**Determination of detonation velocity and Plate Dent properties of PBXW-11 with 30 wt.% aluminium**

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|---|---|
| a) DPX-5 | a) DPX-5 |
| b) Detonation Velocity | b) detonasjonshastighet |
| c) Plate Dent | c) Plate Dent |
| d) | d) |
| e) | e) |

THESAURUS REFERENCE:

8) ABSTRACT

Studied composition PBXW-11with 30wt.% aluminium class 7 powder is a Norwegian produced explosive equal to the American PBXIH-18 composition. By slightly modification of the aluminium content the studied composition will also be equal to Chemring Nobel’s DPX-5 composition.

To determine the detonation velocity for PBXW-11 with 30wt.% aluminium class 7 powder pellets with 25.5 mm diameter have been pressed to a density of 97.4 % of TMD. 11 pellets were glued together to charges of approximately 430 mm in length and a distance between the start and stop sensors of 314 mm. The experimentally determined detonation velocity was found to be 8273 m/s, which is approximately 300 m/s higher than theoretically calculated by use of Cheetah 2.0 code.

Detonation pressure determined by use of Plate Dent test gave an average pressure of 255 kbar. This result is in accordance with theoretically calculated pressure obtained by use of the Cheetah 2.0 code.

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**CONTENTS**

# Determination of detonation velocity and Plate Dent properties of PBXW-11 with 30 wt.% aluminium

## 1 INTRODUCTION

M72 LAW (Light Antiarmour Weapon) has been redesigned with a new warhead for urban warfare. M72 ASM-RC (Anti-Structure Munition Reduced Caliber) has as the name indicates a new warhead for combat of light buildings. This requires a main charge explosive different from those used in shaped charge warheads. Studied composition is of the same family as the newly qualified composition DPX-6 (1), and is an aluminized PBX which is press filled into the warhead. In Norway Chemring Nobel AS (earlier Dyno Nobel ASA) use the name DPX-5 while in US it has the name PBXIH-18. Studied composition under the name DPX-5 is not qualified, and before it can be used in weapons it has to be qualified according to STANAG 4170 (2) and accompanying AOP-7 (3). Detonation velocity is an important property of explosives since it has influence on the performance.

To determinate the detonation velocity experimentally we have used a cylindrical charge with two sensors of twisted Copper wires. The first sensor was placed 8 cm from the booster to register the start and the second sensor 4 cm from the opposite end of the charge to register the stop. After measuring the distance between the start and stop points and the time the reaction front used between these two points, we easily can calculate the detonation velocity.

To determine the detonation pressure we used the same charges as for detonation velocity measurement to perform the Plate Dent test. In addition have we performed theoretical calculations of detonation properties by use of the Cheetah 2.0 code (4).

## 2 EXPERIMENTALLY

### 2.1 Composition

For tested composition PBXW-11 with 30% Aluminium, Ch 07/05, is the content given in Appendix A. For comparison is the nominal content of DPX-5: 64.4±2.0 wt.% HMX, 30.0±2.0 wt.% Al-powder, 1.4±0.5 wt% Hytemp binder and 4.2±1.0 wt.% DOA (5).

### 2.2 Detonation Velocity

The tested PBXW-11 charges consist of single pellets glued together to a length of 430 mm. The used pellets were pressed by Chemring Nobel AS. Dimensions, weight and density of single pellets are given in Appendix B. We did receive 33 pellets and used them to produce three test items. As sensors or measuring probes we used twisted copper wires (6).The Copper wire had a diameter of 0.15 mm and a 0.005 mm thick layer of lacquer. Two wires were twisted together and at the ends was the lacquer removed to obtain contact. We used two measuring probes, start probe placed between the second and third pellet and the stop probe between the two last ones. The position of the start measuring probes was selected to get a stable detonation front/velocity before starting the measurements, and the position of the stop was selected not to influence the Dent.

To initiate the charges we use a 16 g RDX/wax booster and a detonator No 8. A picture of the test items is given in Figure 3.3.

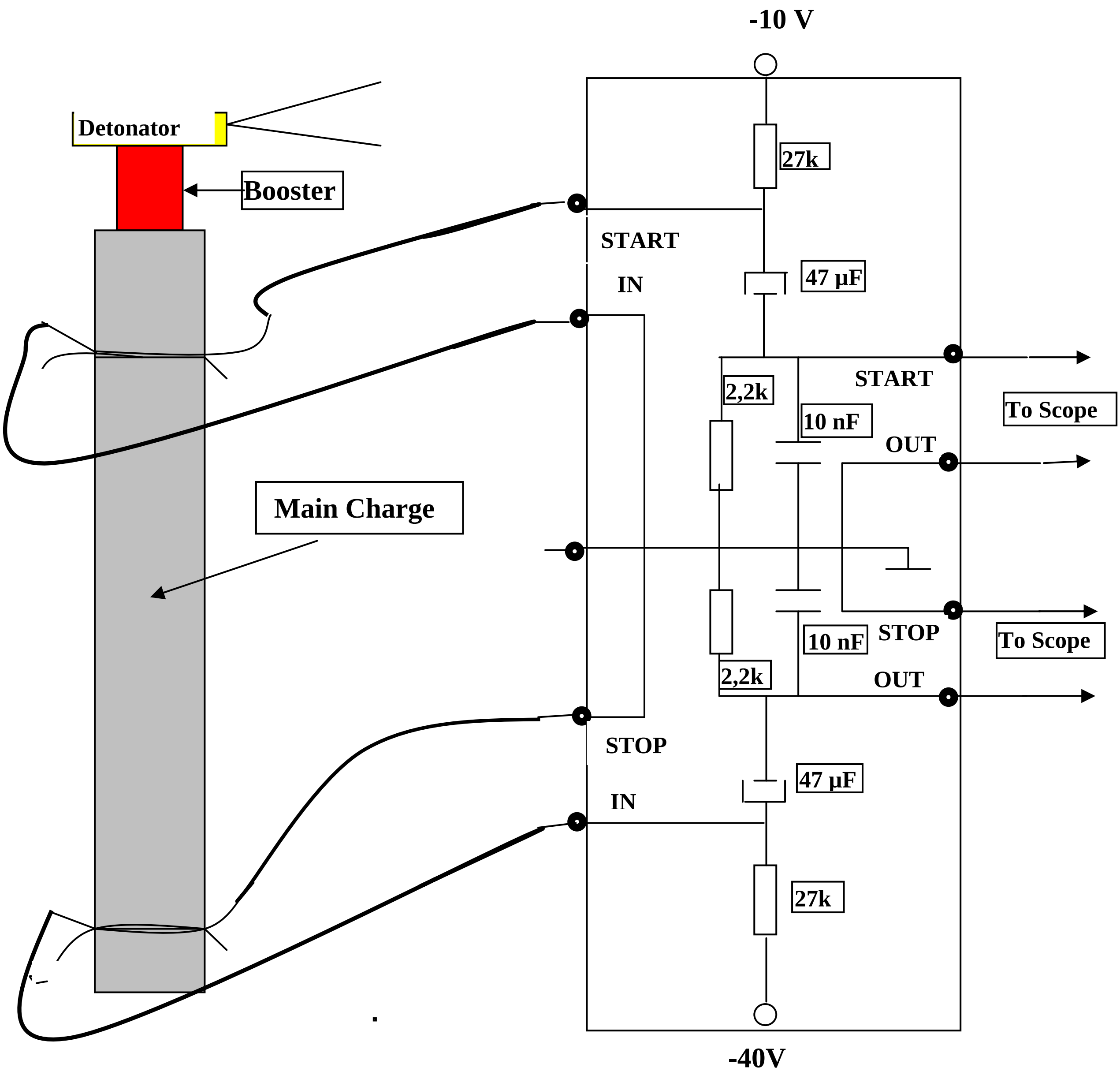


*Figure 2.1 Sketch of the instrumentation for measuring the detonation velocity.*

To measure the velocity we used the set up shown in Figure 2.1 in addition to two power supplies and a scope of type: HEWLETT PACKARD 54510A, Digitizing Oscilloscope, 250 MHz 1G Sa/s, Figure 2.2. When the detonation front passes the start sensor there will go a

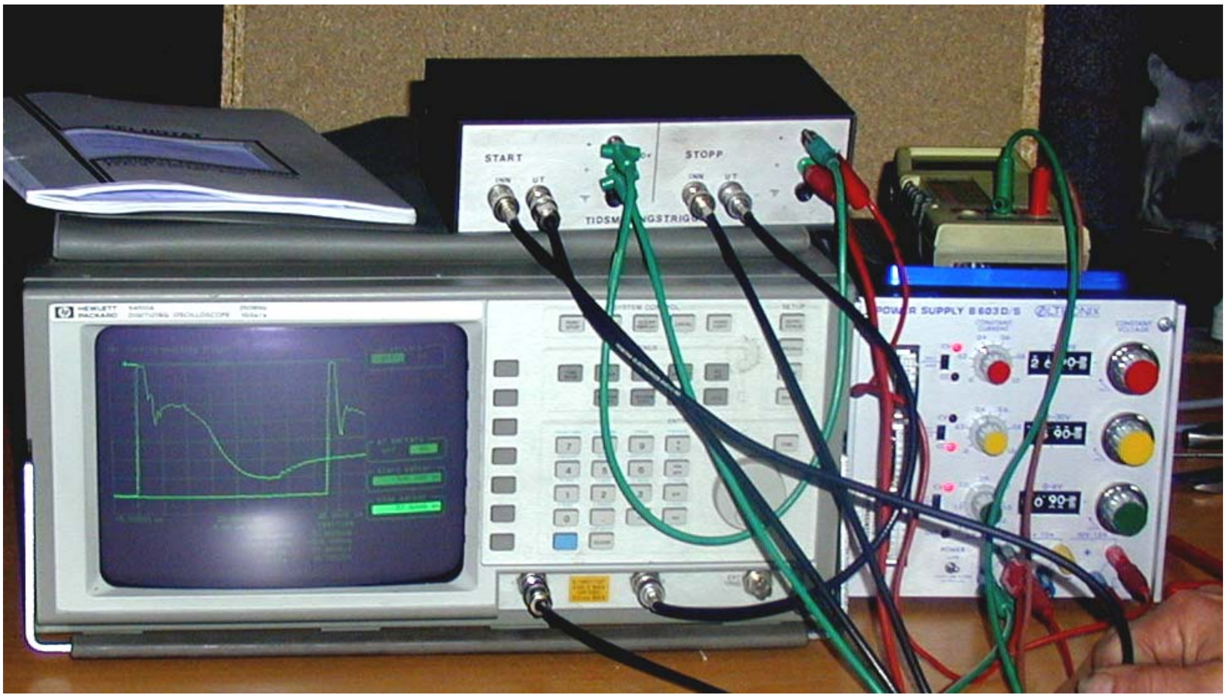


*Figure 2.2 Picture of the used oscilloscope.*

current through the circuit and a signal is observed on the oscilloscope. The same will happen when the detonation front reaches the stop probe. It is the time between these two signals that is used to calculate the detonation velocity since we know the distance between the two sensors.

