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Journal of Hazardous Materials 141 (2007) 536–539

Journal of Hazardous Materials

www.elsevier.com/locate/jhazmat

Detonation velocity of pure and mixed CHNO explosives at maximum nominal density

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Received 17 May 2006; received in revised form 8 July 2006; accepted 10 July 2006
Available online 1 August 2006

Abstract

In this paper, a simple approach is introduced to predict detonation velocity of pure and mixed explosives at maximum nominal density. This technique may be applied to any pure or mixed explosives that contain elements of carbon, hydrogen, nitrogen and oxygen. The new method requires only elemental composition and some specific structural parameters. The introduced correlation can easily be applied for determining maximum expected detonation velocity of any new CHNO explosive without using its crystal density. Calculated detonation velocities by this procedure for both pure and composite explosive formulations show good agreement with respect to measured detonation velocity at maximum nominal density.

Keywords: Performance; Detonation velocity; CHNO explosives; Correlation; Maximum nominal density

1. Introduction

It is important to obtain better theoretical and empirical models for the behavior of energetic materials and an improved diagnostic capability to measure the complex chemical and hydrodynamic process during detonation. Determination of detonation parameters and thermochemical properties of new high explosives from a given molecular structure identifies any poor candidate, which reduces the costs associated with synthesis, test and evaluation of the materials. Reliable determination of detonation properties are very important to chemists concerned with the synthesis of new high energetic compounds as well as to explosive user.

The amount of energy available in an explosive and the rate of its release in detonation can characterize its effectiveness. Detonation velocity, pressure, temperature and heat may be measured experimentally or calculated from theory to determine the effectiveness of different explosives. They are important detonation performance parameters so that some new methods [1–14] have been recently introduced for simple their evaluation. They also can be calculated by a computer code, e.g. TIGER [15], assuming an equation of state and known parameters such as heat of formation and the density of the explosive. However, reliable experimental data are always preferred over values obtained by computer codes or estimation procedures but all too often reliable data are not available in the field of energetic materials. To compare the relative performance of one explosive with another, empirical prediction methods are more convenient and useful.

Detonation velocity is typically measured to within a few percent at various charge diameters and extrapolated to an "infinite diameter". Since it is the easiest Chapman–Jouguet (C–J) state parameter to measure accurately, its knowledge is important. Numerous studies have also been performed to relate chemical structure and either theoretical maximum density or loading density to detonation velocities [8–10,16,17–25]. Explosives with higher density are preferred for warheads because its higher detonation velocity as well as compactness of warheads used in missiles and ammunitions. Thus, predicting of detonation velocity at maximum nominal or theoretical density is very important in armament design. The purpose of this work was to correlate detonation velocity at maximum nominal density with the explosive's elemental composition and some structural parameters. The new procedure can easily be used for any pure or mixed CHNO explosives. The results will be compared with some well-known pure and mixtures of explosives as well as two new explosives, namely CL-20 and K-6. Since maximum

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doi:10.1016/j.jhazmat.2006.07.060

initial density and the heat of formation are rarely known experimentally, for the new explosive of interest, the present method for estimating maximum detonation velocity at its crystal density is of significant value.

2. Prediction of detonation velocity at maximum nominal density

Rothstein and Petersen [24,25] found that detonation velocities for CHNOF explosives at theoretical maximum density can be related to a factor F, which is dependent only on the chemical composition and the structure of high explosive. They found the following relationship:

$$D' = \frac{F - 0.26}{0.55} = D_0 + 3.0(\rho_{TM} - \rho_0) \quad (1)$$

where ρ_{TM} is the theoretical maximum density, ρ_0 the initial density, D_0 the experimental detonation velocity at ρ_0 and D' the detonation velocity at ρ_{TM}. Factor F depends on some structural parameters such as the number of oxygen atoms in excess to those available to form CO_2 and H_2O and/or the number of

Table 1
Comparison of predicted detonation velocity (km/s) by new (D_{new}) and Rothstein and Petersen (D_{RP}) methods at maximum nominal density with the experimental data

