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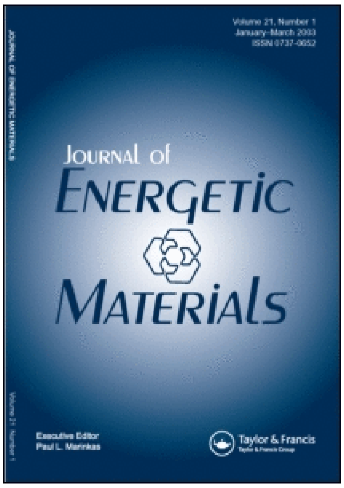

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UNDERWATER PERFORMANCE OF POLYURETHANE - PETN EXPLOSIVES

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ABSTRACT

Detonation velocities and pressures for Polyurethane Foam - PETN charges at a density of 0.6 g/cm^3 have been determined experimentally and compared to theoretical predictions obtained by the TIGER code, using the BKW equation of state with the RDX fit and a new fit developed for low density explosives. It was found that the explosive exhibits a non-ideal performance at small charge diameters. In order to determine the equation of state of the

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detonation products of the explosive in underwater applications, aquarium experiments were conducted and compared with hydrodynamic calculations performed by the TDL code. HOM equation of state parameters were obtained by using a trial and error approach so that good agreement is observed between experimental detonation velocities and gas expansion histories underwater. Using this technique, HOM parameters were obtained in three different charge diameters. It was found that at a diameter of 70 mm the detonation behaviour of the explosive is ideal while non-ideal performance is exhibited at the smaller diameters of 19 mm and 45 mm.

INTRODUCTION

The detonation characteristics of very low density condensed explosive systems have been investigated by Tulis and Austing who examined nitrocellulose, foamed PETN and foamed nitrocellulose / nitroglycerine at densities of 0.25 g/cm^3 and lower(1,2).

Xeuguo(3) examined the detonation parameters of polyurethane / PETN foams at PETN concentrations between 40% and 50% and densities between 0.3 g/cm^3 and 0.9 g/cm^3.

Anderson(4) obtained detonation parameters of polyurethane / PETN mixes at a PETN concentration of 60% and densities between 0.15 g/cm^3 and 0.7 g/cm^3. The recorded detonation velocities of foam slabs were between 1500 and 3300 m/s.

The present study examines a polyurethane / PETN system at a

PETN concentration of 60% and a density of 0.6 g/cm^3 in order to establish equation of state parameters for modelling underwater performance.

For most explosives of military interest and a number of commercial emulsion explosives, which exhibit ideal detonation performance, equations like the Becker - Kistiakowsky - Wilson and the Jacobs - Cowperthwaite - Zwisler have been used to calculate detonation properties assuming complete reaction and chemical equilibrium. Fits of the results obtained by these equations are also used in hydrodynamic codes to model explosive performance. This is for example the case with the HOM equation of state for gases(5) which calculates pressure and temperature, given the internal energy, specific volume and mass fraction of the undecomposed material. Another method which has been popular in performance calculations using hydrodynamics is the calibration of an equation of state of the detonation products by means of an experiment. A typical example is the Jones - Wilkins - Lee (JWL) equation which is calibrated by a cylinder test and a trial and error approach.

The modelling of the performance of low density polyurethane - PETN explosives requires special attention because the explosive can exhibit non-ideal behaviour which cannot be modelled by the previous techniques. The behaviour of the explosive at different diameters has to be examined first by comparing measured and theoretical values of the detonation velocity and pressure.

Equation of state parameters can be determined later, using the previous findings.

EXPERIMENTAL DETERMINATION OF DETONATION PARAMETERS

a. Detonation Velocity

Detonation velocities of cylindrical charges of the polyurethane / PETN solid foam at a density of 0.6 g/cm^3 were determined at a variety of diameters by using streak camera photography.

The charges were primed by 50g of Detasheet C and their length was 30 cm except for one of the 5.1 cm diameter charges and the charge having a diameter of 10cm which had a length of 90 cm.

The results of the tests are shown in Table 1. The detonation velocity varied according to the test diameter. The critical diameter appears to be close to 19mm while the maximum velocity observed was close to 3600 m/s for charges having diameters larger than 51 mm.

b. Detonation Pressure

The detonation pressure of the solid explosive foam was measured at various diameters by means of the aquarium technique.

The experimental set up is shown in Figure 1. In this experiment, the velocity of detonation in the explosive charge and the initial transmitted shock velocity in the liquid are measured.

TABLE 1

Detonation Velocity Measurements with the Streak Camera Method

Diameter (mm)	Density (g/cm^3)	Velocity of Detonation (m/s)
19	0.55	2704
19	0.60	2750
19	0.60	failed
25	0.58	3248
25	0.54	3054
51	0.58	3183
51	0.60	3362
51	0.60	3155
51	0.60	3311
51	0.60	3650
70	0.60	3404
70	0.60	3486
70	0.60	3569
102	0.60	3550

From the transmitted shock velocity in the liquid and the known Hugoniot of the liquid, the initial pressure in the liquid can be calculated. The corresponding detonation pressure can be calculated by the following relationship(6):

$$P_d = P_l \times \frac{\rho_l \times U_{sl} + \rho_e \times U_{se}}{2 \times \rho_l \times U_{sl}} \qquad (1)$$

where P_d is the detonation pressure

P_l is the pressure in the liquid

ρ_e is the initial density of the explosive

ρ_l is the initial density of the liquid

U_{sl} is the initial shock velocity in the liquid

U_{se} is the detonation velocity of the explosive.

