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Research Article

Specific Power of Explosive and its Effect on Nanodiamonds

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Abstract: To determine the dependence of the yield of detonation nanodiamonds on the power of the explosives used, a new concept was introduced—the specific power of explosives (with which the detonation rate and pressure of gases in the Chapman-Jouguet plane are related), which is equal to the ratio of the heat of explosion to the unit of mass and time. The dependence of the yield of detonation nanodiamonds on the detonation velocity and pressure in the Chapman-Jouguet plane was determined. The optimum (> 5% (by mass)) yield of detonation nanodiamonds occurs at a value of the specific explosive power of 30000–60000 kJ/(kg × s), detonation velocity of 7300–8000 m/s, and pressure in the Chapman- Jouguet plane of 21-28 GPa.

***Keywords*:** detonation nanodiamonds; explosive power; pressure in Chapman-Jouguet plane; yield of nanodiamonds; detonation velocity; heat of explosion; composition of explosives

1. Introduction

At present, the process of synthesis of detonation nanodiamonds (DNA) from charges of TNT (Trinitrotoluene) and hexogen mixture is well enough studied, the optimal empirical values of the main control parameters of synthesis are known: charge composition TG (~ 60% TNT and ~ 40% hexogen), charge density (1,6 – 1,7 g/cm^3) [1], optimal oxygen balance (-35 – (-60)) [1], the presence of aqueous or water-salt armoring of the charge [2], a non-oxidizing, or better, a reducing environment of detonation [3], pressure (>17 GPa) and temperature (at least 3000 K) in the chemical reaction zone (CRZ) [4]. However, the quantitative dependence of the DNA yield on the real power of mixed and individual explosives (IE), on the pressure of detonation products (DP) in the Chapman-Jouguet plane, and on the detonation velocity of explosive charges has not been established. The determination of these dependencies is the purpose of the present work.

2. Experimental part

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The paper is devoted to the theoretical processing of previously obtained data, both by the authors of the paper and other authors. No special experiments were performed for this paper. All necessary references [4-10, 12-15] are given in the table.

For the compositions from the table: TNT, TG (TNT/Hexogen) 60/40, TG 50/50, TG 40/60, hexogen, tetryl the DNA production was carried out as follows: in a steel hermetic chamber with a volume of 2,14m^3 "Alpha-2M" was placed a charge of explosive or a mixture of explosives weighing 0,5 kg. Each charge was preliminarily placed in a biodegradable plastic bag with 5 kg of 5% aqueous solution of urotropine to create a reducing environment in the chamber during detonation.

Blended explosive compositions were prepared by mechanical mixing of initial explosives in a given ratio, then pressed at 2000 atm. The obtained charge cylinders had the following dimensions: Ø60 mm, length from 106 to 121 mm depending on the charge density. Each experiment corresponded to five explosions of the same charge composition.

The obtained aqueous suspension of diamond-containing charge (DC) after the fifth detonation was automatically removed from the explosion chamber into the receiving container and was separated on a centrifuge into a solid part (DC) and an aqueous solution of urotropine. The solid part was sent for drying and the aqueous solution of urotropine was disposed of.

Dry DC was chemically purified by treatment with 40% nitric acid at 225±5°C and 80-100 atm pressure. The obtained DNA were washed with distilled water and dried.

DNA from charges TG 70/30, TG 36/64, TG 30/70 were obtained in the same way, but without a shell of water or aqueous solution. Nitrogen at a pressure of 3 - 5 atm was used as an inert medium in the explosion chamber.

3. Discussion of the results

According to the authors, the most universal characteristic for explosives is the explosive power and the associated yield of DNA (all other things being equal). However, the accepted definition of explosive power in «TNT equivalent» evaluates the work of detonation products (DP) of explosives (hight explosiveness and brisance of explosives) and is not a scientific definition of explosive power in the process of DNA synthesis.

Power, defined in explosion engineering as the heat released in an explosion per unit mass, also cannot be used for precise calculations and is not the classical definition of power, which is the release of energy per unit time.

It is postulated that in the process of DNA synthesis, the time of chemical reaction equal to the time of matter passage from the detonation wave front to the Champman-Jouguet plane (i.e., from the beginning to the end of the chemical reaction zone) can be taken as the unit 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 CRZ is of crucial importance, as it allows us to determine the real power of explosives, which is very different for different types of explosives or their mixtures and affects the yield of DNA, all other things being equal. Therefore, it was proposed to define the explosive power as the ratio of the heat of explosion of a unit mass to a unit time:

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

where W is the power of explosives, kJ/(kg·mcs); Q is the heat of explosion, kJ/kg; 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, mcs. 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 [5, 6]; the time of existence of DNA is quite accurately determined in [7, 8]. However, the yield of DNA strongly depends on the conditions of the detonation synthesis process.