Explosive	p_0	D_{exp}	D_{new}	%dev	D_{RP}	%dev
ABH	1.78	7.6 [30]	7.53	−0.90	7.47	−1.69
BTF	1.86	8.49 [31]	8.70	2.48	8.42	−0.81
DATB	1.788	7.52 [31]	7.85	4.44	7.69	2.27
DEGN	1.38	6.76 [31]	7.11	5.18	6.97	3.11
DIPAM	1.79	7.5 [31]	7.88	5.13	7.57	0.88
EXP D	1.55	6.85 [31]	6.89	0.57	7.58	10.69
HMX	1.9	9.1 [30]	8.95	−1.67	9.04	−0.63
HNAB	1.6	7.31 [31]	7.47	2.20	7.64	4.45
HNB	1.97	9.3 [31]	9.15	−1.66	9.10	−2.12
HNS	1.74	7.13 [30]	6.90	−3.21	6.83	−4.21
NG	1.6	7.7 [31]	8.08	4.96	7.48	−2.91
NM	1.13	6.35 [31]	6.49	2.17	5.50	−13.36
NONA	1.78	7.56 [30]	7.55	−0.16	7.31	−3.31
NQ	1.78	8.59 [31]	8.36	−2.65	8.26	−3.82
ONT	1.8	7.33 [31]	7.00	−4.57	6.96	−4.99
PETN	1.77	8.3 [30]	7.87	−5.16	8.08	−2.69
PICRIC ACID	1.76	7.57 [31]	7.56	−0.11	7.36	−2.79
RDX	1.8	8.754 [30]	8.63	−1.41	8.94	2.12
TACOT	1.85	7.25 [31]	7.17	−1.05	7.06	−2.63
TATB	1.895	7.86 [30]	8.04	2.26	7.86	0.01
TETRYL	1.73	7.72 [31]	7.80	1.10	7.77	0.67
TNM	1.64	6.36 [31]	6.31	−0.82	6.75	6.12
TNT	1.64	6.95 [30]	7.07	1.70	6.66	−4.10
TNTAB	1.74	8.58 [30]	8.56	−0.23	9.44	10.05
COM B	1.72	7.92 [31]	7.82	−1.22		
COM B-3	1.72	7.89 [31]	7.83	−0.82		
COM C-3	1.6	7.63 [31]	7.87	3.15		
Composition B	1.713	8.03 [30]	8.30	3.31		
Cyclotol-77/23	1.743	8.25 [30]	8.45	2.46		
Cyclotol-70/30	1.73	8.06 [31]	7.90	−2.01		
Cyclotol-65/35	1.72	8.04 [31]	7.86	−2.21		
Cyclotol-60/40	1.74	8.09 [31]	7.83	−3.23		
Cyclotol-50/50	1.63	7.66 [31]	7.76	1.27		
EDC-11	1.782	8.213 [30]	7.83	−4.67		
EDC-24	1.776	8.713 [30]	8.48	−2.68		
LX-01	1.24	6.84 [31]	6.74	−1.51		
LX-14	1.81	8.76 [30]	8.69	−0.77		
95/5 NQ/estane	1.705	8.3 [30]	8.34	0.43		
Octol-76.3/23.7	1.809	8.476 [30]	8.70	2.66		
PBX-9011	1.767	8.5 [30]	8.40	−1.16		
PBX-9501	1.841	8.826 [30]]	8.80	−0.29		
PBX-9007	1.64	8.09 [31]	7.83	−3.24		
PBX-9205	1.67	8.17 [31]	7.89	−3.46		
PBXC-116	1.65	7.96 [30]	7.75	−2.63		
PBXC-119	1.635	8.075 [30]	7.72	−4.46		
Pentolite	1.65	7.465 [30]	7.57	1.46		
95/5 PYX/polyethylene	1.556	7.097 [30]	6.99	−1.53		
Average absolute deviation				2.26		3.77

fluorine atoms in excess to those available to form HF, the number of nitrato groups existing either as a nitrate ester or as a nitric acid salt, etc. Chen and coworkers were also used [26] backpropagation neural networks to predict detonation velocity at theoretical maximum density.

The study of detonation velocities of various CHNO pure and mixed explosives show that one can express detonation velocity at maximum nominal density as a function of basic parameters, namely the elemental composition and some structural parameters. Various situations are examined and optimized with experimental data. The results have shown that the following simple equation can provide the suitable pathway for predicting detonation velocity at maximum nominal density:

$$D'(\mathrm{km\,s^{-1}}) = y_1 + y_2 a + y_3 b + y_4 c + y_5 d + \sum_{i=6} y_i \mathrm{SSP}_i \quad (2)$$

where a, b, c, and d are stoichiometric coefficients for an explosive of general formula $C_aH_bN_cO_d$, y_i is adjustable parameter and SSP_i is specific structural parameters. Eq. (2) provides the basis for a simple procedure to estimate detonation velocity at maximum nominal or theoretical density. As shown in Eq. (2), elemental composition and some structural parameters are only input information. Experimental data of detonation velocity of all pure explosives and some composite explosives, which are given in Table 1, were used to obtain the adjustable parameters. Although Eq. (2) contains several adjustable parameters, the study showed that optimization of mentioned parameters with large experimental data, by MATLAB [27], gives good result. Multiple linear regression method [27] was used to find adjustable parameters of Eq. (2). The left-division method for solving linear equations uses the least squares method because the equation set is overdetermined [27]. The final form of the optimized correlation can be given as:

