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Thermochemical Calculations for Some Selected Advanced Plastic Bonded Explosives

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Abstract: The parallel demand of energetic and low sensitive explosive formulations makes it necessary to investigate the explosive properties of many explosive formulations to determine which formulation has the required performance parameters for specific applications. Thermochemical calculations have been used for a long time with considerable success as fast-effective tool to investigate the explosive performance parameters of different types of explosive mixtures that are candidate for a given practical application and to minimize high cost of experimental work needed to evaluate efficiently the performance parameters of new synthesized explosive compositions. In this paper; EXPLO5 steady state equilibrium program was used to calculate the explosive characteristics and performance parameters for a number of plastic bonded explosive (PBXs) formulations. These are mixtures of explosives, either classical or advanced, (RDX, HMX, PETN, CL-20 and Bicyclo HMX) and either inert or energetic binder (HTPB or GAP). Low sensitive and castable plastic bonded explosive formulations which satisfy the required performance parameters are selected. PBXs formulations containing CL-20 showed the highest values of detonation heat, detonation velocity, and brisance.

Keywords: Thermochemical calculations, Plastic bonded explosives, EXPLO5 steady state equilibrium program

1. Introduction

By the end of the first world war, the explosives development took the direction to improve the explosive performance, and as a result the sensitivity of explosives has been increased. Over the years, many accidents happened during handling, transporting, testing, and even manufacturing of explosives at which explosive chemists have always paid attention to increase performance without considering safety aspect. In July 1968 the aircraft carrier USS Forrestal on station in the gulf of tonkin, was conducting normal flight operations when a rocket inadvertently fired from an aircraft on the flight deck. The resulting fire and explosion cost the lives of 134 seamen, 74 million dollars in material damage to the carrier alone and operational loss of vessel for an extended period. In January 1969, a similar incident occurred aboard the USS enterprise, numerous deaths and severe damage occurred as a result of violent reaction of ammunition explosives. These accidents were results of what was termed "cook-off", at which confined explosives in ammunition were exposed to extreme heat such as a fuel fire. As a result, a violent reaction may occur leading to a high order detonation [1].

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The demand for increased safety in explosives handling, storage and transportation has led to the development of Insensitive Munitions (IM). The design of these explosives and weapons decreases the probability of unexpected detonation from external stimuli such as shock, weapon fragments, and heat. This can be achieved by modification of the external weapons system, explosive formulation or a combination of both [2].

The new trend in the field of explosives is to develop plastic bonded explosives with a significantly lower vulnerability to various stimuli than conventional high explosives that suffer from various disadvantages [3]. A plastic bonded explosive (PBX) is a term applied to various explosive mixtures where the crystals of high explosives are coated with a thin layer of polymeric material. PBXs have many advantages including; lower vulnerability and sensitivity to mechanical and thermal stimuli, improved mechanical properties, higher performance and detonation velocity due to safe-pressing to high densities, simplicity of the manufacturing technique (most of them produced by casting technique) and excellent chemical stability and resistance to humidity, so they have increased shelf life. Moreover, PBXs overcome the problems encountered with casted TNT. The first actually castable PBXs were developed in the early 1960s.These formulations were RDX or HMX dispersed in polyester or polyether prepolymers. These formulations were of relatively low viscosity and were processed in conventional mixing kettles. The virtues of these systems were the simplicity of mixing, ease of pouring, relative minor shrinkage during curing and resistance to elevated temperatures after curing [4]. This kind of PBXs was not problem-free. Their first problem was their considerable sensitivity to vibrations, shocks and other such impulses that in turn was directly attributable to the hard, brittle, and friable nature of the fully polymerized end products. Polyurethanes were introduced as binders for RDX or HMX-based explosives which resulted in more rubbery and less shock sensitive explosives. Several energetic binders and plasticizers were also developed to compensate performance loss upon using inert binders [5]. The incorporation of advanced explosive materials such as : CL-20, TATB, NTO, GAP, Bicyclo-HMX and HNS into plastic-bonded formulations was studied by many authors [6,7,8].

In this paper, thermochemical calculations were carried out to investigate the explosive properties of PBXs formulations that use a mixture of either classical or advanced explosives and different types of either inert or energetic binders to choose explosive formulations which satisfy the required performance parameters needed for the application of PBXs.

