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Some properties of explosive mixtures containing peroxides
Part I. Relative performance and detonation of mixtures
with triacetone triperoxide

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Abstract

This study concerns mixtures of triacetone triperoxide (3,3,6,6,9,9-hexamethyl-1,2,4,5,7,8-hexoxonane, TATP) and ammonium nitrate (AN) with added water (W), as the case may be, and dry mixtures of TATP with urea nitrate (UN). Relative performances (RP) of the mixtures and their individual components, relative to TNT, were determined by means of ballistic mortar. The detonation energies, E_0, and detonation velocities, D, were calculated for the mixtures studied by means of the thermodynamic code CHEETAH. Relationships have been found and are discussed between the RP and the E_0 values related to unit volume of gaseous products of detonation of these mixtures. These relationships together with those between RP and oxygen balance values of the mixtures studied indicate different types of participation of AN and UN in the explosive decomposition of the respective mixtures. Dry TATP/UN mixtures exhibit lower RP than analogous mixtures TATP/AN containing up to 25% of water. Depending on the water content, the TATP/AN mixtures possess higher detonability values than the ANFO explosives. A semi-logarithmic relationship between the D values and oxygen coefficients has been derived for all the mixtures studied at the charge density of $1000 \, \text{kg m}^{-3}$. Among the mixtures studied, this relationship distinguishes several samples of the type of "tertiary explosives" as well as samples that approach "high explosives" in their performances and detonation velocities.
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1. Introduction

At present, properties of triactone triperoxide (3,3,6,6,9,9-hexamethyl-1,2,4,5,7,8-hexoxonane, TATP) are well known and published in encyclopedias [1,2]. However, its mixtures with ammonium nitrate and urea nitrate have not been sufficiently described yet. The first representatives of such mixtures were suggested, e.g., for blasting jobs in coal mines [3], and at present they are misused by terrorists in their attacks (e.g., Marocco on 16 May 2003) [4]. The mixtures of TATP with urea nitrate (UN) are not attractive; applications of TATP as initiators of UN have attracted attention of assassinators, e.g., in the Middle East [5]. TATP has not found technological applications due to its low

physical stability (high volatility and its tendency to recrystallize while stored creating large crystals). However, performance and detonation characteristics of TATP and its mixtures with oxidizing agents were not studied so far.

In this paper, therefore, attention is focused on relative performance (RP), detonation parameters of the said TATP mixtures. The RP values were evaluated on the basis of measurements using the ballistic mortar and compared to theoretical values calculated by CHEETAH code [6].

2. Experimental

2.1. Substances

2.1.1. Triacetone triperoxide

The triacetone triperoxide (TATP) was prepared by reaction of acetone with hydrogen peroxide. The reaction was catalyzed

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by hydrochloric acid. After its separation from reaction mixture by filtration on the papery filter (Filtrak 388), TATP was not dried, and was immediately used for preparing the TATP mixtures. Quality of this product was checked by differential thermal analysis.

2.1.2. Nitrates

Ammonium nitrate was a product of Synthesia Ltd., Pardubice; it was sieved and the fraction below 0.5 mm was used for preparation of the mixtures. Urea nitrate was prepared from water solution of urea and nitric acid.

2.2. Preparation of mixtures

Wet TATP was carefully mixed with dry ammonium nitrate and the explosive mixture was immediately filled into the tin foil (RP measurement) or plastic tube (mixture no. VII). The casings of charges were made from PVC tubes (inner diameter 12.3, 16.5, 28, 46 and 105 mm; wall thickness 1.8–2.2 mm). The composition of the mixtures and their codes are listed in Table 1. Unlike TATP/AN/W mixtures dry TATP and UN were used for preparation of TATP/UN mixtures.

2.3. Relative performance of TATP mixtures

The relative performance values (RP) were determined by measurements in ballistic mortar [7,8] and the values are reported as a relative performance of TNT (RP). For the measurement, the tested explosive was wrapped in a tin foil and initiated by detonator no. 8. Three tests were carried out for each sample. The averaged values are summarized in Tables 2 and 3.

