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Journal of Hazardous Materials A137 (2006) 1328–1332

Journal of Hazardous Materials

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Velocity of detonation at any initial density without using heat of formation of explosives

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Received 15 March 2006; received in revised form 2 May 2006; accepted 2 May 2006
Available online 9 May 2006

Abstract

The simplest method is introduced for reliable estimating the detonation velocity of large class of CHNO explosives based elemental composition and specific structural groups. There is no need to use heat of formation and the other experimental data for calculation of detonation velocity in the new procedure. Only elemental composition and the number of special structural groups without using heat of formation of explosive is sufficient for reliable desk calculation of detonation velocity. The results show good agreement with experimental values with respect to computed results obtained by complex computer code using BKWS and BKWR equations of state. Predicted velocities of detonation have root-mean-square (rms) percent deviation of 2.2, 5.9 and 5.3 from experimental data for new method, BKWS and BKWR equations of state, respectively.

Keywords: Velocity of detonation; CHNO explosives; Elemental composition; Loading density

1. Introduction

One of the major challenges to chemical industry is the search for new energetic materials with a given performance. Simple reliable prediction of the performance of new energetic materials from a given molecular structure and the known or estimated crystal density is highly desirable to chemist for the expenditure connected with the development and synthesis of new and formulation of energetic materials. Prediction of the performance of new energetic materials should be evaluated prior their actual synthesis because it reduces the costs associated with synthesis and test as well as evaluation of the materials. Due to the difficulty of synthesis and the instability of energetic material, not so many experimental studies have been done. The spending connected with the development and synthesis of new energetic materials also necessitates connected with the development of theoretical methods.

Detonation velocity as one of the important performance parameters can be used for measuring the effectiveness of different explosives. It can typically be measured to within a few percent at various charge diameters and extrapolated to an infinite diameter for comparison with steady state calculation. It can be calculated by some computer codes such as BKW [1] and RUBY [2] and latter's offspring TIGER [3], CHEQ [4] and CHEETAH [5] (a C version of TIGER) with an appropriate empirical equation of state such as Becker–Kistiakosky–Wilson (BKW-EOS) [6], the Jacobs–Cowperthwaite–Zwisler (JCZ-EOS) [7,8] and Kihara–Hikita–Tanaka (KHT-EOS) [9]. The BKW-EOS, in spite of its weak theoretical basis, is used extensively to calculate detonation properties of high explosives. Hobbs and Baer [10] give the historical background and molecular covolumes for the BKW-EOS:

$$\frac{PV}{RT} = 1 + X\,\mathrm{e}^{\beta X} \quad \text{with} \quad X = \frac{\kappa \sum n_i k_i}{V(T+\theta)^{\alpha}} \tag{1}$$

where P, V, R, T and n_i represent pressure, molar gas volume, gas constant, absolute temperature and mole fraction of the ith gaseous component, respectively. The summation extends over

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doi:10.1016/j.jhazmat.2006.05.002

Table 1
Comparison of detonation velocity (km/s) of the new correlation, Eq. (2), as well as BKWS-EOS and BKWR-EOS with measured values [11]

