



Relative Explosive Strength and Detonation Characteristics of Some Explosive Mixtures Containing Urea and Peroxides

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Abstract. Several mixtures, based on urea, urea hydrogen peroxide complex (UHP), triacetone triperoxide (TATP) with some inorganic oxidants were studied by means of ballistics mortar with TNT as a reference standard. The detonation pressure, P , detonation velocity, D , detonation heat, Q , and volume of gaseous product at standard temperature and pressure conditions (STP condition) were calculated by the mean of Explo5 V6.3. The relatively high explosive strength of some samples relative to the TNT charge, focuses on the positive influence of hydrogen peroxide presence in these mixtures, with advantage in the form of its complex with urea (i.e. as UHP).

This influence connects with hydroxi-radical in the mixture under its initiation (as the first intermediate of this initiation reaction).

Keywords: urea, hydrogen peroxide, perchlorate, nitrates, ballistic mortar, Explo5

1. INTRODUCTION

Mixtures on the basis of ammonium nitrate (AN) and urea (U) are used as liquid nitrogen fertilizers, referred to as UAN, [1] with melting point from -18 till -5°C (depending on a content of water) and as intermolecular castable industrial explosives named Carbatols [2, 3] with relatively high density, detonation velocity and resistibility against initiation [2]. A subject of the practical interest, also mixtures on the basis urea nitrate (UN) are [4, 5], unfortunately not seldom from the point of view of their criminal misuse [6-8]. Globally, commercial availability of urea hydrogen peroxide (UHP) and its explosive performance when mixed with the same inorganic salts were not studied till now, therefore, in this paper attention is paid to them in comparison to several other mixtures with peroxides [8-11] and/or ammonium nitrate content.

2. EXPERIMENTAL

2.1. Materials

From the used substances the urea hydrogen peroxide complex (UHP) has not been studied in more detail yet from the point of view of its using in explosive compositions. Density of UHP is 1.4 g cm^{-3} , it is a white crystalline substance that melts with decomposition at $80-90^{\circ}\text{C}$. Thermal decomposition kinetic study of UHP gave activation energy of 113 kJ mol^{-1} with a frequency factor of 10^{-13} s^{-1} [12]. UHP is well known commercially as, hydrogen peroxide carbamide, Exterol, Hydroperit, Hyperol, Orti2on, Percarbamid, Percarbamide, Perhydrit, Perhydrol-Urea, and Thenardol [13]. It is mainly used in the cosmetics and pharmaceutical industry as a disinfecting and bleaching agent. It has been employed as the active ingredient in tooth whiteners [14] and dentifrice formulations which are sold in the United States as over-the-counter drugs. It is used as a topical disinfectant and mouthwashes, as earwax remover and as a hairdresser's bleaches [15].

2.2. Preparation of mixtures

Each the urea (U) and/or UHP embankment was mixed mechanically with ammonium nitrate (AN), ammonium perchlorate (APc) and sodium nitrate (SN). By mixing of the U, Al, and AN components results relatively homogenous mixtures were obtained. The actual wt % was introduced in Table 1.

These mixtures were mixed to have oxygen balance (OB) near zero which provided high power and low toxicity of generated gaseous product.

Four mixtures based on triacetone triperoxide (3,3,6,6,9,9-hexamethyl-1,2,4,5,7,8-hexoxonane, TATP) with AN and different percentage of water (4.2, 9.9, 15.5 and 24.5%, respectively) were previously studied [9,10] and compared with the studied mixtures.

2.3. Calculations of detonation characteristic

The theoretical detonation characteristics (i.e. detonation velocity, detonation energy and volume of gaseous products) of the tested mixtures were calculated by the use of the Explo5 code, version V6.3. The calculation of detonation parameters is based on the chemical equilibrium steady-state ideal detonation model. The state of gaseous detonation products is described by the Exp-6 equation of state, based on the statistic mechanical theories and Exp-6 potential. The detonation velocity, detonation energy and amount of gaseous detonation products calculated by Explo5 are summarized in Table 1.

It is very likely that some of the tested explosives mixtures have non-ideal detonation behavior, particularly those containing aluminum and ammonium nitrate. However, in this study we calculated detonation properties assuming ideal detonation model for all the mixtures (such calculation gives theoretically maximum detonation properties, i.e. properties at infinite explosive charge diameter), except for aluminum containing mixtures for which we carried out calculation in two ways; assuming that Al completely reacts at the CJ state (this gives higher D , p , Q , T values) and assuming that Al does not react, i.e., remains as solid Al.

2.4. Relative explosive strength measurement

A ballistic mortar test was used for the determination of the relative explosive strength of the samples studied, using TNT as reference [16-18]. It substitutes the Trauzl test in the lead block, which was used in the past but had some disadvantages such as high cost, using toxic lead and rupturing of a lead block [16]. A fixed amount of a tested explosive (10 g) was wrapped in polypropylene foil and inserted into the mortar enclosed by a steel projectile and fired using a nonelectric detonator (No. 8). For each measurement, a part of the non-electric detonator is inserted in the sample and fired by match. Three measurements were made for each sample and the mean values are reported in Table 1. The determination is based on measuring the swing angle of the pendulum and by comparing the measurement with a calibration curve for the standard explosive (TNT) at different masses.