$$D'(\mathrm{km\,s^{-1}}) = 7.678 - 0.1977a - 0.1105b + 0.2940c + 0.0742d - 0.6347n_{\mathrm{NR}} - 0.7354n_{\mathrm{mN}} \quad (3)$$

where n_{NR} is the number of –N=N– or NH_4^+ in explosive and n_{mN} is the number of nitro groups ($–NO_2$) attached to carbon in nitrocompounds in which $a = 1$. R^2 value or the coefficient of determination of this correlation is 0.92 [27]. Eq. (3) provides the simplest empirical procedure to estimate detonation velocities of pure and composite explosives. It should be mentioned that Eq. (3) can be used only for nitro, nitrate and nitramine energetic compounds. As seen in Table 1, detonation velocities for 47 underoxidized and overoxidized pure as well as mixed explosives are calculated and compared with corresponding measured values. The percent error, [(predicted − measured)/measured] × 100, are also given in Table 1. The good agreement with experimental values may be taken as appropriate validation test of the new method with pure and mixed $C_aH_bN_cO_d$ explosives. The average percent absolute deviation in Table 1 for new method is 2.26% meanwhile for Rothstein and Petersen [24,25] method in the case of pure explosives is 3.77%.

The new method can be applied for any new $C_aH_bN_cO_d$ energetic compounds. As representative examples, the new method was used to find detonation velocities of two new explosives CL-20 [28] and K-6 [29] at their crystal densities. CL-20 and K-6 have crystal densities 2.04 and 1.932 g/cc, respectively. Their calculated detonation velocities are 10.14 km/s for CL-20 and 9.17 km/s for K-6 [14] at mentioned crystal densities, which are close to calculated values from Eq. (3), 10.25 and 9.15 km/s for CL-20 and K-6 respectively.

3. Conclusions

The main aim of this study was to develop a simple method to calculate detonation velocity of an explosive at its crystal density or maximum nominal density. The developed method is suitable way to estimate maximum detonation velocity of a pure or composite explosive without using initial density and heat of formation of energetic compound. The results are remarkable because the required data are only the elemental composition and molecular structure of explosive. This method is much simpler to user as compared with methods of Rothstein and Petersen [24,25] or Chen and coworkers [26]. Since a few percent errors can generally be attributed to experimental measurements of detonation velocity, the agreement between calculated and measured velocities is very good. Therefore, the new simple method appears to give accurate detonation velocities at maximum nominal density.

Acknowledgements

I would like to thank the research committee of Malek-ashtar University of Technology (MUT) for supporting this work. This research was supported in part by Institute of Chemical and Science Technology, Tehran, Iran Research Council Grant (No. ICST-8I03-2136).

Appendix A

Glossary of compound names

1. ABH: Azobis (2,2′,4,4′,6,6′-hexanitrobisphenyl) ($C_{24}H_6N_{14}O_{24}$)
2. BTF: Benzotris [1,2,5] oxadiazole, 1, 4, 7-trioxide ($C_6N_6O_6$)
3. COMP B: 63/36/1 RDX/TNT/wax ($C_{2.03}H_{2.64}N_{2.18}O_{2.67}$)
4. COMP B-3: 60/40 RDX/TNT ($C_{2.04}H_{2.50}N_{2.15}O_{2.68}$)
5. COMP C-3: 77/4/10/5/1/3 RDX/TNT/DNT/MNT/NC/TETRYL ($C_{1.90}H_{2.83}N_{2.34}O_{2.60}$)
6. Composition B: 64/36 RDX/TNT ($C_{6.851}H_{8.750}N_{7.650}O_{9.3}$)
7. Cyclotol-77/23: 77/23 RDX/TNT ($C_{5.045}H_{7.461}N_{6.786}O_{7.753}$)
8. Cyclotol-70/30: 70/30 RDX/TNT ($C_{1.87}H_{2.56}N_{2.29}O_{2.68}$)
9. Cyclotol-65/35: 65/35 RDX/TNT ($C_{1.96}H_{2.53}N_{2.22}O_{2.68}$)
10. Cyclotol-60/40: 60/40 RDX/TNT ($C_{2.04}H_{2.50}N_{2.15}O_{2.68}$)
11. Cyclotol-50/50: 50/50 RDX/TNT ($C_{2.22}H_{2.45}N_{2.01}O_{2.67}$)
12. DATB: 1,3-Diamino-2,4,6-trinitrobenzene ($C_6H_5N_5O_6$)
13. DEGN: Diethyleneglycol dinitrate ($C_4H_8N_2O_7$)

