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Replacement of PETN by Bicyclo-HMX in Semtex 10*

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Abstract. Bicyclo-HMX (BCHMX) was studied in the form of a plastic explosive bonded by the plastic matrix of the explosive Semtex 10 and the results were compared with the original Semtex 10 which contains PETN as an explosive filler. The tests included measurements in the sensitivity to impact and friction. The thermal stability was studied using differential thermal analysis (DTA) with the evaluation of the outputs using the Kissinger method. The detonation velocity was measured experimentally and the detonation characteristics were calculated by means of EXPLO 5 code and the Kamlet & Jacobs method. On the basis of mutual comparison of all the obtained results, it was concluded that replacement of PETN by Bicyclo-HMX enhances the friction sensitivity, thermal stability and the detonation parameters of the explosive Semtex 10, while the impact sensitivity is approximately the same. Calculated results of EXPLO 5 code showed good agreement with the experimental detonation velocities.
Keywords: chemical engineering, plastic explosive, detonation characteristics

1. INTRODUCTION

BCHMX (cis-1,3,4,6-tetranitrooctahydroimidazo-[4,5-d]imidazole or BCHMX) [1] is an attractive compound with TMD = 1.86 g/cm^3, it has

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a theoretical detonation velocity = 9050 m/s, detonation pressure = 37 GPa and explosion heat = 6,518 MJ/kg [2]. It has a friction sensitivity in the same range as HMX and impact sensitivity in the range of PETN (penthrite or Pentaerythritol tetranitrate) [2]. BCHMX was studied as an explosive filler with the C-4 matrix, where the results showed the ability of the plastic matrix of composition C-4 to decrease the sensitivity of the pure BCHMX and keep its performance higher than Composition C-4 [3, 4]. Semtex 10 is a plastic explosive for special uses, created on the basis of an inert plasticizer with PETN as an active component. Semtex 10 is used for special destruction and blasting works, underwater blasting works; it can be shaped well and has good adhesive properties [5].

The goal of this work is to evaluate the possible enhancement of Semtex 10 by replacement of the active compound PETN with a more powerful and less sensitive alternative BCHMX without significant increase in the price. Sensitivity, thermal stability and the detonation characteristics of the prepared mixture were determined and compared with the original Semtex 10 in addition to the individual explosives [6, 2]. The calculations of the detonation parameters of all the samples were done by EXPLO 5 code [7] and modification of the Kamlet and Jacobs method [8].

2. THE EXPERIMENT

2.1. Preparation of plastic explosives

The plastic explosives were prepared in the Explosia Company (Research institute of industrial chemistry). BCHMX was prepared at IEM in a 2-stage method for its synthesis (unpublished). The matrix of the binder contains rubber with non energetic plasticizer (unpublished). The explosives 85% wt. were mixed with the binder matrix 15% wt. at 70ºC for 70 min under vacuum using a computerized Plastograph mixer. It was observed that the temperature of the mixer and the time of mixing affects the characteristics of the prepared samples. The prepared samples were extruded to obtain cylinder shaped blocks of plastic explosives with a length of 200 mm and a diameter of 16 mm.

2.2. Elemental analysis

A Fisons – EA-1108 CHNS-O elemental analyzer was used to detect the % of C, H and N in the prepared samples which were needed for the theoretical calculation of the detonation parameters for all of the prepared samples. The results of the elemental analysis were recalculated to match the N content to the individual explosive and reported in Tables 1 and 1a. The summary formula calculated in this way was used as if it was an individual explosive and was used in the different methods for calculation of the detonation parameters.

2.3. Heat of combustion

An MS10A Automatic Combustion Calorimeter was used for measuring of the combustion heat of the samples. The samples were prepared and placed in a bomb filled by excess of oxygen [9] where the data obtained from the measurements was reported in Table 1. This data was used for calculation of the heat formation for the samples which were used for the calculation of the detonation parameters.