Table 1. Energetic mixtures and their characteristics

Sample No.	Content of individual components in the mixture (in % of wt.)							
	Urea	UHP	AN	APc	NaNO ₃	H ₂ O	TATP	Al
A ^a	-	-	66.7 ^a	-	-	24.5 ^a	8.8 ^a	-
B ^a	-	-	78.8 ^a	-	-	9.9 ^a	11.3	-
C ^a	-	-	51.5 ^a	-	-	15.5 ^a	33.0	-
D ^a	-	-	90.9 ^a	-	-	4.2 ^a	4.9 ^a	-
E	-	37.0	63.0	-	-	-	-	-
F	-	37.0	-	63.0	-	-	-	-
G	-	56.5	-	-	43.5	-	-	-
H	20.0	-	80.0	-	-	-	-	-
I	29.8	-	-	70.2	-	-	-	-
J	37.0	-	-	-	63.0	-	-	-
N	10.2	-	80.8	-	-	-	-	9
N1	10.2	-	80.8	-	-	-	-	9
UHP	-	100	-	-	-	-	-	-
UN	-	-	-	-	-	-	-	-
TNT	-	-	-	-	-	-	-	-

Sample No.	Exper. density (g.cm ⁻³)	RS % TNT	Calculated detonation parameters				Oxygen balance OB (%)
			P (GPa)	D (m s ⁻¹)	Q _v (kJ kg ⁻¹)	V (dm ³ kg ⁻¹)	
A ^a	1.10	72.0 ^a	7.8	5587	2898	1118	0.02
B ^a	1.10	100.5	8.9	5838	3876	1063	-1.33
C ^a	1.10	78.7 ^a	9.7	5997	3615	1002	-39.60
D ^a	1.10	100.5	7.6	5461	2739	1066	10.76
E	1.06	108.2	7.6	5497	3362	1059	0.00
F	1.04	121.0	6.0	4821	3026	937	8.86
G	1.25	88.5	6.8	4978	3035	744	1.12
H	1.15	100.6	9.4	5972	3297	1059	0.00
I	1.38	114.1	14.0	6539	3614	922	0.08
J	1.64	0	12.6	6269	2915	603	0.07
N	1.1	113.4	6.0	4910	2218	967	0.19
N1	1.1	113.4	7.76	5370	4804	909	0.19
UHP	0.94	0	12.8	4567	1617	953	-34.01
UN	0.9	90.7	4.6	4547	2735	981	-6.50
TNT	1.0	100.0	7.2	5145	3825	567	-59.34

Notes: ^{a)} taken from Ref. 9

Data for the mixture N were calculated taking aluminum as an inert admixture, for the mixture N1 this aluminum has reacted fully in the CJ point.

The explosive strength of the tested explosive was thus expressed relative to TNT (relative explosive strength, RS as % TNT) and compared with previously studied TATP samples from Ref [10]. Three measurements were made for each sample and the mean values are reported in Table 1.

3. RESULTS AND DISCUSSION

3.1. Explosive strength versus detonation pressure

In the PBX explosives uniquely proportional dependence of the Relative Explosive Strength (RS) on the product ρD^2 exists [17]; the product is a representative of detonation pressure and the RS values were in this case also determined by ballistics mortar [17]. But, in the studied mixtures only lines I and II in Fig. 1 correspond to the same course of the mentioned dependence; the TNT data (1.0 g cm^{-3}) are situated on line II. For further discussion it should be stated here, that thermal decomposition of hydrogen peroxide, i.e. homolysis of the peroxide HO-OH bond, has been identified as the dominant chain-branching reaction [19] that controls given charge ignition.

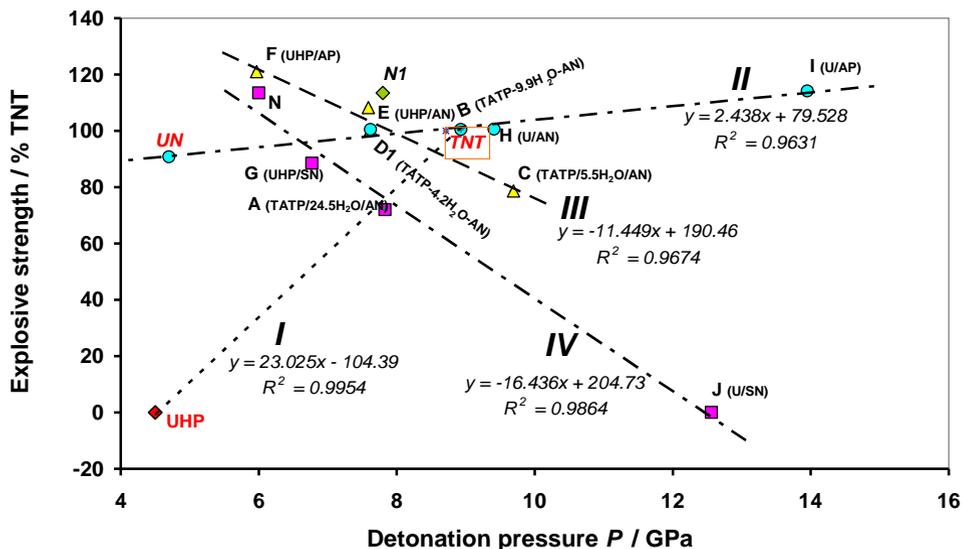


Fig. 1. Mutual relationship between experimental relative explosive strength and calculated detonation pressure of the studied mixtures

