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DETONATION AND INCINERATION PRODUCTS OF PBX EXPLOSIVES

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Abstract

A series of experiments are planned to determine detonation product gases that are released into the environment when high explosives are tested. These experiments will be done in a 1.8-m-diam confinement vessel at ambient air pressure and partial vacuum. A matrix of four shots of PBX 9501, three shots of PBX 9502 and one shot of LX-10 are analyzed to determine the reproducibility and mass balance of materials in the detonation. This paper will only report on the detonation product gases as other experiments are planned.

Introduction

Open-air testing of explosives is and has been an integral part of weapons development process at Los Alamos National Laboratory since the Laboratory's inception. Of growing concern today are the emissions from these tests as judged by the regulations of the New Mexico Air Quality Act, the Federal Clean Air Act, and the EPA restrictions. These regulations are also judged by good and conscientious management practice. Numerous measurements have been made regarding the presence of residual gasses from detonation and burning of explosives in air. This study is an attempt to determine the nature and composition of these gases. The first of a three-part series of experiments is to develop a technique for determination and mass balance of elements from detonations. A 1.8-m-diam confinement vessel is used to contain the shots. Product gases are measured by mass spectrometry. The second part is to determine chlorine and fluorine compositions. A third segment is planned for the open-air burning of explosives. Only results from the first series of experiments are reported here.

Experimental procedure

Six confined shots have been done in both air and vacuum. This shot matrix was designed to determine the best conditions for analysis and reproducibility of the technique. Two compositions, PBX 9501 and 9502, were tested in a 1.8-m-diam confinement vessel that has a volume of 3040 liters. The charges were suspended in the center of the vessel and fired with a SE-1 detonator, which has 0.625 g of PETN, a booster pellet of 2.6 g of PBX 9407, and a 17-g phenolic detonator holder (see Fig 1).

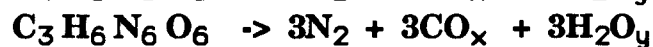
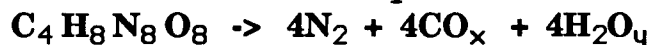
Approximately three different charge weights were used. Gas samples were collected in an evacuated two-liter volume. The shots in air were at ambient pressure and vacuum shots were done at a pressure of approximately 700 microns of mercury. The results of gas analysis from these shots are presented in Tables II, III and IV. Table I is a description of the explosive compositions including the binders, empirical formulas and the assumed detonation equations. Two other shots of PBX 9502 and LX-10 were done in open air. The product gases were sampled in an evacuated glass volume when the shock wave from detonation broke a glass seal. Samples from these shots were concentrated for analysis of the minor constituents and the results are presented in Table V.

Results and discussion

TABLE I
EXPLOSIVE DESCRIPTION

Formulation	Composition Wt %	Empirical Formula
PBX 9501	95/2.5/2.5 :HMX/NP/Estane	HMX- $C_4 H_8 N_8 O_8$ NP- $C_{7.5} H_{13} N_4 O_8$ Estane- $C_{24} H_{34} N O_8$
PBX 9502	95/5 :TATB/KelF-800	TATB- $C_6 H_6 N_6 O_6$ KelF- $(C_5 H F_5 Cl_2)_n$
PBX 9407	94/6 : RDX/Exon 461	RDX- $C_3 H_6 N_6 O_6$ Exon- $(C_4 H_2 F_3 Cl_3)_n$
LX-10	95/5 : HMX/Viton	HMX- $C_4 H_4 N_4 O$ Viton- $(C_5 H_2 F_8)_n$
Detonator Holder	Phenolic polymer	$C_7 H_7 O$

Assume Detonation Equation



Where $x = 0, 1$ or 2 and $y = 0$ or 1 depending on reaction conditions.
Binders and detonator holder are assumed to participate in the reaction also producing gaseous products.

TABLE II
GAS SAMPLE COMPOSITION OF CONFINED SHOTS
(RELATIVE VOLUME %)*

Sample	Sample wt. (grams)	N ₂	O ₂	Ar	CO	CO ₂	H ₂	H ₂ O	NO _x
Background Air		77.8	20.2	.92	-	.07	.02	0.9	-
1-9501 (air)	540	77.6	12.4	.84	-	8.3	.03	0.3	.07
2-9501 (air)	540	77.7	12.8	.84	-	8.2	.01	0.3	.10
3-9501 (vac)	540	35.1	0.06	.02	28.7	12.6	19.8	3.7	.02
4-9501 (vac)	135	42.5	0.15	.21	28.0	11.4	13.8	3.9	.02
1-9502 (air)	1000	78.0	0.11	.78	1.2	21.0	0.2	0.6	.19
2-9502 (vac)	564	27.2	0.03	.02	42.0	6.3	22.6	1.5	.02

Values are averages of at least two analyses on the same gas sample. Reproducibility was at least +/- 1% of the values for the major components, +/- 10% for the minor components, and +/- 50% for the trace (<0.1%) components.