2.4. Thermal stability

The DTA 550 Ex apparatus was used for thermal analysis [9] of explosives. The measurements were carried out at the level of atmospheric pressure, with the tested sample being in direct contact with air. The tested sample (0,05 g) was placed in a test tube made of Simax glass, 5 mm in diameter and 50 mm long. The reference standard was 0,05 g aluminum oxide. A linear heating rate of 5ºC/min was used. The results are presented in Fig. 1, where the exothermic effects of the thermal decomposition and the endothermic peaks of the prepared samples were observed. Peak temperatures of exothermic thermal decomposition at a linear heating rate of 5°C/min for all samples are presented in Table 1. Outputs obtained from the measurements of all the samples at different linear heating rates (10 and 15ºC/min in addition to the 5ºC/min which was measured) were processed using the Kissinger method [10] with the results presented in Fig. 2. The slopes of the Kissinger relationship (E_aR^{-1}), which were taken as the characteristics of thermal reactivity [11, 12] were reported in Table 1a.

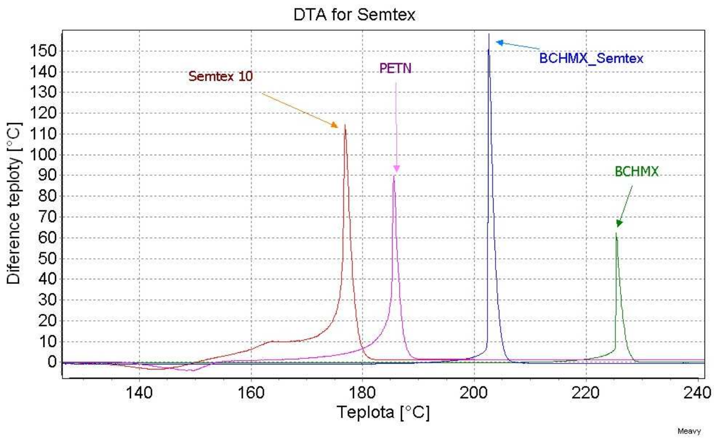

Fig. 1. The typical DTA curves for the studied samples (at a heating rate of 5°C/min)

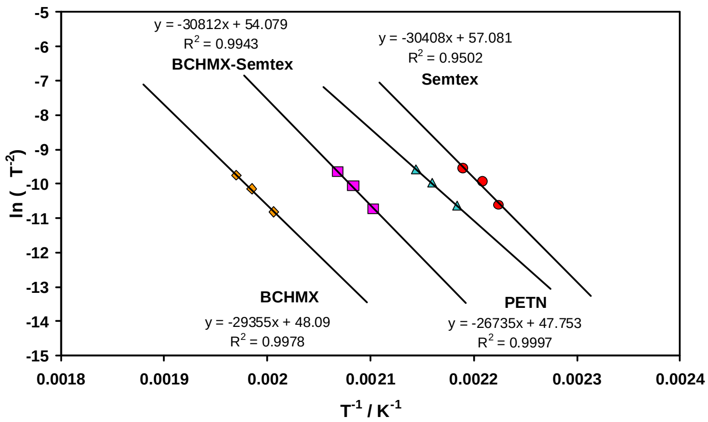

Fig. 2. Evaluation of DTA outputs using the Kissinger method

2.5. Impact sensitivity measurements

The standard impact tester (Julius Peter [13]) was used with an exchangeable anvil, the amount of tested substance being 40 mm^3. 2 and 5 kg weight drop hammers were used for the test. The probit analysis [14] was used to determine the probability levels of the initiation. The obtained sensitivity was expressed as the drop energy (E_d) versus percentage of initiation. Only the 50% probability of initiation is used in this article and is reported in Table 1.

2.6. Friction sensitivity measurements

BAM friction test apparatus was used to determine the sensitivity to friction by applying the standard test conditions [13]. Sensitivity to friction was determined by spreading about 0,01 g of the dry explosive on the surface of the porcelain plate in the form of a thin layer. Different loads were used to change the normal force between the porcelain pin and the plate. The sample initiation was observed through sound, smoke appearance, or by the characteristic smell of the decomposition products. Using the probit analysis [14], only the normal force at which 50% of initiation occurs is reported as the friction sensitivity as in shown in Table 1a.

