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Predictive estimation of detonation nanodiamond yield based on the characteristics of carbon-containing explosives

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Abstract: The paper gives a predictive estimate of detonation nanodiamond (DND) yield depending on the value of oxygen balance, zone length, and chemical reaction time of explosives. The dependences of the main characteristics of explosives on each other are determined. It is shown that practically any characteristic of explosives (e.g., detonation velocity) can be used to calculate other characteristics of explosives, as well as the DND yield during their synthesis. The DND yield from hydrogen-free benzotrifuroxane (1.88 wt. %) was determined for the first time. According to the data of the Institute of Hydrodynamics named after M.A. Lavrentiev (Russia, Novosibirsk), such nanodiamonds have a spherical shape (diameter ~100 nm) due to a very high temperature (4300 K) and pressure of 36 GPa. Moreover, the thermal effect of combustion and the thermal effect of the explosion can be accurately calculated based on the elemental composition of explosives. From there, the specific power of the explosives and all other characteristics, including the DND yield, can be determined. Predictive evaluation does not exclude the need for experimental work, but determines its feasibility.

Keywords: detonation nanodiamonds; yield; explosives; oxygen balance; detonation velocity; pressure; reaction time; chemical reaction zone length.

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Прогнозная оценка выхода детонационных наноалмазов на основе характеристик углеродсодержащих взрывчатых веществ

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Аннотация: Дана прогнозная оценка выхода детонационных наноалмазов (ДНА) в зависимости от значения кислородного баланса, длины зоны и времени химической реакции взрывчатых веществ (ВВ). Определены зависимости основных характеристик ВВ друг от друга. Показано, что практически любой параметр ВВ (например, скорость детонации) может быть использован для расчета других их характеристик, а также выхода

ДНА при их синтезе. Впервые определен выход ДНА из безводородного бензотрифуроксана (1,88 мас. %). Такие наноалмазы по данным Института гидродинамики им. М. А. Лаврентьева (Россия, Новосибирск) имеют сферическую форму (диаметр ~100 нм) из-за очень высокой температуры (4300 К) и давления 36 ГПа. По элементному составу ВВ рассчитаны тепловой эффект сгорания, тепловой эффект взрыва, удельная мощность ВВ и все остальные характеристики, включая выход ДНА. Прогнозная оценка не исключает необходимость проведения экспериментальных работ, но определяет их целесообразность.

Ключевые слова: детонационные наноалмазы; выход; взрывчатые вещества; кислородный баланс; скорость детонации; давление; время реакции; длина зоны химической реакции.

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1. Introduction

Detonation nanodiamonds (DND) are currently one of the most sought-after allotropies of carbon, with attention being paid to the development of technologies for obtaining various types of DND, selection of initial explosives for their production, investigation of properties, and most importantly, their application in various fields of industry, medicine, and agriculture [1–16].

As a rule, explosive is a polynitro compound that contains in each molecule both a “fuel” (carbon, hydrogen) and an “oxidizer” (oxygen), with oxygen bonded to nitrogen. The exothermic reactions of oxidation of carbon to CO and CO_2; hydrogen to H_2O – represent the source of energy of the explosion. When there is a shortage of oxygen (negative oxygen balance (OB)), free carbon appears in detonation products (DP), which can be in the form of DND and non-diamond carbon of various allotropic forms.

The composition of DP depends largely on the equilibrium position of the two reactions:

$$2CO \leftrightarrow CO_2 + C;$$

$$H_2 + CO \leftrightarrow H_2O + C.$$

According to [7] the equilibrium of the second reaction is shifted to the right in all cases, while in the first reaction the equilibrium is shifted to the right only for high initial densities at ρ_0>1.5 g·cm^{-3}. Thus, hydrogen of explosive molecules oxidized to H_2O, and carbon can be oxidized to CO_2 almost completely only for high-density charges with $\rho_0 \to \rho_{max}$, or distributed between CO_2 and CO (for low-density charges). The decomposition of explosives is a complex multistage set of reactions in series and in parallel. The course of reactions and the composition of reaction products can change with the changes in temperature and pressure.

By now, the process of DND synthesis from charges of TNT and hexogen mixture is well enough studied, and the optimal empirical values of the main control parameters of synthesis are known [17]. Charge composition (~60 % TNT and ~40 % hexogen), charge density (1,6–1,7 g·cm^{-3}), optimal oxygen balance (–35÷–60), presence of water or water-salt armor of the charge, non-oxidizing, or better, reducing medium of detonation. At the same time, the pressure in the chemical reaction zone (CRZ) should exceed 17 GPa, and the temperature should be at least 3000 K.

The output and quality of the DND depend on a variety of parameters:

1. Composition of the explosive charge and its specific power.
2. Oxygen balance of explosives.
3. Charge density.
4. Composition and heat capacity of the medium in the explosion chamber (EC).
5. Charge form.
6. The armor (shell) of the charge.
7. Charge mass to explosive chamber (EC) volume ratio.
8. Modification of the charge composition by doping elements or substances.
9. The magnitude of the pulse and the location of charge initiation.
10. EC design and its wall material.

Given the presence of such a large number of influencing factors, it is clear that reference in multiple works to only the same composition cannot guarantee the same yield of nanodiamonds in these studies. Moreover, the basic explosion parameters for the same explosives for charges of the same density do not guarantee the identity of the values of detonation velocity, pressure in the Chapman-Jouguet plane, time, length (width) of the chemical reaction zones (CRZ), and the DND yield. The value of the parameters is influenced not only by the skill of the performers, but also by the availability of hardware capabilities.

However, all of the above is not a hindrance to predictive and evaluative determination with all the above optimized parameters to determine the

feasibility of working with a particular explosive, which was undertaken in this paper.

The paper aims to study the inter-relationship between the main characteristics of carbon-containing high explosives (oxygen balance, detonation velocity *D*, pressure *P* in the Chapman-Jouguet plane, residence time τ, and CRZ length *L* and their influence on the DND yield.