## 2.3 Plate Dent test

The Plate Dent test as described in (7) was performed for all three shots. As witness plate was used round steel diameter 150 mm with thickness 50 mm of ST-37 material.

## 2.4 Theoretical Calculations

The theoretical calculations were performed with Cheetah 2.0 code (4).

# 3 RESULTS

## 3.1 Theoretical Calculations

To calculate the performance of PBXW-11with 30 wt.% Aluminium we have used the Cheetah 2.0 code (4) and the BKWC products database. These calculations have been performed for different densities from TMD (theoretical maximum density) down to 95 %TMD. PBXW-11 with 30 wt.% Aluminium is a composition that is filled by pressing and normally will TMD not be obtained. The pellets used for detonation velocity testing and Plate Dent Test have for instance a density of 1.949$\pm$0.003g/cm$^3$ or 97.37$\pm$0.15 %TMD, Appendix B.

In Appendix C.1 is the complete printout for a standard Cheetah run at TMD given, and it shows that all the aluminium do react. In Appendix C.2 are given Cheetah summary reports for different densities. Table 3.1 summaries the properties at the C-J conditions for PBXW-11 with 30 wt.% Aluminium of different density. From the table it can be seen that a reduction in density of the filling by less than 5% gives a reduction in the C-J pressure of close to 13% or 3.62 GPa, a lower reduction than for DPX-6 which was 20 % or 4.46 GPa (8). From the same density reduction we have a reduction in the detonation velocity for PBXW-11 with 30 wt.% Aluminium of 460 m/s while for DPX-6 it was 750 m/s.

| The C-J Conditions | Density (g/cm$^3$) | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | **2.0016** | **1.992** | **1.982** | **1.972** | **1.962** | **1.952** | **1.942** | **1.932** | **1.922** | **1.912** | **1.902** |
| **%TMD** | **100.00** | **99.5** | **99.0** | **98.5** | **98.0** | **97.5** | **97.0** | **96.5** | **96.0** | **95.5** | **95.0** |
| **The pressure (GPa)** | 28.18 | 27.79 | 27.41 | 27.03 | 26.66 | 26.3 | 25.94 | 25.59 | 25.24 | 24.90 | 24.56 |
| **The volume (cc/g)** | 0.395 | 0.396 | 0.398 | 0.400 | 0.402 | 0.403 | 0.405 | 0.407 | 0.409 | 0.410 | 0.412 |
| **The density (g/cc)** | 2.533 | 2.522 | 2.512 | 2.501 | 2.490 | 2.479 | 2.469 | 2.458 | 2.447 | 2.437 | 2.426 |
| **The energy (kJ/cc)** | 2.96 | 2.92 | 2.89 | 2.86 | 2.83 | 2.80 | 2.77 | 2.74 | 2.71 | 2.68 | 2.66 |
| **Temperature (K)** | 5837 | 5828 | 5818 | 5809 | 5799 | 5790 | 5780 | 5771 | 5761 | 5751 | 5742 |
| **Shock velocity (m/s)** | 8190 | 8143 | 8096 | 8049 | 8002 | 7956 | 7910 | 7865 | 7820 | 7775 | 7730 |
| **Particle velocity (m/s)** | 1719 | 1714 | 1709 | 1704 | 1699 | 1694 | 1689 | 1685 | 1680 | 1676 | 1671 |
| **Speed of sound (m/s)** | 6472 | 6429 | 6387 | 6345 | 6304 | 6262 | 6221 | 6180 | 6140 | 6099 | 6059 |
| **Gamma** | 3.765 | 3.752 | 3.739 | 3.725 | 3.711 | 3.697 | 3.683 | 3.669 | 3.654 | 3.640 | 3.625 |

*Table 3.1 Calculated properties at C-J conditions for different densities of PBXW-11 (28.2 wt% Al).*

## 3.2 Detonation Velocity

Three charges containing 11 pellets was glued together with the sensor between the second and third pellets for registration of the start signal and between the last two pellets for registration of the stop signal. Figure 3.2 gives a picture of the three charges before testing. To test that the equipment functioned as expected we used a detonating cord shown in Figure 3.1.

| Shot No | Material | Measuring Distance (cm) | Time (μs) | Velocity (m/s) |
|---|---|---|---|---|
| 2 | PBXW-11 | 31.355 | 37.9 | 8273 |
| 1 | Det.cord | 60.0 | 82.4 | 7282 |

*Table 3.2 Results from determination of detonation velocity.*

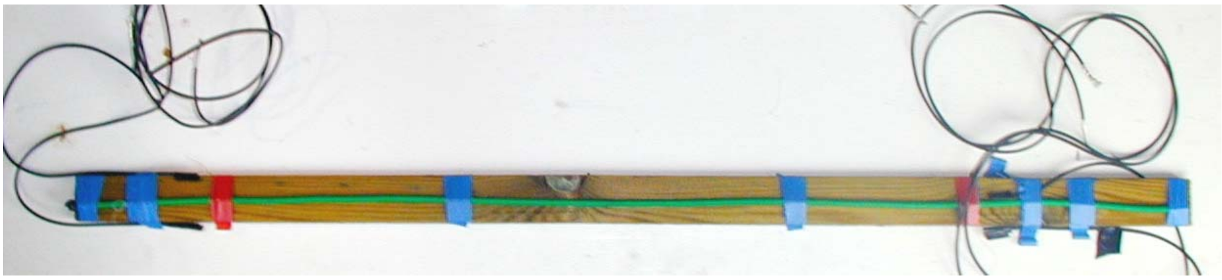

*Figure 3.1 Picture of the detonating cord used to test registration equipment and cabling.*

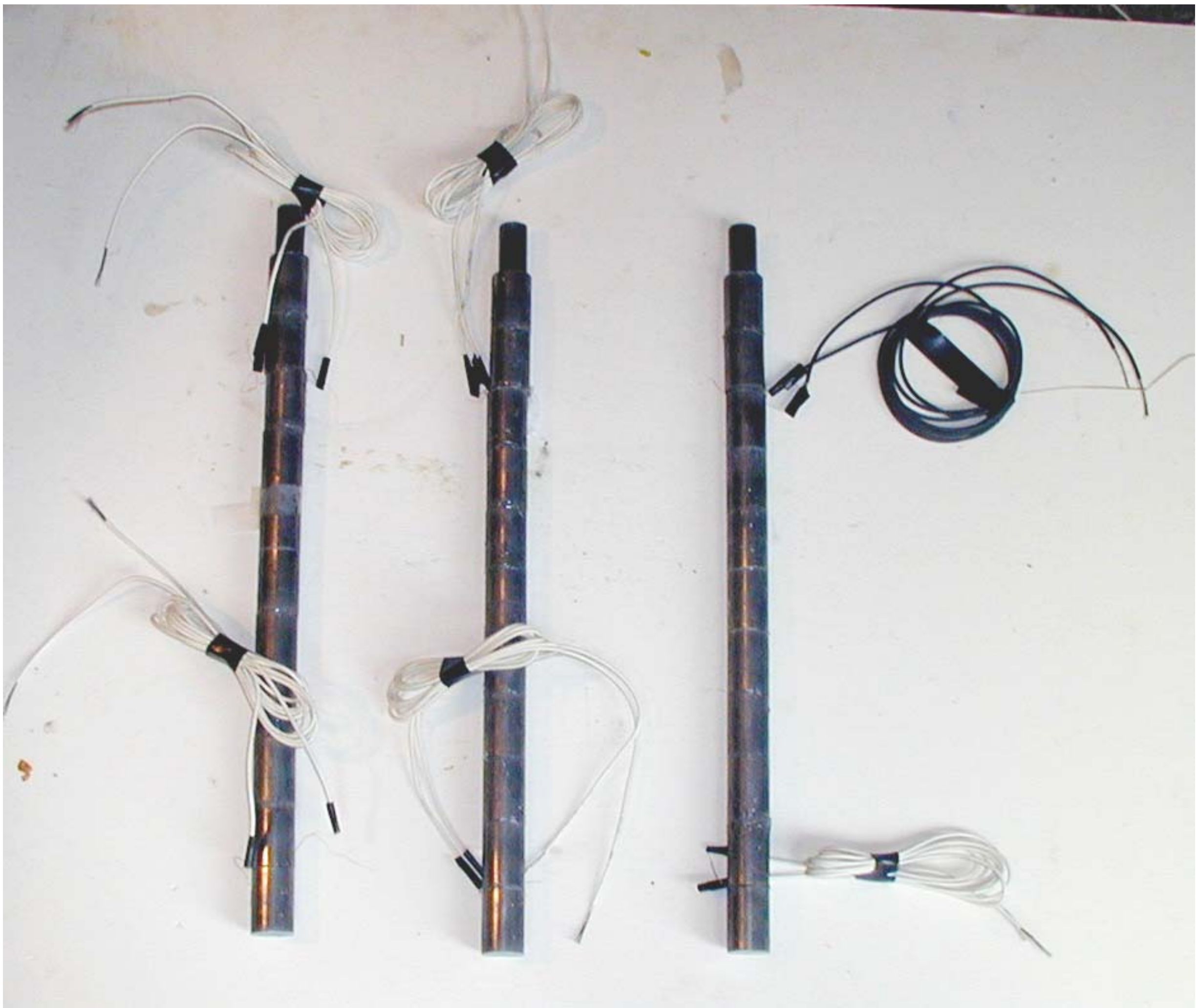

*Figure 3.2 Picture of the charges before testing.*

The test of the equipment went well. The obtained velocity is identical to what we obtained in (8) with the same detonating cord. For the main charges we did obtain results only for one of the charges. The obtained velocity of 8273 m/s is higher than for DPX-6 of 7854 m/s and also higher than what Cheetah gives.

Figure 3.3 show the registration of the start and stop signal when everything goes as expected. For two of the shots we lost the start or the stop signal, and therefore were not able to determine the detonation velocity.