In the case of the aquarium experiments for the solid foam explosive, water was selected as the gauge liquid. The Hugoniot of water is well known(5) and it can be expressed as:

$$U_s = 1483 + 2.0 \times U_p \tag{2}$$

where both shock and particle velocities are in m/s.

According to calculations by the Tiger code, the detonation pressure for the explosive foam should be 27Kbar, the detonation velocity 3796 m/sec and the particle velocity 1100m/sec. At this particle velocity the pressure in the water is higher than 27 Kbar indicating that the reflected wave in the explosive is a weak shock increasing the pressure slightly above the C-J point. This means that the error associated with the assumption of linearity of the Hugoniot of the explosive (P-U_p plane) is negligible; thus water is a good selection of a gauge liquid.

The results of the aquarium experiments are shown in Table 2.

TABLE 2

Detonation Pressure Measurements

Charge Diameter (mm)	Density (g/cm^3)	Pressure (Kbar)
51	0.6	25
51	0.6	25
70	0.6	23
70	0.6	25

The detonation pressure for both 51 and 70 mm charge diameters are about 25 Kbar. Although more tests were performed, the detonation pressures are not reported because the streak camera records were not clear and could not be interpreted reliably. It is suspected that the unclear records were due to jetting which was unavoidable because of the nature of the foam.

The observed detonation pressures did not vary significantly between the various tests. This was expected because the detonation velocities in the diameters of 51 and 70mm are close. From the measured detonation velocity and pressure for the 70mm charge the value for the foam can be calculated by using the following equation(5):

$$\gamma_{CJ} = \frac{\rho \times D^2}{P_{CJ}} - 1 \qquad (3)$$

Therefore $\gamma = 2.06$ which is in agreement with published experimental data (5,7).

THEORETICAL DETERMINATION OF DETONATION PARAMETERS

Detonation parameters for the polyurethane foam / PETN explosive were calculated and compared to the experimental data to estimate the extend of the non-ideality of the explosive. The calculations were based on the assumptions of chemical equilibrium and complete reaction and were performed by the TIGER code(8).

In the runs for the polyurethane - PETN explosive, the BKW equation of state with various sets of parameters and compatible libraries of thermodynamic data for the detonation products as well as the JCZ3 equation of state with the library of thermodynamic data adopted by Queen's University(9) were used.

The composition by weight for the explosive was 60% PETN and 40% polyurethane and the density 0.6 g/cm³. The following data were used for the ingredients:

Polyurethane (Estane)(10):

Chemical formula: $C_{5.14}H_{7.50}N_{0.19}O_{1.76}$

Heat of formation: -95000 cal/mole

Density: 0.8744 g/cm³

PETN(11):

Chemical formula: $C_5H_8N_4O_{12}$

Heat of formation: -127199 cal/mole

Density: 1.76 g/cm³

The results of the calculations are shown in Table 3.

TABLE 3

Predicted Ideal Detonation Parameters for the Polyurethane Foam / PETN Explosive

Equation of State	Library of Data	Detonation Velocity (m/s)	Detonation Pressure (Kbar)
BKW (Original)	SRI	3827	26.9
BKW (Original)	LLNL	4127	30.6
BKW (RDX fit)	Queen's	3796	26.2
JCZ3	Queen's	3660	21.7

The detonation parameters calculated with the BKW equation with the RDX fit and the Queen's Library are very close to the experimental values obtained in the case of the large diameter charges. The results obtained with the SRI values were similar while there were significant discrepancies in the case of the LLNL data and the JCZ3 equation of state.

TABLE 4

Experimental and Calculated Results for Low Density PETN

Density (g/cm^3)	Experimental Detonation Velocity (m/s)	Experimental Detonation Pressure Kbar	Calculated Detonation Velocity (m/s)	Calculated Detonation Pressure (Kbar)	Equation of State
0.5	3600	24	3644	20.0	JCZ3
0.6	3970		4057		
1.0	5541	87	5734	88.0	
0.5	3600	24	4237	29.5	SRI-BKW
0.6	3970		4543	39.5	
1.0	5541	87	5702	95.6	
0.5	3600	24	4428	31.6	LLNL-BKW
0.6	3970		4773	42.0	
1.0	5541	87	6089	106.5	
0.5	3600	24	4096	27.4	QUEEN'S RDX-BKW
0.6	3970		4417	37.1	
1.0	5541	87	5720	94.0	

Similar calculations were conducted for low density PETN experimental data for which could be found in the literature(5). The calculated and experimental values for this case are summarized in Table 4. The BKW equation of state with the LLNL library yields higher detonation velocities than the experimental data while the

JCZ3 equation of state yields lower detonation pressures.

Since the BKW equation with the RDX parameters has been quite successful, it was decided that further calculations would be performed with this equation. Furthermore, it is semi-empirical and has been calibrated on the basis of high density explosives, a separate fit was attempted to improve the calculations for low density compositions.

It was observed that the above equations do not predict the experimental detonation velocity - density relationships for a variety of explosives below 1.0g/cm^3.

For PETN the experimental relationship is$^{(7)}$:

$D = 1854 + 3639\rho$

where D is the detonation velocity (m/s) and

ρ is the initial density of the explosive (g/cm^3).

The calculated relationship obtained by using the parameters fitting RDX and the BKW equation of state is

$D = 2427 + 3307\rho$

which results in high velocities of detonation at the low density regime.