2. Materials and Methods

To carry out the charge explosion we used a steel explosion chamber "Alpha-2M" (Russia) with a capacity of 2.14 m^3. The explosion of charges was carried out in a water shell, the mass ratio of explosives: water – 1 : 10. The explosion medium was gaseous products of previous explosions. The mass of each charge was 0.5 kg, five charges were detonated in each experiment, the charges were made of pentaerythritetetranitrate, 2,4,6-trinitrotoluene, cyclotrimethylenetrinitramine, 2,4,6-trinitrophenol, 2,4,6-trinitro-N-methyl-N-nitroaniline and their mixtures in different ratios. The charges were manufactured and detonated by the same operator. The diamond blend resulting from the explosion was dried, then treated with dilute (Russian Standard 4461-77) nitric acid of concentration 40–50 % at temperature 220–230 °C and pressure 80–100 atm at the pilot plant. Further, the separated nanodiamonds were washed with distilled water in a cascade of countercurrent glass columns. Once the pH of the aqueous medium reached 6–7, the purified nanodiamonds were dried at a temperature of 115–120 °C, the temperature in the drying chamber was maintained by supplying superheated water vapor.

3. Results and Discussion

3.1. Interdependencies of characteristics

Since any use of explosives is a dangerous process and not all potentially suitable substances for producing DND are readily available, it is expedient to theoretically determine the possibility of using a particular explosive to produce DND. At present, only two methods of producing DND are known – from a mixture of TNT and hexogen and from tetryl, but due to the rising cost of raw materials of explosives and their scarcity, it has become necessary to search for new, more affordable types of explosives [18]. The best-known characteristics of explosives are detonation velocity and oxygen balance. In [17], it was found that for some aromatic polynitro compounds of explosives, the optimal oxygen balance for producing DND with an acceptable yield ≥ 5 % of the mass of explosives was –35÷–60 %. These data, with a significant degree of probability, can be used by relating this value to the velocity of detonation of explosives, since [19] showed the dependence of the DND yield on the detonation velocity of a number of aromatic polynitro compounds (mainly mixtures of TNT and hexogen) with an optimum of 7250–8000 $m \cdot s^{-1}$ (DND yield ≥ 5 % of the mass of explosives).

The explosion parameters and the achieved yield from a range of explosives are shown in Table 1.

However, tabular material is difficult to perceive without graphical representation. In Fig. 1, in the coordinates of detonation velocity to OB, the region bounded by oxygen balance –35÷–60 % and optimum D = 7250–8000 $m \cdot s^{-1}$ is highlighted.

Table 1. Detonation velocity, oxygen balance and DND yield depending on the type of explosives [3, 7, 17, 18]

No.	Explosives	D, $m \cdot s^{-1}$	Oxygen balance, %	DND yield, %
1	2	3	4	5
1	Aminotrinitrobenzene (trinitroaniline)	8100	–56.16	
2	BTF	8610	–38.08	1.88
3	Hexogen	8383	–21.6	~1.0
		8850		
4	Hexanitrodiphenyl	7100	–52.8	
5	Hexyl	7145	–52.8	
6	1,3-diamino-2,4,6-trinitrobenzene	7450	–55.97	
7	Octogen	9124	–21.6	~1.0
8	TEN	8142	–10.1	0.15
		8277		
		8590		
9	Tetranitroaniline	7630	–32.2	
10	Tetranitrobenzene	8000	–31	
11	Tetryl	7573	–47.4	7.6

Continuation of the Table 1

1	2	3	4	5
12	TATB	7606 7970	–55.8	4.1
13	Trinitroanisole	7640	–62.5	
14	Trinitrobenzene	7350	–56.3	
15	Trinitrophenol (picricacid)	7350	–45.4	~1.5
16	TNT	7000	–73.9	~1.0
17	EDNA	7570 7750	–32	
18	TH 70/30	7420	–58.3	4.7
19	TH 60/40	7510	–53	8.5
20	TH 50/50	7670	–47.8	6.0
21	TH 40/60	7850	–42.6	5.8
22	TH 36/64 (pres.)	8000	–40.5	5.4
23	TH 30/70	8052	–37.3	4.4
24	GNAB	7311	–49.6	6.63
25	Z-TACOT	7250	–74.2	3.34

BTF: Benzotrifuroxane;
Hexogen: cyclotrimethylenetrithramine;
Hexyl: hexanitrodiphenylamine, dipicrylamine;
Octogen: cyclotetramethylenetetranitramine, 1,3,5,7-tetranitro-1,3,5,7-tetrazacyclooctane;
TEN: pentaerythritetetranitrate, pentrithritol;
Tetryl: 2,4,6-trinitro-N-methyl-N-nitroaniline, methylpicrylnitramine, N-methyl-2,4,6-trinitrophenylnitramine;
TATB: 1,3,5-triamino-2,4,6-trinitrobenzene
EDNA: ethylene-N,N′-dinitramine, ethylenedinitramine, gallium;
GNAB: bis-(2,4,6-trinitrophenyl)-diazine;
Z-TACOT: 2,4,8,10-tetranitro-5H-benzotriazolo-[2,1-a]-benzotriazol-6-um;
TH: alloys or mixtures of TNT and hexogen.

