CTH Simulation of PBX-9501 Taylor Tests
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CTH Simulation of PBX-9501 Taylor Tests

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Abstract

During March-May 2011, multiple Taylor impact tests were conducted at LANL, examining the behavior of PBXN-9 and PBX-9501 under rapid loading. Subsequently, a computational hydrodynamics code (CTH) model was developed to mimic the deformation behavior observed in these impact tests with PBX-9501. Once suitably developed, additional simulations were performed with this model to determine the velocity range at which PBX-9501 would likely initiate upon impact. Also examined was whether an inert slug behind the explosive would lead to initiation at lower, more easily attainable velocities. The simplified model used here showed a minimum velocity for ignition of 530 m/s which was unchanged by the addition of a plastic slug behind the sample. The use of a lead slug did lower the minimum velocity to 460 m/s. These values are likely more qualitative at this point because multiple simplifications are currently used in the materials properties and test geometry. The results do show that this approach is capable of determining ignition due to Taylor impact.

The model used for these simulations is a modified version of the *steinberg.in* input file supplied with CTH, which simulated a Taylor impact of a Tantalum cylinder. Modifications were made to the sample dimensions, mechanical and thermodynamic properties of the material, and impact velocity. All other parameters were essentially unchanged. The dimensions of the CTH material sample were made to match the dimensions of the real specimens used in the Taylor tests (cylinder with a diameter of 1.6 cm, and a length of 7 cm). The thermodynamic EOS selected for this simulation was the History Variable Reactive Burn (HVRB) model for PBX-9501, which is included in the CTH database. The HVRB model uses a pressure-dependent rate law for modeling the reaction of the energetic material being simulated, and triggers the reaction when a specified density or temperature is reached. Finally, the elastic-plastic properties consisted of a preset input for HTPB rubber, with the fracture parameters changed to favor crumbling behavior, as observed in PBX-9501. These parameters were used because CTH does not provide an elastic-plastic model for PBX-9501 or its binders.
Assorted pressure maps are shown for various velocities throughout this summary. At velocities too slow for initiation to occur, an impact wave can be seen propagating through the material, but no ignition occurs. The material subsequently deforms and breaks apart as the impact progresses. Velocities shown are 150 m/s for Figure 1 and 500 m/s for Figure 2. Despite the significant difference in velocity and consequent deformation rate, the qualitative behavior between the two tests is quite similar.

Fig. 1. Impact profiles at 150 m/s, which is easily attainable with the Taylor gun in WX-7 at LANL. Pressure wave is visible in plot on left, taken shortly after impact.

Fig. 2. Impact profiles at 500 m/s. Pressure wave is shorter and more pronounced, but otherwise the deformation behavior is similar to what is seen in Fig. 1.
The impact velocity at which initiation first occurs in this model is ~530 m/s. At this velocity, all parameters given in the HVRB model are satisfied, and the pressure wave transitions to a self-sustaining detonation wave traveling through the material. Due to the rapidly decreasing density and increasing volume, CTH abruptly quits shortly after the material finishes burning. Pressure maps for this test are shown in Figure 3.

![Impact profiles at 530 m/s. Transition from compression wave to detonation wave is clearly visible (begins at 12 microseconds).](image)

Additional simulations were performed with an inert tamper replacing some of the explosive, with ignition at lower velocities as the desired outcome. This was done with Teflon (a possible real-world experiment) and lead (maximum mass). Some results for an impact with a Teflon tamper are shown in Figure 4.
Fig. 4. Impact tests at 530 m/s with Teflon tampers (white) behind the PBX-9501 (grey).

With the Teflon tamper, the minimum velocity for ignition remained unchanged (530 m/s) regardless of the thickness of the tamper relative to the explosive. Furthermore, a similar configuration with a lead tamper still required a minimum impact velocity of 460 m/s for ignition to occur. This is not a significant improvement, considering the maximum velocity for the gas gun is ~220 m/s.

It is worth mentioning that this is a relatively unsophisticated model with multiple simplifications that can lead to a deviation from reality. Compressive heating of air voids in the material, fracture of HMX crystals, and friction between HMX crystals are all ignored in this model. Any of these conditions could prove favorable for ignition at lower impact velocities.
PBXIN_Taylor.in input file with annotations.

Note: PBX_Taylor.in is another input file almost identical to this one, but it doesn’t include inert materials.

************************************************************************

*eor* cthin
************************************************************************

* cthin input for Taylor Cylinder Test
*
*   |<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<<
*   rigid  PBX-9501 at 1.2e4 cm/s
*
Taylor Test: PBX-9501 with inert slug
*
control
   tstop = 100.0e-6               Stop time in seconds.
     mmp0
endcontrol
*
mesh
   block 1  geom=2dc    type=e
     x0=0.0
     x1  n=100  w=8.0  dxf=0.08
   endx
     y0=0.0
     y1  n=100  w=8.00  dyf=0.08
   endy
   xaction=0., 1.600
   yaction=0., 7.000
   endb
endmesh
*
************************************************************************

