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Research Article

Simple correlation for predicting detonation velocity of ideal and non-ideal explosives

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ABSTRACT

This paper describes a simple method for prediction of detonation velocity of ideal and non-ideal explosives. A non-ideal aluminized and nitrated explosive can have Chapman–Jouguet detonation velocity significantly different from that expected from existing thermodynamic computer codes for equilibrium and steady-state calculations. Detonation velocity of explosives with general formula $C_aH_bN_cO_dAl_e$ can be predicted only from values of *a*, *b*, *c*, *d*, *e* and a specific structural parameter without using any assumed detonation products, heat of formation and experimental data. Predicted detonation velocities by this procedure for ideal and non-ideal explosives show good agreement with respect to experimental values as compared to computed results of BKWR and BKWS equations of state.

1. Introduction

An ideal explosive is one whose performance can be described adequately for engineering purpose by steady-state detonation calculations using appropriate equations of state. Ideal explosives like HMX, RDX and TNT should have short reaction zone and have small failure diameters, which are suitable for practical applications. A non-ideal explosive has significantly different detonation properties than those predicted by some computer codes such as BKW [1], RUBY [2] and latter's offspring TIGER [3], CHEQ [4], and CHEETAH [5] (a C version of TIGER) which use empirical equations of state such as Becker–Kistiakosky–Wilson (BKW-EOS) [6], Jacobs–Cowperthwaite–Zwisler (JCZ-EOS) [7] or Kihara–Hikita–Tanaka (KHT-EOS) [8]. Aluminized composite explosives and explosive nitrate salts are two common non-ideal explosives. Physical separation of the fuel and oxidizer in non-ideal explosives results in extended chemical reaction zone. However, diffusion may play a major role in experimentally determined detonation properties.

Aluminum powder is a common ingredient in solid propellants because it is a high-energy combustible material. Moreover, it increases the energy and raises the flame temperature in rocket propellants. Thus, it is widely used in rocket propellants, fuel–air and aluminized explosives. It is also incorporated into explosives in order to raise reaction temperature, enhance heat of detonation, increase bubble energies in underwater weapons, improve air blast and create incendiary effect. To explain the role of aluminum powder in the detonation process of aluminized explosives, some investigations have been done [9–13]. Ammonium nitrate-based explosives are the important explosive nitrate salts which have been widely used as industrial explosives or energetic compositions such as ANFO (ammonium nitrate and fuel oil), emulsion explosives or Amatol, etc. Explosive nitrate salts are known as non-ideal explosives because their detonation velocities do not easily reach theoretically predicted values. Their non-ideal behavior causes a wide reaction zone in combination with lateral heat losses and refraction waves which extinguish the decomposition reactions. This can be explained by the low decomposition rate of ammonium nitrate.

The purpose of this work is to introduce a simple general correlation for calculating detonation velocity of ideal and non-ideal explosives, i.e. aluminized composite explosives or explosive nitrate salts, at any loading density only from data on molecular structure of explosives without the use of heat of formation and detonation products. It is shown here how detonation velocity of pure and mixture of CHNO explosives as well as aluminized or nitrated explosives with formula $C_aH_bN_cO_dAl_e$ can be predicted using their molecular structures. The calculated detonation velocity will also be tested on some well-known explosives as well as compared with computed results of two appropriate equations of state.

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2. Theory

2.1. Predicting detonation velocity

Prediction of detonation properties of new energetic materials should be done prior to their actual synthesis. Due to the difficulty of synthesis and the instability of energetic material, theoretical methods reduce the costs associated with synthesis, test and evaluation of the materials. Predicting detonation velocity is very important in armament design. Its measurements are probably good (within a few percent), since it is the easiest Chapman–Jouguet (C–J) state parameter to measure accurately. As mentioned before, it can be predicted by some complicated computer codes with an appropriate empirical equation of state. The BKW-EOS in spite of its weak theoretical basis is used extensively and the BKWC-EOS [5], BKWS-EOS [14] and BKWR-EOS [15] are three different parameterizations of the BKW-EOS. Some simple methods have also been used for simple evaluation of detonation velocity of explosives through different approaches [16].