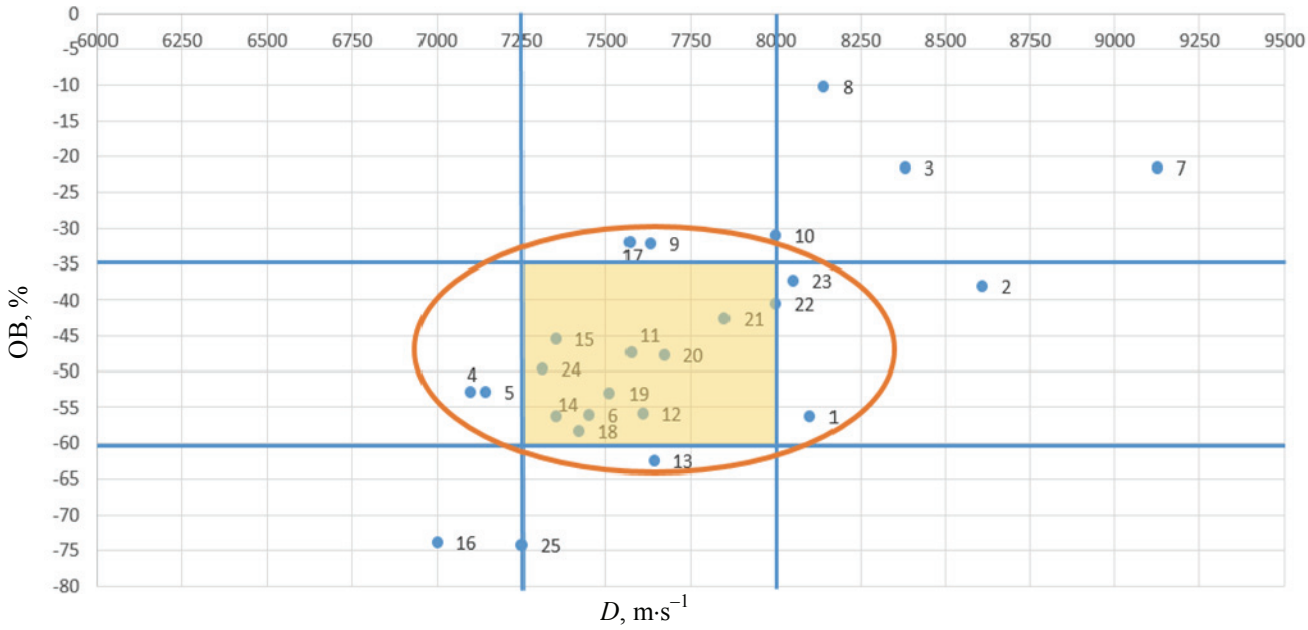

Fig. 1. Detonation velocity *D* and OB of explosives optimal for producing DND with yield ≥ 5 % of the mass of explosives

All explosives inside this region (as well as those lying immediately beyond it) are likely to provide an acceptable yield of DND (≥ 5 wt. %). These new initial explosives can include: hexyl (hexanitrodiphenylamine), hexanitrodiphenyl, tetranitroaniline, tetranitrobenzene, trinitroaniline, trinitroanisole, 1,3-diamino-2,4,6-trinitrobenzene, trinitrobenzene and their mixtures, i.e. polynitroaromatic compounds. The dependences obtained below with a high degree of probability can be extended only to powerful polyaromatic explosives. In addition, the value of DND yield obtained under different conditions for one and the same type of explosives can significantly differ from each other for different researchers.

In Fig. 1, the ellipse highlights the region with explosives that can theoretically provide an acceptable yield of DND (~5 wt. %).

It is equally important to trace the dependences of the DND yield on the other explosion parameters listed in Table 2.

Table 2 shows experimental and literature data reflecting the main parameters of the detonation process. Table 2 shows how much the specific explosive power differs – up to ~6 times, in contrast to the thermal effect – the maximum difference is only 1.35 times [17]. Part of the heat of explosion was calculated by additivity (by the proportional contribution of individual explosives constituting the mixture). It was preliminarily established by well-known thermal effects of mixed explosives that this technique gives an error of 1.4–1.8 %, which is insignificant.

Table 2. Explosion parameters and the DND yield depending on the type of explosives [7, 17, 19, 20]

No.	Explosive	Specific charge density ρ, $g \cdot cm^{-3}$	Heat of explosion Q, $kJ \cdot kg^{-1}$	Specific power W, $kJ \cdot (kg \cdot \mu s)^{-1}$	Detonation velocity D, $m \cdot s^{-1}$	Pressure in flat. of Chapman-Jouget P, GPa	Chemical reaction time τ, μs	Length of the chemical reaction zone L, mm	DND yield Y, wt. %
1	TNT pres.	1.61	4190	22053	6611	**17.1 (7)**	0.19	1.25	**0.6–2.1 1.4 (1)**
2	TH 80/20 molded	1.64	4440	**34154-55500 (8)**	7200	21.5	**0.13 (6)**	**0.65 (8)**	7.88
3	TH 70/30	1.64	4565	57063	7420	21.4	0.08	0.44	**7.61 (1)**
4	TH 60/40 molded 1	1.67	4690	33500	7510	24.4	0.14	0.72	**5.46 (1)**
5	TH 60/40 molded 2	1.64	4690	39083	7500	22.2	**0.12 (6)**	0.4	**7.92 (1)**
6	TH 50/50	1.68	4815	37003	7670	25.9	0.13	0.64	**6.07 (1)**
7	TH 40/60 pres.	1.61	4940	44909	7850	22.8	0.11	0.50	**7.15 (1)**
8	TH 30/70 pres.	1.60	5065	42208	8052	27.6	0.12	**0.5 (3)**	**5.0 (1)**
9	Z-TACOT	1.85	4103	32564	7250	26.3	**0.126 (6)**	**0.57 (3) – 0.60 (6)**	**3.44 (2) – 6.61 (1)**
10	Z-TACOT/Octogen80/20	1.58	4388	27425	8040	22.2	0.16	**0.71 (1)**	**6.38 (1)**
11	Hexogen	1.78	5440	77714	8670	34.5	0.07	0.36	1.1
12	TH 36/64	1.73	4990	49900	7920	28	0.10	0.60	**6.38 (1)**
13	TEN	1.76	6318	78975	8260	30.8	0.08	0.42	0.15
14	TATB	1.88	3473	14475	7350	29.7	0.24	1.18	**1.9 (1) – 4.43 (2)**
15	TATB/Octogen 70/30	1.85	3536	25257	**8129 (5)**	**23.8 (4)**	**0.14 (9)**	**0.71 (1)**	5.3
16	Octogen	1.91	5526	138150	8920	**34.4 (6)**	0.04	0.25	
17	Octogen/TH T 90/10		5392	77028	8790	**33.4 (6)**	0.07	0.37	
18	TNT	1.73	4609	46090	7500	26.7	0.10	0.33	7.6

Bold indicate calculated data obtained using formulas (1) – (9), the number of the formula used for calculation is indicated in parentheses.

Table 2 presents the data of DND yield and such difficult-to-determine explosion parameters as the length of the chemical reaction zone (from the detonation wave front to the Chapman-Jouguet plane) and its time. By determining the time of the chemical reaction or the length of the chemical reaction zone, it is possible to predict the DND yield.