2.7. Detonation velocity measurements

The detonation velocity of all the prepared plastic explosives were measured by the ionization copper probe method [13] where the data were reported on the oscilloscope (Tektronix TDS 3012). The samples were prepared in the form of cylinders with a 16 mm diameter and 200 mm in length. The copper probes were connected to the oscilloscope via coaxial cable.

Charges were set off using a booster charge (Semtex 1A which had a mass = 3 g and diameter = 16 mm) initiated by standard industrial no. 8 electric detonator. The tests were done in triplicate with variation between readings being lower than 68 m/s and reported in Tables 2 and 2a.

2.8. Calculation of the detonation characteristics

The theoretical detonation characteristics (detonation velocity *D*, heat of explosion or detonation *Q*, detonation pressure *P*) of the prepared samples as well as the pure explosives were calculated by the use of EXPLO5 code [7] and the Kamlet & Jacobs method [8]. In the case of the EXPLO5 code, the BKWS set of parameters for the BKW EOS was applied, these parameters are: α = 0,5, β = 0,298, κ = 10,50, Θ = 6620. The calculated detonation characteristics of all the tested explosives are reported in Tables 2 and 2a.

TABLE 1. The data obtained from the experimental measurements

Sample		Formula	Mol. Weight [g/mol]	Heat of combustion [J/g]	Heat of formation [kJ/mol)
No.	Code designation				
1	BCHMX cryst.	$C_4H_6N_8O_8$	294,17	-9124	236,5
2	BCHMX-Semtex	$C_{6.66}H_{10.86}N_8O_{8.39}$	337,25	-12784	125,3
3	PETN	$C_5H_8N_4O_{12}$	316,15	-8182	-538,7
4	Semtex 10	$C_{8.05}H_{12.64}N_4O_{12.37}$	363,38	-11942	-646,8

TABLE 1a. The data obtained from the experimental measurements

Sample		Formula	Impact Sensitivity [J]	Friction sensitivity [N]	DTA peak [5ºC/min]	Kissinger slope EaR^{-1} [K]
No.	Code designation					
1	BCHMX cryst.	$C_4H_6N_8O_8$	3,2	88	225,3	-29355
2	BCHMX-Semtex	$C_{6.66}H_{10.86}N_8O_{8.39}$	16,8	258	202,5	-30812
3	PETN	$C_5H_8N_4O_{12}$	2,90	46	184,7	-26735
4	Semtex 10	$C_{8.05}H_{12.64}N_4O_{12.37}$	15,7	204	176,6	-30408

TABLE 2. Results of the experimental and calculated detonation characteristics

Sample		Experimental		Kamlet & Jacobs calculation		
No.	Code designation	Density [g/cm^3]	Detonation velocity *experiment* [m/s]	Detonation velocity *calculated* [m/s]	Detonation pressure [GPa]	Heat of explosion max. [kJ/kg]
1	BCHMX cryst.	1,79*	8650*	8843	34,5	6620
2	BCHMX-Semtex	1,57	7824	7617	23,6	5999
3	PETN	1,70**	8400**	8448	30,5	6340
4	Semtex 10	1,53	7486	7370	21,7	5708

TABLE 2a. Results of the experimental and calculated detonation characteristics

Sample		Experimental		EXPLO5		
No.	Code designation	Density [g/cm^3]	Detonation velocity *experiment* [m/s]	Detonation velocity *calculated* [m/s]	Detonation pressure [GPa]	Heat of detonation [kJ/kg]
1	BCHMX cryst.	1,79*	8650*	8755	32,8	6433
2	BCHMX-Semtex	1,57	7824	7869	23,1	5868
3	PETN	1,70**	8400**	8318	28,5	6160
4	Semtex 10	1,53	7486	7529	21,0	5545

* Reference [2]
** ICT thermochemical Data base, Pfinztal 2004

3. RESULTS AND DISCUSSION

According to the sensitivity tests, it is obvious from Table 1 that the drop energy needed to initiate the explosive crystals which were coated by the Semtex matrix is approximately 5 times higher than that needed to initiate the pure BCHMX and PETN.