2.2. Non-ideal explosives and prediction of their detonation velocities

Ideal explosives should have short reaction zones and have small failure diameters, which are suitable for practical applications. Non-ideal explosives can have C–J detonation pressure and velocity significantly different from that expected from a computer code such as BKW for equilibrium and steady-state calculations [19]. Two important characteristics of non-ideal explosives include high degree of inhomogeneity and secondary reactions occurring in the detonation products expanding behind the detonation zone.

Aluminized composite explosives and explosives containing nitrate salts are two well-known non-ideal explosives. Finely dispersible aluminum powders can be used in explosives to increase their performances. Aluminum not only increases the heat of explosion but also acts as intermediate sensitive agent. It can be generally assumed that combustion of aluminum particles in explosives occurs behind the reaction front, during the expansion of gaseous detonation products. However, aluminum particles do not participate in the reaction zone but act as inert ingredients. Thermodynamic calculations of detonation parameters are carried out by assuming a certain degree of aluminum oxidation because its value in the C–J point for mixture of high explosives with aluminum is not clear. Decomposing ammonium nitrate lowers the temperature that determines how much ammonium nitrate is decomposed near the C–J plane. In contrast, the burning aluminum raises the temperature, which could lead to an increase in the rate of aluminum burning until it is completely burned near the C–J plane.

For non-ideal explosives, the amount of reacted material may be a function of the reaction zone length. To predict detonation properties for non-ideal explosives, as a simple approximation, partial equilibrium rather than a complex reacting mechanism can be used. Partial equilibrium is invoked by specifying the amount of the initial aluminum or ammonium nitrate that is assumed to react. Inert aluminum atoms were included in the product species database of computer codes that could only form solid, liquid or gaseous aluminum. This prevents Al reacting with oxygen or other reactive species. Decreasing in the amount of condensed carbon and increasing the number of gaseous products can be improved by prevention of aluminum from forming such products as aluminum oxide. It should be noted that detonation pressure and velocity increase with the higher gas yield [16]. Due to the large negative heat of formation of aluminum oxide, the high-temperature oxidation of aluminum produces a hot, fuel rich gas phase and more solid carbon. However, more condensed aluminum oxide is produced if complete equilibrium is reached, forcing oxygen to react with aluminum rather than carbon.

Ammonium nitrate is one of the major components of the most nitrate-based explosives. It has large values for the minimum diameter and relatively small values for the critical diameter. For the most practical conditions as predicted by hydrodynamic theory, it will never reach the ideal behavior. Since explosive nitrate salts are non-ideal explosives, it can be assumed that either complete reaction or no reaction of the ammonium nitrate with the rest of reaction products exhibits large differences between observed and calculated performances. For computation of detonation velocity by a computer code such as BKW [1], some percentage of ammonium nitrate is assumed to decompose and the rest is intact. For example, the experimental values of detonation velocities in Amatex and Amatol can be obtained by BKW computer code if 50% and 19% of ammonium nitrate decompose in them, respectively [1]. However, the Amatex detonation temperatures are higher and more ammonium nitrate decomposition occurs at the higher temperatures.

Some new methods have been recently introduced to predict detonation performance of aluminized and nitrated explosives [13,16,17]. But their application to a wide range of ideal and non-ideal explosives is rather limited.

3. Results and discussion

The velocity of a detonation shock wave passing through the charge is an important detonation parameter. Its measurements are probably good (within a few percent), besides there are enough data for various explosives. For non-ideal explosives, detonation velocities are significantly different from those predicted by equilibrium, one-dimensional and steady-state calculations.

Experimental data of the most ideal and non-ideal explosives reveal that detonation velocity is roughly proportional to loading density [18]. Recent works have also shown that elemental composition of different explosives including aluminized composite explosives or explosive nitrate salts can be correlated to detonation parameters [13,16,17] without using assumed composition of detonation products. However, it can be assumed that detonation velocity of any explosive can be expressed as a function of basic parameters, e.g. the elemental composition, oxygen balance, heat of formation and initial density of mixture. It was found that detonation velocity (D) of those explosives that do not contain Al and/or nitrate salts can be selected as core correlation and can be revised according to the presence of Al and nitrate salt for non-ideal explosives:

$$D = D_{\text{core}} + y_7 n'_{\text{Al}} + y_8 n'_{\text{NO}_3\text{ salt}} \tag{1a}$$

$$D_{\text{core}} = y_1 + y_2\rho_0 + y_3 a + y_4 c + y_5 d + y_6 n_{-\text{NRR}'} \tag{1b}$$

where a, c, d and $n_{-\text{NRR}'}$ are the number of moles of carbon, oxygen, nitrogen and a specific group in explosives; n'_{Al} and $n'_{\text{NO}_3\text{ salt}}$ are two functions of the number of Al and nitrate salt moles, respectively, which are dependent on oxygen to carbon and hydrogen ratios; y_1–y_8 are adjustable parameters. The variables of D_{core} are very closely related to previous work for prediction of detonation velocities of CHNO explosives [19]. The specific group $-\text{NRR}'$ of D_{core} includes $-\text{NH}_2$, NH_4^+ and five member ring with three (or four) nitrogens in any explosive as well as five (or six) member ring in cage nitramines. All experimental data of various explosives, which are listed in Tables 1 and 2 , were used to find adjustable parameters (R-squared value or the coefficient of determination [20] = 0.983). To find adjustable parameters (y_1–y_8), multiple linear regression method [20] was used. It should be mentioned that multiple linear regression can fit a set of data in the least squares sense between two or more variables and a response variable. There are more

Table 1
Comparison between detonation velocities (in km/s) calculated by means of the new correlation for explosives that do not contain Al or nitrate salt with BKWS-EOS, BKWR-EOS and measured values.