* spy
   Save("VOLM,VX,VY,P");
   SaveTime(0, 2e-6);              Data acquisition interval in seconds.
   PlotTime(0, 2e-6);
*
define main()
{
  printf(" PLOT: Cycle=%d, Time=%e\n",CYCLE,TIME);
  XBMirror(ON);
  XLimits(-4,4);
  YLimits(0,8);
  Image("PBX-Pressure",WHITE);
  Window(0.05,0,0.8,1);
  MatColors(DIM_GRAY);
  Plot2DMats;
  ColorMapRange(1e4,1e12,LOG_MAP);
  ColorMapClipping(ON,OFF);
  DrawColorMap("P (dyn/cm^2^)",0.85,0.4,0.99,0.8);
  Label(sprintf("Time=%5.1f ~m~s",TIME*1E6));
  Plot2D("P");
  ResetMirrors;
  XBMirror(ON);
  Draw2DTracers(3);
  Draw2DMatContour;
}
EndImage;
Image("PBX-Density","WHITE");
Window(0.05,0,0.8,1);
MatColors(DIM_GRAY);
ColorMapRange(1e-2,1e1,LOG_MAP);
ColorMapClipping(ON,OFF);
DrawColorMap("Dens (g/cm^3^)",0.85,0.4,0.99,0.8);
Label(sprintf("Time=%5.1f ~m~s",TIME*1E6));
Plot2D("DENS");
ResetMirrors;
XBMirror(ON);
Draw2DTracers(3);
Draw2DMatContour;
EndImage;

%    Image("PBX-Mats");
%      Window(0.05,0,0.8,1);
%      MatColors(DIM_GRAY);
%      Label(sprintf("Time=%5.1f ~m~s",TIME*1E6));
%      Plot2DMats;
%    EndImage;

SaveHis("GLOBAL,VX,P,DENS,YLD,PSR");
SaveTracer(ALL);
HisCycle(0,1);

define spyhis_main()
{
    HisLoad(1,"hsctch",OFF);
    HisImageName("steinberg_history");

    TPlot("EK",1,ON);

    Label("Yield Stress");
    AutoScale(1,"TIME","YLD.1");
    VMaxAutoScale(1,"YLD.2");
    TPlot("YLD.1",1,OFF);
    Set1DLineProperties(2,1,SDASH,BLACK);
    TDraw("YLD.2",1);

    Set1DLineProperties(2,1,SOLID,BLACK);
    Label("Plastic Strain-Rate");
    AutoScale(1,"TIME","PSR.1");
    VMaxAutoScale(1,"PSR.2");
    TPlot("PSR.1",1,OFF);
    Set1DLineProperties(2,1,LDASH,BLACK);
    TDraw("PSR.2",1);

    Set1DLineProperties(2,1,SOLID,BLACK);
    Label("Plastic Strain");
    AutoScale(1,"TIME","Q1.1");
    VMaxAutoScale(1,"Q1.2");
    TPlot("Q1.1",1,OFF);
    Set1DLineProperties(2,1,LDASH,BLACK);
    TDraw("Q1.2",1);
}
endspy
*
************************************************************************
*
diatoms
package 'cylinder'
 material 1
    iter 4
    xvel 0.0
    yvel -5.3e4
    insert box
        p1 0.0 0.5
        p2 0.8 4.0
    endinsert
endpackage
package 'cylinder'
 material 2
    iter 4
    xvel 0.0
    yvel -5.3e4
    insert box
        p1 0.0 4.0
        p2 0.8 7.5
    endinsert
endpackage
* package 'cylinder'
* material 3
* iter 4
* xvel 0.0
* yvel -5.5e4
* insert box
*    p1 0.4 0.5
*    p2 0.8 4.0
* endinsert
* endpackage
enddiatoms
*
************************************************************************
*
tracer
*Cylinder center:
    add 0.000 0.060
*Cylinder edge:
    add 0.321 0.060
endt
*
************************************************************************
*
eos
    mat1 HVRB PBX9501
    mat2 MGR PTFE
*    mat3 MGR PTFE
endeos
*
************************************************************************
*
epdata
    vpsave
    matep 1 vep htpb
    matep 2 vep rm
*    matep 3 vep rm
    mix 3
ende
*
************************************************************************
*
Sample velocity in m/s.
Sample dimensions (radius in left column, height in right column, both in cm).
Inert slug behind explosive (optional).
Velocity of inert backing. This *MUST* match the velocity of the explosive.
Additional inert (required for “co-ax” tamper).
As before, the velocities must all match.
EOS for explosive and inert(s).
Material properties for explosive and inert(s).
Convct
  interface=high_resolution
endc
*
*************************************************************************
* discard
  mat 1 dens=0.01 press=1e6
endd
*************************************************************************
* edit
  shortc
    cy = 00    , dc = 1000
  ends
  longt
    time = 1.e-6  , dt = 1.0
  endl
  plott
    time  0.0  dtfrequency  50e-6
  endp
ende
*************************************************************************
* fracts
  stress
    pfrac1=-2.0e7
    pfmix=-2.0e15
    pfvoid=-5.0e6
  endf
*************************************************************************
* boundary
  bhydro  * rigid boundaries all around
    block 1
      bxbot = 0  , bxtop = 0
      bybot = 0  , bxtop = 0
    endb
  endh
endb
*