Table 1
Content of the triacetone triperoxide (TATP), ammonium nitrate (AN), urea nitrate (UN) and water in the studied mixtures

Code of mixture	Content of the components (wt.%)			
	TATP	AN	UN	Water
I	4.9	90.9	–	4.2
II	8.8	66.7	–	24.5
III	11.3	78.8	–	9.9
IV	11.3	88.7	–	–
V	11.7	88.3	–	–
VI	22.4	15	–	62.6
VII	26.0	54.0	–	20.0
VIII	33.0	51.5	–	15.5
IX	42.2	21.2	–	36.6
X	42.6	14.3	–	43.1
XI	44.5	34.5	–	21.0
XII	53.6	21.2	–	25.2
XIII	57.9	14.8	–	27.3
XIV	2.0	–	98.0	–
XV	4.1	–	95.9	–
XVI	10.0	–	90.0	–
XVII	15.0	–	85.0	–
XVIII	20.0	–	80.0	–
XIX	40.0	–	60.0	–
XX	60.0	–	40.0	–
XXI	80.0	–	20.0	–

2.4. Determination of detonation velocities

The tests were performed in accordance with the binding procedure approved by the Czech Mining Authority [7]. Four to six sensors (depending on the length of charge) at the distances of 40 mm were introduced into the explosive substance through the casing of charge. The individual sensors were interconnected by means of coaxial cables with the RC circuit, which was connected with an oscilloscope Tektronix RDS 3014B. The initiation of mixture VII was accomplished by means of Initiator no. 8 with the priming charge of 50 g Semtex. The results are presented in Table 3. For comparison, we also used the detonation velocities of charges of ANFO explosive composed of 5.5% of fuel oil and 94.5% of AN (placed in steel tubes), taken from ref. [9].

2.5. Calculation of detonation characteristics

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 CHEETAH code [6]. CHEETAH is a computer program for calculating the thermodynamic properties of non-ideal heterogeneous systems of known atomic composition described by arbitrary equations of state. The physical properties of gaseous species are described by the Becker–Kistiakowsky–Wilson (BKW) [10] equation of state (EOS). For the determination of equilibrium composition, the method based on the minimization of free energy is used. The allowed thermodynamic states behind a detonation wave are intersections of the Rayleigh line (expressing conservation of mass and momentum), and the Hugoniot shock adiabate (expressing conservation of energy). The Chapman–Jouguetr (CJ) theory states that a stable detonation occurs when the Rayleigh line is tangent to the shock adiabate.

In this work, the BKWC set of parameters for the BKW EOS was applied in calculations: $\alpha = 0.5$, $\beta = 0.403$, $\kappa = 10.8$, $\Theta = 5441$ [6]. The detonation velocity, detonation energy [11] and amount of gaseous products of detonation were estimated from CHEETAH calculations. The results are summarized in Tables 2 and 3.

2.6. Oxygen balance

For the purposes of this paper, the oxygen balance (OB) of energetic material with summary formula $C_aH_bN_cO_d$ is expressed as a dimensionless oxygen coefficient α [25]

$$\alpha = \frac{d}{2a + 0.5b} \tag{1}$$

Zero oxygen balance corresponds with $\alpha = 1$.

3. Results and discussion

3.1. Aspects of evaluation of relative performance by ballistic mortar

According to Taylor and Morris [12] the ballistic mortar permits the "strength" of an explosive to be expressed in absolute

Table 2
Calculated detonation velocities, detonation energies, oxygen coefficients and theoretical volumes of gaseous product of detonation, frozen at 1800 K, and measured values of relative performance for TATP/AN mixtures