Name[a]	ρ_0 (g/cm^3)	D_{exp}[b]	D_{new}	%Dev new	$D_{BKWR-EOS}$	%Dev BKWR-EOS	$D_{BKWS-EOS}$	%Dev BKWS-EOS
ABH	1.64	7.2	6.96	−3.3	7.28	1.1	7.14	−0.8
BTF	1.86	8.49	8.56	0.8	8.43	−0.7	8.4	−1.1
	1.76	8.26	8.19	−0.8	8.14	−1.5	8.14	−1.5
CL-20	2.04	9.38	9.56	1.9	–	–	–	–
COM B	1.72	7.92	8.00	1.1	8.12	2.5	8.2	3.5
COM B-3	1.72	7.89	8.00	1.4	8.08	2.4	8.16	3.4
COM C-3	1.6	7.63	7.60	−0.4	7.77	1.8	7.74	1.4
CYCLOTOL-78/22	1.76	8.31	8.22	−1.1	8.4	1.1	8.53	2.6
CYCLOTOL-77/23	1.74	8.25	8.14	−1.3	8.33	1.0	8.44	2.3
CYCLOTOL-75/25	1.76	8.3	8.21	−1.1	8.37	0.8	8.49	2.3
	1.62	7.95	7.69	−3.2	7.91	−0.5	7.95	0.0
CYCLOTOL-70/30	1.73	8.06	8.08	0.2	8.22	2.0	8.31	3.1
CYCLOTOL-65/35	1.72	8.04	8.02	−0.3	8.13	1.1	8.22	2.2
CYCLOTOL-60/40	1.74	8.09	8.07	−0.2	8.15	0.7	8.24	1.9
CYCLOTOL-60/40	1.72	7.9	8.00	1.3	8.08	2.3	8.16	3.3
CYCLOTOL-50/50	1.63	7.66	7.63	−0.4	7.69	0.4	7.71	0.7
DATB	1.8	7.6	7.63	0.4	7.92	4.2	7.86	3.4
	1.78	7.6	7.56	−0.6	7.85	3.3	7.79	2.5
DEGN	1.38	6.76	6.64	−1.7	7.08	4.7	7.19	6.4
DIPM	1.76	7.4	7.26	−1.9	7.62	3.0	7.56	2.2
EXP D	1.55	6.85	6.93	1.2	7.02	2.5	6.91	0.9
	1.48	6.7	6.68	−0.3	6.78	1.2	6.66	−0.6
HMX	1.89	9.11	9.25	1.5	9.08	−0.3	9.35	2.6
	1.6	7.91	8.19	3.5	8.1	2.4	8.14	2.9
	1.4	7.3	7.46	2.2	7.45	2.1	7.41	1.5
	1.2	6.58	6.73	2.3	6.85	4.1	6.78	3.0
	1.0	5.8	6.00	3.4	6.31	8.8	6.2	6.9
	0.75	4.88	5.09	4.2	5.54	13.5	5.42	11.1
HNAB	1.6	7.31	7.27	−0.6	7.22	−1.2	7.09	−3.0
HNB	1.97	9.3	9.19	−1.2	8.89	−4.4	8.47	−8.9
HNS	1.6	6.8	6.76	−0.6	6.96	2.4	6.88	1.2
	1.7	7	7.13	1.8	7.26	3.7	7.22	3.1
LX-14	1.84	8.83	8.56	−3.1	8.86	0.3	9.04	2.4
MEN-II	1.02	5.49	5.36	−2.3	5.97	8.7	6	9.3
NG	1.6	7.7	7.78	1.0	7.94	3.1	8.01	4.0
NONA	1.7	7.4	7.17	−3.1	7.35	−0.7	7.26	−1.9
NQ	1.78	8.59	8.55	−0.5	8.83	2.8	8.53	−0.7
	1.62	7.93	7.97	0.4	8.17	3.0	7.82	−1.4
	1.55	7.65	7.71	0.8	7.89	3.1	7.52	−1.7
OCTOL-78/22	1.82	–	8.39	−0.7	8.59	–	8.76	–
OCTOL-76/23	1.81	8.45	8.39	−1.1	8.54	1.1	8.7	3.0
OCTOL-75/25	1.81	8.48	8.29	1.6	8.53	0.6	8.69	2.5
OCTOL-60/40	1.8	8.16	8.26	−2.9	8.34	2.2	8.47	3.8
PA	1.76	7.57	7.88	4.1	7.69	1.6	7.71	1.8
	1.71	7.26	7.70	6.0	7.69	5.9	7.71	6.2
	1.6	7.1	7.29	2.7	7.69	8.3	7.71	8.6
PBX-9011	1.77	8.5	8.57	−3.0	8.56	0.7	8.65	1.8
PBX-9501	1.84	8.83	7.84	1.1	8.87	0.5	9.07	2.7
PETN	1.76	8.27	8.33	0.7	8.23	−0.5	8.67	4.8
	1.7	8.07	8.11	0.5	8.02	−0.6	8.43	4.5
	1.6	7.75	7.74	−0.1	7.7	−0.6	8.03	3.6
	1.45	7.18	7.20	0.2	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	0.7	6.01	9.7	5.99	9.3
	0.88	5.06	5.11	1.1	5.65	11.7	5.61	10.9
	0.48	3.6	3.65	1.5	4.24	17.8	4.12	14.4
	0.3	2.99	3.00	0.2	3.57	19.4	3.44	15.1
	0.25	2.83	2.81	−0.6	3.38	19.4	3.25	14.8
PENTOLITE	1.71	7.75	7.80	3.6	7.72	−0.4	7.91	2.1
	1.7	7.53	7.73	1.0	7.69	2.1	7.87	4.5
	1.68	7.65	7.58	0.7	7.63	−0.3	7.8	2.0
	1.64	7.53	7.78	1.0	7.51	−0.3	7.65	1.6
RDX	1.8	8.75	8.74	−0.1	8.77	0.2	8.96	2.4
	1.77	8.7	8.63	−0.8	8.67	−0.3	8.84	1.6
	1.72	8.46	8.45	−0.1	8.5	0.5	8.63	2.0
	1.66	8.24	8.23	−0.1	8.3	0.7	8.38	1.7
	1.6	8.13	8.01	−1.4	8.1	−0.4	8.15	0.2
	1.46	7.6	7.50	−1.3	7.64	0.5	7.63	0.4
	1.4	7.46	7.28	−2.4	7.45	−0.1	7.42	−0.5
	1.29	7	6.88	−1.7	7.12	1.7	7.06	0.9

Table 1 (*Continued*)

