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CONTRIBUTION TO DETONATION ABILITY OF EXPLOSIVES

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By investigating a set of 40 substances, a possibility has been shown of estimate of their detonation ability from the calculated detonation energy and oxygen balance. The calculations have shown that substances with detonation energies below 3 kJ cm^{-1} will probably be able to detonate only if their geometry exceeds the critical diameter, or the detonation will fail at all. Also discussed are the effects of density and initiation pressure.

Introduction

In the context of research into preparation and properties of nano-structure energetic materials (NEM) there arises a question of the conditions at which, and the ratios between oxidant and fuel for which, a particular mixture prepared can detonate. The theory of detonation specifies three qualitative conditions to be met by the respective substance: (i) sufficiently exothermic reaction, (ii) volume change, (iii) high reaction rate. An additional requirement is a suitable geometry of charge, which is usually expressed by the critical diameter $\varnothing_{CR}$, below which the detonation fails [1,2]. Fundamental influence upon the above-mentioned criteria is exerted by the following factors: the composition of the explosive, heat of formation of the explosive and heats of formation of the detonation products, and the density. It was experimentally proved [3] that an increased addition of inert substance to the explosive (observing the condition of homogeneity of the mixture) results in a decrease in output parameters until total interruption of detonation. At the same time, the critical diameter $\varnothing_{CR}$ rapidly increases. It is also well known that for a detonation to be initiated there must be present a certain initiation pressure P_i, which is lower than the detonation pressure P_{CJ}. If, depending on the composition and density of the explosive, there arises a situation where $P_{CJ} < P_i$, then the detonation will not take place.

For finding the conditions at which a substance is not able to detonate any more, one can start from the oxygen balance of the substance and its detonation energy. Both these criteria can be calculated from the composition of the explosive.

Calculation

Kamlet and Jacobs [4] suggested equations for calculation of detonation velocity D and detonation pressure P on the basis of a simple decomposition equation for explosives having a composition of $C_aH_bN_cO_d$. They start from the parameter Φ in the form

$$\Phi = N\sqrt{MQ} \qquad (1)$$

where N, M and Q are number of moles of gas per gram explosive, the grams of gas per mole of gas and heat of detonation in cal g^{-1}, respectively.

Then the equations for detonation velocity and pressure read as follows

$$D = 1.01\sqrt{\Phi}(1 + 1.3\rho) \qquad (2)$$

$$P = 1.559\Phi\rho^2 \qquad (3)$$

where ρ is density of explosive.

The equation of the balance of oxygen (BO) is

$$BO = \frac{1600(d - 2a - 0.5b)}{mol.\ weight} \qquad (4)$$

and the volume detonation energy E_d [5] is calculated from the equation

$$E_d = \frac{P}{2(\gamma - 1)} \qquad (5)$$

where γ is adiabatic coefficient.

The results of these calculations for 40 explosives are summarised in Table I. The substances are listed in the order of magnitude of their E_d values. The relationship between the volume detonation energy and oxygen balance is presented in Fig. 1. The explosives with the lowest values of volume detonation energy are presented in Fig. 2.

Discussion

The set of substances listed in Table I includes various types of nitro compounds and various types of composition. Besides the most frequently represented types CHNO there are also shown substances without hydrogen (CNO), or without nitrogen (CHO). From Fig. 1 it can be seen that the highest detonation energies are encountered with the substances having levelled oxygen balance, while both increasing and decreasing *BO* is accompanied by a decrease in the detonation energy per volume unit.

A more interesting situation is encountered with substances having large negative *BO*, as it can clearly be seen in Fig. 2. The highlighted (by bold letters) substances NM/A 70/30 and DIN/ACN 61/39 demonstrably fail to detonate [3] and have more negative values of *BO* and E_d than their analogues containing a higher proportion of explosive. In the case of another highlighted substance, BuNENA (analogue of DINA), the detonation ability is not expected, but the magnitude of E_d indicates (see the neighbouring substances) that it probably will detonate if larger amounts of it are used. Similarly, TATP, which has a very negative balance, has sufficient detonation energy and demonstrably detonates. As it can be seen from the E_d data in Table I, there exists a certain limit around the value of 3 kJ cm^{-3}, where it can be stated that the substances with a higher content of E_d exhibit the potential to detonate even if their balance is considerably negative.