14. DIPM: Dipiramide ($C_{12}H_6N_8O_{12}$)
15. EDC-11: 64/4/30/1/1 HMX/RDX/TNT/Wax/trylene ($C_{1.986}H_{2.7825}N_{2.233}O_{2.6293}$)
16. EDC-24: 95/5 HMX/Wax ($C_{5.113}H_{10.252}N_8O_8$)
17. EXP D: Ammonium picrate ($C_6H_6N_4O_7$)
18. HMX: Cyclotetramethylenetetranitramine ($C_4H_8N_8O_8$)
19. HNAB: 2,2′,4,4′,6,6′-Hexanitroazobenzene ($C_{12}H_4N_8O_{12}$)
20. HNB: Hexanitrobenzene ($C_6N_6O_{12}$)
21. HNS: 2,2′,4,4′,6,6′-Hexanitrostilbene ($C_{14}H_6N_6O_{12}$)
22. MEN-II: 72.2/23.4/4.4 Nitromethane/methanol/ethylene diamine ($C_{2.06}H_{7.06}N_{1.33}O_{3.10}$)
23. NG: Nitroglycerine ($C_3H_5N_3O_9$)
24. NM: Nitromethane (CH_3NO_2)
25. NONA: 2,2′,2″,4,4′,4″,6,6′,6″-Nonanitroterphenyl ($C_{18}H_5N_9O_{18}$)
26. NQ: Nitroguanidine ($CH_4N_4O_2$)
27. ONT: 2,2′,4,4′,4″,6,6′,6″-Octanitroterphenyl ($C_{18}H_6N_8O_{16}$)
28. PA: Picric acid ($C_6H_3N_3O_7$)
29. PETN: Pentaerythritol tetranitrate ($C_5H_8N_4O_{12}$)
30. RDX: Cyclomethylene trinitramine ($C_3H_6N_6O_6$)
31. TACOT: 2,4,8,10-Tetranitro-5H-benzotriazolo[2,1,a]-benzotriazol-6-ium, hydroxide, inner salt ($C_{12}H_4N_8O_8$)
32. TATB: 1,3,5-Triamino-2,4,6-trinitrobenzene ($C_6H_6N_6O_6$)
33. TETRYL: *N*-Methyl-*N*-nitro-2,4,6-trinitroaniline ($C_7H_5N_5O_8$)
34. TNM: Tetranitromethane (CN_4O_8)
35. TNT: 2,4,6-Trinitrotoluene ($C_7H_5N_3O_6$)
36. TNTAB: Trinitrotriazidobenzene ($C_6N_{12}O_6$)
37. LX-14: 95/5 HMX/estane ($C_{4.800}H_{9.1365}N_{8.024}O_{8.2811}$)
38. LX-01: 51.7/33.2/15.1 NM/TNM/1-nitropropane ($C_{1.52}H_{3.73}N_{1.69}O_{3.39}$)
39. 95/5 NQ/estane ($C_{1.281}H_{4.3993}N_4O_{2.0987}$)
40. Octol-76.3/23: 76.3/23.7 HMX/TNT ($C_{6.835}H_{10.025}N_{9.215}O_{10.43}$)
41. PBX-9007: 90/9.1/0.5/0.4 RDX/polystyrene/DOP/rosin ($C_{1.97}H_{3.22}N_{2.43}O_{2.44}$)
42. PBX-9011: 90/10 HMX/estane ($C_{5.696}H_{10.476}N_{8.062}O_{8.589}$)
43. PBX-9501: 95/2.5/2.5 HMX/estane/BDNPF ($C_{4.575}H_{8.8678}N_{8.112}O_{8.390}$)
44. PBX-9205: 92/6/2 RDX/polystyrene/DOP ($C_{1.83}H_{3.14}N_{2.49}O_{2.51}$)
45. PBXC-116: 86/14 RDX/binder ($C_{1.968}H_{3.7463}N_{2.356}O_{2.4744}$)
46. PBXC-119: 82/18 HMX/binder ($C_{1.817}H_{4.1073}N_{2.2149}O_{2.6880}$)
47. Pentolite: 50/50 TNT/PETN ($C_{2.332}H_{2.3659}N_{1.293}O_{3.2187}$)
48. 95/5 PYX/polyethylene ($C_{19.33}H_{11.663}N_{11}O_{16}$)

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