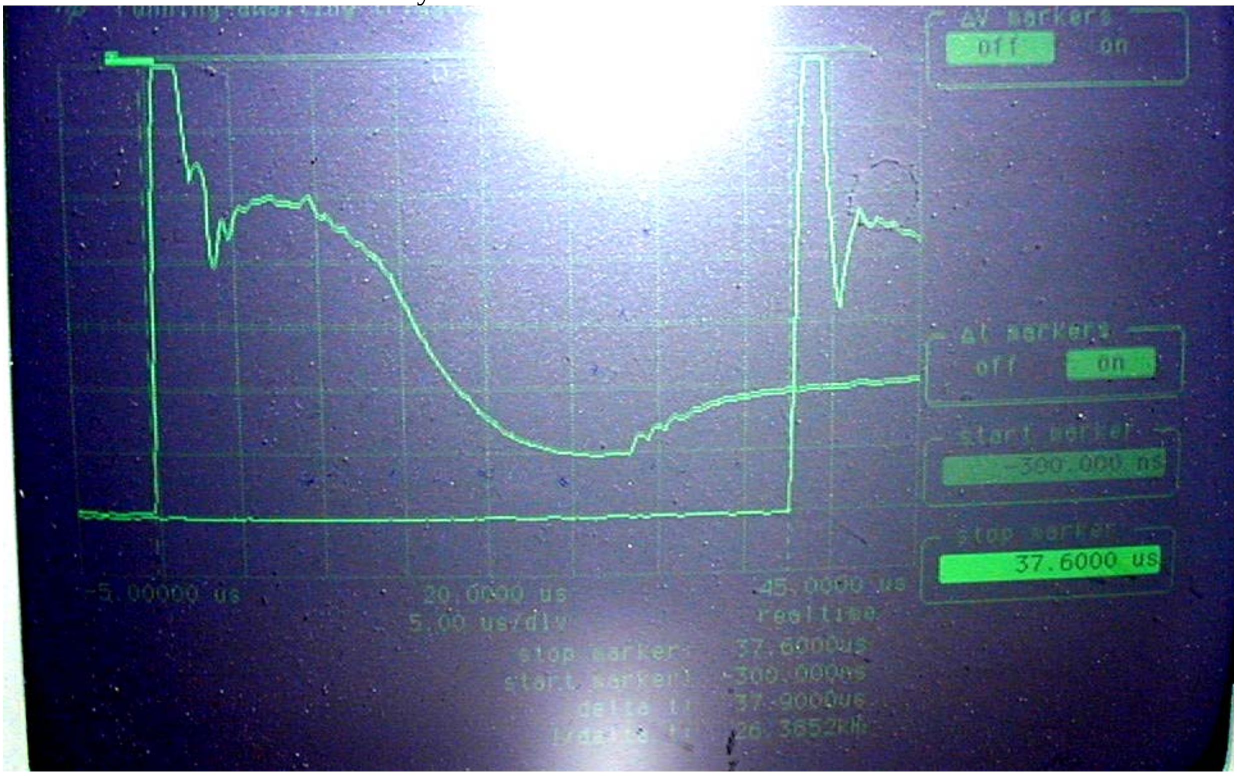


*Figure 3.3  Picture of the scope after firing showing the start and stop signal.*

## 3.3 Plate Dent

Plate Dent test gives results with respect to pressure performance. The depth of the hollow in the witness plate is proportional to the detonation pressure and the diameter of the charge. Figure 3.4 show the set up of the test with the charge in the centre of the witness plate. Figure 3.5 is a picture of the witness plates after firing. The results obtained are given in table 3.3. Comparing the results for PBXW-11 with 30 wt.% Aluminium with earlier tests performed in reference 5 for TNT and other compositions, is our Dent equal to a pressure of approximately 255 kbar. Comparing this result with theoretical calculated pressure in Appendix C.2 or in Table 3.1 gives good agreement between experimentally determined and theoretically calculated J-C pressure. Compared with recently fired comparable charges of

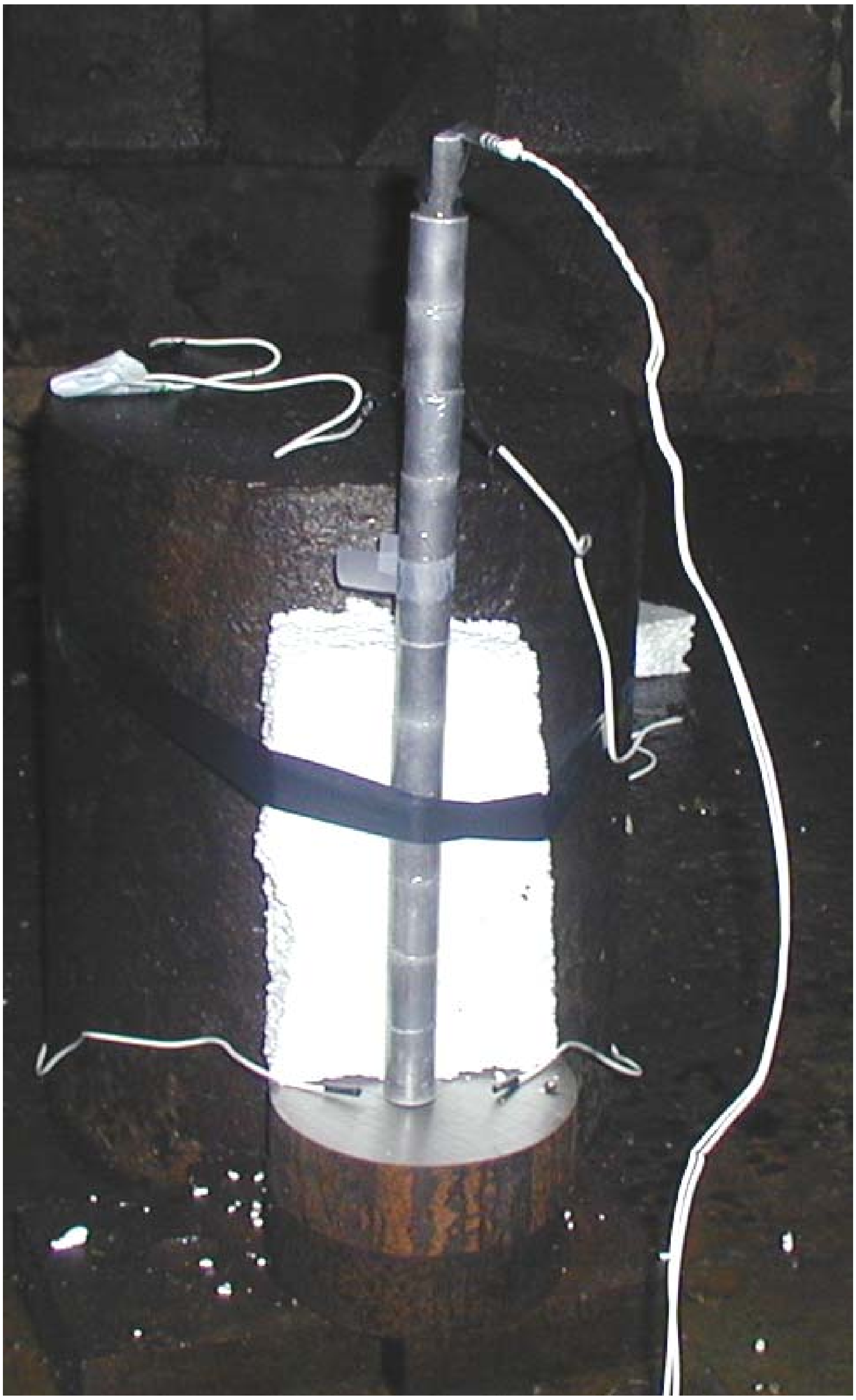

*Figure 3.4 Picture of the test item used for testing of detonation velocity and Plate Dent.*

DPX-6 with the same diameter for which we obtained a Dent depth of 3.79 mm or 205 kbar pressure, PBXW-11 with 30 wt.% Aluminium has 20% higher shock pressure.

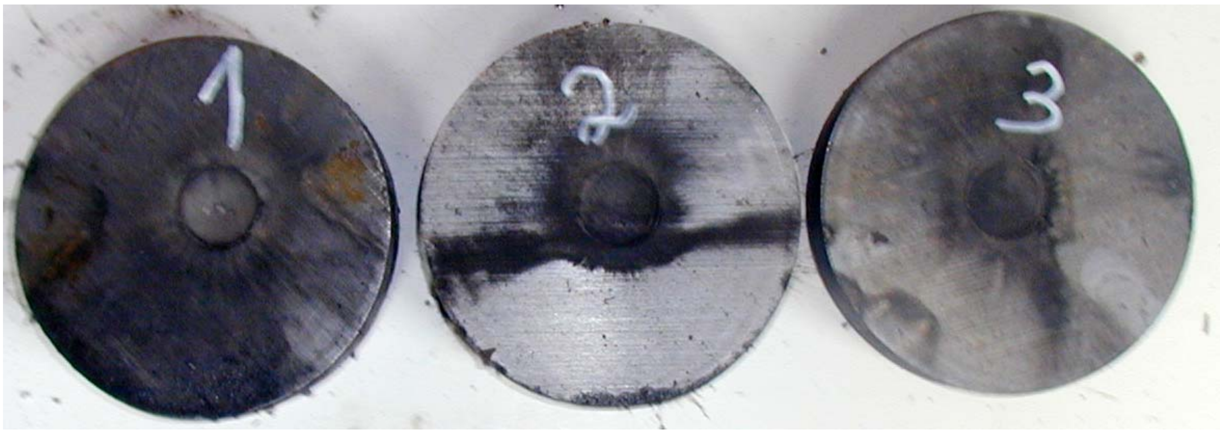


*Figure 3.5 Picture of the Dent witness plates after firing.*

| **Shot No.** | **Charge diameter (mm)** | **Dent Depth (mm)** | **Calculated Detonation Pressure* (kbar)** |
|---|---|---|---|
| 1 | 25.67 | 4.65 | 260 |
| 2 | 25.66 | 4.50 | 252 |
| 3 | 25.66 | 4.54 | 254 |
| **Average** | | **4.56** | **255** |

**From calibration curves with TNT charges (6).*

*Table 3.3 Results for Plate Dent Test of PBXW-11 with 30 wt.% Aluminium charges.*

## 4 SUMMARY

PBXW-11 containing 28.2 wt.% class 7 aluminium powder has been studied with regard to detonation velocity and detonation pressure. The tests have been performed on cylindrical charges pressed to a density of 1.949 g/cm$^3$ or 97.4 % TMD.

Experimentally detonation velocity was measured to 8273 m/s.

The shock pressure was determined by use of Plate Dent Test. Obtained average results from three firings were 255 kbar. Theoretically calculated by Cheetah 2.0 code gave 26.2 GPa.