2. Thermochemical Calculations

2.1 Objective

Thermochemical calculations have been used for a long time with considerable success as an effective and fast tool to investigate the explosive performance parameters of different types of both pure explosives and explosive mixtures. The approach of thermochemical calculations became of great importance for choosing the explosive formulations that are candidate for a given practical application. Also, it is used to minimize high cost of experimental work needed to evaluate the performance parameters of new synthesized explosive compositions efficiently [9,10]. Recently, the parallel demand of energetic and low sensitive explosive formulations makes it necessary to investigate the explosive properties of many explosive formulations including modern types of energetic explosives to determine the explosive formulations that give the required performance parameters of the needed applications. In this work, the detonation parameters for several high explosive formulations proposed as comp- B substitutes were calculated using a computer program named EXPLO5.

2.2 EXPLO05 Program

EXPLO5 program, based on chemical equilibrium and steady-state model of detonation, uses the Becker-Kistiakowsky-Wilson equation of state (BKW EOS) for detonation gaseous products and Cowan-Fickett equation of state for solid products [11]. The input data required to run the program are the composition and density of each explosive formulation, figure (1). Window of start calculations is shown in figure (2). EXPLO5 program was used for calculation of the detonation parameters shown in table (1), while the explosion force (F) and brisance (B) were then calculated according to the following equations [12]

$$\mathbf{f = n\ R\ T_v} \qquad (1)$$

where: f = Explosion force [J/kg]; n = Number of moles of gaseous products / 1kg of explosive;.R = Universal gas constant; T_v = Explosion temperature [K].

And

$$\mathbf{B = f\ \rho\ D} \qquad (2)$$

where: B = Brisance [N/m.s)]; ρ = Density [kg/m^3]; D = Detonation velocity [m/s].