By using a trial and error approach, the following parameters were identified namely:

$\alpha = 0.54$; $\beta = 0.72$; $\kappa = 7.50$ and $\theta = 400$

Tiger with the new BKW equation of state parameters gives the following detonation velocity - density relationship for low density PETN:

$D = 1966 + 3695\rho$

This is very close to the experimental one⁽⁷⁾.

For the Polyurethane foam / PETN explosive, the low density fit resulted in a detonation velocity of 3630 m/s and a detonation pressure of 23 Kbar. These results are very close to the experimental measurements for the large diameter charges.

In addition, for low density (0.732 g/cm^3) TNT, the calculated velocity of detonation was 4248 m/s which is very close to the experimental detonation velocity⁽⁷⁾ of 4240 m/s. Unfortunately most of the data available to the author are for high density explosives; for this reason the new BKW equation of state parameters cannot be extensively verified. However the parameters were tested and were found to be physically correct for explosives having an initial density smaller than 1 g/cm^3. For these cases, $(\partial P/\partial T)_V>0$ and $(\partial P/\partial V)_T<0$ while for higher densities sometimes the derivative $(\partial P/\partial T)_V$ becomes negative which is not physically correct.

EQUATION OF STATE DETERMINATION

From the comparison between calculated and experimental results it follows that the polyurethane foam / PETN explosive behaves non-ideally at diameters smaller than 70 mm. Therefore, it was decided to obtain HOM equation of state parameters for the products of detonation at the various diameters of interest by using a relatively simple test for the calibration. For this purpose an approach similar to the one used by Mader$^{(5,13)}$ was considered. This is outlined in the following.

First, the detonation velocities calculated theoretically using TIGER are compared to the measured detonation velocities. For the smaller diameter charges when the measured detonation velocity is significantly lower than the one predicted, the reaction at the detonation front is considered to be incomplete. Then, additional calculations are performed by varying the amounts of constituents withheld from chemical reaction at the detonation front until agreement is achieved between measured and calculated detonation velocity. The constituents can later on be allowed to react in the expansion zone according to a decomposition model which has to be verified experimentally.

The calculated HOM parameters are then used in a two dimensional Lagrangian code to simulate an aquarium test described in the following section. Calculated product expansion and shock wave histories are compared to the experimental ones and this serves as an indication of the validity of the decomposition model adopted in the expansion zone. The procedure is repeated until a close match between experimental and calculated results is observed.

a. The Aquarium experiment

The aquarium experiment designed for this work is shown in Figure 2. The explosive, foamed inside a plexiglas tube having wall thickness of 3.2 mm, is detonated underwater. The slit of the streak camera is perpendicular to the axis of the tube at a point located away from the initiator (normally 4 diameters from the initiator and 3 diameters from the other free end). Thus the location of the wall of the tube and the shock wave transmitted to the water can be recorded from the cut off of the light produced by an argon filled light bomb, located opposite to the camera. A typical example of a streak camera record is shown in Figure 3. The streak camera records were digitized by an optical digitizer (Stecometer by Carl Zeiss Jena).

b. Hydrodynamic calculations

The aquarium experiments were modelled by using the TDL code(14). The explosive was burnt by using the sharp shock(5) method.

For the simulations, the calculation domain was divided in cells having a size of 1.5875 mm x 1.5875 mm. The detonation starts by assuming that a small part at the bottom end of the explosive cylinder is completely decomposed.

RESULTS

The aquarium experiments conducted with explosive charge diameters of 19, 44 and 70 mm were modelled according to the method outlined previously.

In order to model non-ideal performance by using the TIGER code, constituents must be fixed so that they are withheld from reaction. In calculating the thermodynamic state of the system, the mole numbers of the fixed species must be specified, and the mole numbers of the other species must be calculated using the equilibrium and the stoichiometric conditions. For the approach to work, explosive ingredients have to be able to appear as products.

Since polyurethane is the non explosive ingredient, it was decided that it is the only ingredient which can decompose partially at the diameters of interest. In order to be able to model partial reaction of the polyurethane, data for solid polyurethane had to be provided in the thermodynamic library of the TIGER code (reference state, OLD equation of state)(8).

The relationship between heat capacity at constant pressure and temperature was calculated from the heat capacity at constant volume and the compressibility and thermal expansivity coefficients for polyurethane which were assumed to be 10 (1/Mbar) and 0.0001 (1/K) respectively.

The heat capacity at constant volume as a function of temperature was calculated by using the TDF code provided by Mader(15). For the calculations the Debye theta was estimated to be 1420 in order to match the molar heat capacity of the polyurethane (C_v=35 cal/mole). Heat capacities were calculated for a range of temperatures from 300 K to 4000 K.

For the equation of state of the solid products, the compressibility and thermal expansivity data used previously were used in this case as well. The rest of the coefficients were set to zero. The calculated coefficients for the thermodynamic library of the TIGER code are shown in Table 5.

TABLE 5

Coefficients for the Library of the TIGER code for Polyurethane

C_1	0.341
C_2	-1.296
C_3	-0.341
C_4	-0.031
C_5	-2.095
C_6	-4.263
C_7	0.708
C_8	-0.145040 E+06
C_9	0.219600 E+02
A_{11}	80.0
A_{12}	1.0 E-04
A_{13}	0.0
A_{21}	1.0 E-05
A_{22}	0.0
A_{23}	0.0
A_{31}	0.0
A_{32}	0.0
A_{33}	0.0

Figure 4 compares the experimental and calculated expansion history of the gaseous detonation products for the 19mm diameter charge assuming complete reaction when calculating the HOM parameters. Because the experimental data lie below the calculated curve it is inferred that the reaction is not complete in the detonation wave. detonation wave. The fact that the calculated detonation velocity is larger than the measured one also supports this conclusion.