From the data above, it can be seen that there was a significant amount of argon in shot 4, which indicates a leak in either the vessel or the sample volume. In this shot the pressure in the vessel was not consistent with the predicted pressure, which indicates that this would not be the desired sample size for these experiments. An interesting observation from these data is that hydrogen reacted completely with the available oxygen and produced water which condensed on the walls of the vessel in the air shots. The vacuum shots on the other hand show a considerable amount of free hydrogen. The number of moles of O₂ initially in the vessel before the shot is 19.48. The number of moles after the shot is 13.58 which means that the shot consumed 5.9 moles of oxygen. Assuming that all available carbon in the shot, including binder and phenolic holder, plus all of the oxygen in the PBX explosive burned to CO₂, the total amount of CO₂ produced would be 9.09 moles. Table III represents the product yield in moles of gas for the PBX 9501 shots vs the predicted amount of gas when pressure and temperature of the vessel are known. The difference be-

tween the CO₂ produced in the observed sample and the calculated is 0.17 moles, which may indicate a slight amount of carbon residue deposited on the vessel walls.

TABLE III
PRODUCT YIELD OF PBX 9501 SHOTS
(MOLES OF GAS OBSERVED vs MOLES OF GAS PREDICTED)

Sample	N ₂ *	C O _x	H ₂ O _y	NO _z	Others	Total Moles
1-9501 (air)						
Observed	7.03	8.92	1.06	0.07	-	17.1
Calculated	7.07	9.09	8.28	-	-	24.5
2-9501 (air)						
Observed	7.18	8.87	0.80	0.10	-	7.0
Calculated	7.07	9.09	8.28	-	-	24.5
3-9501 (vac)					(Trace)	
Observed	7.17	8.88	5.05	Trace	HCN/NH ₃	21.1
Calculated	7.07	9.09	8.28	24.5		
4-9501 (vac)					(Trace)	
Observed	1.04	1.60	0.72	Trace	HCN/NH ₃	3.4
Calculated	1.08	3.15	2.53	7.5		

Note x can equal 1 or 2; y = 0 or 1; z = 1/2 (i.e. N₂O) = 1 or 2

*Corrected for presence of air initially in vessel using N₂/Ar= 84.6 from blank. Trace = < 0.01.

From Table III it can be seen that the discrepancy in the number of moles of water observed vs the calculated number is greatest in the air shots. This is because water produced from the shot condensed on the walls of the vessel. This was confirmed by measuring a relative humidity of 44% in the vessel before the shot and a humidity of 90% afterwards. The following Table IV represents product yield of gas from the PBX 9502 shots. In the 1-Kg shot number 1-9502, no pressure was measured in the vessel due to a faulty transducer; therefore the observed moles of gas could not be presented.

TABLE IV
PRODUCT YIELD OF PBX 9502 SHOTS
(MOLES OF GAS OBSERVED vs MOLES OF GAS PREDICTED)

Sample	N ₂ *	C O _x	H ₂ O _y	NO _z	Other (Trace)	Total Moles
1-9502 (air)						
Calculated	11.1	24.1	12.1	.	.	47.3
2-9502 (vac)						
Observed	5.70	10.8	5.37	Trace	C₂/NH₃/HCN	21.9
Calculated	6.26	13.6	6.82	.	.	26.7

Note: x can equal 1 or 2; y= 0 or 1; z= 1/2 (i.e. N₂O) = 1 or 2.

***Corrected for presence of air initially in the vessel using N₂/Ar= 84.6 from blank.**

From this table, the discrepancy in the number of moles of carbon observed and calculated can be explained by the presence of residual carbon deposited on the vessel wall. The exact composition of this residue has not been determined but future tests may try to identify it.

TABLE V
DETECTED TRACE PRODUCTS
(OPEN AIR SHOTS)

Explosive	Product*
PBX 9502 (93 grams)	HCN, NH₃, NO_x, C₂X_n
PBX LX-10 (80 grams)	HCN, NO_x, C₂H₂F₂, HF**

***Estimated to be present in 10 to 200-ppm concentration in sample volume**

****Inferred from presence of SiF₄ resulting from reaction of product gases with glass sample bulb.**

These shots were done in an evacuated glass volume with a glass break seal and concentrated by freezing out the minor components. No attempt was made to quantitate the amount of the trace products that would be released into the environment during open-air testing. But judging from what was seen in the sample volume, it was estimated to be very small.