Code of mixture	Calculated data					Experimental relative performance (% TNT)
	For density (g cm^{-3})	Detonation velocity (m s^{-1})	Detonation energy (J cm^{-3})	Oxygen coefficient, α	Volume of gases at 1800 K (dm^3 kg^{-1})	
I	1.0 1.1	4693 5037	2585 2844	1.234	1070	100.5
II	1.0 1.1	4716 5063	2725 2997	1.018	1119	72.0
III	1.0 1.1	5128 5495	3667 4031	0.974	1080	100.5
IV	0.7 1.0 1.1	4261 5312 5687	2990 4272 4699	1.010	1042	114.0
V	0.7 1.0 1.1	4282 5337 5714	3053 4361 4798	0.998	1041	114.0
VI	1.0 1.1	3177 3430	668 734	0.376	1096 1195	6.5
VII	1.0 1.1	4879 5169	3114 3517	0.604	1114 1102	81.0
VIII	0.9 1.1	4733 5270	3022 3902	0.532	1119 1089	78.7
IX	1.0 1.1	4395 4689	2727 3047	0.341	1087 1082	37.2
X	1.0 1.1	4213 4515	2395 2655	0.269	1095 1093	30.7
XI	0.9 1.1	4565 5097	3027 3913	0.238	1098 1069	59.1
XII	0.9 1.1	4457 5011	3049 3928	0.318	1080 1052	45.0
XIII	0.9 1.1	4410 4978	3055 3929	0.285	1071 1045	53.1

Table 3
Calculated detonation velocities, detonation energies, oxygen coefficients and theoretical volumes of gaseous product, frozen at 1800 K, of detonation and measured values of relative performance for TATP/UN mixtures, AN, UN and TATP

Code of mixture	For density (g cm^{-3})	Calculated data				Experimental relative performance (% TNT)
		Detonation velocity (m s^{-1})	Detonation energy (J cm^{-3})	Volumes of gases at 1800 K (dm^3 kg^{-1})	Oxygen coefficient, α	
XIV	1.0	4850	2713	862	0.846	81.0
XV	1.0	4858	2745	860	0.806	79.4
XVI	1.0	4877	2861	855	0.709	70.3
.XVII	1.0	4890	3002	850	0.642	67.8
XVIII	1.0	4903	3145	840	0.586	66.3
XIX	1.0	4958	3079	820	0.429	62.6
XX	1.0	5032	4261	800	0.333	60.9
XXI	1.0	5115	4806	780	0.269	60.9
AN	1.0	4171	1585	980	1.50	0
UN	1.0	4819	2699	865	0.888	78
TATP	1.0	5199	5347	755	0.222	61.7

Table 4
Results of detonation velocity measurements

Sample	Internal diameter (mm)	Density of charge (g cm^{-3})	Detonation velocity (m s^{-1})
No. VII[a]	12.3	1.29	2520
	16.5	1.29	2880
	28.0	1.19	4110
	46.0	1.16	4400
	105.0	1.28	4810
ANFO[b]	38	[c]	2600
	51		2920
	63		3050
	70		3300
	80		3450
	100		3650
	150		3970

[a] Designation according to Table 1.
[b] Diameters and detonation velocity values taken from Ref. [9].
[c] Not present in the original paper [9].

units. The term "strength" means the maximum mechanical work which the explosive products are capable of performing when utilized most efficiently in a given expansion [12]. Cooper, referring to application of ballistic mortar, points out the following facts [13]. In an ideal explosive, essentially all of the chemical reaction is completed in the Chapman–Jouget (CJ) zone of the detonation wave, and the gases expand isentropically from that point on down. However, in a non-ideal explosive, only a part of the chemical reaction is completed in the CJ zone, the balance of the reaction is completed in the expansion behind the CJ plane. This is markedly seen in the explosive mixtures whose homogeneity is not ideal [14]. This means that the expansion is not isentropic since the chemical reaction is producing additional energy during the expansion. Thus this kind of explosives releases the unstable expansion energy in a way different from TNT or other ideal explosives [13]. RP of explosive is also closely connected with the density of its charge [14]. However, Pagowski and Subocz [15], and later on Buczkowski et al. [16] found and confirmed that the results of measurements obtained with the use of ballistic mortar are not affected by the density of explosive and the degree of its homogeneity. This is due to a relatively long-term retention of gaseous products of explosive decomposition of tested sample in the chamber of ballistic mortar (a consequence of the relatively high mass of projectile); thus, these products have the possibility of perfect mixing and completion of reaction [15] (Table 4).

3.2. Components decomposition pathways

A number of studies show (see Ref. [17] and references herein) that the chemical micro-mechanism of primary splitting of initiation and development of detonation of energetic materials is identical with the primary mechanism of their splitting in low-temperature thermal decomposition.