Following a trial and error approach, the amount of polyurethane withheld from reaction in the TIGER code was adjusted until the calculated and measured detonation velocities were close. For the 19 mm charge diameter, this happened when all of the polyurethane was assumed to be unreacted and in chemical and thermal equilibrium with the PETN detonation products. The resulting calculated expansion history is shown in Figures 5 in which the experimental curve is also included.

However, the agreement between calculated and experimental results is not satisfactory which indicates that some polyurethane must react in the expansion zone. For simplicity, the mass fraction of the polyurethane was assumed to vary linearly with pressure from the effective C-J pressure down to 1Kbar.

It was found by iteration that the agreement between experimental and calculated curves was good when 50% of the polyurethane was allowed to react in this fashion. The calculated expansion history obtained by using the BKW equation with the RDX fit is shown in Figure 6 while that obtained by using the low density fit is given in Figure 7. The corresponding HOM parameters are given in Table 6.

The above procedure was repeated for the charge having a diameter of 45 mm. Results produced with the RDX and the low density fits on the basis of complete reaction before the C-J plane are shown in Figures 8 and 9 respectively. The best match between calculated and experimental expansion histories for the original RDX fit were obtained when 25 % of the polyurethane was allowed to react

TABLE 6

HOM Parameters for the Polyurethane Foam / PETN Explosive when 50% of Polyurethane Reacts Between C-J and 1Kbar

Parameter	Value	
	RDX Fit	Low Density Fit
A	-.432408733823 E+01	-.447447773211 E+01
B	-.145023207994 E+01	-.108462060801 E+01
C	-.616239100216 E-01	-.195403950020 E+00
D	.267025593885 E-01	.467819367075 E-01
E	-.202729869034 E-02	-.307845445832 E-02
K	-.155096425901 E+01	-.115505480809 E+01
L	.276226598098 E+00	.457019626097 E+00
M	.325163613531 E-01	.623887464039 E-01
N	.192313842847 E-02	.409117510658 E-02
O	.432629366378 E-04	.999992454199 E-04
Q	.756153587549 E+01	.756055559270 E+01
R	-.231022900804 E+00	-.208037595351 E+00
S	.283810268281 E-01	.265676506126 E-01
T	-.197007809373 E-02	-.287844517172 E-02
U	.272021727609 E-04	.121418923539 E-03
C_V	.900000000000 E+00	.900000000000 E+00
Z	.100000000000 E+00	.100000000000 E+00

in the detonation wave and 50% behind it. The calculated detonation velocity was 3290 m/s which is close to the experimental one. For the case of the low density fit the best prediction was obtained when 50% of the polyurethane was allowed to react in the detonation wave while the rest was let to react behind it. The calculated detonation velocity was 3300 m/s. Figures 10 and 11 compare the measured and predicted expansion histories. The HOM parameters for both fits are given in Table 7.

For the 70mm diameter charges the calculated and experimental expansion histories are shown in Figures 12 and 13. The calculations were performed by using both the RDX and the low

TABLE 7

HOM Parameters for Polyurethane / PETN with Specified % of Unreacted Polyurethane in the Detonation Wave.

Parameter	Value	
	RDX fit (75% Unreacted)	Low Density Fit (50% Unreacted)
A	-.409177626653 E+01	-.399638556946 E+01
B	-.135979296492 E+01	-.140465444672 E+01
C	-.303467015082 E+00	-.418201038253 E+00
D	.119052035130 E+00	.232786481714 E+00
E	-.833233416081 E-02	-.360546320314 E-01
K	-.230813613345 E+01	-.111089684908 E+01
L	-.273489980917 E+00	.665948991895 E+00
M	-.115904463106 E+00	.156174169443 E+00
N	-.154801581469 E-01	.189888797366 E-01
O	-.713510340904 E-03	.901781763415 E-03
Q	.759538653236 E+01	.761038153857 E+01
R	-.154463855243 E+00	-.158211127477 E+00
S	-.138648400991 E+00	-.145474320584 E+00
T	.946237307333 E-01	.109425527257 E+00
U	-.186872191203 E-01	-.237276688534 E-01
C_v	.900000000000 E+00	.900000000000 E+00
Z	.100000000000 E+00	.100000000000 E+00

density fit for the BKW equation of state and by assuming complete reaction and chemical equilibrium. The HOM parameters are given in Table 8.

The calculated and experimental shock wave histories were also compared in order to find the best fit for the equation of state of the detonation products. The agreement between experimental and calculated results was good for the previously mentioned "best" cases. In general, the shock wave histories did not prove to be very sensitive to the slight variations of the assumed decomposition law. They demonstrated however that decomposition does occur in the

TABLE 8

HOM Parameters for Polyurethane / PETN with Complete Reaction.