Name[a]	ρ_0 (g/cm^3)	D_{exp}	D_{new}	%Dev new	$D_{BKWR\text{-}EOS}$	%Dev BKWR-EOS	$D_{BKWS\text{-}EOS}$	%Dev BKWS-EOS
ABH	1.64	7.2	7.08	−1.6	7.28	1.1	7.14	−0.8
COM B	1.72	7.92	7.93	0.1	8.12	2.5	8.2	3.5
COM B-3	1.72	7.89	7.92	0.4	8.08	2.4	8.16	3.4
COM C-3	1.6	7.63	7.53	−1.3	7.77	1.8	7.74	1.4
CYCLOTOL-78/22	1.76	8.31	8.14	−2.1	8.4	1.1	8.53	2.6
CYCLOTOL-77/23	1.74	8.25	8.06	−2.3	8.33	1.0	8.44	2.3
CYCLOTOL-75/25	1.76	8.3	8.13	−2.1	8.37	0.8	8.49	2.3
	1.62	7.95	7.62	−4.1	7.91	−0.5	7.95	0.0
CYCLOTOL-70/30	1.73	8.06	8.00	−0.8	8.22	2.0	8.31	3.1
CYCLOTOL-65/35	1.72	8.04	7.94	−1.2	8.13	1.1	8.22	2.2
CYCLOTOL-60/40	1.74	8.09	7.99	−1.2	8.15	0.7	8.24	1.9
CYCLOTOL-60/40	1.72	7.9	7.92	0.3	8.08	2.3	8.16	3.3
CYCLOTOL-50/50	1.63	7.66	7.56	−1.3	7.69	0.4	7.71	0.7
DATB	1.8	7.6	7.61	0.2	7.92	4.2	7.86	3.4
	1.78	7.6	7.54	−0.8	7.85	3.3	7.79	2.5
DEGN	1.38	6.76	6.60	−2.4	7.08	4.7	7.19	6.4
DIPM	1.76	7.4	7.30	−1.4	7.62	3.0	7.56	2.2
EXP D	1.55	6.85	6.91	0.9	7.02	2.5	6.91	0.9
	1.48	6.7	6.66	−0.6	6.78	1.2	6.66	−0.6
HMX	1.89	9.11	9.20	0.9	9.08	−0.3	9.35	2.6
	1.6	7.91	8.15	3.1	8.1	2.4	8.14	2.9
	1.4	7.3	7.44	1.9	7.45	2.1	7.41	1.5
	1.2	6.58	6.72	2.1	6.85	4.1	6.78	3.0
	1	5.8	6.00	3.4	6.31	8.8	6.2	6.9
	0.75	4.88	5.10	4.5	5.54	13.5	5.42	11.1
HNAB	1.6	7.31	7.28	−0.4	7.22	−1.2	7.09	−3.0
HNS	1.6	6.8	6.77	−0.4	6.96	2.4	6.88	1.2
	1.7	7	7.13	1.9	7.26	3.7	7.22	3.1
LX-14	1.84	8.83	8.47	−4.0	8.86	0.3	9.04	2.4
MEN-2	1.02	5.49	5.31	−3.3	5.97	8.7	6	9.3
NG	1.6	7.7	7.74	0.5	7.94	3.1	8.01	4.0
NONA	1.7	7.4	7.23	−2.3	7.35	−0.7	7.26	−1.9
NQ	1.78	8.59	8.46	−1.5	8.83	2.8	8.53	−0.7
	1.62	7.93	7.89	−0.5	8.17	3.0	7.82	−1.4
	1.55	7.65	7.64	−0.2	7.89	3.1	7.52	−1.7
OCTOL-78/22	1.82	–	8.35	–	8.59	–	8.76	–
OCTOL-76/23	1.81	8.45	8.31	−1.7	8.54	1.1	8.7	3.0
OCTOL-75/25	1.81	8.48	8.31	−2.0	8.53	0.6	8.69	2.5
OCTOL-60/40	1.8	8.16	8.21	0.6	8.34	2.2	8.47	3.8
PBX-9011	1.77	8.5	8.17	−3.8	8.56	0.7	8.65	1.8
PBX-9501	1.84	8.83	8.48	−3.9	8.87	0.5	9.07	2.7
PENTOLITE	1.71	7.75	7.77	0.2	7.72	−0.4	7.91	2.1
	1.7	7.53	7.73	2.7	7.69	2.1	7.87	4.5
	1.68	7.65	7.66	0.2	7.63	−0.3	7.8	2.0
	1.64	7.53	7.52	−0.2	7.51	−0.3	7.65	1.6
PETN	1.76	8.27	8.29	0.3	8.23	−0.5	8.67	4.8
	1.7	8.07	8.08	0.1	8.02	−0.6	8.43	4.5
	1.6	7.75	7.72	−0.4	7.7	−0.6	8.03	3.6
	1.45	7.18	7.18	0.0	7.27	1.3	7.48	4.2
	1.23	6.37	6.39	0.3	6.71	5.3	6.76	6.1
	0.99	5.48	5.52	0.8	6.01	9.7	5.99	9.3
	0.88	5.06	5.13	1.4	5.65	11.7	5.61	10.9
	0.48	3.6	3.69	2.5	4.24	17.8	4.12	14.4
	0.3	2.99	3.04	1.8	3.57	19.4	3.44	15.1
	0.25	2.83	2.86	1.2	3.38	19.4	3.25	14.8

Table 1 (*Continued*)