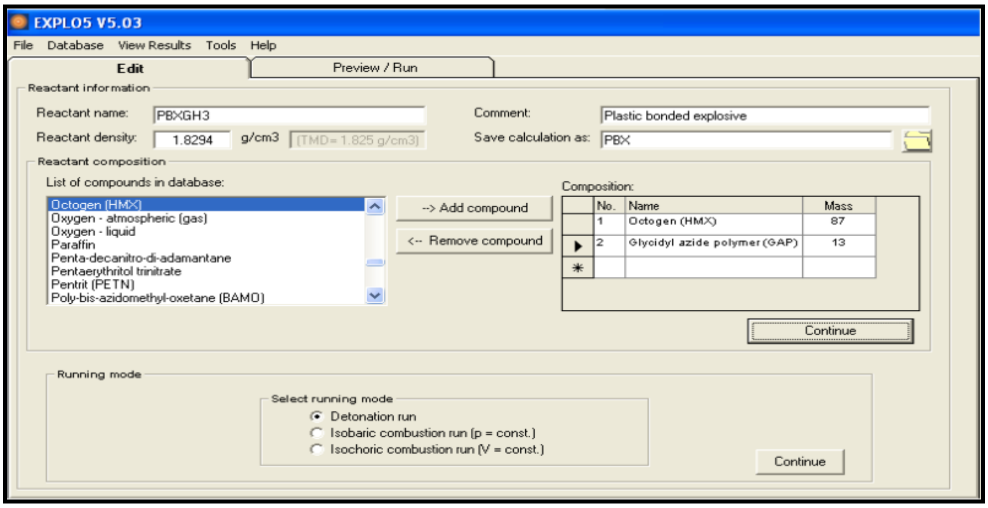

Figure 1: Window of data entry of EXPLO5 program

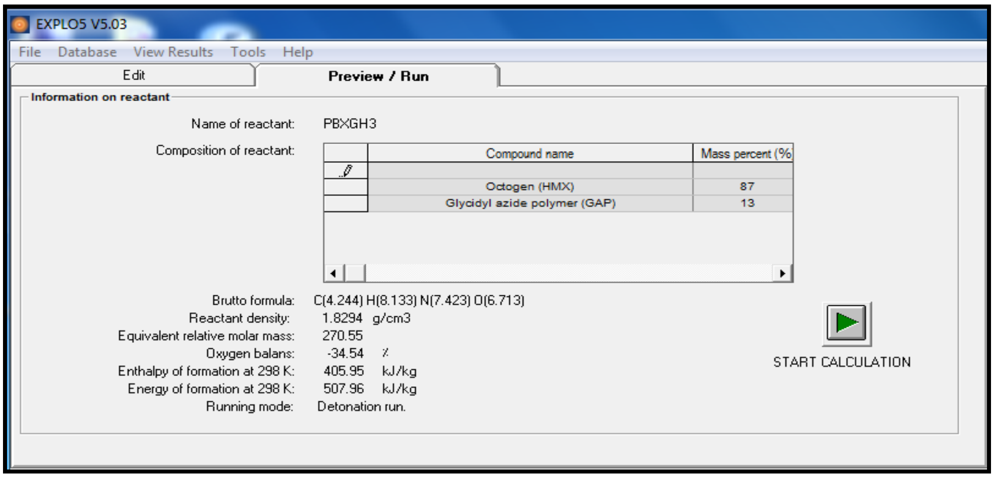

Figure2: Window of start calculations of EXPLO5 program

Table 1: Detonation parameters calculated by EXPLO5

Property	Units
Explosion heat (Q_v)	[kJ/kg]
Explosion temperature (T)	[K]
Explosion pressure (P)	[kbar]
Detonation velocity (D)	[m/s]
Moles of explosion products (n)	[per mole of explosive]
Specific volume (V_o)	l/kg

2.3 Compositions of Examined Plastic Bonded Explosives

Sample abbreviations of the examined formulations are shown in tables (2, 3, 4, 5 and 6). An example of the calculated explosive characteristics using EXPLO5 of PBX formulations containing RDX, HMX, PETN, CL-20 or Bi cyclo-HMX with polyurethane based on either HTPB or GAP is shown in table (7).

Table 2: Sample abbreviations of PBX formulations containing RDX

PBXs abbreviation	RDX (Wt %)	PU based on HTPB (Wt %)	PU based on GAP (Wt %)
PBXRT1	90	10	-
PBXRT2	88	12	-
PBXRT3	86	14	-
PBXRT4	84	16	-
PBXRT5	82	18	-
PBXRT6	80	20	-
PBXRG1	90	-	10
PBXRG2	88	-	12
PBXRG3	86	-	14
PBXRG4	84	-	16
PBXRG5	82	-	18
PBXRG6	80	-	20

Table 3: Sample abbreviations of PBX formulations containing HMX

PBXs abbreviation	**HMX (Wt %)**	**PU based on HTPB (Wt %)**	PU based on GAP (Wt %)
PBXHT1	90	10	-
PBXHT2	88	12	-
PBXHT3	86	14	-
PBXHT4	84	16	-
PBXHT5	82	18	-
PBXHT6	80	20	-
PBXHG1	90	-	10
PBXHG2	88	-	12
PBXHG3	86	-	14
PBXHG4	84	-	16
PBXHG5	82	-	18
PBXHG6	80	-	20

Table 4: Sample abbreviations of PBX formulations containing PETN

PBXs abbreviation	PETN (wt %)	PU based on HTPB (wt %)	PU based on GAP (wt %)
$PBXPT_1$	90	10	-
$PBXPT_2$	88	12	-
$PBXPT_3$	86	14	-
$PBXPT_4$	84	16	-
$PBXPT_5$	82	18	-
$PBXPT_6$	80	20	-
$PBXPG_1$	90	-	10
$PBXPG_2$	88	-	12
$PBXPG_3$	86	-	14
$PBXPG_4$	84	-	16
$PBXPG_5$	82	-	18
$PBXPG_6$	80	-	20

Table 5: Sample abbreviations of PBX formulations containing CL-20

PBXs abbreviation	CL-20 (Wt %)	PU based on HTPB (wt %)	PU based on GAP (wt %)
$PBXCT_1$	90	10	-
$PBXCT_2$	88	12	-
$PBXCT_3$	86	14	-
$PBXCT_4$	84	16	-
$PBXCT_5$	82	18	-
$PBXCT_6$	80	20	-
$PBXCG_1$	90	-	10
$PBXCG_2$	88	-	12
$PBXCG_3$	86	-	14
$PBXCG_4$	84	-	16
$PBXCG_5$	82	-	18
$PBXCG_6$	80	-	20

Table 6: Sample abbreviations of PBX formulations based on Bicyclo-HMX

PBXs abbreviation	Bicyclo-HMX (wt%)	PU based on HTPB (wt%)	PU based on GAP (wt%)
$PBXBT_1$	90	10	-
$PBXBT_2$	88	12	-
$PBXBT_3$	86	14	-
$PBXBT_4$	84	16	-
$PBXBT_5$	82	18	-
$PBXBT_6$	80	20	-
$PBXBG_1$	90	-	10
$PBXBG_2$	88	-	12
$PBXBG_3$	86	-	14
$PBXBG_4$	84	-	16
$PBXBG_5$	82	-	18
$PBXBG_6$	80	-	20

