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Initiation of propagating detonations

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Abstract--The initiation of propagating detonation in PBX 9404, PBX 9502, and X0219 by hemispheric initiators of PBX 9404, 1.8 g/cm³-TATB, and X0351 is described numerically, using the two-dimensional Lagrangian code, 2DL, and the Forest Fire rate to describe the heterogeneous explosive shock initiation process. The initiation of propagating detonation in the insensitive explosive PBX 9502 by triple-shock-wave interaction from three initiators has been modeled using the three-dimensional, reactive, Eulerian hydrodynamic code, 3DE.

1. Introduction

The initiation of propagating, diverging detonation is usually accomplished by small conventional initiators; however, as the explosive to be initiated becomes more shock insensitive, the initiators must have larger diameters (~2.5 cm) to be effective.

The $^{12}$C camera was used to examine the nature of the diverging detonation waves formed in PBX 9404 (94/3/3 HMX/nitrocellulose/Tris-8-chloroethyl phosphate), X0290 or PBX 9502 (95/5 TATB/Kel-F at 1.894 g/cm³) and X0219 (90/10 TATB/Kel-F at 1.914 g/cm³) by hemispheric initiators.† The geometries of the initiators were (1) a 6.35-mm-radius hemisphere of PBX 9407

†These data were supplied by James R. Travis, Los Alamos National Laboratory Group M-3.
(94/6 RDX/Exon at 1.61 g/cm³) surrounded by a 6.35-mm-thick hemisphere of PBX 9404, (2) a 6.35-mm-radius hemisphere of 1.7-g/cm³ TATB surrounded by a 19.05-mm-thick hemisphere of 1.8-g/cm³ TATB, or (3) a 16-mm-radius hemisphere of X0351 (15/5/80 HMX/Kel-F/TATB at 1.89 g/cm³).

We have numerically examined systems with similar geometries by use of the hydrodynamic code 2DL [1] and the Forest Fire rate [1] to describe the shock initiation process. As the explosive to be initiated becomes more shock insensitive, the initiators must have larger diameters or some other method must be used to achieve the required high pressures of adequate duration. High pressures are achieved if two or more shock waves interact to form regular or Mach shock reflections. We will investigate propagating detonation initiation in the insensitive high explosive PBX 9502 by the double- and triple-wave interaction of shock waves formed by initiators that are too weak to initiate propagating detonation individually.

2. Numerical modeling of initiation by single initiators

The two-dimensional, reactive, Lagrangian hydrodynamic code 2DL was used to describe the reactive fluid dynamics. The Forest Fire description of heterogeneous shock initiation was used to describe explosive burn. The HOM equation of state and Forest Fire rate constants for PBX 9502, PBX 9404, and X0219 were identical to those described in Ref. [1]. The Pop plots are shown in Fig. 1 and the Forest Fire rates in Fig. 2. The BKW detonation product equation-of-state constants for X0351 and for 1.7- and 1.8-g/cm³ TATB are given in Ref. [2].

The calculations were done in cylindrical geometry with Lucite confinement rather than the air confinement present in the experimental study. The Lucite confinement prevents the mesh distortion that can be fatal to Lagrangian calculations.
The central 6.35-mm region of the detonator is initially exploded, which initiates the remaining explosive in the detonator using a C-J volume burn. For any given mesh size and time step, the viscosity must be adjusted to give a peak pressure at the detonation front near the effective C-J pressure. The parameters used are as follows.

<table>
<thead>
<tr>
<th>Calculation</th>
<th>Initiator</th>
<th>Acceptor</th>
<th>Mesh Size (cm)</th>
<th>Time Step (μs)</th>
<th>Viscosity Coefficient</th>
</tr>
</thead>
<tbody>
<tr>
<td>PBX 9407/PBX 9404</td>
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<td></td>
<td>0.05</td>
<td>0.02</td>
<td>4.0</td>
</tr>
<tr>
<td>PBX 9407/PBX 9404</td>
<td>PBX 9502</td>
<td></td>
<td>0.05</td>
<td>0.02</td>
<td>5.0</td>
</tr>
<tr>
<td>PBX 9407/PBX 9404</td>
<td>X0219</td>
<td></td>
<td>0.05</td>
<td>0.02</td>
<td>4.2</td>
</tr>
<tr>
<td>1.7 TATB/1.8 TATB</td>
<td>PBX 9502</td>
<td></td>
<td>0.1</td>
<td>0.02</td>
<td>5.0</td>
</tr>
<tr>
<td>X0351</td>
<td>PBX 9502</td>
<td></td>
<td>0.1</td>
<td>0.02</td>
<td>5.0</td>
</tr>
</tbody>
</table>

The pressure and mass fraction contours are shown for a PBX 9404 hemisphere initiating PBX 9404 in Fig. 3, PBX 9502 (X0290) in Fig. 4, and X0219 in Fig. 5. The experimental and calculated position of the leading wave as a function of distance from the origin is shown in Fig. 6.