We are just discussing the DND yield here, and as previously stated, the found dependences of DND yield on different explosion parameters are only applicable to polynitroaromatic compounds and their combinations; they are not applicable for calculations for nitroolefins and nitroheterocycles. There is a correlation between the other characteristics of different explosives. For example, octogen is an analog of hexogen, and subsequently after detonation of octogen the DND yield of more than 1 % follows (exp. 16). Addition of 10 wt. % to TNT octogen cannot practically affect the DND yield (exp. 17).

In [19], it was postulated that in the process of DND synthesis, the chemical reaction time equal to the time of matter passage from the detonation wave front to the Chapman-Jouguet plane (i.e., from the beginning to the end of the chemical reaction zone) can be taken as the unit of time of energy release in an explosion. This time is tenths and hundredths of a microsecond. For many practical calculations, the exact time of existence of the CRZ is of critical importance, since it allows us to establish the real explosive power, which differs greatly for different types of explosives or their mixtures and affects the DND yield under other equal conditions. Therefore, it was proposed to determine the explosive power as the ratio of the heat of explosion of a unit mass to a unit time, i.e.

$$W = \frac{Q}{m\,\tau},$$

where W is the power of explosives, kJ·(kg·μs)$^{-1}$; Q is the heat of explosion, kJ·kg^{-1}; m is the mass of explosives, kg or g-mol; τ is the time of energy release from the detonation wave front to the Chapman-Jouguet plane, μs. The heat of explosion of individual types of explosives and their mixtures has been determined many times and depends slightly on the methodology of determination and specific performers [18]; the time of existence of CRZ is quite accurately determined in [20, 21]. However, the DND yield strongly depends on the conditions of the detonation synthesis process.

Table 2 also shows the specific power of explosives, then the graphical dependencies of the DND yield on various explosion parameters and their dependencies on each other, as well as the mathematical dependencies (formulas) describing the graphical material are presented.

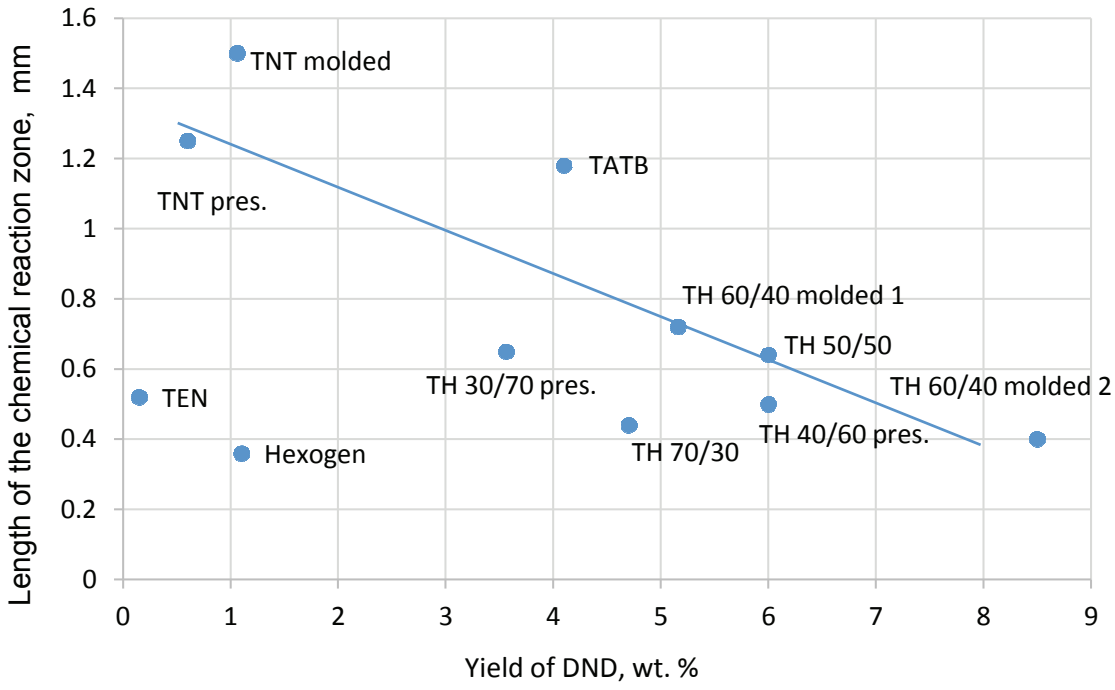

Fig. 2. Dependence of the DND yield on the length of the chemical reaction zone

The equation (Fig. 2) of the best linear approximation (without taking into account the points of the corresponding heating elements and hexogen) of the dependence DND yield, wt. %. (Y) from the length of chemical reaction zone, mm (L)

$$Y = -7.7L + 11. \quad (1)$$

The equation (Fig. 3) of the best approximation by a parabola (excluding the points of the corresponding TEN, hexogen, TNT pres. and TATB) of the dependence of yield of DND, wt. % (Y) on the chemical reaction time, μs (τ):

$$Y = 1.97(\tau - 0{,}15)^{0.5} + 4.25. \quad (2)$$

But the length of the CRZ of the recommended explosives can be determined very accurately by the dependence of the CRZ length on the pressure in the Chapman-Jouguet plane (a parameter that is known for many explosives).