In the case of TATP, methods of quantum chemistry were utilized to predict the primary products of its thermal decomposition [18], i.e. oxygen, acetone and unstable acetone monoperoxide, whose formation is preceded by primary homol-

ysis of –O–O– bond [18]. By means of a *ReaxFF* monomolecular molecular-dynamic cookoff simulation it was found [19] that the initiation of TATP decomposition in the condensed phase is dominated by a monomolecular process [19]. This simulation demonstrates that this initiation is entropy-driven, since the initial reaction is almost energy-neutral [19].

The decomposition mechanism of the best known oxidizer, ammonium nitrate (AN), is given below. In the solid state, AN is dissociated according to the following equilibrium [20,21]:

$$NH_4NO_{3(s)} \rightleftharpoons NH_{3(g)} + HNO_{3(g,1)} \tag{2.1}$$
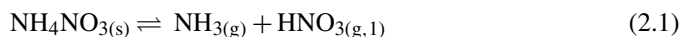
Another decomposition of AN takes place through nitration of ammonia [20,21]:

$$NH_{3(g)} + HNO_{3(g,1)} + H^+$$
$$\rightarrow H_2O + NH_3NO_2^+ \rightarrow H_2O + H_3O^+ + N_2O \tag{2.2}$$
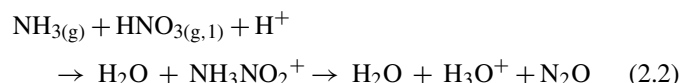
and the main decomposition can be accompanied by side reactions [20]

$$NH_4NO_3 \rightarrow N_2 + 0.5O_2 + 2H_2O \tag{2.3}$$

$$NH_4NO_3 \rightarrow 0.8N_2 + 1.8O_2 + 0.4HNO_3 \tag{2.4}$$
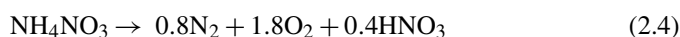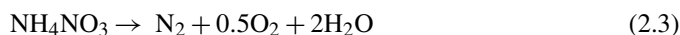
Quantum-chemical methods were used to study the mechanism of primary thermal decomposition of urea nitrate [22,23]. Nitric acid plays a catalytic role for the (1,3)-H-shifts in urea by acting as a donor of the first and an acceptor of the second proton-transfers in a relay fashion. The double proton transfer takes place in the carbonyl/hydrogen bond complex, and its result is breakdown of the urea moiety of UN giving HNCO and NH$_3$ fragments [23].

Depending on the pressure and temperature, two main decomposition pathways are suggested on the basis of experimental data [22,23] (a mechanism of the eight-center pathway of HNO$_3$-catalyzed UN transformation in the sense of Scheme 3.1; see in Ref. [23])

$$[(NH_2)_2COH]NO_3 \rightarrow NH_4NO_3 + HNCO \tag{3.1}$$

$$[(NH_2)_2COH]NO_3 \rightarrow N_2O + CO_2 + NH_3 + H_2O \tag{3.2}$$
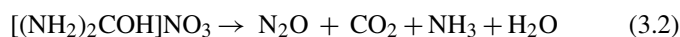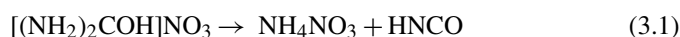
TATP represents the most reactive component in the mixtures TATP/AN and TATP/UN. The radicals resulting from the homolysis of –O–O– bonds (or also ozone, as the case may be, one of the final products in this decomposition [18]) should primarily react with NH$_3$ (this is also the reaction on which a method of liquidation of ozone is based [24]); in the presence of pressure impulse, thus the decomposition of oxidizer (AN or UN) would be initiated. On the basis of the mentioned pieces of knowledge about primary processes in decomposition of AN and UN, the former should be more accessible for the TATP splitting fragments and – in this sense – more reactive.