Parameter	Value	
	RDX fit	Low Density Fit
A	-.34848879570 E+01	-.35355302590 E+01
B	-.21496823562 E+01	-.23278450535 E+01
C	.20194652205 E+00	.32257681601 E+00
D	-.15569431476 E-01	-.38126666323 E-01
E	.33220066970 E-03	.16683854555 E-02
K	-.13941390613 E+01	-.15433094523 E+01
L	.36810532862 E+00	.29739491105 E+00
M	.47617810518 E-01	.37615413695 E-01
N	.30692213786 E-02	.24473720358 E-02
O	.75006958360 E-04	.60403994705 E-04
Q	.77637845496 E+01	.77195044801 E+01
R	-.45278527117 E+00	-.40687233905 E+00
S	.10781549629 E-00	.10706406241 E+00
T	-.14329755850 E-01	-.14090928022 E-01
U	.68939603493 E-03	.71131905489 E-03
C_v	.90000000000 E+00	.90000000000 E+00
Z	.10000000000 E+00	.10000000000 E+00

expansion zone as can be shown in Figures 14 and 15 where the measured and predicted shock wave histories for 19 mm diameter charge are compared.

CONCLUSIONS

The detonation parameters of cylindrical charges of polyurethane / PETN foams at a PETN concentration of 60% by weight and a density of 0.6 g/cm^3 have been established for both ideal and non-ideal detonation conditions. A new low density PETN fit for the BKW equation of state was also derived. In addition the gaseous HOM equation of state parameters for the ideal and two non-ideal detonation cases were determined using aquarium experiments and hydrodynamic calculations.

Reasonably good agreement between calculated results and experimental measurements was achieved by the adopted method of solution. Charges of 70 mm diameter detonated almost ideally, as was evident by comparison of both the calculated and measured velocities of detonation and the expansion histories of the detonation products. The detonation for the 45 mm and the 19mm diameter charges was shown to be non-ideal. In the non-ideal detonation cases it was demonstrated that additional reaction occurs in the expansion zone.

The developed low density fit for the BKW equation of state resulted in predictions of the expansion histories which were comparable to the ones obtained with the RDX fit. However, the calculated detonation velocities were closer to the measured ones for the new low density PETN fit.

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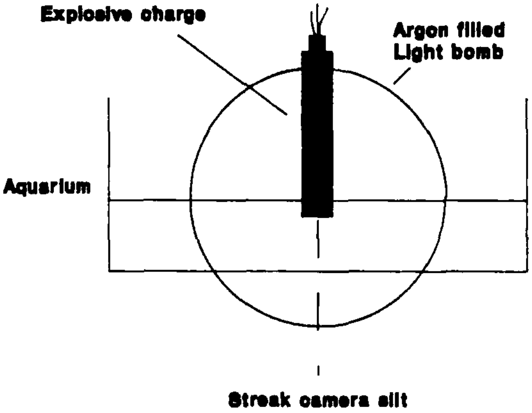

FIGURE 1

Experimental arrangements for measuring detonation pressures by the aquarium technique.

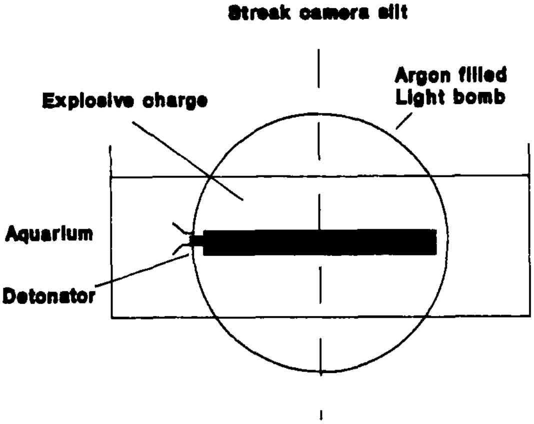

FIGURE 2

Aquarium experiment for measuring shock wave and expansion histories in water resulting from the detonation of the foamed PETN explosive.

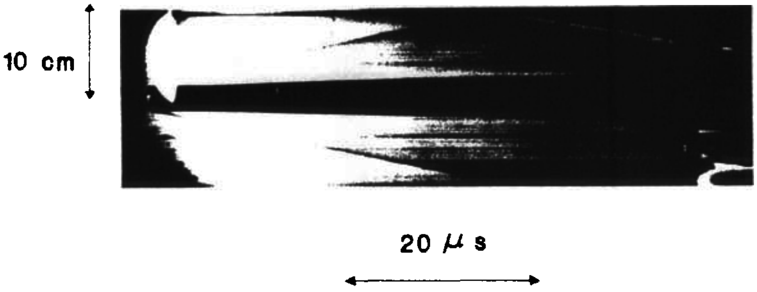

FIGURE 3

Typical streak camera record from the aquarium experiment (19mm charge).

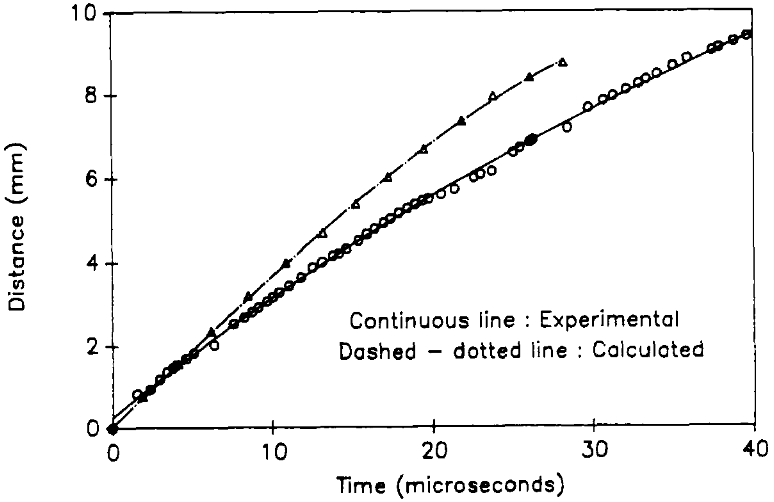

FIGURE 4

Detonation product expansion histories for the 19mm diameter charge when complete reaction is assumed (BKW fit).