Name[a]	ρ_0 (g/cm^3)	D_{exp}[b]	D_{new}	%Dev new	$D_{BKWR-EOS}$	%Dev BKWR-EOS	$D_{BKWS-EOS}$	%Dev BKWS-EOS
RDX	1.2	6.77	6.55	−3.2	6.86	1.3	6.79	0.3
	1.1	6.18	6.19	0.1	6.58	6.5	6.49	5.0
	1	6.1	5.82	−4.5	6.32	3.6	6.21	1.8
	0.95	5.8	5.64	−2.8	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	4.22	4.1	4.84	19.5	4.72	16.5
TACOT	1.85	7.25	7.43	2.5	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	7.64	−0.3	8.18	6.8	8.07	5.4
TETRYL	1.73	7.72	7.91	2.4	7.75	0.4	7.81	1.2
	1.71	7.85	7.83	−0.2	7.69	−2.0	7.74	−1.4
	1.68	7.5	7.73	3.0	7.6	1.3	7.63	1.7
	1.61	7.58	7.47	−1.5	7.39	−2.5	7.38	−2.6
	1.36	6.68	6.56	−1.8	6.67	−0.1	6.59	−1.3
	1.2	6.34	5.97	−5.8	6.24	−1.6	6.15	−3.0
TNT	1.64	6.93	7.27	4.9	7.2	3.9	7.19	3.8
	1.45	6.5	6.57	1.1	6.6	1.5	6.51	0.2
	1.36	6.2	6.24	0.7	6.32	1.9	6.22	0.3
	1	5	4.93	−1.4	5.3	6.0	5.21	4.2
	0.8	4.34	4.20	−3.2	4.79	10.4	4.74	9.2
TNTAB	1.74	8.58	8.82	2.8	8.44	−1.6	8.39	−2.2
R.m.s. percent deviation				2.1		5.9		5.3

[a] See Appendix A for glossary of compound name.
[b] All experimental data taken from Ref. [14] except CL-20 that was obtained from Ref. [21].

independent equations than unknowns that give overdetermined system. The matrix inverse method and Cramer's method will not work for such a system [20]. Thus, we can make use of the fact that the left-division method for solving linear equations uses the least squares method when the equation set is overdetermined [20]. Since the contribution of the number of hydrogen moles in Eq. (1) is small because the value of *R*-squared value does not change, it was neglected. Final optimized correlation can be given as follows:

Table 2
Comparison between detonation velocities calculated by means of the new correlation for aluminized composite explosives and explosives containing nitrate salts with BKWS-EOS (using full and partial, 50%, interaction of aluminum and nitrate salt with detonation products) [14] and measured values.