The impact sensitivity of the plastic BCHMX-Semtex is slightly lower than Semtex 10. The Semtex matrix decreases impact sensitivity of BCHMX from 3,2 to 16,8 J just as it decreases the impact sensitivity of PETN from 2,9 to 15,7 J in case of Semtex 10. These results prove the efficiency of the Semtex matrix to decrease the impact sensitivity of the pure explosives. Regarding to the friction sensitivity, plastic BCHMX-Semtex has lower friction sensitivity than the original Semtex 10 as shown in Table 1a, where the Semtex matrix decreased the friction sensitivity of the pure explosives by approximately 3 to 4 times than in case of the corresponding crystalline explosives. From the measurements of the sensitivities for the prepared samples, it is obvious that plastic BCHMX-Semtex has a lower sensitivity to impact and friction than the original Semtex 10 as shown in Figure 3.

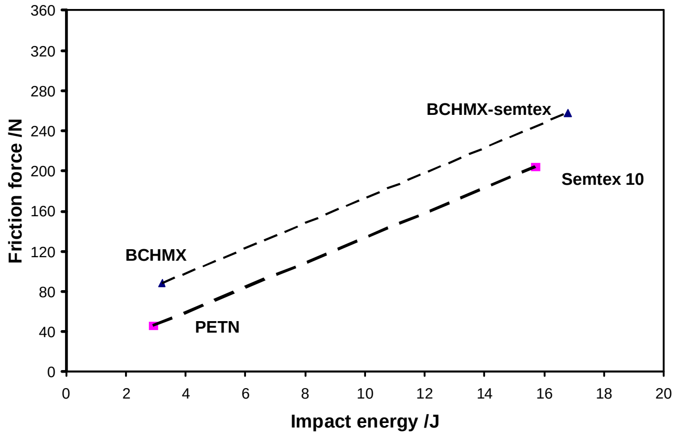

Fig. 3. Relation between the friction force for initiation and the impact energy for initiation of the samples

From the DTA results of the studied samples, it is observed from Figure 1 that the peak temperatures of the prepared mixtures are lower than that of pure explosives; this is most likely due to the presence of the inert plasticizer in the binder matrix which acts as a solvent for the pure explosives and decreases its thermal stability as reported in [15]. Experimentally determined detonation velocity of the plastic BCHMX-Semtex is higher than the original Semtex 10 by more than 300 m/s, in the mean time, BCHMX and its plastic composition are more thermally stable than PETN and Semtex 10 as shown in Fig. 4.

Regarding to the calculated detonation parameters, a linear relationship represented by a straight line was found between the calculated detonation pressure according to EXPLO 5 code and the experimentally determined ρD^2 of the studied explosives as shown in Fig. 5, which proves the correspondence between the experimental and the calculated results.

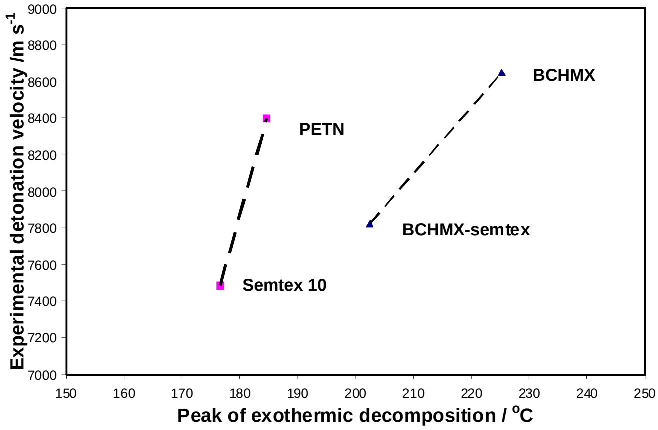

Fig. 4. Relationship between the experimental detonation velocities and DTA-peak temperatures (at 5°C/min)

