Ramsay[4] demonstrated that very thin thicknesses of confining materials greatly reduce the failure thickness of PBX 9502 detonation waves and that the size of the reduction increases with the impedance of the confining material. First the effect of 1 mm aluminum confinement was calculated for a 2 mm to 8 mm thick prism. The experimental failure thickness was approximately 1.5 mm. The Ignition and Growth calculation showed detonation throughout this prism, indicating that the calculated failure thickness would be less than 2 mm. A 1 mm to 7 mm thick prism was then constructed and calculated. Failure began at the 1 mm thickness edge. Stability was reached after a few millimeters. At the end of the 5 cm prism, the predicted failure thickness was approximately 1.2 mm, compared with the experimental value of 1.5 mm. Figure 4 shows particle velocity contours near the end of this run using the same scale as in Figure 3. The blue (dark) region on the left hand side indicates failure, while the yellow/green (bright) region implies detonation propagation through most of the prism. The confinement layer is not show.

The PBX 9502 overall reaction zone length is approximately 3 mm or 0.4 μs time duration.[13] One mm thick aluminum supplies a high impedance boundary for a sufficient time (about 0.3 μs) for the main exothermic gaseous product formation reaction to occur before a rarefaction wave lowers the

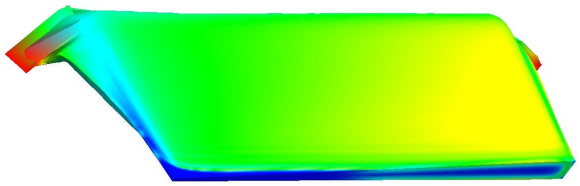

FIGURE 4. PBX 9502 PARTICLE VELOCITY CONTOURS IN A CONFINED PRISM TEST CALCULATION. THE ALUMINUM CONFINEMENT LAYER IS NOT SHOWN.

pressure and temperature quenching the reaction. The detonation wave continues to propagate at smaller thicknesses than in the cases of no confinement, weaker confinement, or thinner aluminum confinement.

CONCLUSIONS

The Ignition and Growth PBX 9502 detonation reactive flow model was shown to accurately simulate a two-dimensional "Hockey Puck" corner turning experiment and several unconfined and confined three-dimensional trapezoidal prism experiments. The model can be used with some confidence to predict 2D and 3D detonation propagation in scenarios that cannot be tested. However, a great deal more modeling effort is required to simulate the great wealth of prism test data available for PBX 9502 under various initial conditions of confinement and temperature.

ACKNOWLEDGEMENTS

*This work was performed under the auspices of the United States Department of Energy by the University of California, Lawrence Livermore National Laboratory under Contract No. W-7405-ENG-48.

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TABLE 1. IGNITION & GROWTH PARAMETERS FOR PBX 9502 AND ULTRAFINE TATB

A. PBX 9502	r_o =1.895 g/cm^3	
UNREACTED JWL	PRODUCT JWL	REACTION RATES
A=778.1 Mbar	A=13.6177 Mbar	I=4.0x10^6 ms^{-1}
B= -0.05031 Mbar	B=0.7199 Mbar	a=0.214
R_1=11.3	R_1=6.2	b=0.667
R_2=1.13	R_2=2.2	x=7.0 F_{igmax}=0.025
w=0.8938	w=0.5	G_1=4613 Mbar^{-2}ms^{-1}
C_V=2.487x10^{-5} Mbar/K	C_V=1.0x10^{-5} Mbar/K	c=0.667
T_o = 298°K	E_o=0.069 Mbar	d=1.0
Shear Modulus=0.0354 Mbar		y=3.0 F_{G1max}=0.8
Yield Strength=0.002 Mbar		G_2=30 Mbar^{-1}ms^{-1}
		e=0.667 z=1.0
		g=0.667 FG2min=0.8
B. ULTRAFINE TATB	ρ_o =1.80 g/cm^3	
UNREACTED JWL	PRODUCT JWL	REACTION RATES
A=632.07 Mbar	A=12.05026 Mbar	I=4.0x10^{6}ms^{-1}
B= -0.04472 Mbar	B=0.602513 Mbar	a=0.22
R_1=11.3	R_1=6.2	b=0.667
R_2=1.13	R_2=2.2	x=7.0 F_{igmax}=0.071
w=0.8938	w=0.5	G_1=2200 Mbar^{-2}ms^{-1}
C_V=2.487x10^{-5} Mbar/K	C_V=1.0x10^{-5} Mbar/K	c=0.667
T_o = 298°K	E_o=0.069 Mbar	d=1.0
Shear Modulus=0.03 Mbar		y=2.0 F_{G1max}=1.0
Yield Strength=0.002 Mbar		G_2=60 Mbar^{-1}ms^{-1}
		e=0.667 z=1.0
		g=0.667 F_{G2min}=0.8

TABLE 2. C-J DETONATION AND JWL PARAMETERS FOR PBX 9501

Initial density ρ_o = 1.835 g/cm^3; Detonation velocity D = 0.88 cm/μs; C-J Pressure P_{CJ} = 0.340 Mbars; A = 16.689 Mbars; B = 0.5969 Mbars; R_1 = 5.9; R_2 = 2.1; ω = 0.45; Eo = 0.102 Mbar-cc/cc-g

TABLE 3. GRUNEISEN EQUATION OF STATE PARAMETERS FOR INERT MATERIALS

$$P = \rho_o c^2 \mu[1+(1-\gamma_o/2)\mu - a/2\mu^2]/[1-(S_1-1)\mu - S_2\mu^2/(\mu+1) - S_3\mu^3/(\mu+1)^2]^2 + (\gamma_o + a\mu)E,$$

where $\mu = (\rho/\rho_o - 1)$ and E is thermal energy

INERT	ρ_o(g/cm^3)	c(mm/ms)	S_1	S_2	S_3	g_o	a
Al 6061	2.703	5.24	1.4	0.0	0.0	1.97	0.48
Steel	7.90	4.57	1.49	0.0	0.0	1.93	0.5
PMMA	1.186	2.57	1.54	0.0	0.0	0.85	0.0
Copper	8.93	3.94	1.489	0.0	0.0	2.02	0.47