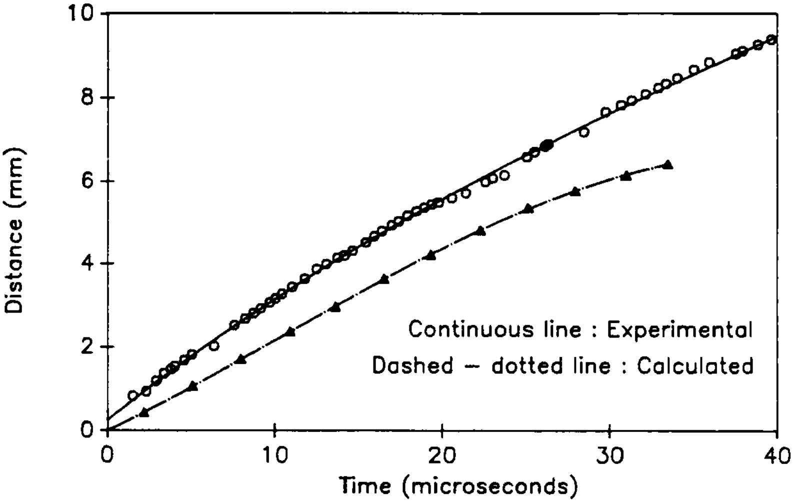

FIGURE 5

Detonation product expansion histories for the 19mm diameter charge when polyurethane is assumed unreacted (BKW fit).

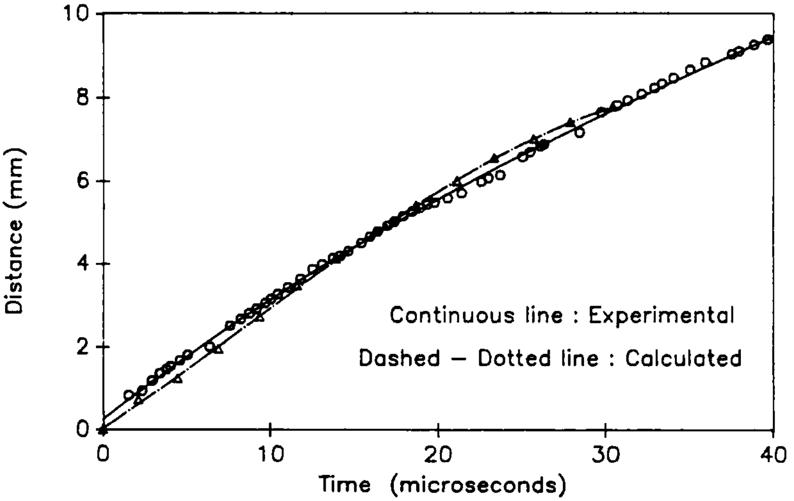

FIGURE 6

Detonation product expansion histories for the 19mm diameter charge when 50% of the polyurethane reacts in the expansion zone (BKW fit).

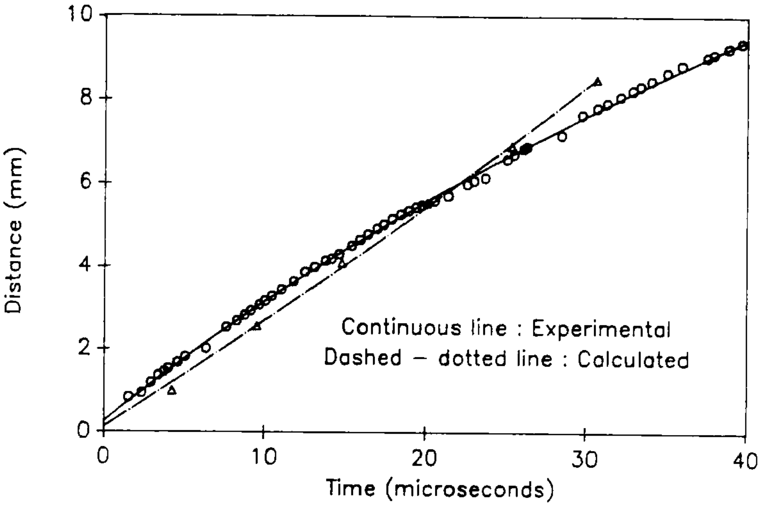

FIGURE 7

Detonation product expansion histories for the 19mm diameter charge when 50% of the polyurethane reacts in the expansion zone (Low Density fit).