3.3. Relationship between relative performance and energy of detonation

Cooper, using a set of 62 explosives of chemically different types, showed that their CJ pressure and PV energy in CJ zone
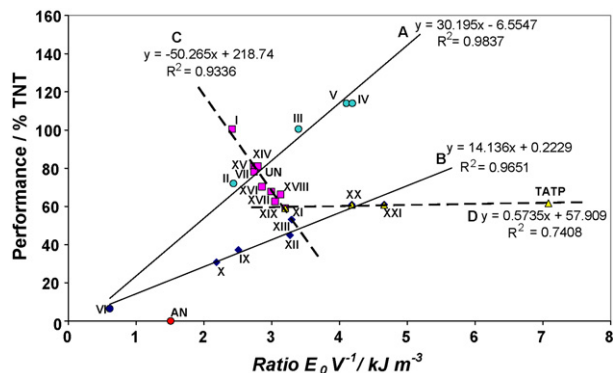
Fig. 1. Relationship between relative performance of the studied mixtures and the ratio of detonation energy, E_0, and volume, V, of gaseous detonation products frozen at 1800 K.

Fig. 2. Relationship between the relative performance and oxygen coefficient α of the studied mixtures.

do not correlate with the results of measurements carried out on ballistic mortar [13]. In our case the relationships between energy of detonation and relative performance is possible to find. However, for deriving the dependences of RP we chose the ratio of E_0 values and volumes of detonation products, V; this approach is a modification of the evaluation method used for permissible explosives, where one of the characteristics is the ratios of heats of explosion, Q, and the values of V [25]. The thing is that the majority of studied TATP mixtures contain water, i.e. a cooling component. High-nitrogen compounds, such as nitrates of urea derivatives, or guanidine, have low Q values and (to a certain extent) act as cooling components in the explosive mixtures containing them [25].

The values of ratios E_0V^{-1} of the TATP mixtures investigated (the values of E_0 for the charge density of $1000\,\mathrm{kg\,m^{-3}}$) correlate with the found relative performances in the sense of Fig. 1. It can be seen that line A includes data of the mixtures with the AN content predominating over the TATP content. On the other hand, line B corresponds to the TATP/AN mixtures whose TATP content predominated over the AN content. The data of mixture VI correlate with both the lines mentioned; however, the detonation ability of this mixture is very doubtful (at the experimental conditions its sample probably underwent a thermal explosion). Dry mixtures TATP/UN are represented in Fig. 1 by a two-segment line: C (UN content above 50%) and D (TATP content above 50%). The data of mixtures containing an excess of TATP (XX, XXI) approach line B. The data of UN and its high-percentage mixtures XIV and XV correlate with line A. Mixture I on the basis of AN with positive oxygen balance ($\alpha = 1.234$) correlates with line C (here might be some similarity between decompositions 2.4 and 3.2).

The opposite course of relationship C as compared with the relationships for TATP/AN mixtures in Fig. 1 is probably connected with the low heat of explosion of UN and its possible effect upon the degree of completion of reaction of the products of primary splitting in the chamber of ballistic mortar (it is also connected with the differences between the courses of primary splitting of AN and UN molecules). This is also confirmed by the relationship of performance values and the oxygen coefficient α in Fig. 2 (for nitro compounds, nitramines, nitrate esters and aluminized explosives see in Ref. [10]): curve H for dry
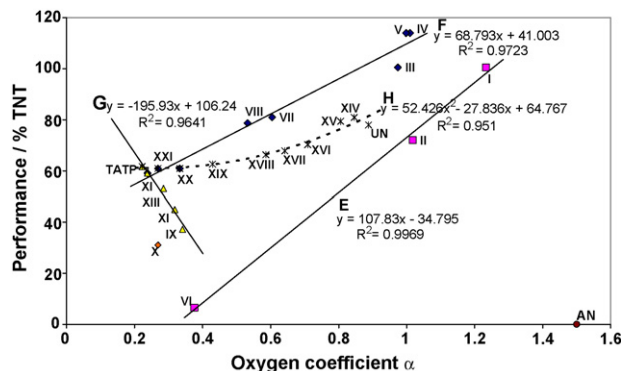
TATP/UN mixtures supports the idea of different mechanism of the course of their explosive transformation as compared with that of the TATP/AN mixtures; it should be pointed out that these mixtures exhibit lower performances than those observed with the TATP/AN mixtures containing up to 12% of TATP and up to 25 wt.% of water (line F). The data of the TATP/UN mixtures with high TATP content, namely XX and XXI, correlate with line F. The data of pure TATP lie on line G valid for TATP/AN mixtures containing over 40 wt.% of TATP and over 20 wt.% of water: the relatively high water content results in negative slope of line G. The thermochemical aspects of explosive decomposition result in the existence of line E.