The burn can become unstable when it turns a corner. The instability is apparently numerical because it can be eliminated by using an average of nearby cell pressures for the Forest Fire burn rather than the individual cell pressure.

The pressure and mass fraction contours are shown in Fig. 7 for the 1.8-g/cm³ TATB hemisphere initiating PBX 9502. Very little undecomposed explosive was observed experimentally, in agreement with the calculated results. The contours are shown in Fig. 8 for an X0351 hemisphere initiating PBX 9502. The experimental and calculated regions of partially decomposed PBX 9502 are shown in Fig. 9.
3. Numerical modeling of initiation by multiple initiators

The three-dimensional Eulerian hydrodynamic computer code, 3DE, [3] was used to model numerically the interaction of shock waves in PBX 9502 formed by initiators that are too small to initiate propagating detonation. The calculations were performed on the CRAY computer. The Forest Fire model of heterogeneous explosive shock initiation was used to describe the explosive burn.

The geometry studied is shown in Fig. 10. Two or three initiator cubes of 7 by 7 by 7 cells are placed symmetrically in a PBX 9502 cube with continuum boundaries on its sides. The initiator cube centers were 1.6 cm apart and 1.09 cm from the cube bottoms. The indices i, j, and k designate the position of the x-, y-, and z-coordinates. The total cube height is k of 31, i is 29, and j is 25. The initiator cubes were initially decomposed PBX 9502 with a 2.5-g/cm³ initial density, which has an initial pressure of 245 kbar. This sends a diverging ~100-kbar shock into the surrounding PBX 9502. The computational cell size used was 0.114 cm, and the time step was 0.022 µs. The computer time for the 22,475 cells was about 50 minutes for 150 cycles.

The expected wave interactions are sketched in Fig. 11. The sketch shows the waves, just after double-wave interaction, as dashed lines, and the dark region shows the double-wave interactions. The solid lines and dotted regions show the waves after triple-wave interaction.

The pressures from the diverging double-wave interaction in inert PBX 9502 are about 200 kbar, and those from the triple-wave interaction are about 300 kbar.

The calculated three-dimensional pressure and mass fraction contours for two initiators are shown in Fig. 12 and for three initiators in Fig. 13.
The isobar and mass fraction cross sections for layer j of 9 (across the detonator centers) are shown for two initiators in Fig. 14 at 1.34 µs, in Fig. 15 at 1.78 µs, and in Fig. 16 at 2.66 µs. The isobar and mass fraction cross sections for layer j of 11 (across the edge of the detonators) for three initiators are shown in Fig. 17 at 1.78 µs, in Fig. 18 at 3.10 µs, and in Fig. 19 at 4.42 µs.

Although two initiators cause double-wave interaction that results in considerable decomposition, propagating detonation does not result.

Three initiators fail to initiate propagating detonation at the double-wave interaction points but do at the triple-wave interaction region. The higher triple-wave interaction pressure results in a shorter run to detonation. The detonation can be maintained long enough to become a propagating, diverging detonation.

4. Conclusions

The initiation of propagating detonation in sensitive (PBX 9404) and insensitive (PBX 9502 and X0219) explosives by hemispheric initiators can be described numerically using the two-dimensional Lagrangian code 2DL and the Forest Fire rate. Large regions of partially decomposed explosive occur even when insensitive explosives are initiated by large initiators.

The three-dimensional Eulerian hydrodynamic computer code, 3DE, has been used to examine the interaction of two and three shock waves from initiators in PBX 9502. The dynamics of initiating propagating detonation in an insensitive explosive by multiple shock-wave interactions has been modeled numerically.