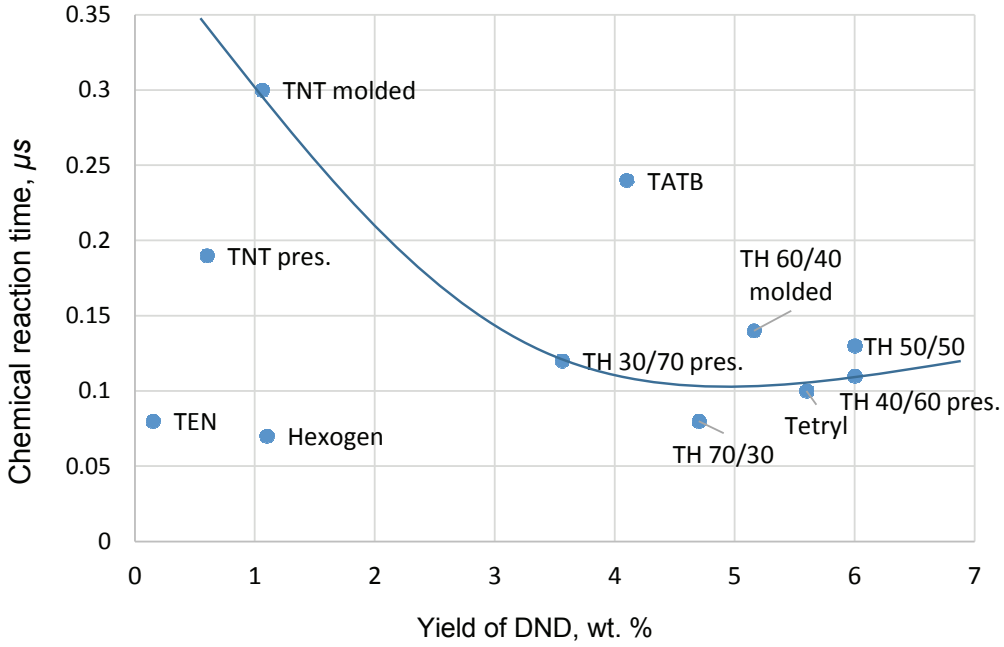

Fig. 3. Dependence of the DND yield on chemical reaction time

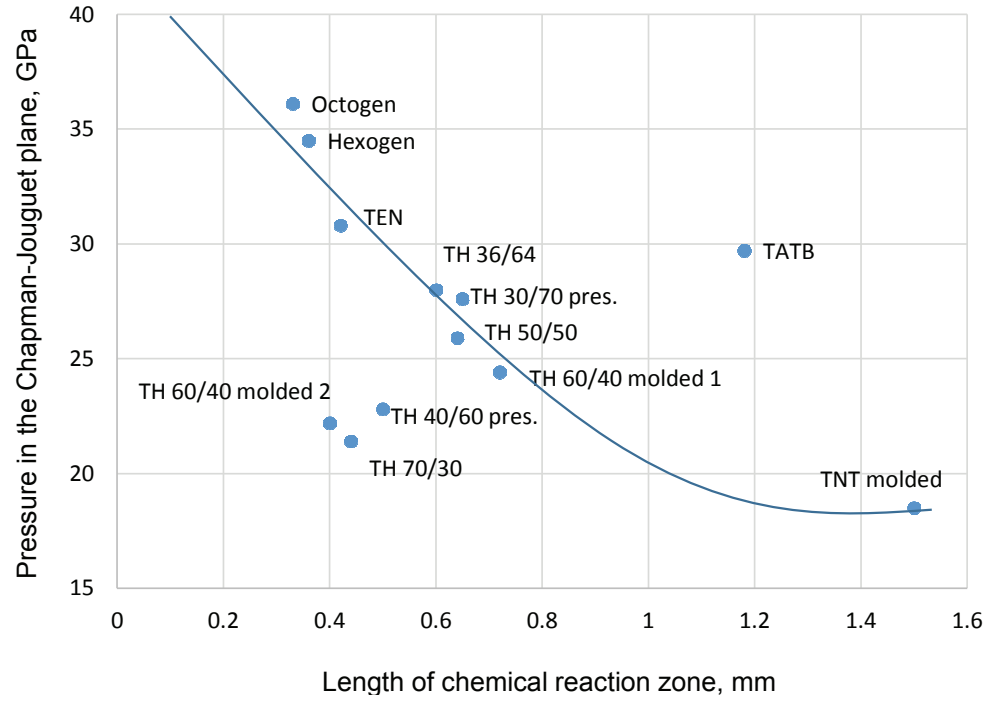

Fig. 4. Dependence of the CRZ length on pressure in the Chapman-Jouguet plane

The equation (Fig. 5) of the best approximation by hyperbola (excluding the points of the corresponding TH 70/30, TH 60/40 molded 2 and TATB) of the dependence CRZ length, mm (L) on P in the Chapman-Jouguet plane, GPa, (P):

$$L = -5.84 + 770/(P + 93.8). \quad (3)$$

The equation (Fig. 5) of the best approximation by hyperbola (excluding the points corresponding TH 70/30, TH 60/40 molded 2 and TATB) of the dependence of P in the Chapman-Jouguet plane, GPa, (P) on the CRZ length, mm (L):

$$P = -93.8 + 770/(L + 5.84). \quad (4)$$

It is more straightforward to determine the CRZ length from widely known values of the detonation velocity, which is first determined by the explosion parameters for new explosives and their mixtures according to Fig. 5. This dependence is expressed very clearly. The dropout of the TH 36/64 composition from the series, with high probability, indicates an incorrect determination: either of the detonation velocity, or of the CRZ length, or of the anomalously high (low) value of the specific density of the compacted charge.

The equation of the best approximation by a parabola (excluding the points corresponding to TH 60/40 molded 2, TH 70/30 and TATB) of the dependence of the detonation velocity, m/s (D) on the CRZ length, mm (L):

$$D = 1000L^2 - 2500L + 9400. \quad (5)$$

The dependence of the chemical reaction time on the detonation velocity is also informative (Fig. 6). There is also a well-defined dependence here, which makes it easy (from the detonation velocity) to determine the time of the LCR. The dropout of TATB and TEN from this series may indicate "over compressed" detonation at too high a charge density.