Name[a]	ρ_0 (g/cm^3)	D_{exp}	D_{new}	%Dev new	$D_{BKWR-EOS}$	%Dev BKWR-EOS	$D_{BKWS-EOS}$	%Dev BKWS-EOS
PA	1.76	7.57	7.83	3.5	7.69	1.6	7.71	1.8
	1.71	7.26	7.65	5.4	7.69	5.9	7.71	6.2
	1.6	7.1	7.26	2.2	7.69	8.3	7.71	8.6
RDX	1.8	8.75	8.68	−0.8	8.77	0.2	8.96	2.4
	1.77	8.7	8.57	−1.4	8.67	−0.3	8.84	1.6
	1.72	8.46	8.39	−0.8	8.5	0.5	8.63	2.0
	1.66	8.24	8.18	−0.7	8.3	0.7	8.38	1.7
	1.6	8.13	7.96	−2.0	8.1	−0.4	8.15	0.2
	1.46	7.6	7.46	−1.8	7.64	0.5	7.63	0.4
	1.4	7.46	7.25	−2.9	7.45	−0.1	7.42	−0.5
	1.29	7	6.85	−2.1	7.12	1.7	7.06	0.9
	1.2	6.77	6.53	−3.6	6.86	1.3	6.79	0.3
	1.1	6.18	6.17	−0.2	6.58	6.5	6.49	5.0
RDX	1	6.1	5.81	−4.8	6.32	3.6	6.21	1.8
	0.95	5.8	5.63	−3.0	6.19	6.7	6.06	4.5
	0.7	4.65	4.73	1.7	5.36	15.3	5.25	12.9
	0.56	4.05	4.23	4.4	4.84	19.5	4.72	16.5
TACOT	1.85	7.25	7.45	2.8	7.79	7.4	7.62	5.1
TATB	1.88	7.76	7.74	−0.2	8.28	6.7	8.19	5.5
	1.85	7.66	7.63	−0.3	8.18	6.8	8.07	5.4
TETRYL	1.73	7.72	7.87	2.0	7.75	0.4	7.81	1.2
	1.71	7.85	7.80	−0.6	7.69	−2.0	7.74	−1.4
	1.68	7.5	7.69	2.6	7.6	1.3	7.63	1.7
	1.61	7.58	7.44	−1.8	7.39	−2.5	7.38	−2.6
	1.36	6.68	6.54	−2.1	6.67	−0.1	6.59	−1.3
	1.2	6.34	5.97	−5.9	6.24	−1.6	6.15	−3.0
TNT	1.64	6.93	7.22	4.2	7.2	3.9	7.19	3.8
	1.45	6.5	6.54	0.6	6.6	1.5	6.51	0.2
	1.36	6.2	6.21	0.2	6.32	1.9	6.22	0.3
	1	5	4.92	−1.6	5.3	6.0	5.21	4.2
	0.8	4.34	4.20	−3.2	4.79	10.4	4.74	9.2
BTF	1.86	8.49	8.52	0.4	8.43	−0.7	8.4	−1.1
	1.76	8.26	8.16	−1.2	8.14	−1.5	8.14	−1.5
HNB	1.97	9.3	9.18	−1.3	8.89	−4.4	8.47	−8.9
TNTAB	1.74	8.58	8.81	2.7	8.44	−1.6	8.39	−2.2
rms percent deviation				2.2		5.9		5.3

[a] See Appendix A for glossary of compound name.

all components of the gaseous mixture. The covolume factors, k_i, represent excluded volume [10]. The parameters α, β, κ and θ are also empirical constants. The parameters α, β, κ, θ and k_i are adjusted to fit measured detonation properties. However, the BKWC-EOS [5], BKWS-EOS [10] and BKWR-EOS [11] are three different parameterizations of the BKW-EOS. Some theoretical methods have also been used for simple evaluation of detonation velocity of explosives using heat of detonation at loading density greater than 1 g/cm^3 [12,13] or any loading density [14], approximate detonation temperature [15] and gas phase heat of formation [16]. Calculated detonation velocity using different mentioned methods usually requires the heat of formation and the density of the explosive.

The purpose of this work is to introduce the simplest method for calculating detonation velocity of CHNO explosives at any loading density only from structure of explosives without the use of heat of formation and detonation products. The new procedure introduces a new simple correlation for desk calculation of detonation velocity of explosives as function of elemental composition and some specific groups. Another goal of this work is to provide insight to understanding suitable mixture of high explosives which are responsible for higher detonation velocity and which are not. In this paper, the influence of chemical composition and initial densities of explosives for determining their detonation velocities are of particular importance. The calculated detonation velocity will compare with measured values for some well-known pure and mixed explosives over a wide range of loading densities. The results will be also compared with the computed values using BKWS-EOS and BKWR-EOS.