# APPENDIX

## A CONTROL REPORT FOR USED COMPOSITION

**DYNO**
High Energy Materials

**Kontrollrapport**
etter EN 10204 – 2.3

| | | |
|---|---|---|
| Kjøper / Mottaker<br>Nammo Raufoss AS<br>Postboks 162<br>2831 Raufoss | Bestillingsnummer<br>53840-0/SOL/3<br><br>Bestillingsdato<br>03.10.05 | Rapportnummer<br>RD-26/05<br><br>Kontroll dato<br>30.11.05 |
| Produsent<br>Dyno Nobel ASA<br>N-3476 Sætre<br>NORGE | Produksjonsdato<br>29.11.05 | Offentlig oppdragsnummer |
| Lot nummer<br>DDP05K0009E | Mengde<br>10 kg | |
| Sprengstofftype<br>PBXW-11 med 30 % Aluminium (kl 7) | Leveringsbetingelser/Teknisk underlag<br>Kun informative verdier, 30 % aluminium | |

**Analyseresultater**

| | Sammensetning | | | | Fuktighet | Volumvekt |
|---|---|---|---|---|---|---|
| | HMX | Aluminium | HyTemp | DOA | | |
| KRAV | Informativ | Informativ | Informativ | Informativ | ≤ 0,10 % | Informativ |
| RESULTAT<br>Ch 07/05 | 68,4 | 28,2 | 0,8 | 2,6 | 0,02 | 1,10 |

| | Granulatfordeling, % gjennom USSS Nr. | | | | | |
|---|---|---|---|---|---|---|
| | 6 (3350 µ) | 8 (2360 µ) | 12 (1700 µ) | 18 (1000 µ) | 25 (710 µ) | 40 (425 µ) |
| KRAV | Informativ | Informativ | Informativ | Informativ | Informativ | Informativ |
| RESULTAT<br>Ch 07/05 | 100 | 100 | 100 | 68 | 21 | 1 |

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Forsker

## B DENSITY OF PBXW-11 (WITH 30% ALUMINIUM) PELLETS

| | Diameter (mm) | Radius (mm) | Height (mm) | Volume ($mm^3$) | Weight (g) | Density ($g/cm^3$) |
|---|---|---|---|---|---|---|
| 1 | 25.68 | 12.840 | 39.12 | 20261.835 | 39.468 | 1.948 |
| 2 | 25.70 | 12.850 | 39.09 | 20277.845 | 39.4348 | 1.945 |
| 3 | 25.69 | 12.845 | 39.13 | 20282.801 | 39.4655 | 1.946 |
| 4 | 25.67 | 12.835 | 39.10 | 20235.707 | 39.4432 | 1.949 |
| 5 | 25.66 | 12.830 | 39.05 | 20194.087 | 39.4727 | 1.955 |
| 6 | 25.68 | 12.840 | 39.05 | 20225.579 | 39.4142 | 1.949 |
| 7 | 25.66 | 12.830 | 39.03 | 20183.744 | 39.4338 | 1.954 |
| 8 | 25.66 | 12.830 | 39.05 | 20194.087 | 39.4765 | 1.955 |
| 9 | 25.68 | 12.840 | 39.12 | 20261.835 | 39.4444 | 1.947 |
| 10 | 25.67 | 12.835 | 39.13 | 20251.233 | 39.4769 | 1.949 |
| 11 | 25.72 | 12.860 | 39.09 | 20309.418 | 39.4931 | 1.945 |
| 12 | 25.66 | 12.830 | 39.14 | 20240.629 | 39.4278 | 1.948 |
| 13 | 25.63 | 12.815 | 39.15 | 20198.488 | 39.3874 | 1.950 |
| 14 | 25.67 | 12.835 | 39.14 | 20256.408 | 39.4309 | 1.947 |
| 15 | 25.68 | 12.840 | 39.07 | 20235.938 | 39.4515 | 1.950 |
| 16 | 25.67 | 12.835 | 39.14 | 20256.408 | 39.4678 | 1.948 |
| **Average** | | | | | | **1.949±0.003** |

*Table B. 1 Measured dimensions and weight of pellets used for detonation velocity and Plate Dent test.*

Calculated average density in Table-App. 1 of 1.949 $g/cm^3$ corresponds to 97.37 %TMD. Chemring Nobel AS has given for all 31 pellets an average density of 97.2±0.2 %TMD.

# C THEORETICAL CALCULATIONS

## C.1 Complete printout with BKWC

```
Product library title: bkwc
Executing library command: gas eos, bkw
Executing library command: set, bkw, alpha, 0.499123809964
Executing library command: set, bkw, beta, 0.402655787895
Executing library command: set, bkw, theta, 5441.84607543
Executing library command: set, bkw, kappa, 10.8636743138
Reactant library title:# Version 2.0 by P. Clark Souers
```

The Composition

| Name | % wt. | % mol | % vol. | Heat of formation (cal/mol) | Standard volume (cc/mol) | Standard entropy (cal/K/mol) | Mol. wt. | Formula |
|---|---|---|---|---|---|---|---|---|
| Al | 28.20 | 81.19 | 20.91 | 0 | 9.99 | 0.000 | 26.98 | $Al_1$ |
| Hytemp | 0.80 | 0.33 | 1.60 | -205067 | 188.60 | 0.000 | 188.60 | $C_{10}H_{15.46}O_{3.307}$ |
| DOA | 2.60 | 0.55 | 5.63 | -290392 | 400.60 | 0.000 | 370.56 | $C_{22}H_{42}O_4$ |
| HMX | 68.40 | 17.94 | 71.87 | 17866 | 155.47 | 0.000 | 296.17 | $C_4H_8N_8O_8$ |

```
Heat of formation =     12.187 cal/gm
Standard volume   =      0.500 cc/gm
Standard entropy  =      0.000 cal/k/gm
Standard energy   =     12.175 cal/gm

The elements and percent by mole
     al            12.886
     c             13.816
     h             27.221
     o             23.298
     n             22.779
The average mol. wt. =  77.674 g/mol
Input>library file, bkwc.chl
Product library title: bkwc
Executing library command: gas eos, bkw
Executing library command: set, bkw, alpha, 0.499123809964
Executing library command: set, bkw, beta, 0.402655787895
Executing library command: set, bkw, theta, 5441.84607543
Executing library command: set, bkw, kappa, 10.8636743138
Input>composition, al, 28.2, hytemp, 0.8, doa, 2.6, hmx, 68.4, weight
```

The Composition

| Name | % wt. | % mol | % vol. | Heat of formation (cal/mol) | Standard volume (cc/mol) | Standard entropy (cal/K/mol) | Mol. wt. | Formula |
|---|---|---|---|---|---|---|---|---|
| Al | 28.20 | 81.19 | 20.91 | 0 | 9.99 | 0.000 | 26.98 | $Al_1$ |
| Hytemp | 0.80 | 0.33 | 1.60 | -205067 | 188.60 | 0.000 | 188.60 | $C_{10}H_{15.46}O_{3.307}$ |
| DOA | 2.60 | 0.55 | 5.63 | -290392 | 400.60 | 0.000 | 370.56 | $C_{22}H_{42}O_4$ |
| HMX | 68.40 | 17.94 | 71.87 | 17866 | 155.47 | 0.000 | 296.17 | $C_4H_8N_8O_8$ |

```
Heat of formation =     12.187 cal/gm
Standard volume   =      0.500 cc/gm
Standard entropy  =      0.000 cal/k/gm
Standard energy   =     12.175 cal/gm

The elements and percent by mole
     al            12.886
     c             13.816
     h             27.221
     o             23.298
     n             22.779
```

```
The average mol. wt. =  77.674 g/mol
Input>standard run, rho, 2.001571
The initial equation error was huge: 16445.534331
The hugoniot reference state:
P0 = 1.000000 ATM, V0 = 0.499608 cc/gm, E0 = 12.174692 cal/gm
The initial equation error was huge: 21018.806942
The initial damping was too small
Using  128466 ATM as a lower bound for the C-J pressure
Using  321165 ATM as an upper bound for the C-J pressure
The C-J point was bracketed in cjbrent
The CJ state was found in 6 iterations
                              The C-J condition

The shock velocity    =   8.19034e+003 m/s
The particle velocity =   1.71878e+003 m/s
The speed of sound    =   6.47155e+003 m/s

P0 =       1 atm, V0 =  0.49961 cc/gm, E0 =  12.17469 cal/gm

                         Reference state = reactants
               H(R) = H-12.19, E(R) = E-12.17, S(R) = S- 0.00

         P          V        T       H(R)      E(R)      S(R)     VGS
       (ATM)     (CC/GM)    (K)    (CAL/GM)  (CAL/GM) (CAL/K/GM) (CC/GM)
 1.)  278086.0     0.3948   5837.0   3011.65    353.05    1.581    0.2428

Product concentrations
         Name   (mol/kg) (mol gas/mol explosive)
       n2  Gas   9.197e+000  7.144e-001
      h2o  Gas   3.678e+000  2.857e-001
     c2h4  Gas   2.361e+000  1.834e-001
      ch4  Gas   1.192e+000  9.255e-002
       co  Gas   2.864e-001  2.225e-002
      h3n  Gas   7.770e-002  6.035e-003
       h2  Gas   7.377e-002  5.730e-003
    ch3oh  Gas   3.111e-002  2.416e-003
      co2  Gas   1.685e-002  1.309e-003
       no  Gas   4.268e-003  3.315e-004
    ch2o2  Gas   2.870e-003  2.229e-004
     ch2o  Gas   3.953e-004  3.071e-005
     c2h6  Gas   3.007e-004  2.336e-005
      ch3  Gas   2.728e-004  2.119e-005
       o2  Gas   3.840e-005  2.983e-006
      alo  Gas   9.296e-007  7.221e-008
      no2  Gas   1.575e-011  1.223e-012
       *c  solid 4.954e+000  3.848e-001
    al2o3  solid 4.953e+000  3.847e-001
      *al  solid 5.471e-001  4.250e-002
    al2o3 liquid 0.000e+000  0.000e+000
      *al liquid 0.000e+000  0.000e+000

     Total Gas   1.692e+001  1.314e+000
     Total Cond. 1.045e+001  8.120e-001
                               The C-J Adiabat

                         Reference state = reactants
               H(R) = H-12.19, E(R) = E-12.17, S(R) = S- 0.00

         P          V        T       H(R)      E(R)      S(R)     VGS
       (ATM)     (CC/GM)    (K)    (CAL/GM)  (CAL/GM) (CAL/K/GM) (CC/GM)
 1.)  123185.1     0.4996   5068.6   1373.99   -116.48    1.581    0.3445

Product concentrations
         Name   (mol/kg) (mol gas/mol explosive)
       n2  Gas   9.146e+000  7.104e-001
      h2o  Gas   2.578e+000  2.003e-001
     c2h4  Gas   2.060e+000  1.600e-001
      ch4  Gas   1.735e+000  1.348e-001
       co  Gas   1.599e+000  1.242e-001
```

| | | | |
|---|---|---|---|
| h2 | Gas | 5.044e-001 | 3.918e-002 |
| h3n | Gas | 1.813e-001 | 1.408e-002 |
| co2 | Gas | 5.325e-002 | 4.136e-003 |
| ch3oh | Gas | 3.134e-002 | 2.434e-003 |
| ch2o2 | Gas | 6.232e-003 | 4.841e-004 |
| ch3 | Gas | 6.093e-003 | 4.733e-004 |
| ch2o | Gas | 4.493e-003 | 3.490e-004 |
| c2h6 | Gas | 3.839e-003 | 2.982e-004 |
| no | Gas | 3.448e-003 | 2.678e-004 |
| o2 | Gas | 1.879e-005 | 1.459e-006 |
| alo | Gas | 9.917e-006 | 7.703e-007 |
| no2 | Gas | 4.677e-010 | 3.633e-011 |
| al2o3 | solid | 4.854e+000 | 3.770e-001 |
| *c | solid | 3.642e+000 | 2.829e-001 |
| *al | solid | 7.446e-001 | 5.784e-002 |
| al2o3 | liquid | 0.000e+000 | 0.000e+000 |
| *al | liquid | 0.000e+000 | 0.000e+000 |
| Total | Gas | 1.791e+001 | 1.391e+000 |
| Total | Cond. | 9.240e+000 | 7.177e-001 |