All data on the yield of DNA were determined by the authors of this work, all detonations were carried out in an Alpha-2-M explosion chamber with a capacity of 2,14 m^3, charges were made and detonated by the same operator, and detonations were carried out in water armor.

The main parameters of the detonation process of DNA production (experimental and from literature sources) are given in the table. It can be seen that the power for different types of explosives or their mixtures differs by a factor of ~6, but the amount of released heat is maximally only by a factor of 1,35.

The heat of explosion was also calculated by additivity (by the proportional contribution of individual explosives making up the mixture). Preliminary on well-known thermal effects of mixed explosives it was established that such calculation gives an error of 1,5 – 2,0 %, which in this case is insignificant.

All below given figures № 1 - 4 were digitized, in the received formulas the following designations are accepted:

x – yield of DNA (in %);

W – specific power of explosive (in kJ/(kg·mcs));

p – pressure in the Chapman-Jouguet plane at explosion of explosives (in GPa);

v – velocities of detonation of explosives (in m/s).

Fig. 1 shows the dependence of yield of DNA on the specific power of explosives. If we assume the optimum yield of DNA ≥ 5 % (by mass), it is necessary to use explosives having a power of 30 – 60 kJ/(kg·mcs). The best result was obtained using TG 60/40 composition detonated in water armor. At the same time, TG 50/50, TG 40/60, TG 36/64 and tetryl charges can be used. The formula describing this process is the dependence of yield of DNA (x in %) on the power of the explosives. (W in kJ/(kg·mcs)):

$$x = -0{,}36 \cdot 10^{-8} \cdot W^2 + 3{,}24 \cdot 10^{-4} \cdot W - 1{,}31$$

Using the dependence of yield of DNA on PD pressure in the Chapman-Jouguet plane shows that the PD pressure should be in the range of 21 – 28,5 GPa (Fig. 2). The formula describing this dependence is the dependence of yield of DNA (x in %) on the pressure in the Chapman-Jouguet plane at explosion of explosives (p in GPa):

$$x = -0{,}049 \cdot p^2 + 2{,}4 \cdot p - 23{,}4$$

This formula is obtained in the approximation of the obvious (see Figure 4) linear approximation, taking into account the totality of the data in the Table. The linear correlation coefficient in this case is 0,879. However, if we do not take into account the data on TG70/30, the suspiciousness of which has already been indicated above, the formula remains practically unchanged, but the correlation coefficient increases to 0 ,963.

Table 1. Detonation process parameters of TNT-hexogen and tetryl charges

explosive or mixture composition	oxygen balance, %	charge density, g/cm^3	Q, kJ/(kg·mcs)	τ, mcs	W, kJ/(kg·mcs)	yield of DNA, % (by mass)	detonation velocity, mcs	Pressure in the plan Chapman-Jouguet, GPa
TNT (cast)	–74	1,62	4232 [5, 6]	0,29 [8]	14593	1,06	6850 [7]	ср. 18,5 [13]
TG 70/30	–58,3	1,61	4684*	0,08 [8]	58550	4,7	7420 [5]	27,6 [13]
TG 60/40	–53,0	1,66	4835*	0,14 [8]	34540	7,2	7510 [5]	22,3 [9]
TG 50/50	–47,8	1,62	4944 [5]	0,13 [8]	38031	6,0	7670 [8]	24,6 [10]
TG 40/60	–42,6	1,66	5137*	0,11 [8]	46700	5,8	7850 [12]	26,0 [4]
TG 36/64 (pressed)	–40,5	1,68	5197*	0,10 [7]	51970	5,4	8000 [7]	ср. 28,1 [13]
TG 30/70	–37,3	1,60	4969 [6]	0,08 [8]	66100	4,4	8052 [5]	21,4 [15]
Hexogen (RDX)	–21,6	1,68	5740 [12]	0,07 [8]	82000	1,1	8670 [12]	34,5 [12];
Tetryl	–47,4	1,65	4602 [5]	0,10 [7]	46000	5,6	7500 [7]	26,7 [13]

*The known values of the heat of explosion of TNT and hexogen can be easily determined by the method of additivity to determine the heat of explosion of these mixtures [6].