Name	ρ_0 (g/cm^3)	D_{exp} (km/s)	D_{new} (km/s)	%Dev new	$D_{BKWS-EOS}$ (km/s), full	%Dev BKWS-EOS full	$D_{BKWS-EOS}$ (km/s), partial	%Dev BKWS-EOS partial
Alex 20	1.801	7.53 [1]	7.66	1.8	–	–	–	–
Alex 32	1.88	7.3 [1]	7.49	2.6	–	–	–	–
Amatex-20	1.66	7.55 [14]	7.46	−1.2	8.05	6.6	7.53	−0.3
Amatex-40	1.61	7.01 [14]	6.95	−0.8	7.97	13.7	6.84	−2.4
Amatol-60/40	1.6	5.76 [14]	5.83	1.3	8.05	39.8	6.24	8.3
Amatol-80/20	1.6	5.2 [14]	5.34	2.7	8.46	62.7	5.65	8.7
AN	1.05	4.5 [1]	4.41	−2.0	–	–	–	–
90/10 AN/Al	1.05	5.6 [1]	5.64	0.7	–	–	–	–
80/20 AN/Al	1.05	5.8 [1]	5.52	−4.9	–	–	–	–
70/30 AN/Al	1.05	5.4 [1]	5.40	0.0	–	–	–	–
ANFO-6/94	0.88	5.5 [1]	5.66	3.0	–	–	–	–
Destex	1.68	6.65 [1]	6.53	−1.8	–	–	–	–
H-6	1.71	7.194 [1]	7.32	1.8	7.22	−0.4	7.49	−4.1
HBX-1	1.72	7.224 [1]	7.43	2.9	7.18	−6.1	7.38	2.1
HBX-3	1.81	6.917 [1]	6.78	−2.0	6.27	−9.4	6.91	−0.1
HMX/Al(90/10)	1.76	8.3 [14]	8.28	−0.2	8.32	0.2	8.41	1.3
HMX/Al(80/20)	1.82	8.3 [14]	8.20	−1.2	7.93	−4.5	8.22	−1.0
HMX/Al(70/30)	1.86	8 [14]	7.92	−1.0	7.27	−9.1	7.82	−2.3
HMX/Al(60/40)	1.94	7.7 [14]	7.66	−0.5	6.86	−10.9	7.46	−3.1
70/30 Hydrazine/hydrazine nitrate	1.14	8.025 [1]	8.13	1.3	–	–	–	–
21/79 Hydrazine/hydrazine nitrate	1.4418	8.6 [1]	8.39	−2.5	–	–	–	–
Hydrazine nitrate	1.626	8.691[1]	8.75	0.7	–	–	–	–
PBXC-117	1.75	7.7 [1]	7.66	−0.5	–	–	–	–
PBXN-1	1.77	7.93 [1]	7.66	−3.4	–	–	–	–
RDX/Al(90/10)	1.68	8.03 [14]	7.99	−0.5	8.02	−0.12	8.08	0.6
RDX/Al(80/20)	1.73	7.77 [14]	7.87	1.3	7.60	−2.2	7.81	0.5
RDX/Al(70/30)	1.79	7.58 [14]	7.66	1.1	7.03	−7.3	7.49	−1.2
RDX/Al(60/40)	1.84	7.2 [14]	7.30	1.3	6.42	−10.8	6.93	−3.8
RDX/Al(50/50)	1.89	6.81 [14]	6.71	−1.4	5.78	−15.1	6.02	−11.6
TNETB/Al(90/10)	1.75	8.12 [14]	8.12	0.0	7.85	−3.3	7.91	−2.6
TNETB/Al(80/20)	1.82	7.99 [14]	8.08	1.1	7.53	−5.8	7.73	−3.3
TNETB/Al(70/30)	1.88	7.84 [14]	7.87	0.3	6.99	−10.8	7.43	−5.2
TNT/Al(89.4/10.6)	1.72	7.05 [14]	6.94	−1.6	7.02	−0.4	7.12	1.0
TNT/Al(78.3/21.7)	1.8	7.05 [14]	7.10	0.7	6.59	−6.5	6.94	−1.6
TNT/Al(67.8/32.2)	1.89	7.05 [14]	6.94	−1.5	4360	5.94	−15.7	−4.8
Torpex	1.81	7.495 [1]	7.79	3.9	–	–	–	–
Tritonal	1.72	6.475 [1]	6.71	3.6	–	–	–	–
R.m.s. percent deviation				1.9		17.7		4.3

Table 3
Comparison between detonation velocities calculated by means of the new correlation for new explosives and measured values.

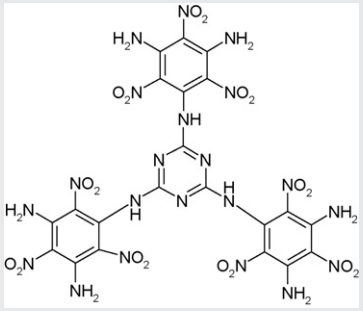
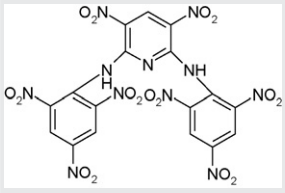
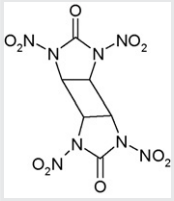
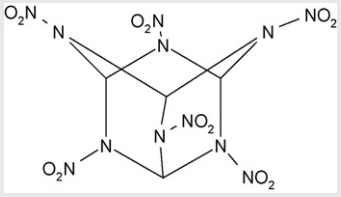
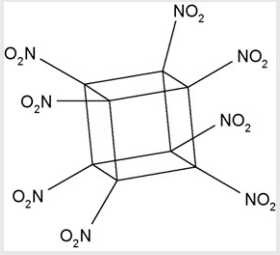
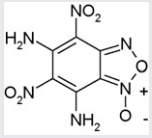
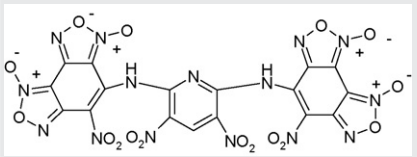
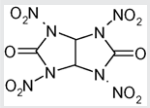
Molecular structure	ρ_0 (g/cm^3)	D_{exp} (km/s)	D_{new} (km/s)	%Dev new
	2.01	7.861 [21]	7.53	−4.2
	1.75	7.45 [22]	7.64	2.6
	1.99	8.40 [22]	8.83	5.1
	2.10	9.50 [22]	9.76	2.7
	2.00	9.80 [22]	9.42	−3.9
	1.91	8.05 [22]	8.15	1.2
	1.91	8.63 [22]	8.70	0.8
	1.94	9.07 [22]	8.92	−1.7