The equation of the best approximation by hyperbola (excluding the points of the corresponding TH 70/30, TNT pres. and TATB) of the dependence of chemical reaction time, μs (τ) ondetonation velocity, $m \cdot s^{-1}$ (D) will be

$$\tau = 0.075 + 84/(D - 5600). \quad (6)$$

The equation (Fig. 7) of the best linear approximation (excluding the points of the corresponding TATB, TH 70/30 pres., TH 40/60 pres.) of the dependence of pressure in the Chapman-Jouguet plane, GPa, (P) on detonation velocity, $m \cdot s^{-1}$ (D) will be

$$P = 0.0075D - 32.5. \quad (7)$$

The equation of the best linear approximation (ignoring the point corresponding TNT pres.) of the dependence of CRZ length, mm (L) on chemical reaction time, μs (τ) will be

$$L = 5\tau. \quad (8)$$

The equation of the best linear approximation (excluding the point of the corresponding TNT pres.) of the dependence of chemical reaction time, μs (τ) on CRZ length, mm (L) will be

$$\tau = 0.2L. \quad (9)$$

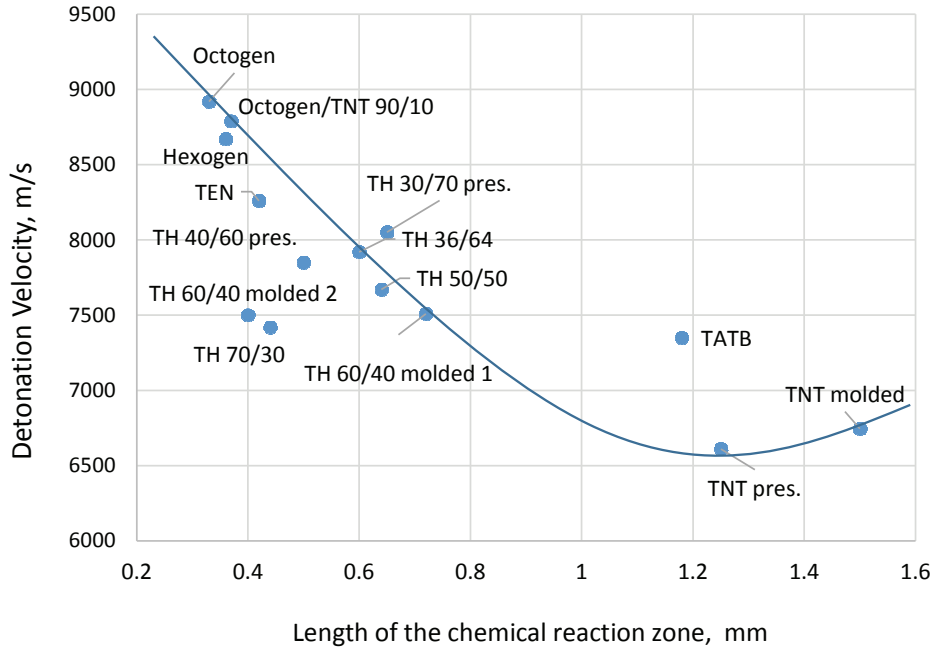

Fig. 5. Dependence of the CRZ length on the detonation velocity

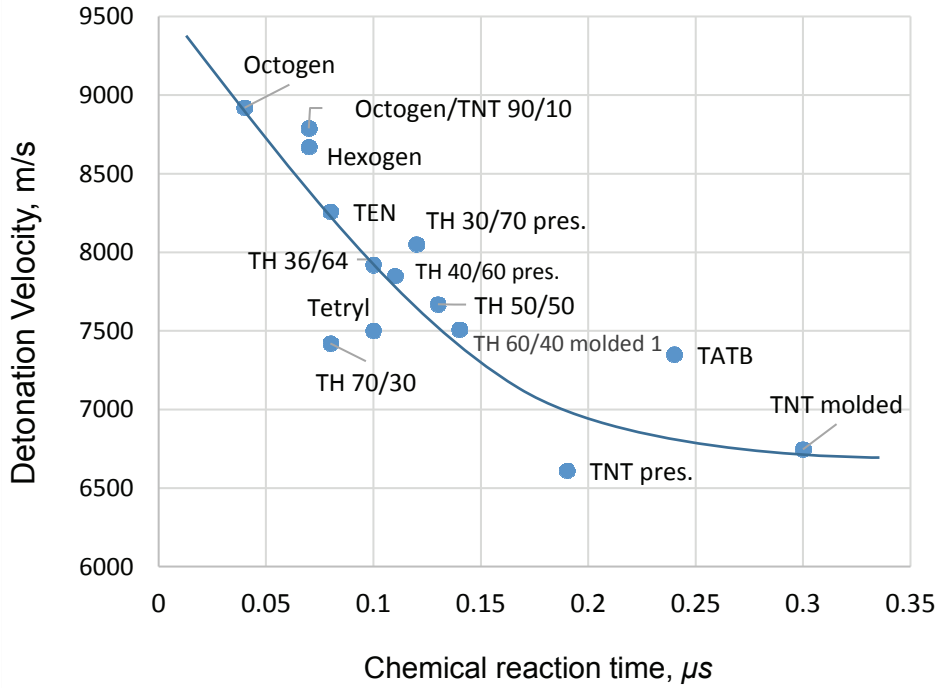

Fig. 6. Dependence of chemical reaction time on detonation velocity

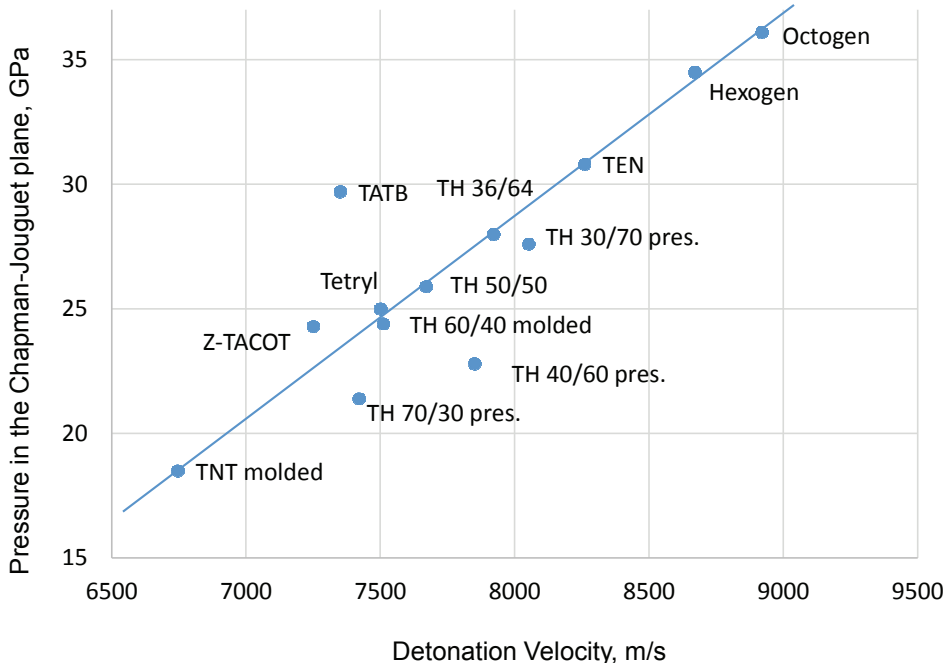

Fig. 7. Dependence of the pressure in the Chapman-Jouguet plane on the detonation velocity

The chemical reaction time, which is natural, correlates reasonably well with the CRZ length (Fig. 8), making it easy to determine one quantity by knowing the other.