However, the same cannot be said about the substances with the E_d values below 3 kJ cm^{-3}. If their density is lower than the theoretically maximum density

Table I Properties of selected explosives

	Compound	H_f kJ mol^{-1}	ρ g cm^{-3}	E_d kJ cm^{-3}	OB %
1	DNAF	581.9	2.00	9.822	0.0
2	HNIW	415.3	2.03	9.684	–11.0
3	HNB	196.7	2.00	9.372	0.0
4	BTNEN	–736.3	1.96	8.861	16.7
5	HMX	74.9	1.90	8.858	–21.6
6	BTNEU	–300.1	1.86	8.657	0.0
7	TNAZ	12.6	1.84	8.614	–16.7
8	RDX	61.5	1.80	8.321	–21.6
9	PETN	–540.0	1.77	8.157	–10.1
10	TNETB	–496.0	1.78	7.976	–4.1
11	DADNE	–134.0	1.88	7.889	–21.6
12	DINA	–309.8	1.67	7.348	–26.7
13	BDNPN	–293.3	1.73	7.343	–34.4
14	NG	–496.9	1.59	7.224	3.5
15	ADNBF	154.0	1.90	7.074	–49.8
16	TEX	–540.8	1.99	6.991	–42.8
17	DNI	20.5	1.67	6.806	–30.4
18	NTO	–129.8	1.93	6.791	–24.6
19	TATB	–139.4	1.94	6.711	–55.8
20	NQ	–92.1	1.77	6.651	–30.8
21	TE	33.5	1.73	6.590	–47.4
22	DATB	–98.8	1.84	6.394	–56.0
23	HNE	119.7	1.85	6.350	42.7
24	TNA	–75.3	1.77	6.131	–56.1
25	PA	–239.9	1.76	6.108	–45.4
26	HNS	67.4	1.74	5.731	–67.6
27	TNB	–103.0	1.68	5.631	–56.3
28	TACOT	460.5	1.77	5.624	–74.2
29	HMTD	–360.0	1.57	5.442	–92.2
30	TNT	–75.3	1.65	5.336	–74.0
31	TNM	38.5	1.63	4.741	49.1
32	NM	–112.8	1.14	4.336	–39.3
33	DNB	–162.0	1.50	4.220	–95.2
34	DNT	–56.5	1.52	3.970	–114.2
35	BuNENA	–192.5	1.22	3.766	–104.2
36	DIN/ACN1	–57.3	1.20	3.720	–85.8
37	TATP	–90.8	1.22	3.575	–150.1
38	DIN/ACN2	–40.1	1.15	3.167	–99.9
39	NM/A1	–245.9	1.05	3.020	–84.7
40	NM/A2	–257.8	1.02	2.730	–93.7

(TMD), for which the values of Table I were calculated, it is evident that the amount of E_d for the given substance is decreased, but its sensitivity is increased, its $\varnothing_{CR}$ is decreased, and the substance could be able to detonate. In such cases, the calculation of both E_d and BO indicates the necessity of experimental verification.

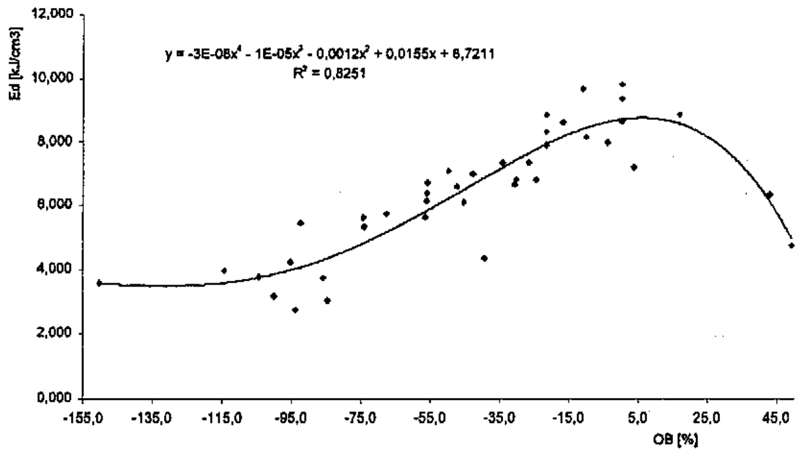

Fig. 1 Relationship between volume detonation energy and oxygen balance for substances listed in Table I (The curve has only illustrative character: it only represents the trend.)