Reference state = reactants
H(R) = H-12.19, E(R) = E-12.17, S(R) = S- 0.00

| | P (ATM) | V (CC/GM) | T (K) | H(R) (CAL/GM) | E(R) (CAL/GM) | S(R) (CAL/K/GM) | VGS (CC/GM) |
|---|---|---|---|---|---|---|---|
| 1.) | 16724.9 | 1.0991 | 3578.0 | -390.16 | -835.35 | 1.581 | 0.8646 |

Product concentrations

| Name | | (mol/kg) | (mol gas/mol explosive) |
|---|---|---|---|
| n2 | Gas | 9.123e+000 | 7.086e-001 |
| h2 | Gas | 4.976e+000 | 3.865e-001 |
| co | Gas | 2.897e+000 | 2.250e-001 |
| ch4 | Gas | 1.974e+000 | 1.534e-001 |
| c2h4 | Gas | 6.529e-001 | 5.071e-002 |
| h2o | Gas | 2.963e-001 | 2.302e-002 |
| h3n | Gas | 2.306e-001 | 1.791e-002 |
| ch3 | Gas | 6.586e-002 | 5.116e-003 |
| c2h6 | Gas | 1.947e-002 | 1.512e-003 |
| co2 | Gas | 8.687e-003 | 6.748e-004 |
| ch2o | Gas | 6.286e-003 | 4.883e-004 |
| ch3oh | Gas | 1.503e-003 | 1.168e-004 |
| ch2o2 | Gas | 1.888e-004 | 1.467e-005 |
| no | Gas | 8.609e-005 | 6.687e-006 |
| alo | Gas | 1.410e-005 | 1.095e-006 |
| o2 | Gas | 2.617e-008 | 2.033e-009 |
| no2 | Gas | 3.117e-011 | 2.421e-012 |
| al2o3 | liquid | 5.226e+000 | 4.059e-001 |
| *c | solid | 4.907e+000 | 3.812e-001 |
| *al | solid | 0.000e+000 | 0.000e+000 |
| *al | liquid | 0.000e+000 | 0.000e+000 |
| al2o3 | solid | 0.000e+000 | 0.000e+000 |
| Total | Gas | 2.025e+001 | 1.573e+000 |
| Total | Cond. | 1.013e+001 | 7.871e-001 |

Reference state = reactants
H(R) = H-12.19, E(R) = E-12.17, S(R) = S- 0.00

| | P (ATM) | V (CC/GM) | T (K) | H(R) (CAL/GM) | E(R) (CAL/GM) | S(R) (CAL/K/GM) | VGS (CC/GM) |
|---|---|---|---|---|---|---|---|
| 1.) | 4923.5 | 2.0484 | 3121.0 | -793.29 | -1037.52 | 1.581 | 1.8148 |

Product concentrations

| Name | | (mol/kg) | (mol gas/mol explosive) |
|---|---|---|---|
| n2 | Gas | 9.179e+000 | 7.129e-001 |
| h2 | Gas | 8.001e+000 | 6.214e-001 |
| co | Gas | 3.122e+000 | 2.425e-001 |
| ch4 | Gas | 1.114e+000 | 8.654e-002 |
| c2h4 | Gas | 2.147e-001 | 1.667e-002 |

```
       h3n  Gas   1.187e-001  9.217e-003
       h2o  Gas   8.785e-002  6.824e-003
       ch3  Gas   5.827e-002  4.526e-003
      c2h6  Gas   8.179e-003  6.353e-004
       co2  Gas   3.099e-003  2.407e-004
      ch2o  Gas   2.908e-003  2.259e-004
     ch3oh  Gas   1.599e-004  1.242e-005
     ch2o2  Gas   1.864e-005  1.448e-006
       alo  Gas   1.325e-005  1.029e-006
        no  Gas   1.210e-005  9.397e-007
        o2  Gas   9.719e-010  7.549e-011
       no2  Gas   2.072e-012  1.610e-013
        *c  solid 6.460e+000  5.018e-001
     al2o3 liquid 5.226e+000  4.059e-001
       *al  solid 0.000e+000  0.000e+000
       *al liquid 0.000e+000  0.000e+000
     al2o3  solid 0.000e+000  0.000e+000

      Total Gas   2.191e+001  1.702e+000
      Total Cond. 1.169e+001  9.077e-001


                        Reference state = reactants
               H(R) = H-12.19, E(R) = E-12.17, S(R) = S- 0.00

          P          V          T        H(R)       E(R)       S(R)      VGS
        (ATM)      (CC/GM)     (K)     (CAL/GM)  (CAL/GM) (CAL/K/GM) (CC/GM)
  1.)    2375.2      3.2474   2901.1   -948.59  -1135.38     1.581    3.0156

Product concentrations
          Name   (mol/kg) (mol gas/mol explosive)
        n2  Gas   9.202e+000  7.147e-001
        h2  Gas   9.114e+000  7.080e-001
        co  Gas   3.164e+000  2.457e-001
       ch4  Gas   7.441e-001  5.779e-002
      c2h4  Gas   1.031e-001  8.010e-003
       h3n  Gas   7.286e-002  5.660e-003
       h2o  Gas   4.930e-002  3.830e-003
       ch3  Gas   3.950e-002  3.068e-003
      c2h6  Gas   3.662e-003  2.844e-004
       co2  Gas   1.926e-003  1.496e-004
      ch2o  Gas   1.624e-003  1.262e-004
     ch3oh  Gas   4.444e-005  3.452e-006
       alo  Gas   8.286e-006  6.436e-007
     ch2o2  Gas   5.325e-006  4.136e-007
        no  Gas   4.039e-006  3.137e-007
        o2  Gas   1.688e-010  1.311e-011
       no2  Gas   3.568e-013  2.771e-014
        *c  solid 7.041e+000  5.469e-001
     al2o3 liquid 5.226e+000  4.059e-001
       *al  solid 0.000e+000  0.000e+000
       *al liquid 0.000e+000  0.000e+000
     al2o3  solid 0.000e+000  0.000e+000

      Total Gas   2.250e+001  1.747e+000
      Total Cond. 1.227e+001  9.529e-001

                        Reference state = reactants
               H(R) = H-12.19, E(R) = E-12.17, S(R) = S- 0.00

          P          V          T        H(R)       E(R)       S(R)      VGS
        (ATM)      (CC/GM)     (K)     (CAL/GM)  (CAL/GM) (CAL/K/GM) (CC/GM)
  1.)    1297.2      4.9961   2735.6  -1051.94  -1208.88     1.581    4.7662

Product concentrations
          Name   (mol/kg) (mol gas/mol explosive)
        h2  Gas   9.723e+000  7.552e-001
        n2  Gas   9.214e+000  7.157e-001
        co  Gas   3.182e+000  2.471e-001
       ch4  Gas   5.290e-001  4.109e-002
```

| | | | |
|---|---|---|---|
| c2h4 | Gas | 5.466e-002 | 4.245e-003 |
| h3n | Gas | 4.765e-002 | 3.701e-003 |
| h2o | Gas | 3.306e-002 | 2.568e-003 |
| ch3 | Gas | 2.539e-002 | 1.972e-003 |
| c2h6 | Gas | 1.718e-003 | 1.335e-004 |
| co2 | Gas | 1.397e-003 | 1.085e-004 |
| ch2o | Gas | 9.672e-004 | 7.513e-005 |
| ch3oh | Gas | 1.598e-005 | 1.241e-006 |
| alo | Gas | 4.368e-006 | 3.393e-007 |
| ch2o2 | Gas | 2.020e-006 | 1.569e-007 |
| no | Gas | 1.649e-006 | 1.281e-007 |
| o2 | Gas | 4.239e-011 | 3.292e-012 |
| no2 | Gas | 7.751e-014 | 6.021e-015 |
| *c | solid | 7.354e+000 | 5.713e-001 |
| al2o3 | liquid | 5.226e+000 | 4.059e-001 |
| *al | solid | 0.000e+000 | 0.000e+000 |
| *al | liquid | 0.000e+000 | 0.000e+000 |
| al2o3 | solid | 0.000e+000 | 0.000e+000 |
| Total | Gas | 2.281e+001 | 1.772e+000 |
| Total | Cond. | 1.258e+001 | 9.772e-001 |

Reference state = reactants
H(R) = H-12.19, E(R) = E-12.17, S(R) = S- 0.00

| | P (ATM) | V (CC/GM) | T (K) | H(R) (CAL/GM) | E(R) (CAL/GM) | S(R) (CAL/K/GM) | VGS (CC/GM) |
|---|---|---|---|---|---|---|---|
| 1.) | 536.0 | 9.9922 | 2513.0 | -1177.56 | -1307.26 | 1.581 | 9.7658 |

Product concentrations

| Name | | (mol/kg) | (mol gas/mol explosive) |
|---|---|---|---|
| h2 | Gas | 1.027e+001 | 7.979e-001 |
| n2 | Gas | 9.225e+000 | 7.166e-001 |
| co | Gas | 3.196e+000 | 2.482e-001 |
| ch4 | Gas | 3.239e-001 | 2.516e-002 |
| h3n | Gas | 2.533e-002 | 1.968e-003 |
| c2h4 | Gas | 2.088e-002 | 1.622e-003 |
| h2o | Gas | 2.052e-002 | 1.594e-003 |
| ch3 | Gas | 1.153e-002 | 8.960e-004 |
| co2 | Gas | 9.651e-004 | 7.497e-005 |
| c2h6 | Gas | 5.239e-004 | 4.069e-005 |
| ch2o | Gas | 4.378e-004 | 3.401e-005 |
| ch3oh | Gas | 3.794e-006 | 2.947e-007 |
| alo | Gas | 1.166e-006 | 9.057e-008 |
| ch2o2 | Gas | 5.379e-007 | 4.178e-008 |
| no | Gas | 4.408e-007 | 3.424e-008 |
| o2 | Gas | 5.892e-012 | 4.577e-013 |
| no2 | Gas | 7.483e-015 | 5.812e-016 |
| *c | solid | 7.630e+000 | 5.927e-001 |
| al2o3 | liquid | 5.226e+000 | 4.059e-001 |
| *al | solid | 0.000e+000 | 0.000e+000 |
| *al | liquid | 0.000e+000 | 0.000e+000 |
| al2o3 | solid | 0.000e+000 | 0.000e+000 |
| Total | Gas | 2.310e+001 | 1.794e+000 |
| Total | Cond. | 1.286e+001 | 9.986e-001 |

Reference state = reactants
H(R) = H-12.19, E(R) = E-12.17, S(R) = S- 0.00

| | P (ATM) | V (CC/GM) | T (K) | H(R) (CAL/GM) | E(R) (CAL/GM) | S(R) (CAL/K/GM) | VGS (CC/GM) |
|---|---|---|---|---|---|---|---|
| 1.) | 236.4 | 19.9843 | 2335.5 | -1276.83 | -1391.25 | 1.581 | 19.7632 |