On opposite course of line III, the reactive radicals might have a strong influence (OH-radicals and radicals, derived from chlorine intermediates of decomposition in the mixture F) with absence of cooling water admixture in the samples F and E, i.e., the decomposition velocity of the mixtures F and E in a chamber of ballistics mortar could have been higher as it is in the case of other mixtures. The mixture C is already “cooled” by the present water and negative oxygen balance (-39.6%).

The said supposition about influence of very reactive radicals (in this case for OH) is possible to show on the basis of mutual comparison of positions in Fig 1 of the mixture couples of F and I, E and H and mainly by the couple G and J.

Course of line IV is influenced by solid particles in decomposition products and in the case of the mixture A by a relatively high content of water. Concerning the aluminized mixture N, the point N1 in Fig. 1 corresponds to assumption that Al completely reacts in CJ point and, on the other hand, the point N to unreacted solid Al. It seems the second one correlates logically with line IV.

3.2. Explosive strength versus heat content of gaseous products of detonation

Interesting is mutual comparison of relative explosion strength and heat content of gaseous products of explosion (i.e. ratio $Q \cdot V^1$) according to Fig. 2; this content is used in appraisal of permissible industrial explosives [2].

In this Figure lines I, II and III correspond to expectation – to increasing RS raising in this heat content corresponds. Line IV in Fig. 2 is as if dividing line between “hot” (above line) and “cold” mixtures; this line practically corresponds to RS of TNT.

Line V in Fig. 2 has opposite running – the mixtures N and J have solid particles in detonation products, all mixtures of this line have relatively low the Q values and three from them contains urea or its derivatives (mixtures N, UN and J).

Similarly to Fig. 1, also in Fig. 2 the data for aluminized mixture with unreacted Al correlates with opposite running of the presented relationship, i. e. here the point N on the line V, while the data for case of the Al reaction in CJ point are outside of all partial relationships of this figure (point N1).

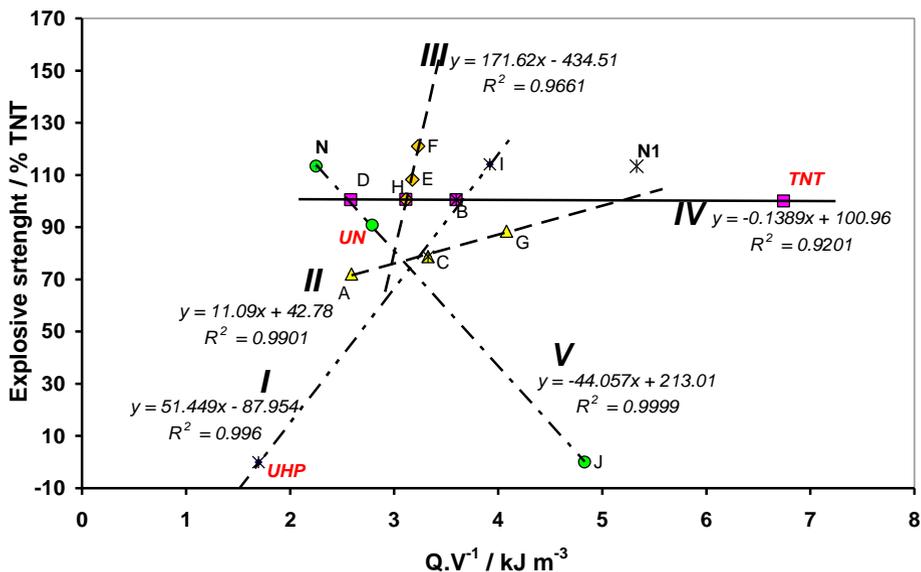


Fig. 2. Mutual relationship between experimental relative explosive strength and heat content of the gaseous products ($Q.V^{-1}$) of the studied mixtures detonation.

4. CONCLUSION

Based on theoretical calculation, it can be concluded that it is possible to prepare explosive mixtures based on urea, with explosive strength better than TNT. Their performance can be perceivably positively influenced by the presence of hydrogen peroxide in their composition, with advantage in form of its complex with urea (UHP). This influence is notable, namely in the application of sodium nitrate as an oxidant in these mixtures. Chemical nature of the mentioned effect lies in the reactive hydroxi-radical formation as the first intermediate in the given mixture initiation.

Theoretical calculation is done assuming ideal detonation model, so calculated detonation properties of the mixtures correspond to theoretical maximum that can be obtained at infinite diameter of explosive charge. In accordance with current knowledge on burning of metal powders in reaction zone, it can be assumed that calculation carried out taking aluminum does not react at the CJ point gives more realistic results for the studied mixtures.

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