The said thermochemical aspects, i.e. the combined effects of oxygen balance and water content in the TATP/AN mixtures upon the performance, are documented in Fig. 3: the x axis represents a dimensionless sum of oxygen coefficient α and molar ratio of water W and AN in the mixture. Line I in this diagram corresponds to the TATP/AN mixtures containing less than 25 wt.% of water. Line J combines data of the mixtures containing more than 20 wt.% of TATP and markedly increasing water content (from 20% in mixture VII to 62.6% in mixture VI). Line K corresponds to the mixtures containing 42.6–57.9% of TATP and 36.6–25.2% of water. Fig. 3 clearly documents the "cooling effect" of water in the mixtures investigated.
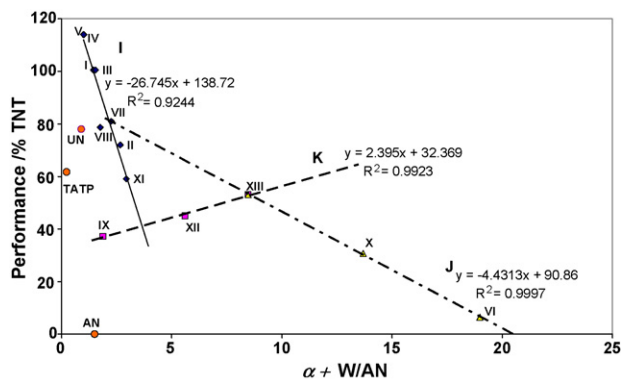

Fig. 3. Demonstration of the combined effect of oxygen balance (here coefficient α) and molar ratio of water (W) and ammonium nitrate (AN) upon the relative performance of the studied mixtures.
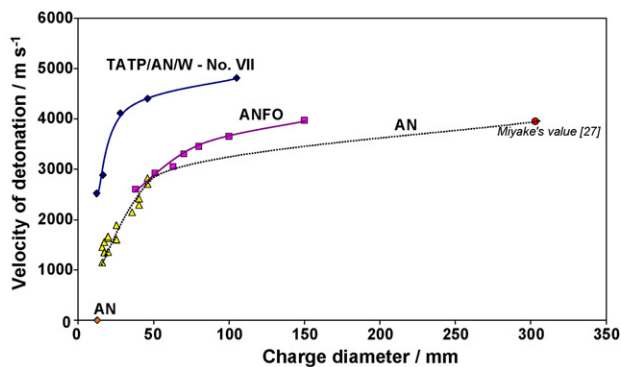
Fig. 4. Approximative relationships between velocity of detonation and charge diameter of the TATP/AN/W mixture VII, ANFO and technical AN.

3.4. Detonation

The effect of charge diameter upon the detonation of TATP/AN mixture was studied using mixture VII, the data of which correlate in Fig. 3 with lines I and J. This mixture is also easily accessible technologically. The results are presented in Fig. 4 for comparison, the figure also presents the data for ANFO [9] and technical-grade AN [26]. In spite of the relatively high water content in mixture VII, the TATP present in it distinctly increases its detonability as compared with ANFO and technical-grade AN.

Fig. 5 presents the relationship between the calculated detonation velocities, D, of the mixtures tested and their oxygen coefficient. The D values apply here to the charge density of $1000 \, \text{kg} \, \text{m}^{-3}$, even though in practice this density is difficult to achieve with loose technical-grade AN: in comparison with the calculated D value in Table 2 the highest experimental D value for ammonium nitrate is $3.95 \, \text{km} \, \text{s}^{-1}$ [27] (in a steel tube of 303 mm diameter and for a charge density of $830 \, \text{kg} \, \text{m}^{-3}$). The detonation velocity of the nitrate extrapolated to an infinite diameter was calculated as $D = 3.85 \, \text{km} \, \text{s}^{-1}$ [28] (Zeman et al. extrapolated their experimental values to $D = 3.81 \, \text{km} \, \text{s}^{-1}$ [29]).