Product concentrations

| Name | | (mol/kg) | (mol gas/mol explosive) |
|---|---|---|---|
| h2 | Gas | 1.057e+001 | 8.210e-001 |
| n2 | Gas | 9.231e+000 | 7.170e-001 |
| co | Gas | 3.203e+000 | 2.488e-001 |
| ch4 | Gas | 2.046e-001 | 1.590e-002 |

```
      h3n  Gas   1.394e-002  1.083e-003
      h2o  Gas   1.394e-002  1.083e-003
     c2h4  Gas   8.400e-003  6.524e-004
      ch3  Gas   5.152e-003  4.002e-004
      co2  Gas   7.195e-004  5.588e-005
     ch2o  Gas   2.056e-004  1.597e-005
     c2h6  Gas   1.636e-004  1.271e-005
    ch3oh  Gas   1.030e-006  7.998e-008
      alo  Gas   2.889e-007  2.244e-008
    ch2o2  Gas   1.657e-007  1.287e-008
       no  Gas   1.324e-007  1.028e-008
       o2  Gas   1.008e-012  7.826e-014
      no2  Gas   8.304e-016  6.450e-017
       *c  solid 7.775e+000  6.039e-001
    al2o3 liquid 4.997e+000  3.881e-001
    al2o3  solid 2.292e-001  1.780e-002
      *al liquid 0.000e+000  0.000e+000
      *al  solid 0.000e+000  0.000e+000

     Total Gas   2.325e+001  1.806e+000
     Total Cond. 1.300e+001  1.010e+000

                         Reference state = reactants
              H(R) = H-12.19, E(R) = E-12.17, S(R) = S- 0.00

          P           V         T       H(R)      E(R)       S(R)     VGS
        (ATM)      (CC/GM)     (K)    (CAL/GM)  (CAL/GM) (CAL/K/GM) (CC/GM)
 1.)     115.2     39.9686   2332.5   -1357.95  -1469.42    1.581   39.7737

Product concentrations
         Name    (mol/kg) (mol gas/mol explosive)
       h2  Gas   1.080e+001  8.390e-001
       n2  Gas   9.235e+000  7.173e-001
       co  Gas   3.211e+000  2.494e-001
      ch4  Gas   1.029e-001  7.994e-003
      h3n  Gas   6.981e-003  5.423e-004
      h2o  Gas   6.765e-003  5.255e-004
     c2h4  Gas   4.211e-003  3.271e-004
      ch3  Gas   3.752e-003  2.914e-004
      co2  Gas   3.488e-004  2.709e-005
     ch2o  Gas   1.027e-004  7.981e-006
     c2h6  Gas   4.189e-005  3.254e-006
      alo  Gas   8.607e-007  6.685e-008
    ch3oh  Gas   2.495e-007  1.938e-008
       no  Gas   9.020e-008  7.006e-009
    ch2o2  Gas   3.958e-008  3.074e-009
       o2  Gas   4.696e-013  3.648e-014
      no2  Gas   2.827e-016  2.196e-017
       *c  solid 7.879e+000  6.120e-001
    al2o3  solid 3.180e+000  2.470e-001
    al2o3 liquid 2.046e+000  1.589e-001
      *al  solid 0.000e+000  0.000e+000
      *al liquid 0.000e+000  0.000e+000

     Total Gas   2.337e+001  1.815e+000
     Total Cond. 1.311e+001  1.018e+000

                       Reference state = reactants
              H(R) = H-12.19, E(R) = E-12.17, S(R) = S- 0.00

          P           V         T       H(R)      E(R)       S(R)     VGS
        (ATM)      (CC/GM)     (K)    (CAL/GM)  (CAL/GM) (CAL/K/GM) (CC/GM)
 1.)      55.4     79.9372   2272.4   -1438.57  -1545.86    1.581   79.7608

Product concentrations
         Name    (mol/kg) (mol gas/mol explosive)
       h2  Gas   1.091e+001  8.474e-001
       n2  Gas   9.236e+000  7.174e-001
       co  Gas   3.214e+000  2.497e-001
      ch4  Gas   5.682e-002  4.414e-003
```

```
      h2o  Gas   3.864e-003  3.002e-004
      h3n  Gas   3.654e-003  2.838e-004
      ch3  Gas   2.227e-003  1.730e-004
     c2h4  Gas   1.960e-003  1.522e-004
      co2  Gas   2.058e-004  1.598e-005
     ch2o  Gas   5.058e-005  3.929e-006
     c2h6  Gas   1.154e-005  8.965e-007
      alo  Gas   8.760e-007  6.804e-008
    ch3oh  Gas   6.598e-008  5.125e-009
       no  Gas   4.666e-008  3.624e-009
    ch2o2  Gas   1.099e-008  8.536e-010
       o2  Gas   1.601e-013  1.244e-014
      no2  Gas   6.542e-017  5.081e-018
       *c  solid 7.928e+000  6.158e-001
    al2o3  solid 5.226e+000  4.059e-001
      *al  solid 0.000e+000  0.000e+000
    al2o3 liquid 0.000e+000  0.000e+000
      *al liquid 0.000e+000  0.000e+000

     Total Gas   2.343e+001  1.820e+000
     Total Cond. 1.315e+001  1.022e+000
The initial equation error was huge: 14155.062966

                             The End of the Adiabat

                          Reference state = reactants
                  H(R) = H-12.19, E(R) = E-12.17, S(R) = S- 0.00

           P           V          T        H(R)       E(R)       S(R)      VGS
         (ATM)      (CC/GM)      (K)    (CAL/GM)  (CAL/GM) (CAL/K/GM) (CC/GM)
 1.)       1.0   2772.6050   1438.8  -1782.26  -1849.39     1.581 2772.4306

Product concentrations
         Name   (mol/kg) (mol gas/mol explosive)
       h2  Gas   1.100e+001  8.544e-001
       n2  Gas   9.238e+000  7.175e-001
       co  Gas   3.213e+000  2.496e-001
      ch4  Gas   1.774e-002  1.378e-003
      h2o  Gas   4.163e-003  3.233e-004
      co2  Gas   5.215e-004  4.051e-005
      h3n  Gas   3.631e-004  2.820e-005
     c2h4  Gas   1.219e-005  9.471e-007
      ch3  Gas   5.080e-006  3.946e-007
     ch2o  Gas   1.283e-006  9.967e-008
     c2h6  Gas   1.014e-007  7.873e-009
    ch3oh  Gas   4.588e-010  3.563e-011
    ch2o2  Gas   3.039e-010  2.361e-011
       no  Gas   1.064e-011  8.262e-013
      alo  Gas   3.877e-015  3.012e-016
       o2  Gas   2.133e-018  1.657e-019
      no2  Gas   4.365e-023  3.390e-024
       *c  solid 7.974e+000  6.194e-001
    al2o3  solid 5.226e+000  4.059e-001
      *al  solid 0.000e+000  0.000e+000
    al2o3 liquid 0.000e+000  0.000e+000
      *al liquid 0.000e+000  0.000e+000

     Total Gas   2.347e+001  1.823e+000
     Total Cond. 1.320e+001  1.025e+000
                 The Products at room temperature and pressure

                          Reference state = reactants
                  H(R) = H-12.19, E(R) = E-12.17, S(R) = S- 0.00


           P           V          T        H(R)       E(R)       S(R)      VGS
         (ATM)      (CC/GM)      (K)    (CAL/GM)  (CAL/GM) (CAL/K/GM) (CC/GM)
 1.)       1.0    401.2137    298.0  -2361.17  -2370.87     0.848  401.0458
```

```
Product concentrations
          Name   (mol/kg) (mol gas/mol explosive)
        n2  Gas   9.238e+000  7.175e-001
       ch4  Gas   3.930e+000  3.053e-001
       h2o  Gas   3.178e+000  2.469e-001
       co2  Gas   2.032e-002  1.578e-003
       h3n  Gas   6.640e-004  5.158e-005
        h2  Gas   2.824e-004  2.193e-005
      c2h6  Gas   4.894e-008  3.802e-009
        co  Gas   1.713e-011  1.331e-012
     ch2o2  Gas   8.711e-015  6.767e-016
     ch3oh  Gas   1.387e-016  1.078e-017
      c2h4  Gas   5.039e-021  3.914e-022
      ch2o  Gas   4.947e-021  3.843e-022
       ch3  Gas   1.378e-032  1.070e-033
       alo  Gas   0.000e+000  0.000e+000
        o2  Gas   0.000e+000  0.000e+000
       no2  Gas   0.000e+000  0.000e+000
        no  Gas   0.000e+000  0.000e+000
        *c  solid 7.255e+000  5.636e-001
     al2o3  solid 5.226e+000  4.059e-001
       *al  solid 0.000e+000  0.000e+000
     al2o3 liquid 0.000e+000  0.000e+000
       *al liquid 0.000e+000  0.000e+000

      Total Gas   1.637e+001  1.271e+000
      Total Cond. 1.248e+001  9.695e-001
The mechanical energy of detonation =    -15.488 kJ/cc
The thermal energy of detonation    =     -4.367 kJ/cc
The total energy of detonation      =    -19.855 kJ/cc

JWL Tail Fit results:
Initial E0 =    -19.704, Final E0 =    -26.760
E0(V=infty) =    -26.760
C =      1.246,  omega =      0.065
Final fitting error = 0.000256
```

| V/V0 | Actual E (kJ/cc) | Fit E (kJ/cc) | Actual P (GPa) | Fit P (GPa) |
|---|---|---|---|---|
| 20.000 | -10.948 | -10.950 | 0.054 | 0.051 |
| 40.000 | -11.651 | -11.645 | 0.024 | 0.025 |
| 80.000 | -12.306 | -12.310 | 0.012 | 0.012 |
| 160.000 | -12.946 | -12.945 | 0.006 | 0.006 |

```
JWL Fit results:
E0(V=infty) =    -26.760
R[1] =      6.374, R[2] =      1.071, omega =      0.065
A    =   2991.237, B    =     17.906, C     =      1.246
Final fitting error = 0.017938
```

| V/V0 | Actual E (kJ/cc) | Fit E (kJ/cc) | Actual P (GPa) | Fit P (GPa) |
|---|---|---|---|---|
| 0.790 | 2.957 | 2.957 | 28.177 | 28.718 |
| 1.000 | -0.975 | -1.031 | 12.482 | 12.482 |
| 2.200 | -6.996 | -6.932 | 1.695 | 2.237 |
| 4.100 | -8.689 | -9.031 | 0.499 | 0.499 |
| 6.500 | -9.508 | -9.739 | 0.241 | 0.187 |
| 10.000 | -10.124 | -10.223 | 0.131 | 0.108 |
| 20.000 | -10.948 | -10.950 | 0.054 | 0.051 |
| 40.000 | -11.651 | -11.645 | 0.024 | 0.025 |
| 80.000 | -12.306 | -12.310 | 0.012 | 0.012 |
| 160.000 | -12.946 | -12.945 | 0.006 | 0.006 |

## C.2 Summary printout for different densities

Product library title: bkwc
Reactant library title: # Version 2.0 by P. Clark Souers