Table 3 summarizes the calculated data based on the obtained dependencies for all eight recommended polynitroaromatic compounds: hexyl (hexanitrodiphenylamine), hexanitrodiphenyl, tetranitroaniline, tetranitrobenzene, trinitroaniline, trinitroanisole, 1,3-diamino-2,4,6-trinitrobenzene, and trinitrobenzene.

The expected DND yield, specific power of explosives, pressure in the Chapman-Jouguet plane, time, and CRZ length (width) were all calculated based on the known value, or detonation velocity.

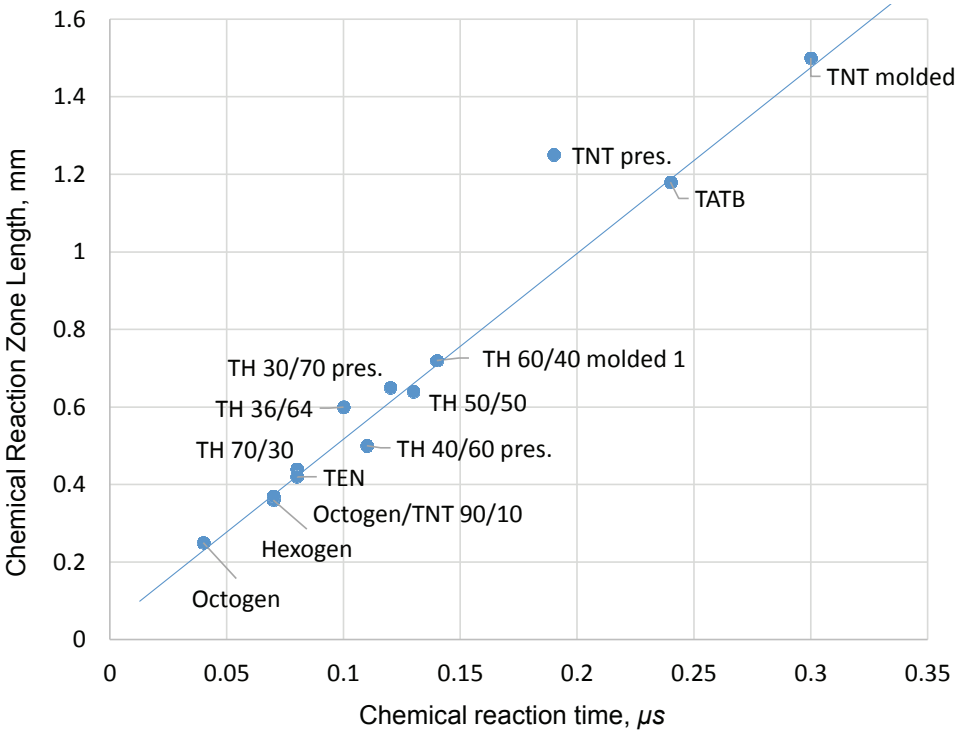

Fig. 8. Dependence of chemical reaction time on the CRZ length

Table 3. Explosion and DND yield parameters for polynitroaromatic compounds

No.	Explosive	Specific charge density ρ, g·cm^{-3}	Heat of explosion Q, kJ·kg^{-1}	Specific power W, kJ·(kg·μs)$^{-1}$	Detonation velocity D, m·s^{-1}	Pressure in flat. of Chapman-Jouget P, GPa	Chemical reaction time τ, μs	Length of the chemical reaction zone L, mm	Yield of DND Y, wt. %	Oxygen balance, %
1	Trinitroaniline	1.762	4148	37709	8100	28.3	0.11	0.47	7.4	–56.16
					(ρ = 1.75)	(7)	(6)	(3)	(1)	
2	Hexanitrodiphenyl	1.61			7100	20.8	0.13	0.88	4.2	–52.8
					(ρ = 1.6)	(7)	(6)	(3)	(1)	
3	Hexyl	1.653	4220	32462	7145	21.1	0.13	0.86	4.4	–52.8
					(ρ = 1.6)	(7)	(6)	(3)	(1)	
4	1,3-diamino-2,4,6-trinitrobenzene	1.8	4278	35650	7450	23.4	0.12	0.73	5.4	–56.0
					(ρ = 1.79)	(7)	(6)	(3)	(1)	
5	Tetranitroaniline	1.867	4261	35508	7630	24.7	0.12	0.66	5.9	–32.2
					(ρ = 1.6)	(7)	(6)	(3)	(1)	
6	Tetranitrobenzene	1.82			8000	27.5	0.11	0.51	7.1	–31.0
					(ρ = 1.82)	(7)	(6)	(3)	(1)	
7	Trinitroanisole	1.61			7640	24.8	0.12	0.65	6.6	–62.6
					(ρ = 1.6)	(7)	(6)	(3)	(1)	
8	Trinitrobenzene	1.688	4600	38333	7300	22.3	0.12	0.79	4.9	–56.3
					(ρ = 1.65)	(7)	(6)	(3)	(1)	

In [22] it was shown that the calculation of the value of heat of combustion (HC) (low calorific value Q_{low}, considering heat losses with water vapor) of elements, organic and inorganic substances with negative oxygen balance, including explosive, is carried out by a simple formula:

$$Q_{low} = 0.1387\ (OB).$$

From here, knowing the gross formula of the substance, it is easy to calculate the heat of combustion.