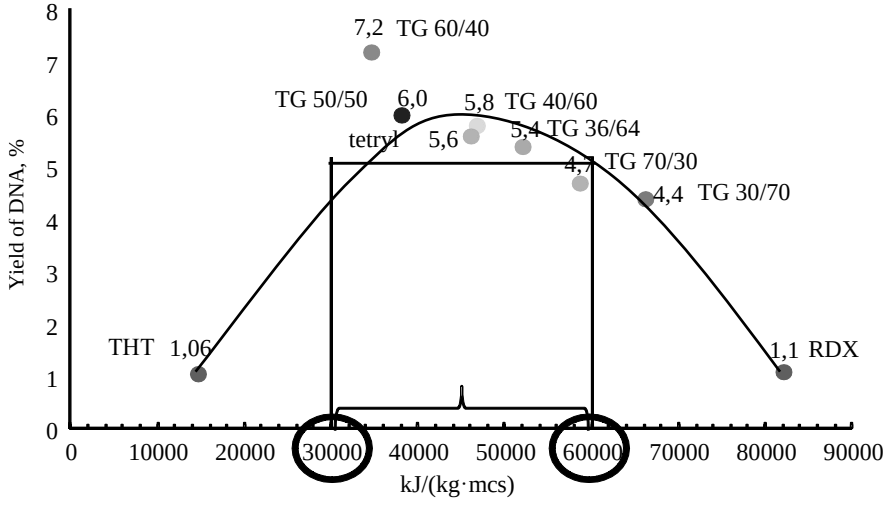

Figure 1. Dependence of yield of DNA on the specific power of explosives

The dependence of yield of DNA on detonation velocity (integral index) shows (Fig. 3) that it is necessary to use explosives having detonation velocity from 7300 to 8000 m/s, i.e., knowing the detonation velocity of explosives or the composition of their mixture, it is possible to estimate the yield of DNA from these products with sufficient accuracy.

The formula describing this dependence of yield of DNA (x in %) on the velocity of detonation of explosives (v in m/s):

$$x = -4{,}45 \cdot 10^{-6} \cdot \mathrm{v}^2 + 68{,}5 \cdot 10^{-3} \cdot \mathrm{v} - 158$$

Fig. 4 shows an almost directly proportional relationship between the detonation velocity of explosives and their power. Thus, knowing the detonation velocity, it is possible to determine quite accurately the specific power of explosives and their compositions. However, the data on the power of TG 70/30 [8] fall out of this dependence unreasonably strongly; probably, the time of the chemical reaction in this case was much shorter than in the real process.

The formula describing the power dependence of the BB. (W in kJ/(kg·mcs)) on the velocity of detonation of the explosive (v in m/s).

$$W = 0{,}116\,\mathrm{v} - 7{,}04$$

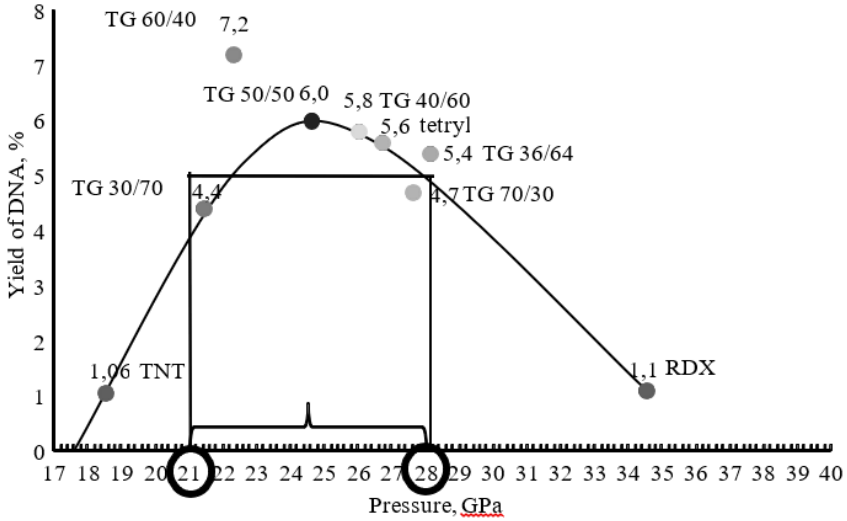

Figure 2. Dependence of yield of DNA on pressure in the Chapman-Jouguet plane at explosion of explosives