3. Results of Thermochemical Calculations

3.1 Heat of explosion (Q_v)

The measurement of the heat of explosion is analogous to the determination of the heat exchange in various chemical or physical processes. It is one of the most important characteristics of the explosive because it determines the efficiency of the explosive. It is clear from figures (3, 4) that the heat of explosion of PBXs formulations decreases as the weight percentage of PU binder increases. When comparing the values of explosion heat of the prepared PBXs formulations based on PU binder based on (HTPB or GAP), it was found that the formulations based on GAP have higher explosion heat than those formulations based on HTPB due to high oxygen balance, figures (5, 6).

3.2 Detonation velocity (D)

Detonation velocity of explosives represents the rate of energy delivery through explosive conversion. It has a great importance in fragmentation warheads at which there is a direct relation between the detonation velocity and fragment velocity. It is clear from figures (7, 8) that the detonation velocity of the PBXs formulations decreases as the weight percentage of PU binder increases, which confirms the fact that PU binder will not directly represent a reaction partner in the detonation zone; therefore PU reduces the reacting molecules in the detonation front. Explosive formulations based on PU/GAP give higher results than that based on PU/HTPB and from technological point of view, 14% binder is the minimum percentage that could be casted, e.g. for PBXCT3, detonation velocity decreased by approximately 8% compared with that of pure CL-20 but for PBXCG3 the decrease is approximately 4% compared with that of pure CL-20. This may be attributed to the higher density of GAP and to GAP energetic groups (Azide groups, oxygen atoms) and hence its higher conversion rate than that of HTPB, which contains only carbon and hydrogen atoms. Therefore, the comparison will be between the formulations based on 14% PU/GAP or PU/HTPB. From figures (9, 10) it is clear that the formulation PBXCG3 give the highest detonation velocity among other formulations.

3.3 Explosion force (F)

Explosion force represents the output work capacity of the decomposition gaseous products. It is also an important term in the calculation of brisance. The explosion force is calculated by equation (1). It is clear from figures (11, 12) that the explosion forces of PBXs formulations decreases as the weight percentage of PU binder increases. From figures (13, 14) it is clear that the formulation PBXBG3 give the highest explosion force among other formulations.

3.4 Brisance (B)

Brisance of an explosive is a very important term which represents the ability of explosives to disintegrate and fragment the solid object surrounding the explosive charge. The brisance of an explosive depends mainly on explosive density, detonation velocity (rate of energy delivery), composition of gaseous products, and explosion temperature. The brisance is calculated by equation (2). It is clear from figures (15, 16) that the brisance of the PBXs formulations decreases as the weight percentage of PU binder increases. Such behavior mainly due to the decrease in detonation velocity as the weight percentage of PU binder increases. Explosive formulations based on HTPB produce values of brisance much less than that of pure explosive, e.g for PBXCT3, the brisance decreased by about 54% compared with that of pure CL-20. This may be explained by the decrease of the brisant high explosive content (CL-20) and hence the decrease of oxygen balance (more negative), number of moles of gaseous products and detonation velocity of the prepared PBXs formulations. A better situation was obtained for the formulations based on GAP, where values of brisance were not much decreased, e.g PBXCG3, the brisance decreases by about 32% compared with that of pure CL-20. The values of brisance for formulations based on GAP are higher than those corresponding to compositions based on HTPB. From figure (17, 18), it is clear that the formulation PBXCG3 gives the highest brisance among other formulations.

4. Conclusion

From thermochemical calculation results, it can be concluded that PBX formulations based on 10% binder have the best performance parameters, but from technological point of view, 14% binder content is the minimum percentage that could be casted. Theoretical calculations obtained from EXPLO5 program showed that PBXs formulations containing PU based on GAP have the highest performance characteristics among other formulations containing PU based on HTPB because GAP is denser and more energetic since it has higher calorific value than HTPB. Formulations based on GAP have the highest values of heat of explosion, detonation velocity and brisance than those based on HTPB. Moreover, since CL-20 has high of formation and density (its performance is approximately 20% higher than standard explosives), then PBX formulations based on both CL-20 and GAP (PBXCG3) are good candidate explosives for air to air rockets provided with fragmentation warheads.

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