References


Figure captions

1. The distance of run to detonation as a function of the shock pressure.
2. The Forest Fire decomposition rates as a function of shock pressure.
3. The pressure and mass fraction contours at various times for a hemi-spheric initiator of 6.35-mm-radius PBX 9407 surrounded by 6.35 mm of PBX 9404 initiating PBX 9404. The pressure contour interval is 50 kbar and the mass fraction contour is 0.1.
4. The pressure and mass fraction contours at various times for a hemi-spheric initiator of 6.35-mm-radius PBX 9407 surrounded by 6.35 mm of PBX 9404 initiating PBX 9502 (X0290). The pressure contour interval is 50 kbar and the mass fraction contour is 0.1.
5. The pressure and mass fraction contours at various times for a hemi-spheric initiator of 6.35-mm-radius PBX 9407 surrounded by 6.35 mm of PBX 9404 initiating X0219. The pressure contour interval is 50 kbar and the mass fraction contour is 0.1.
6. The experimental and calculated position of the leading wave from the top of the explosive block as a function of the distance of the leading front of the wave from the origin.
7. The pressure and mass fraction contours at various times for a hemi-spheric initiator of 6.35-mm-radius TATB at 1.7 g/cm³ surrounded by 19.05 mm of TATB at 1.8 g/cm³ initiating PBX 9502. The pressure contour interval is 50 kbar and the mass fraction contour is 0.1.
8. The pressure and mass fraction contours at various times for a hemi-spheric initiator of 16-mm-radius X0351 initiating PBX 9502. The pressure contour interval is 50 kbar and the mass fraction contour is 0.1.
9. The calculated and experimental region of partially decomposed PBX 9502 when initiated by an X0351 initiator.
Figure captions (cont)

10. A PBX 9502 cube with three embedded rectangular initiators.

11. The expected double- and triple-wave interactions from three initiators.

   The dashed lines and dark regions show the double-wave interaction.

   The solid lines and dotted regions show the triple-wave interaction.

12. The calculated three-dimensional pressure and mass fraction contours

   for two initiators in PBX 9502. The pressure contours are shown for

   200, 150, and 100 kbar at 0.4, 1.5, and 2.7 μs. The mass fraction

   contours are 0.8 and 0.5.

13. The calculated three-dimensional pressure and mass fraction contours

   for three initiators in PBX 9502. The pressure contours are shown

   for 200, 150, and 100 kbar at 1.5, 3.1, and 4.5 μs. The mass fraction

   contours are 0.8 and 0.5.

14. The isobar and mass fraction cross sections for layer j of 9 are shown

   for two initiators at 1.34 μs. The isobar interval is 50 kbar. The

   mass fraction interval is 0.1.

15. The isobar and mass fraction cross sections for layer j of 9 are shown

   for two initiators at 1.78 μs. The isobar interval is 50 kbar. The

   mass fraction interval is 0.1.

16. The isobar and mass fraction cross sections for layer j of 9 are shown

   for two initiators at 2.66 μs. The isobar interval is 50 kbar. The

   mass fraction interval is 0.1.

17. The isobar and mass fraction cross sections for layer j of 11 are shown

   for three initiators at 1.78 μs. The isobar interval is 50 kbar. The

   mass fraction interval is 0.1.

18. The isobar and mass fraction cross sections for layer j of 11 are shown

   for three initiators at 3.10 μs. The isobar interval is 50 kbar. The

   mass fraction interval is 0.1.
Figure captions (cont)

19. The isobar and mass fraction cross sections for layer j of 11 are shown for three initiators at 4.42 $\mu$s. The isobar interval is 50 kbar. The mass fraction interval is 0.1.
Rate = $\frac{1}{w} \frac{dw}{dt}$ (µ/sec⁻¹)

Pressure (kbar)

PBX 9404
Comp. B
X0219
X0290

Fig. 2 - Trace
Distance From Origin (mm)

Position Of Leading Wave From Top (mm)

- Travis PBX 9502 data
- Travis X0219 data
- Calculated PBX 9502
- Calculated X0219
压力（兆巴）

燃烧质量分数
Figure 18 - Graphs of Pressure (left) and Burn Mass Fraction (right) with specified parameters.

Pressure (Megabars) J: 11

Burn Mass Fraction J: 11

Parameters:
- Time: 3.102E+00 MS
- Cycle: 141
- Delta: 5.000E-02
- Time: 3.102E+00 MS
- Cycle: 141
- Delta: 1.000E-01
Pressure (Megabars)  $J = 11$

Burn Mass Fraction  $J = 11$