The calculation of OB is based on the assumption that the combustibles in a substance

molecule (carbon and hydrogen) are oxidized during combustion or explosion by an oxidizer (oxygen in the molecule) to higher oxides – carbon to CO_2, and hydrogen to H_2O. In reality, some carbon is oxidized to carbon monoxide (CO), with less energy released. In addition, experimentally determined Q_{low} is not a constant, the accuracy of its determination is influenced by the method of determination, the peculiarities of the apparatus and the qualification of the experimenter, sometimes Q_{low} differs from each other (in different reference books) significantly. Considering the "ideality" of the Q_{low} calculation, it should be expected that the calculation and Q_{low}, as a rule, should give a higher value than the experimentally determined TC. It is to be expected that the smaller the difference between the calculated Q_{low} value (by OB) and the experimentally determined one, the more accurate the experimental data will be.

It is clear that at explosion due to incompleteness of redox reactions the heat of explosion (Q_{exp}) will be less than Q_{low}. Calculated and experimental data of explosions given in Table 3 [22] show that on average Q_{exp} Less, for dinitroaromatic compounds – by 5 times; for trinitroaromatic compounds – by 1.7 times. For tetranitroaromatic compounds by a factor of 1.05.

Thus, proceeding from the gross formula of explosive it is possible to determine with satisfactory accuracy Q_{low}, further – Q_{exp} (multiply reducing Q_{low}). Knowing the time of the CRZ existence, by the formula denoted earlier: $W = Q/m\,\tau$, we determine W. Then by the formula

$$Y = 0.36 \cdot 10^{-3} W^2 + + 3.24 \cdot 10^{-4} W - 1.31$$

– we determine the DND yield.

3.2. On deviations from approximation ratios and curves

Consider the deviations from the approximation relationships and curves for Z-TACOT/octogen 80/20 explosives (No. 10 in Table 2). The only known value that is included in the formulas and graphs, and even then without indication of the measurement error, is the DND yield, $Y = 6.28$ wt. %.

From the band of acceptable values, it can be found that the corresponding CRZ length, L, lies in the range from 0.4 to 1.0 mm (Fig. 2). This corresponds well to the value $L = 0.8$ mm found by the approximation relation (1) $Y = -7.7\,L + 11$, with a correlation of at least 50 %.

By the band of acceptable values, it can be found that the corresponding chemical reaction time lies in the range from 0.12 to 0.16 μs (Fig. 3). This corresponds well to the value of $\tau = 0.16$ μs found by the approximation relation (2) $Y = 1.97\,(\tau - -0.15)^{0.5} + 4.25$, with a correlation of at least 75 %.

From the band of valid values for the calculated value of L = 0.8 mm, it can be found that the corresponding Chapman-Jouguet plane pressure P lies in the range of 22 to 26 GPa (Fig. 4). This corresponds well to the value $P = -93.8 + + 770 / (L + 5.84)$ found by the approximation relation (4) to be $P = 22.2$ GPa, with a correlation of at least 84 %. Note that for the values of L corresponding to the edges of its band of acceptable values from 0.4 to 1.0 mm the value of P lies in the range from 31 to 21 GPa, giving a correlation of about 50 %.

From the band of acceptable values for the calculated value of $L = 0.8$ mm, it can be found that the corresponding detonation velocity D, lies in the range of 7400 to 8000 $m \cdot s^{-1}$ (Fig. 5). This corresponds to the value $D = 8040$ $m \cdot s^{-1}$ found by the approximation relation (5) $D = 1000\,L^2 - - 2500\,L + 9400$, with a correlation of at least 90 %. Note that for the values of L corresponding to the edges of its band of admissible values from 0.4 to 1.0 mm the value of D lies in the range from 8700 to 6800 $m \cdot s^{-1}$, giving a correlation of about 85 %.

From the band of acceptable values for the calculated value of $\tau = 0.16$ μs, it can be found that the corresponding detonation velocity D, lies in the range of 6800 to 7200 $m \cdot s^{-1}$ (Fig. 6). This corresponds to the value $D = 8040$ $m \cdot s^{-1}$ found by the approximation relation (6) $\tau = 0.075 + 84 / (D - 5600)$, with a correlation of at least 85 %. Note that for values of τ corresponding to the edges of its bandwidth of 0.12 to 0.16 μs the value of D lies between 7200 and 7800 $m \cdot s^{-1}$, giving a correlation of about 85 %.

Calculating the correlation in Fig. 7 for P from D and the correlation in Fig. 8 for L from τ requires determining the band of acceptable values of the first parameter from the band of acceptable values of the second. Such calculations will contain a significant error.

4. Conclusion

Using widely known data on explosives (detonation velocity, oxygen balance), a predictive evaluation of the applicability of explosives for DND production was carried out, and using the found complex of dependencies, it became possible to

determine various characteristics of explosives, including the DND yield, knowing at least one of the characteristics.

Thus, by the formula $Y = -\ 7.7L + 11$, where Y is the DNDyield and L is the CRZ length (mm), we determine the nanodiamond yield.

Using the formula $Y = 1.97(\tau - 0.15)^{0.5} + 4.25$, where τ is the chemical reaction time (μs), we also determine the nanodiamond yield.

The CRZ length (mm) is related to the pressure in the Chapman-Jouguet plane (P, GPa), by the following dependence $L = -5.84 + 770/(P + 93.8)$.

The pressure in the Chapman-Jouguet plane is related to the CRZ length by the formula $P = -93.8 + 770/(L + 5.84)$.

The detonation velocity ($m \cdot s^{-1}$) correlates with the length of the chemical reaction zone by the equation $D = 1000\ L^2 - 2500L + 9400$.

The chemical reaction time is related to the detonation velocity $\tau = 0.075 + 84/(D - 5600)$.

The pressure in the Chapman-Jouguet plane is related to the detonation velocity by the equation $P = 0.0075D - 32.5$.

The CRZ length correlates with the chemical reaction time by the formula $L = 5\tau$, and the chemical reaction time from the CRZ length, respectively, as $\tau = 0.2L$.

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6. Conflict of interest

The authors declare no conflict of interests.

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