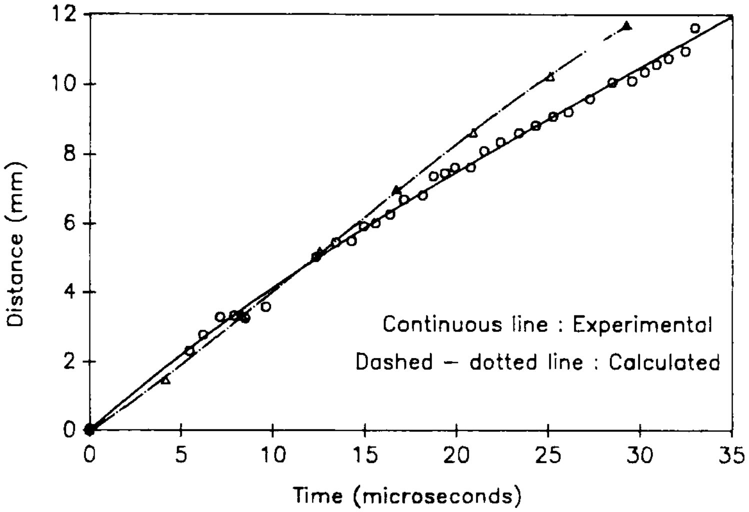

FIGURE 8

Detonation product expansion histories for the 45mm diameter charge when the polyurethane is assumed completely reacted (BKW fit).

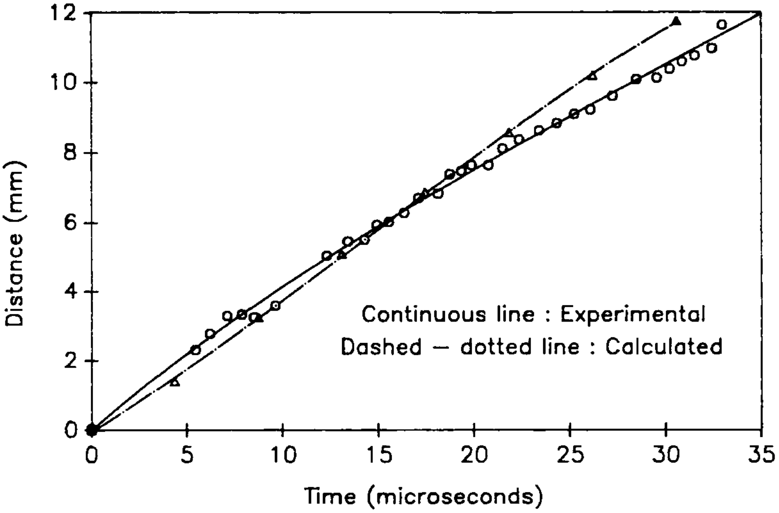

FIGURE 9

Detonation product expansion histories for the 45mm diameter charge when the polyurethane is assumed completely reacted (Low density fit).

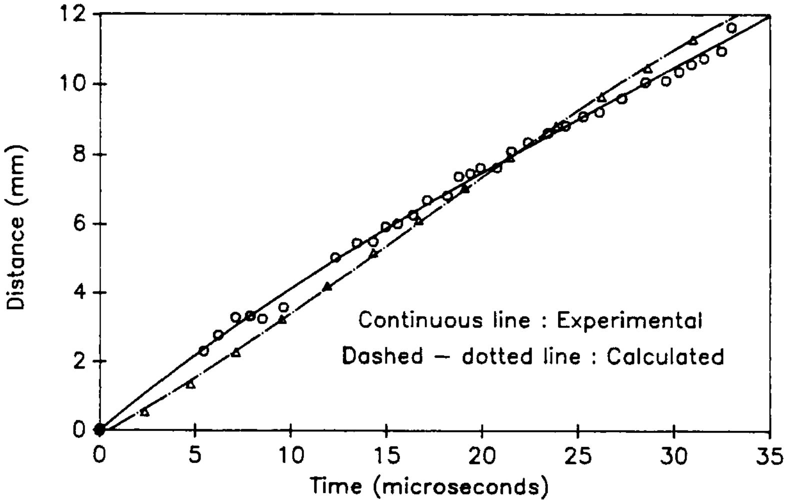

FIGURE 10

Detonation product expansion histories for the 45mm diameter charge when 25% of the polyurethane reacts in the detonation wave and 50% in the expansion zone (BKW fit).

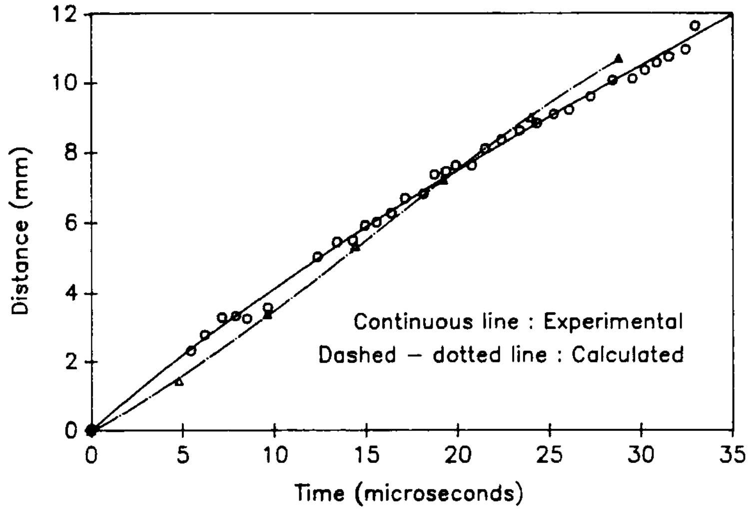

FIGURE 11

Detonation product expansion histories for the 45mm diameter charge when 50% of the polyurethane reacts in the expansion wave and 50% in the expansion zone (Low density fit).