Table 3 (*Continued*)

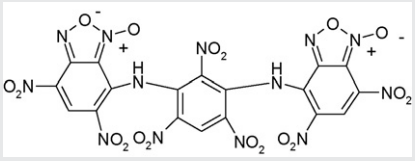
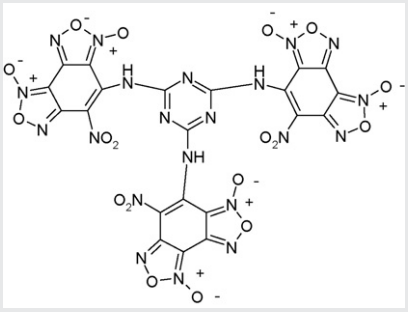
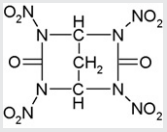
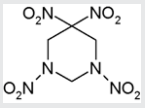
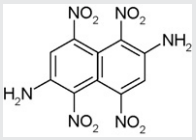
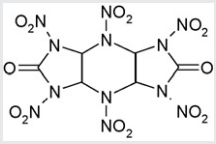
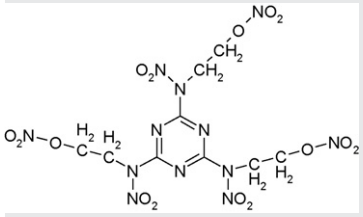
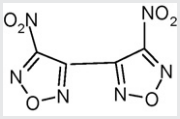
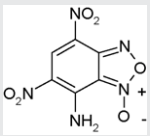
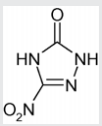
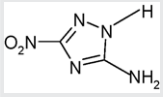
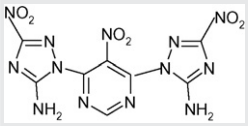
Molecular structure	ρ_0 (g/cm^3)	D_{exp} (km/s)	D_{new} (km/s)	%Dev new
	1.92	8.57 [22]	8.44	−1.5
	1.90	8.695 [22]	8.90	2.4
	1.98	9.03 [22]	8.93	−1.1
	1.82	8.73 [22]	8.76	0.3
	1.78	7.00 [22]	7.21	3.0
	2.07	9.70 [22]	9.75	0.5
	1.73	8.70 [22]	8.73	0.4
	1.92	8.70 [22]	8.93	2.6
	1.90	7.91 [22]	8.29	4.8
	1.93	8.51 [22]	8.59	0.9

Table 3 (*Continued*)

Molecular structure	ρ_0 (g/cm^3)	D_{exp} (km/s)	D_{new} (km/s)	%Dev new
	1.82	8.46 [22]	8.09	−4.4
	1.86	8.20 [22]	8.06	−1.7

$$D = D_{core} - 0.620n'_{Al} - 1.41n'_{NO_3\ salt} \quad (2a)$$

$$D_{core} = 1.64 + 3.65\rho_0 - 0.135a + 0.117c + 0.0391d - 0.295n_{-NRR'} \quad (2b)$$

where D and D_{core} are expressed in km/s; n'_{Al} is equal to the number of moles of aluminum except that its value can be changed according to the following conditions:

(i) If $d \le a + 0.1$, then $n'_{Al} = 0.75n_{Al} + 1.00$.
(ii) If $d \ge a + b/2$, then $n'_{Al} = n_{Al} - 0.375$,

and $n'_{NO_3\ salt}$ is equal to the number of moles of nitrate salt with the exception of:
(iii) If $d \le a + 3b/5$ then $n'_{NO_3\ salt} = n_{NO_3\ salt} - 1.50$.
(iv) If $d \ge 2a + b/4$ then $n'_{NO_3\ salt} = 1.75n_{NO_3\ salt}$.