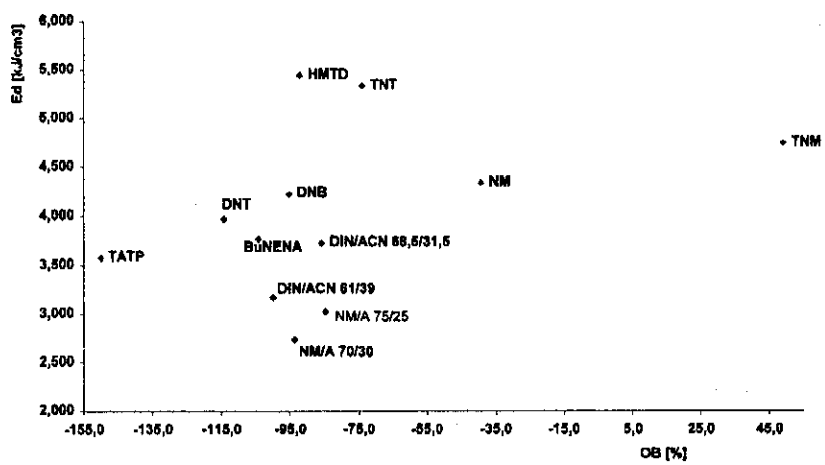

Fig. 2 Relationship between volume detonation energy and oxygen balance for the substances with the lowest E_d values

As it is seen from Fig. 1, a similar situation can also be encountered even with positive oxygen balance, where the E_d value is decreased. The calculation in this case is somewhat more complex; it is necessary to take into account the reactions producing nitrogen oxides, and the finding of equilibrium is more complicated. However, it is possible to presume that the calculated E_d values higher than 3 kJ cm^{-3} can also mean that the substance will be able to detonate, but its critical diameter will probably be large.

Conclusion

On the basis of known composition of an explosive it is possible to make an estimate of potential ability of the substance to detonate from the calculated volume energy and oxygen balance. In the evaluation of detonation ability it is necessary to take into account also the geometry of charge expressed by its critical diameter.

Acknowledgements

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Abbreviations:

1. DNAF 4,4′-dinitro-3,3′-diazenofuroxane
2. HNIW 2,4,6,8,10,12-hexanitro-2,4,6,8,10,12-hexaazatetracyclo[5.5.0.0^{5,9}.0^{3,11}] dodecane
3. HNB hexanitrobenzene
4. BTNEN bis(2,2,2-trinitroethyl)nitramine
5. HMX 1,3,5,7-tetranitro-1,3,5,7-tetraazacyclooctane
6. BTNEU bis(2,2,2-trinitroethyl)urea
7. TNAZ 1,3,3-trinitroazetidine
8. RDX 1,3,5-trinitro-1,3,5-triazacyclohexane
9. PETN pentaerithritol tetranitrate
10 TNETB 2,2,2-trinitroethyl-4,4,4-trinitrobutyrate
11. DADNE 1,1-diamino- 2,2-dinitroethene
12. DINA bis(nitratoethyl)nitramine
13. BDNPN bis(2,2-dinitroprapyl)nitramine
14. NG glycerol trinitrate
15. ADNBF 7-amino-4,6-dinitrobenzofuroxane
16. TEX 4,10-dinitro-4,10-diaza-2,6,8,12-tetraoxatetracyclo[5.5.0.0^{5,9}.0^{3,11}]dodecane
17. DNI 2,4-dinitroimidazole

18. NTO 3-nitro-1,2,4-triazol-5-one
19. TATB 1,3,5-triamino-2,4,6-trinitrobenzene
20. NQ nitroguanidine
21. TE *N*-methyl-2,4,6,*N*-tetranitroaniline
22. DATB 1,3-diamino-2,4,6-trinitrobenzene
23. HNE hexanitroethane
24. TNA 1-amino-2,4,6-trinitrobenzene
25. PA 1-hydroxy-2,4,6-trinitrobenzene
26. HNS 2,2′,4,4′,6,6′-hexanitrostilbene
27. TNB 1,3,5-trinitrobenzene
28. TACOT tetranitro-2,3,5,6-dibenzo-1,3a,4,6a-tetraazapentalene
29. HMTD hexamethylenetriperoxide diamine
30. TNT 2,4,6-trinitrotoluene
31. TNM tetranitromethane
32. NM nitromethane
33. DNB 1,3-dinitrobenzene
34. DNT 2,4-dinitrotoluene
35. BuNENA n-butyl-nitratoethylnitramine
36. DIN/ACN1 DINA/acetonitrile 68,5/31,5
37. TATP triacetone triperoxide
38. DIN/ACN2 DINA/acetonitrile 61/39
39. NM/A1 NM/acetone 75/25
40. NM/A2 NM/acetone 70/30