The composition:

| Name | % wt. | % mol | % vol | Heat of formation (cal/mol) | Mol. wt. | TMD (g/cc) | |
|---|---|---|---|---|---|---|---|
| al | 28.20 | 81.19 | 20.91 | 0 | 26.98 | 2.70 | $Al_1$ |
| hytemp | 0.80 | 0.33 | 1.60 | -205067 | 188.60 | 1.00 | $C_{10}H_{15.46}O_{3.307}$ |
| doa | 2.60 | 0.55 | 5.63 | -290392 | 370.56 | 0.93 | $C_{22}H_{42}O_4$ |
| hmx | 68.40 | 17.94 | 71.87 | 17866 | 296.17 | 1.91 | $C_4H_8N_8O_8$ |

Product library title: bkwc
Reactant library title: # Version 2.0 by P. Clark Souers

The composition:

| Name | % wt. | % mol | % vol | Heat of formation (cal/mol) | Mol. wt. | TMD (g/cc) | |
|---|---|---|---|---|---|---|---|
| al | 28.20 | 81.19 | 20.91 | 0 | 26.98 | 2.70 | $Al_1$ |
| hytemp | 0.80 | 0.33 | 1.60 | -205067 | 188.60 | 1.00 | $C_{10}H_{15.46}O_{3.307}$ |
| doa | 2.60 | 0.55 | 5.63 | -290392 | 370.56 | 0.93 | $C_{22}H_{42}O_4$ |
| hmx | 68.40 | 17.94 | 71.87 | 17866 | 296.17 | 1.91 | $C_4H_8N_8O_8$ |


**Density = 2.0016 g/cc   Mixture TMD =  2.0016 g/cc   % TMD = 100.0000**

```
The C-J condition:
The pressure          =          28.18 GPa
The volume            =          0.395 cc/g
The density           =          2.533 g/cc
The energy            =          2.96  kJ/cc explosive
The temperature       =          5837  K
The shock velocity    =          8.190 mm/us
The particle velocity =          1.719 mm/us
The speed of sound    =          6.472 mm/us
Gamma                 =          3.765
```

Cylinder runs:   % of standards

| V/V0 (rel.) | Energy (kJ/cc) | TATB 1.83g/cc | PETN 1.76g/cc | HMX 1.89g/cc | CL-20 2.04g/cc | TRITON 1.70g/cc |
|---|---|---|---|---|---|---|
| 1.00 | -0.98 | | | | | |
| 2.20 | -7.00 | 144 | 110 | 94 | 77 | 160 |
| 4.10 | -8.69 | 150 | 113 | 98 | 82 | 157 |
| 6.50 | -9.51 | 153 | 115 | 101 | 85 | 156 |
| 10.00 | -10.12 | 155 | 117 | 104 | 88 | 154 |
| 20.00 | -10.95 | 159 | 120 | 107 | 92 | 153 |
| 40.00 | -11.65 | 163 | 123 | 111 | 96 | 151 |
| 80.00 | -12.31 | 167 | 126 | 115 | 100 | 149 |
| 160.00 | -12.95 | | | | | |

```
The mechanical energy of detonation =    -15.488 kJ/cc
The thermal energy of detonation    =     -4.367 kJ/cc
The total energy of detonation      =    -19.855 kJ/cc

JWL Fit results:
E0   =   -26.760 kJ/cc
A    =  2991.24 GPa, B  =  17.91 GPa , C     =  1.25 GPa
R[1] =     6.37,   R[2] =   1.07,      omega =  0.06
RMS fitting error = 1.79 %
```

**Density = 1.9916 g/cc   Mixture TMD =  2.0016 g/cc   % TMD = 99.5000**

The C-J condition:
The pressure = 27.79 GPa
The volume = 0.396 cc/g
The density = 2.522 g/cc
The energy = 2.92 kJ/cc explosive
The temperature = 5828 K
The shock velocity = 8.143 mm/us
The particle velocity = 1.714 mm/us
The speed of sound = 6.429 mm/us
Gamma = 3.752

Cylinder runs: % of standards

| V/V0 (rel.) | Energy (kJ/cc) | TATB 1.83g/cc | PETN 1.76g/cc | HMX 1.89g/cc | CL-20 2.04g/cc | TRITON 1.70g/cc |
|---|---|---|---|---|---|---|
| 1.00 | -0.97 | | | | | |
| 2.20 | -6.93 | 143 | 109 | 93 | 77 | 159 |
| 4.10 | -8.61 | 148 | 112 | 97 | 82 | 156 |
| 6.50 | -9.43 | 151 | 114 | 100 | 85 | 154 |
| 10.00 | -10.04 | 154 | 116 | 103 | 87 | 153 |
| 20.00 | -10.87 | 158 | 119 | 107 | 91 | 152 |
| 40.00 | -11.57 | 162 | 122 | 110 | 95 | 150 |
| 80.00 | -12.22 | 166 | 125 | 114 | 99 | 148 |
| 160.00 | -12.86 | | | | | |

The mechanical energy of detonation = -15.394 kJ/cc
The thermal energy of detonation = -4.362 kJ/cc
The total energy of detonation = -19.756 kJ/cc

JWL Fit results:
E0 = -20.313 kJ/cc
A = 2837.06 GPa, B = 17.61 GPa , C = 1.53 GPa
R[1] = 6.33, R[2] = 1.12, omega = 0.11
RMS fitting error = 1.49 %

**Density =1.9816 g/cc  Mixture TMD =  2.0016 g/cc   % TMD = 99.0000**

The C-J condition:
The pressure = 27.41 GPa
The volume = 0.398 cc/g
The density = 2.512 g/cc
The energy = 2.89 kJ/cc explosive
The temperature = 5818 K
The shock velocity = 8.096 mm/us
The particle velocity = 1.709 mm/us
The speed of sound = 6.387 mm/us
Gamma = 3.739

Cylinder runs: % of standards

| V/V0 (rel.) | Energy (kJ/cc) | TATB 1.83g/cc | PETN 1.76g/cc | HMX 1.89g/cc | CL-20 2.04g/cc | TRITON 1.70g/cc |
|---|---|---|---|---|---|---|
| 1.00 | -0.96 | | | | | |
| 2.20 | -6.87 | 142 | 108 | 92 | 76 | 158 |
| 4.10 | -8.54 | 147 | 111 | 96 | 81 | 155 |
| 6.50 | -9.35 | 150 | 113 | 99 | 84 | 153 |
| 10.00 | -9.96 | 153 | 115 | 102 | 87 | 152 |
| 20.00 | -10.78 | 157 | 118 | 106 | 91 | 150 |
| 40.00 | -11.48 | 161 | 121 | 110 | 95 | 149 |
| 80.00 | -12.13 | 165 | 124 | 113 | 98 | 147 |
| 160.00 | -12.77 | | | | | |

The mechanical energy of detonation = -15.300 kJ/cc
The thermal energy of detonation = -4.357 kJ/cc
The total energy of detonation = -19.657 kJ/cc

```
JWL Fit results:
E0   =  -26.142 kJ/cc
A    = 2863.96 GPa, B    =  17.61 GPa , C     =  1.24 GPa
R[1] =    6.37,     R[2] =   1.07,      omega =  0.07
RMS fitting error = 1.80 %
```

**Density = 1.9715 g/cc   Mixture TMD =  2.0016 g/cc   % TMD = 98.5000**

```
The C-J condition:
The pressure          =          27.03 GPa
The volume            =          0.400 cc/g
The density           =          2.501 g/cc
The energy            =          2.86  kJ/cc explosive
The temperature       =          5809  K
The shock velocity    =          8.049 mm/us
The particle velocity =          1.704 mm/us
The speed of sound    =          6.345 mm/us
Gamma                 =          3.725
```

Cylinder runs: % of standards

| V/V0 (rel.) | Energy (kJ/cc) | TATB 1.83g/cc | PETN 1.76g/cc | HMX 1.89g/cc | CL-20 2.04g/cc | TRITON 1.70g/cc |
|---|---|---|---|---|---|---|
| 1.00 | -0.95 | | | | | |
| 2.20 | -6.81 | 140 | 107 | 91 | 75 | 156 |
| 4.10 | -8.47 | 146 | 110 | 96 | 80 | 153 |
| 6.50 | -9.28 | 149 | 112 | 98 | 83 | 152 |
| 10.00 | -9.88 | 152 | 114 | 101 | 86 | 151 |
| 20.00 | -10.70 | 156 | 117 | 105 | 90 | 149 |
| 40.00 | -11.40 | 159 | 120 | 109 | 94 | 147 |
| 80.00 | -12.04 | 163 | 123 | 112 | 98 | 146 |
| 160.00 | -12.68 | | | | | |

```
The mechanical energy of detonation =    -15.206 kJ/cc
The thermal energy of detonation    =     -4.351 kJ/cc
The total energy of detonation      =    -19.557 kJ/cc

JWL Fit results:
E0   =   -19.873 kJ/cc
A    =  2713.23 GPa, B   =   17.33 GPa , C     =  1.54 GPa
R[1] =    6.33,     R[2] =    1.12,      omega =  0.12
RMS fitting error = 1.49 %
```

**Density = 1.9615 g/cc   Mixture TMD =  2.0016 g/cc   % TMD = 98.0000**

```
The C-J condition:
The pressure          =          26.66 GPa
The volume            =          0.402 cc/g
The density           =          2.490 g/cc
The energy            =          2.83  kJ/cc explosive
The temperature       =          5799  K
The shock velocity    =          8.002 mm/us
The particle velocity =          1.699 mm/us
The speed of sound    =          6.304 mm/us
Gamma                 =          3.711
```

Cylinder runs: % of standards

| V/V0 (rel.) | Energy (kJ/cc) | TATB 1.83g/cc | PETN 1.76g/cc | HMX 1.89g/cc | CL-20 2.04g/cc | TRITON 1.70g/cc |
|---|---|---|---|---|---|---|
| 1.00 | -0.94 | | | | | |
| 2.20 | -6.74 | 139 | 106 | 90 | 75 | 155 |
| 4.10 | -8.39 | 144 | 109 | 95 | 79 | 152 |
| 6.50 | -9.20 | 148 | 111 | 98 | 83 | 151 |
| 10.00 | -9.81 | 150 | 113 | 100 | 85 | 149 |
| 20.00 | -10.62 | 155 | 116 | 104 | 89 | 148 |
| 40.00 | -11.32 | 158 | 119 | 108 | 93 | 146 |
| 80.00 | -11.96 | 162 | 122 | 112 | 97 | 145 |
| 160.00 | -12.59 | | | | | |

The mechanical energy of detonation = -15.112 kJ/cc
The thermal energy of detonation = -4.346 kJ/cc
The total energy of detonation = -19.458 kJ/cc

JWL Fit results:
E0 = -19.642 kJ/cc
A = 2653.33 GPa, B = 17.19 GPa , C = 1.54 GPa
R[1] = 6.33, R[2] = 1.12,omega = 0.12
RMS fitting error = 1.48 %