2. New predicting method of velocity of detonation

The velocity at which the detonation shock wave proceeds through a charge is an important detonation parameter so that detonation velocity is one the most important detonation parameters. Its measurements are probably good to within few

percent as well as enough data for various explosives [1]. However, its knowledge is important because it is the easiest Chapman–Jouguet (C–J) state parameter to measure accurately. Moreover, some useful equations relate the detonation velocity to the other C–J state parameters [1].

To establish a correlation between molecular properties and measured data, finding reliable data would be needed. One can express detonation velocity as a function of basic parameters, namely the elemental composition, oxygen balance, heat of formation and initial density of mixture. However, it is found that the detonation velocity can be related to its elemental composition and some specific groups. To express detonation velocity as a function of mentioned parameters, various combinations of them were studied and optimized with experimental data. The results showed that the following model can provide the suitable pathway to obtain prediction of detonation velocity:

$$D = z_1 + z_2\rho_0 + \sum_{i=3} z_i ns_i \quad (2)$$

where ρ_0 is the loading density, z_i the adjustable parameters and ns_i is the number of carbon, hydrogen, nitrogen, oxygen and specific functional groups. Experimental data of various pure explosives, which are listed in Table 1, were used to find adjustable parameters (R-squared value or the coefficient of determination [17], 0.989). Final correlation can be given as follows:

$$D\,(\text{km/s}) = 1.6439 + 3.5933\rho_0 - 0.1326a - 0.0034b + 0.1206c + 0.0442d - 0.2768n_{-\text{NRR}'} \quad (3)$$

where a, b, c, d and $-\text{NRR}'$ are the number of moles of carbon, hydrogen, oxygen, nitrogen and specific group in explosives. The specific group $-\text{NRR}'$ includes $-NH_2$, NH_4^+ and  groups. Calculated detonation velocities of well-known pure and mixed explosives are given in Table 1. The results are compared with experimental data as well as computed values of BKWS-EOS and BKWR-EOS. As seen in Table 1, the new hand calculated detonation velocities show surprisingly very good agreement with experimental data especially at loading densities less than 1 g/cm^3 as compared to the results of complicated computation outputs. Comparison of the calculated results with experimental data may be taken as appropriate validation test of the introduced simple correlation for overoxidized and underoxidized explosives.

3. Limitations of new correlation

The new correlation has two restrictions for predicting detonation velocities of various CHNO explosives: (i) deviation from experimental data increases with non-energetic additives in the case of mixture of explosives and (ii) this correlation cannot be used for very high overoxidized explosives, e.g. TNM, and their mixtures with the other components, e.g. LX-01.

4. Conclusions

A new method has introduced for calculating detonation velocities of CHNO explosive so that there is no need to use any experimental data, assumed detonation products and heat of formation. Calculated detonation velocities by new method for most pure and mixed well-known explosives show good agreement with experimental values with respect to computed results obtained by two complex BKWS-EOS and BKWR-EOS computations. As indicated in Table 1, this method gives good detonation velocity predictions for loading density less than 1 g/cm^3. The new correlation requires no prior knowledge of any measured, estimated or calculated physical, chemical or thermochemical properties of explosive and assumed detonation products.

The new approach is the simplest method for reliable quick estimation of detonation velocity and, at the same time, gives results that are comparable with predicted values from the other methods involving the equation of state of the products. Since few percent deviations generally attributed to experimental measurements, the agreement between calculated and measured detonation velocity is satisfactory. One can estimate detonation velocities of new or mixture of high explosives to within about a few percent from the given chemical formula and molecular structure. The results of this work are remarkable because the necessary data for this method is only elemental composition of explosive and determining specific group.

In brief, the introduced simple hand calculated empirical correlation for determining detonation velocities of CHNO explosives show surprisingly very good agreement with experimental values at given loading density which may be taken as appropriate validation tests of the new method.

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-8I03-2131).