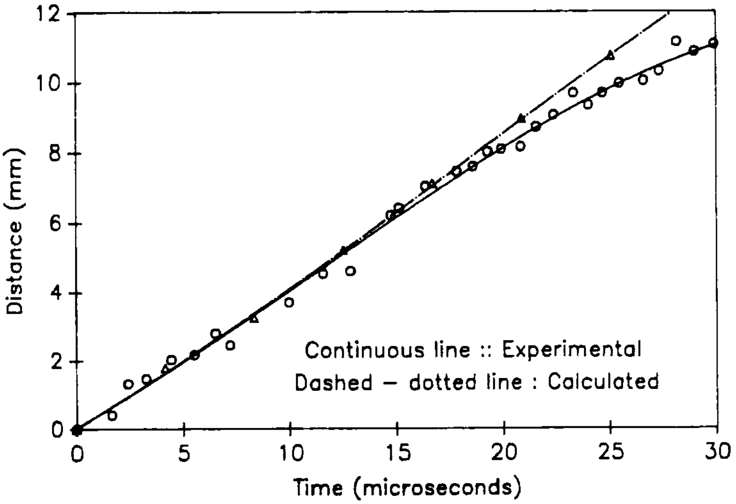

FIGURE 12

Detonation product expansion histories for the 70mm diameter charge when complete reaction is assumed (BKW fit).

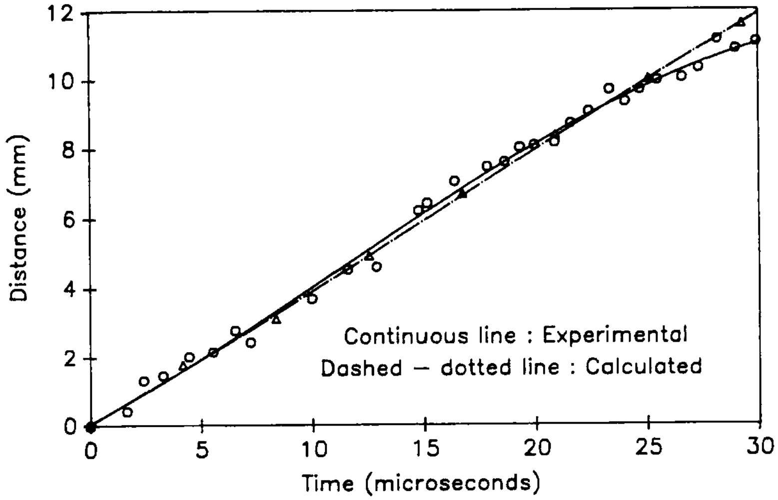

FIGURE 13

Detonation product expansion histories for the 70mm diameter charge when complete reaction is assumed (Low density fit).

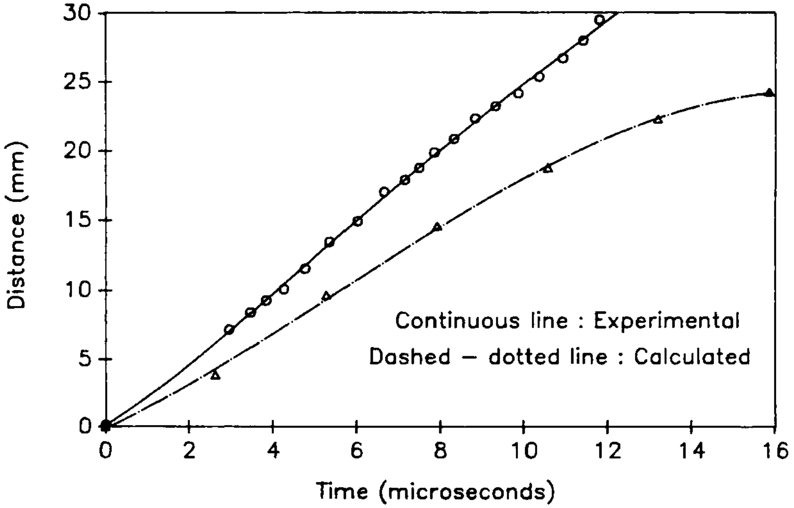

FIGURE 14

Shock wave histories for the 19mm diameter charge when the polyurethane is assumed unreacted (BKW fit)

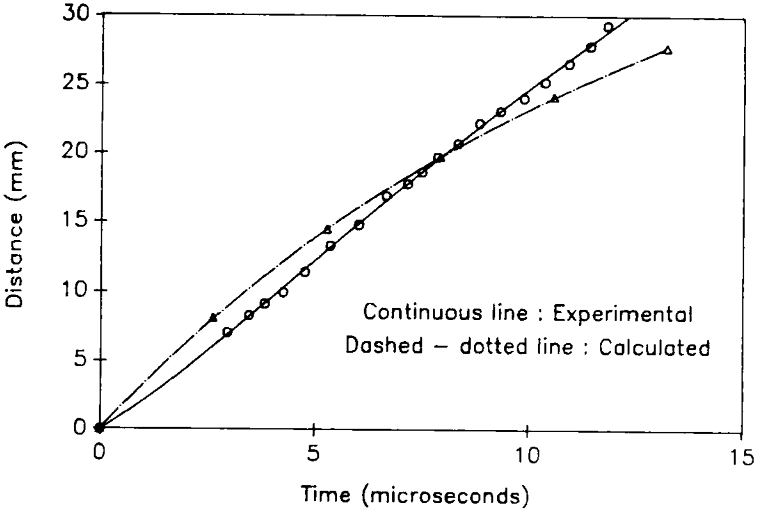

FIGURE 15

Shock wave histories for the 19mm diameter charge when 50% of the polyurethane reacts in the expansion zone (BKW fit)

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