**Density = 1.9515 g/cc Mixture TMD = 2.0016 g/cc % TMD = 97.5000**

The C-J condition:
The pressure = 26.30 GPa
The volume = 0.403 cc/g
The density = 2.479 g/cc
The energy = 2.80 kJ/cc explosive
The temperature = 5790 K
The shock velocity = 7.956 mm/us
The particle velocity = 1.694 mm/us
The speed of sound = 6.262 mm/us
Gamma = 3.697

Cylinder runs: % of standards

| V/V0 (rel.) | Energy (kJ/cc) | TATB 1.83g/cc | PETN 1.76g/cc | HMX 1.89g/cc | CL-20 2.04g/cc | TRITON 1.70g/cc |
|---|---|---|---|---|---|---|
| 1.00 | -0.93 | | | | | |
| 2.20 | -6.68 | 138 | 105 | 89 | 74 | 153 |
| 4.10 | -8.32 | 143 | 108 | 94 | 79 | 151 |
| 6.50 | -9.12 | 146 | 110 | 97 | 82 | 149 |
| 10.00 | -9.73 | 149 | 112 | 99 | 85 | 148 |
| 20.00 | -10.54 | 153 | 115 | 103 | 89 | 147 |
| 40.00 | -11.23 | 157 | 118 | 107 | 92 | 145 |
| 80.00 | -11.87 | 161 | 122 | 111 | 96 | 144 |
| 160.00 | -12.50 | | | | | |

The mechanical energy of detonation = -15.019 kJ/cc
The thermal energy of detonation = -4.340 kJ/cc
The total energy of detonation = -19.359 kJ/cc

JWL Fit results:
E0 = -19.421 kJ/cc
A = 2593.96 GPa, B = 17.05 GPa , C = 1.54 GPa
R[1] = 6.33, R[2] = 1.13, omega = 0.12
RMS fitting error = 1.48 %

**Density = 1.9415 g/cc Mixture TMD = 2.0016 g/cc % TMD = 97.0000**

The C-J condition:
The pressure = 25.94 GPa
The volume = 0.405 cc/g
The density = 2.469 g/cc
The energy = 2.77 kJ/cc explosive
The temperature = 5780 K
The shock velocity = 7.910 mm/us
The particle velocity = 1.689 mm/us
The speed of sound = 6.221 mm/us
Gamma = 3.683

Cylinder runs: % of standards

| V/V0 (rel.) | Energy (kJ/cc) | TATB 1.83g/cc | PETN 1.76g/cc | HMX 1.89g/cc | CL-20 2.04g/cc | TRITON 1.70g/cc |
|---|---|---|---|---|---|---|
| 1.00 | -0.92 | | | | | |
| 2.20 | -6.62 | 137 | 104 | 89 | 73 | 152 |
| 4.10 | -8.25 | 142 | 107 | 93 | 78 | 149 |
| 6.50 | -9.05 | 145 | 109 | 96 | 81 | 148 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 10.00 | -9.65 | 148 | 111 | 99 | 84 | 147 |
| 20.00 | -10.46 | 152 | 114 | 103 | 88 | 146 |
| 40.00 | -11.15 | 156 | 117 | 106 | 92 | 144 |
| 80.00 | -11.79 | 160 | 121 | 110 | 95 | 143 |
| 160.00 | -12.41 | | | | | |

The mechanical energy of detonation = -14.925 kJ/cc
The thermal energy of detonation = -4.334 kJ/cc
The total energy of detonation = -19.259 kJ/cc

JWL Fit results:
E0 = -19.217 kJ/cc
A = 2535.45 GPa, B = 16.91 GPa , C = 1.54 GPa
R[1] = 6.33, R[2] = 1.13, omega = 0.12
RMS fitting error = 1.48 %

**Density = 1.9315 g/cc Mixture TMD = 2.0016 g/cc % TMD = 96.5000**

The C-J condition:
The pressure = 25.59 GPa
The volume = 0.407 cc/g
The density = 2.458 g/cc
The energy = 2.74 kJ/cc explosive
The temperature = 5771 K
The shock velocity = 7.865 mm/us
The particle velocity = 1.685 mm/us
The speed of sound = 6.180 mm/us
Gamma = 3.669

Cylinder runs: % of standards

| V/V0 (rel.) | Energy (kJ/cc) | TATB 1.83g/cc | PETN 1.76g/cc | HMX 1.89g/cc | CL-20 2.04g/cc | TRITON 1.70g/cc |
|---|---|---|---|---|---|---|
| 1.00 | -0.91 | | | | | |
| 2.20 | -6.56 | 135 | 103 | 88 | 72 | 150 |
| 4.10 | -8.18 | 141 | 106 | 92 | 77 | 148 |
| 6.50 | -8.97 | 144 | 108 | 95 | 81 | 147 |
| 10.00 | -9.57 | 147 | 110 | 98 | 83 | 146 |
| 20.00 | -10.38 | 151 | 113 | 102 | 87 | 145 |
| 40.00 | -11.07 | 155 | 117 | 106 | 91 | 143 |
| 80.00 | -11.70 | 159 | 120 | 109 | 95 | 142 |
| 160.00 | -12.32 | | | | | |

The mechanical energy of detonation = -14.832 kJ/cc
The thermal energy of detonation = -4.328 kJ/cc
The total energy of detonation = -19.160 kJ/cc

JWL Fit results:
E0 = -18.995 kJ/cc
A = 2478.39 GPa, B = 16.77 GPa , C = 1.55 GPa
R[1] = 6.33, R[2] = 1.13, omega = 0.12
RMS fitting error = 1.47 %

**Density = 1.9215 g/cc Mixture TMD = 2.0016 g/cc % TMD = 96.0000**

The C-J condition:
The pressure = 25.24 GPa
The volume = 0.409 cc/g
The density = 2.447 g/cc
The energy = 2.71 kJ/cc explosive
The temperature = 5761 K
The shock velocity = 7.820 mm/us
The particle velocity = 1.680 mm/us
The speed of sound = 6.140 mm/us
Gamma = 3.654

Cylinder runs: % of standards

| V/V0 (rel.) | Energy (kJ/cc) | TATB 1.83g/cc | PETN 1.76g/cc | HMX 1.89g/cc | CL-20 2.04g/cc | TRITON 1.70g/cc |
|---|---|---|---|---|---|---|
| 1.00 | -0.90 | | | | | |
| 2.20 | -6.50 | 134 | 102 | 87 | 72 | 149 |
| 4.10 | -8.10 | 139 | 105 | 91 | 77 | 147 |
| 6.50 | -8.89 | 143 | 107 | 94 | 80 | 146 |
| 10.00 | -9.49 | 146 | 109 | 97 | 83 | 145 |
| 20.00 | -10.30 | 150 | 112 | 101 | 87 | 144 |
| 40.00 | -10.99 | 154 | 116 | 105 | 90 | 142 |
| 80.00 | -11.62 | 158 | 119 | 108 | 94 | 141 |
| 160.00 | -12.23 | | | | | |

The mechanical energy of detonation = -14.739 kJ/cc
The thermal energy of detonation = -4.322 kJ/cc
The total energy of detonation = -19.061 kJ/cc

JWL Fit results:
E0 = -18.781 kJ/cc
A = 2421.95 GPa, B = 16.64 GPa , C = 1.55 GPa
R[1] = 6.32, R[2] = 1.13, omega = 0.13
RMS fitting error = 1.47 %

**Density = 1.9115 g/cc Mixture TMD = 2.0016 g/cc % TMD = 95.5000**

The C-J condition:
The pressure = 24.90 GPa
The volume = 0.410 cc/g
The density = 2.437 g/cc
The energy = 2.68 kJ/cc explosive
The temperature = 5751 K
The shock velocity = 7.775 mm/us
The particle velocity = 1.676 mm/us
The speed of sound = 6.099 mm/us
Gamma = 3.640

Cylinder runs: % of standards

| V/V0 (rel.) | Energy (kJ/cc) | TATB 1.83g/cc | PETN 1.76g/cc | HMX 1.89g/cc | CL-20 2.04g/cc | TRITON 1.70g/cc |
|---|---|---|---|---|---|---|
| 1.00 | -0.90 | | | | | |
| 2.20 | -6.44 | 133 | 101 | 86 | 71 | 148 |
| 4.10 | -8.03 | 138 | 104 | 91 | 76 | 146 |
| 6.50 | -8.82 | 142 | 106 | 94 | 79 | 144 |
| 10.00 | -9.42 | 144 | 108 | 96 | 82 | 144 |
| 20.00 | -10.22 | 149 | 112 | 100 | 86 | 142 |
| 40.00 | -10.90 | 153 | 115 | 104 | 90 | 141 |
| 80.00 | -11.53 | 156 | 118 | 108 | 93 | 140 |
| 160.00 | -12.14 | | | | | |

The mechanical energy of detonation = -14.646 kJ/cc
The thermal energy of detonation = -4.316 kJ/cc
The total energy of detonation = -18.962 kJ/cc

JWL Fit results:
E0 = -18.474 kJ/cc
A = 2368.72 GPa, B = 16.52 GPa , C = 1.56 GPa
R[1] = 6.32, R[2] = 1.13, omega = 0.13
RMS fitting error = 1.46 %

**Density = 1.9015 g/cc   Mixture TMD =  2.0016 g/cc   % TMD = 95.0000**

The C-J condition:

| | | |
|---|---|---|
| The pressure | = | 24.56 GPa |
| The volume | = | 0.412 cc/g |
| The density | = | 2.426 g/cc |
| The energy | = | 2.66 kJ/cc explosive |
| The temperature | = | 5742 K |
| The shock velocity | = | 7.730 mm/us |
| The particle velocity | = | 1.671 mm/us |
| The speed of sound | = | 6.059 mm/us |
| Gamma | = | 3.625 |

Cylinder runs: % of standards

| V/V0 (rel.) | Energy (kJ/cc) | TATB 1.83g/cc | PETN 1.76g/cc | HMX 1.89g/cc | CL-20 2.04g/cc | TRITON 1.70g/cc |
|---|---|---|---|---|---|---|
| 1.00 | -0.89 | | | | | |
| 2.20 | -6.38 | 131 | 100 | 85 | 70 | 146 |
| 4.10 | -7.96 | 137 | 103 | 90 | 75 | 144 |
| 6.50 | -8.74 | 140 | 105 | 93 | 79 | 143 |
| 10.00 | -9.34 | 143 | 107 | 95 | 81 | 142 |
| 20.00 | -10.14 | 148 | 111 | 99 | 85 | 141 |
| 40.00 | -10.82 | 151 | 114 | 103 | 89 | 140 |
| 80.00 | -11.45 | 155 | 117 | 107 | 93 | 139 |
| 160.00 | -12.06 | | | | | |

The mechanical energy of detonation = -14.553 kJ/cc
The thermal energy of detonation = -4.310 kJ/cc
The total energy of detonation = -18.862 kJ/cc

JWL Fit results:
E0 = -18.414 kJ/cc
A = 2311.34 GPa, B = 16.35 GPa , C = 1.55 GPa
R[1] = 6.32, R[2] = 1.13, omega = 0.13
RMS fitting error = 1.46 %

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