Conclusions

The results of these experiments show that reasonable agreement between predicted and observed detonation product gases can be obtained by firing in a confinement vessel. Trace compounds of environmental interest are generated by the explosives and are detectable in these experiments. However, better collection and concentration procedures are needed to characterize and quantitate these products. It is likely that several of these trace compounds react with the vessel wall thereby changing the composition that will reduce their detection limit and estimated concentration.

As mentioned in the PBX 9501 air shots, the amount of O₂ consumed from the vessel air can be nearly accounted for by assuming that the carbon atoms in the explosives are partitioned equally in the products between C and CO₂, the C then burned to CO₂. The other organic components, i.e. phenolic, NP, and Estane, also burned to CO₂ and water. Very little residual carbon is visible in the vessel after the shots in air.

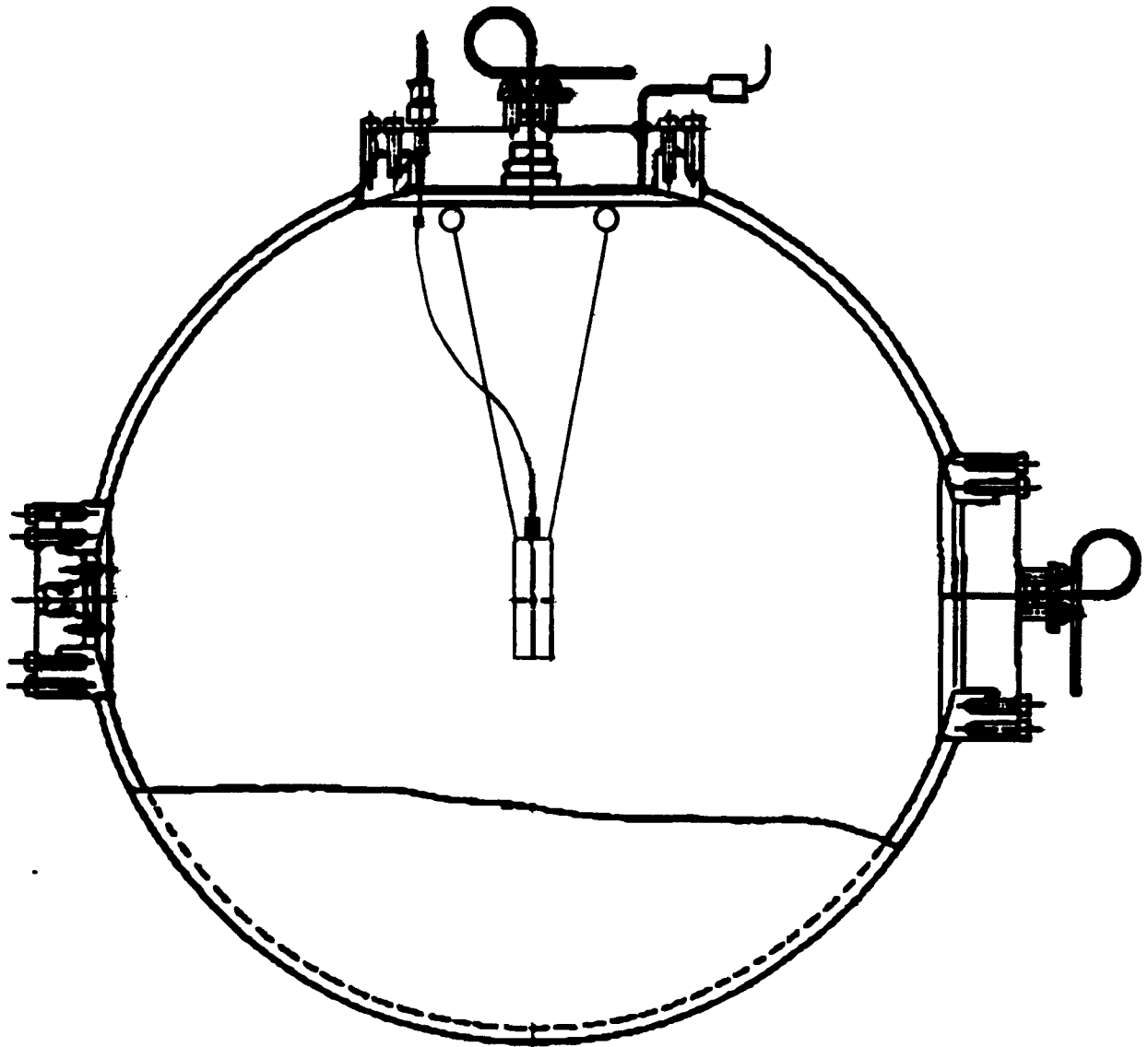


Figure 1. 1.8 Meter diameter confinement vessel

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