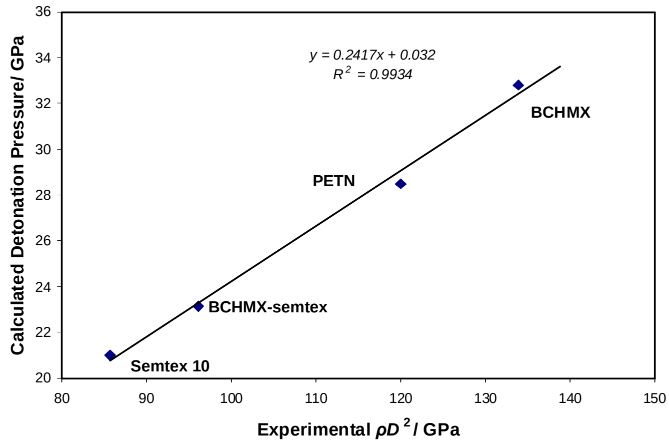

Fig. 5. Relationship between the calculated detonation pressure by EXPLO 5 code and experimental square of detonation velocity multiplied by initial density

It was observed from Fig. 6 that the addition of Semtex 10 matrix to the pure explosives increases its heat of combustion by approximately one and half times just as it decreases the heat of detonation, also the heat of combustion and the heat of detonation of plastic BCHMX-Semtex are higher than Semtex 10.

In Fig. 7, one can see a good linear relationship between the detonation pressures calculated by EXPLO 5 code and the calculated detonation pressure according to the Kamlet and Jacobs method while we observed higher calculated detonation pressure in case of the Kamlet & Jacobs method.

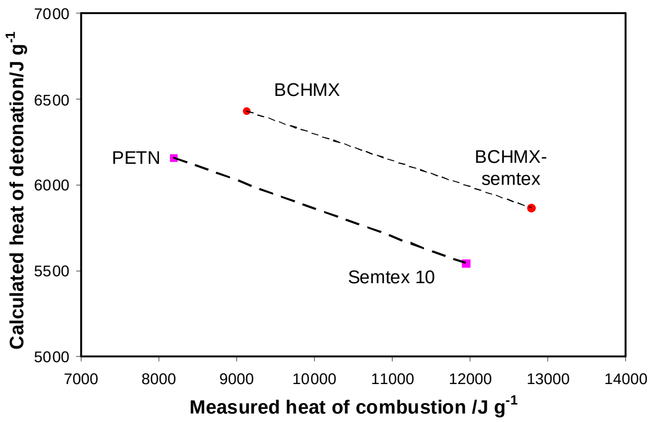

Fig. 6. Relation between calculated heat of detonation by EXPLO 5 and the measured heat of combustion

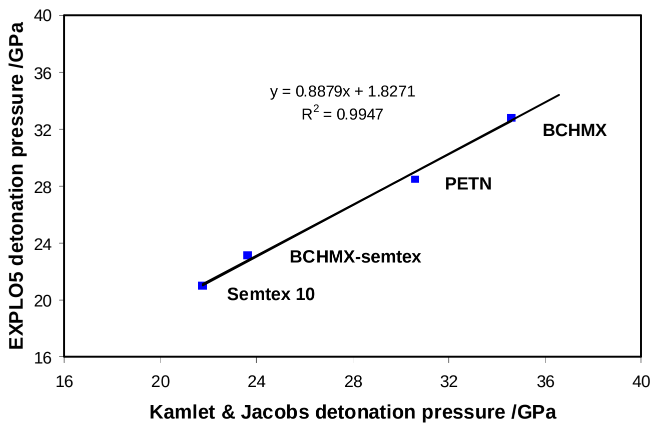

Fig. 7. Mutual comparison of the calculated values of detonation pressures by EXPLO5 with those from application of the Kamlet & Jacobs method

4. CONCLUSION

From this study it was concluded that the new plastic explosive which contains BCHMX as an explosive filler and a Semtex 10 matrix as a binder, has lower sensitivity to impact and friction than the original Semtex 10 and at the same time is more thermally stable. Also, the experimental measurements showed that the detonation velocity of the plastic BCHMX-Semtex is higher than that of the original Semtex 10 by more than 300 m/s and has higher heat of combustion. It was observed from the calculated detonation parameters that the heat of detonation, detonation pressure and detonation velocity of the new plastic BCHMX-Semtex are higher than Semtex 10. All the results indicate that replacement of PETN by BCHMX enhances all characteristics of the Semtex 10 plastic explosive.

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