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. DATB: 1,3-Diamino-2,4,6-trinitrobenzene ($C_6H_5N_5O_6$)
4. DEGN: Diethyleneglycol dinitrate ($C_4H_8N_2O_7$)
5. DIPM: Dipiramide ($C_{12}H_6N_8O_{12}$)
6. EXP D: Ammonium picrate ($C_6H_6N_4O_7$)
7. HMX: Cyclotetramethylenetetranitramine ($C_4H_8N_8O_8$)
8. HNAB: 2,2′,4,4′,6,6′-Hexanitroazobenzene ($C_{12}H_4N_8O_{12}$)
9. HNB: Hexanitrobenzene ($C_6N_6O_{12}$)
10. HNS: 2,2′,4,4′,6,6′-Hexanitrostilbene ($C_{14}H_6N_6O_{12}$)
11. NG: Nitroglycerine ($C_3H_5N_3O_9$)

12. MEN-II: 72.2/23.4/4.4 nitromethane/methanol/ethylene diamine ($C_{2.06}H_{7.06}N_{1.33}O_{3.10}$)
13. NONA: 2,2′,2″,4,4′,4″,6,6′,6″-Nonanitroterphenyl ($C_{18}H_5N_9O_{18}$)
14. NQ: Nitroguanidine ($CH_4N_4O_2$)
15. PA: Picric acid ($C_6H_3N_3O_7$)
16. PETN: Pentaerythritol tetranitrate ($C_5H_8N_4O_{12}$)
17. RDX: Cyclomethylene trinitroamine ($C_3H_6N_6O_6$)
18. TACOT: 2,4,8,10-Tetranitro-5H-benzotriazolo[2,1,*a*]-benzotriazol-6-ium, hydroxide, inner salt ($C_{12}H_4N_8O_8$)
19. TATB: 1,3,5-Triamino-2,4,6-trinitrobenzene ($C_6H_6N_6O_6$)
20. TETRYL: *N*-Methyl-*N*-nitro-2,4,6-trinitroaniline ($C_7H_5N_5O_8$)
21. TNM: Tetranitromethane (CN_4O_8)
22. TNT: 2,4,6-Trinitrotoluene ($C_7H_5N_3O_6$)
23. TNTAB: Trinitrotriazidobenzene ($C_6N_{12}O_6$)
24. COMP B: 63/36/1 RDX/TNT/wax ($C_{2.03}H_{2.64}N_{2.18}O_{2.67}$)
25. COMP B-3: 60/40 RDX/TNT ($C_{2.04}H_{2.50}N_{2.15}O_{2.68}$)
26. COMP C-3: 77/4/10/5/1/3 RDX/TNT/DNT/MNT/NC/TETRYL ($C_{1.90}H_{2.83}N_{2.34}O_{2.60}$)
27. CYCLOTOL-78/22: 78/22 RDX/TNT ($C_{1.73}H_{2.59}N_{2.40}O_{2.69}$)
28. CYCLOTOL-77/23: 77/23 RDX/TNT ($C_{1.75}H_{2.59}N_{2.38}O_{2.69}$)
29. CYCLOTOL-75/25: 75/25 RDX/TNT ($C_{1.78}H_{2.58}N_{2.36}O_{2.69}$)
30. CYCLOTOL-70/30: 70/30 RDX/TNT ($C_{1.87}H_{2.56}N_{2.29}O_{2.68}$)
31. CYCLOTOL-65/35: 65/35 RDX/TNT ($C_{1.96}H_{2.53}N_{2.22}O_{2.68}$)
32. CYCLOTOL-60/40: 60/40 RDX/TNT ($C_{2.04}H_{2.50}N_{2.15}O_{2.68}$)
33. CYCLOTOL-50/50: 50/50 RDX/TNT ($C_{2.22}H_{2.45}N_{2.01}O_{2.67}$)
34. LX-14: 95.5/4.5 HMX/Estane 5702-F1 ($C_{1.52}H_{2.92}N_{2.59}O_{2.66}$)
35. OCTOL-78/22: 77.6/22.4 HMX/TNT ($C_{1.74}H_{2.59}N_{2.39}O_{2.69}$)
36. OCTOL-76/23: 76.3/23.7 HMX/TNT ($C_{1.76}H_{2.58}N_{2.37}O_{2.69}$)
37. OCTOL-75/25: 75/25 HMX/TNT ($C_{1.78}H_{2.58}N_{2.36}O_{2.69}$)
38. OCTOL-60/40: 60/40 HMX/TNT ($C_{2.04}H_{2.50}N_{2.15}O_{2.68}$)
39. PBX-9011: 90/10 HMX/Estane ($C_{1.73}H_{3.18}N_{2.45}O_{2.61}$)
40. PBX-9501: 95/2.5/2.5 HMX/Estane/EDNPA-F ($C_{1.47}H_{2.86}N_{2.60}O_{2.69}$)
41. PENTOLITE: 50/50 TNT/PETN ($C_{2.33}H_{2.37}N_{1.29}O_{3.22}$)

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