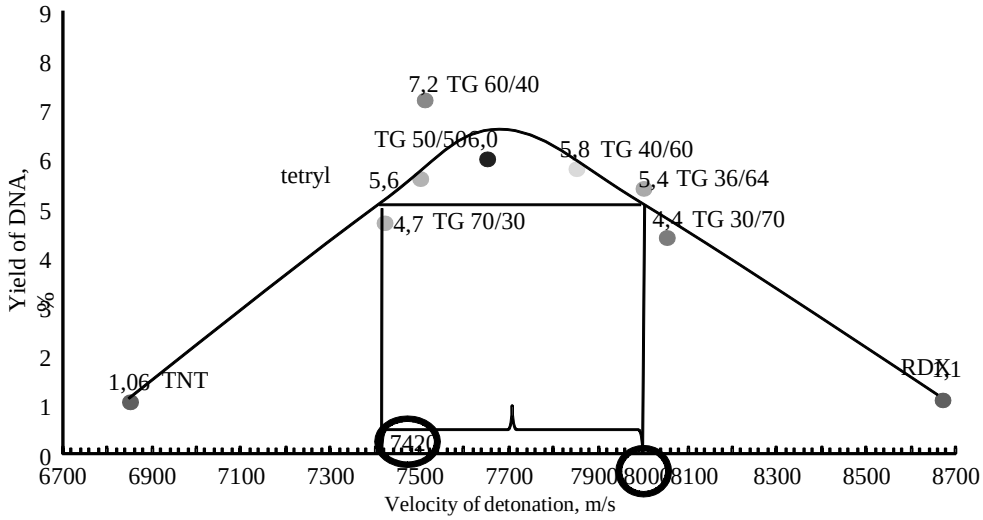

Figure 3. Dependence of yield of DNA on the velocity of detonation of explosives

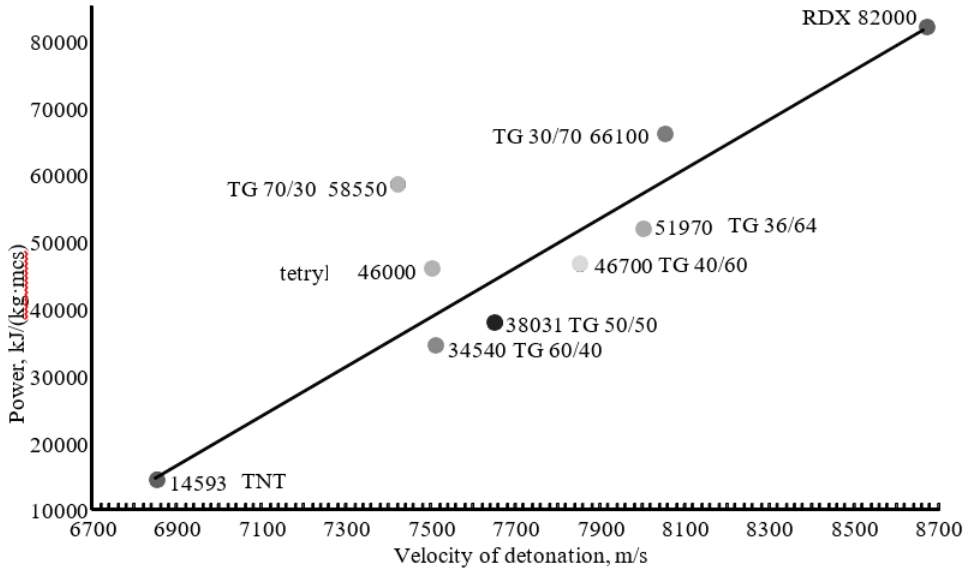

Figure 4. Dependence of explosive power on the velocity of detonation of explosives

From the data in the table and Fig. 4 shows that an increase in the heat and specific explosion power leads to an increase in the detonation velocity.

4. Conclusions

In order to produce yields of DNA with a sustained yield of 5% or more, it is necessary for the explosive or mixture composition to meet the following conditions:

- the specific power of the of the explosive should be 30-60 kJ/(kg·mcs);
- pressure of PD in the Chapman-Jouguet plane - in the range of 21-28 GPa;
- detonation velocity – 7300 – 8000 mcs.

The dependence of the detonation velocity on the specific explosive power is close to being directly proportional.

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