The relationship between D values of explosives and their oxygen balance values (OB) was dealt with, e.g., by Martin and Yallop [30] and Pagowski [31]. They derived relatively com-
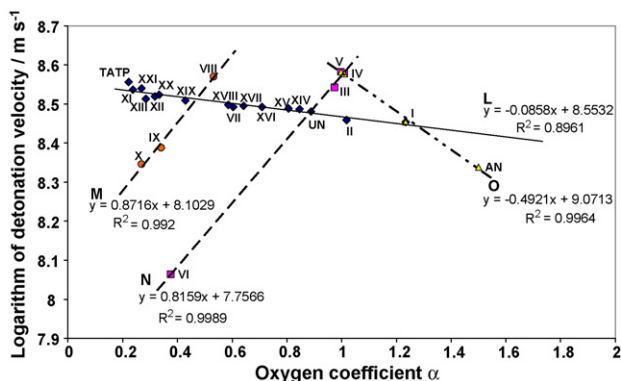
plex relationships, also including the charge density (Martin and Yallop also included the heat of formation). A partial result obtained by Pagowski for a single value of charge density is his linear relationship between the D values and oxygen balance [31]. In our case, the closest correlation between the D and α values is expressed by the semi-logarithmic relationship given in Fig. 5. In this diagram, straight line L unifies the data of detonating explosives containing a cooling component (water or UN); this set also includes TATP with its highly negative OB as well as mixture I with positive OB. The mixtures whose data lie below this line (AN, VI, X a XI) should belong among the so-called "tertiary explosives" (an unofficial classification according to monograph [32]), which are brought to detonation by a very strong primer and in charges of larger diameter; a typical "tertiary explosive" is AN. The data lying above straight line L correspond to mixtures of the type of high explosives. Straight line M corresponds to mixtures TATP/AN containing higher proportion of triperoxide (above 33 wt.%) and a relatively higher content of water (IX and X). Straight line N corresponds to mixtures with a lower TATP content (below 22.4 wt.%); it also includes UN. The data assembled in straight line O correspond to mixtures with positive oxygen balance (inclusive of AN). Hence, even here thermochemical aspects are projected into the classification of the mixtures studied.

4. Conclusions

The admixtures added to triacetone triperoxide (TATP) in the mixtures studied are different: ammonium nitrate (AN) with positive oxygen balance and with simple equilibrium dissociation into ammonia and nitric acid as the first step of its thermal decomposition [21,22]; in contrast to it, urea nitrate (UN) with negative oxygen balance and with the double proton transfer in the carbonyl/hydrogen bond complex preceding the decomposition of its molecule [22,23].

The application of ballistic mortar to determination of relative performances (RP) of tested mixtures should not be affected in the outputs of the respective measurements by the density and homogeneity of the mixtures investigated [15,16]; the relatively long-term retention of decomposition products from tested sample in the chamber of ballistic mortar has the consequence that a low RP can be exhibited also by mixtures that are not capable of detonation (e.g., due to very high water content as it is in sample VI).

The relationship between the RP values determined for the tested mixtures of TATP with additives and the calculated detonation energies related to volume unit of gaseous products of detonation of these mixtures is not unequivocal. Depending on the content of cooling components (water or UN) in the samples studied, this relationship is composed of a number of partial linear equations. The above-mentioned difference between AN and UN results in an opposite course of this dependence for mixtures containing more than 50 wt.% of UN as compared with the TATP/AN mixtures. Also the relationships between the RP values and oxygen balance indicate different (logical) participation of AN and UN in the explosive decomposition of the respective mixtures. The dry TATP/UN mixtures exhibit lower RPs than

Fig. 5. Semi-logarithmic relationship between velocity of detonation and oxygen coefficient of the studied mixtures, TATP, UN and AN.

those of analogous TATP/AN mixtures, which mostly contain up to 12% of TATP and up to 25% of water.

Depending on the water content present in them, the TATP/AN mixtures can exhibit a higher detonability than that of the ANFO explosives. This is documented by mixture VII, which contains 26% of TATP and 20% of water. Including all the mixtures studied at the charge density of $1000 \, \text{kg m}^{-3}$, we have derived a semi-logarithmic relationship between their calculated detonation velocity and oxygen coefficient. Among the mixtures tested, this relationship distinguishes samples of the type of "tertiary explosives" and samples whose performances and detonation velocities approach those of "high explosives".

Acknowledgement

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