To use Eq. (2) for aluminized explosives, 100 g of explosives were taken for calculation of detonation velocity and the number of moles of extra aluminum in explosives with general formula $C_aH_bN_cO_dAl_e$ should be considered, e.g. TNT/Al (89.4/10.6) has formula $C_{2.756}H_{1.968}N_{1.181}O_{2.362}Al_{0.3929}$ on the basis of 100 g mixture of TNT and Al that should be changed to formula $C_{3.084}H_{2.203}N_{1.322}O_{2.643}Al_{1.328}$.

Calculated detonation velocities of well-known pure and mixed explosives as well as aluminized and nitrated explosives are given in Tables 1 and 2. Since detonation velocity increases with an increase in the amount of gaseous products, which depends on the oxygen content of explosive, positive and negative signs appear in correlation coefficients of the number of moles of carbon and hydrogen in Eq. (2b). As shown in Table 1, calculated detonation velocities of explosives are compared with the computed results of the BKWR-EOS and BKWS-EOS. Besides, predicted detonation velocities of aluminized and nitrated explosives are compared with BKWS-EOS using full and partial equilibrium of Al and nitrated salt. In the case of partial equilibrium, only 50% of aluminum is assumed to interact with combustion products. As indicated in Tables 1 and 2, the new hand calculated detonation velocities of different ideal and non-ideal explosives show surprisingly very good agreement with experimental data as compared to the computed results of complicated computer program. The predicted results of Eq. (2) are close to previous methods [13,16,17,19], which use different correlations for ideal and non-ideal explosives, e.g. root-mean-square (r.m.s.) percent deviation is 2.2 from experimental data for CHNO explosives in previous method [19]. New correlation requires no prior knowledge of any measured, estimated or calculated physical, chemical or thermochemical property of explosive and assumed detonation products.

To check the reliability of new method, the calculated values for some further new explosives with complex molecular structures are given in Table 3. As seen in Table 3, the predicted results are also close the measured values.

4. Limitations of the new method

There are some limitations of new method, i.e. (i) The new procedure cannot be used for highly overoxidized explosives, e.g. TNM, and their mixtures with the other components, e.g. LX-01; (ii) deviation from experimental data increases with use of non-energetic additives.

5. Conclusions

A simple theoretical approach complemented by the computer output has been introduced for desk calculation of detonation velocity of any explosive with general formula $C_aH_bN_cO_dAl_e$ only from molecular structure data. There is no need to use any experimental data, assumed detonation products and heat of formation. Although the heat of formation of a solid or liquid explosive is an important factor to predict its performance, there is no need to use it in the present method. Moreover, new method does not require using full or partial oxidation of aluminum that is usually required by a computer code. The agreement between calculated and measured detonation velocity is satisfactory because few percent deviations generally can be attributed to experimental measurements. Given the chemical formula of an ideal or non-ideal composite explosive, one can estimate reliable detonation velocity as a function of loading density which is associated with large uncertainty of detonation velocity.

Acknowledgement

I would like to thank the research committee of Malek-ashtar University of Technology (MUT) for supporting this work.

Appendix A. Glossary of compound names for pure as well as composite explosives on the basis of 100 g for mixture of different compounds

1. ABH: azobis(2,2′,4,4′,6,6′-hexanitrobisphenyl)($C_{24}H_6N_{14}O_{24}$)
2. Alex 20: $C_{1.783}H_{2.469}N_{1.613}O_{2.039}Al_{0.7335}$
3. Alex 32: $C_{1.647}H_{2.093}N_{1.365}O_{1.744}Al_{1.142}$
4. Amatex-20: $C_{1.73}H_{2.99}N_{2.14}O_{2.90}$
5. Amatex-40: $C_{1.44}H_{3.48}N_{2.09}O_{3.12}$
6. Amatol-60/40: $C_{1.23}H_{3.88}N_{2.03}O_{3.31}$
7. Amatol-80/20: $C_{0.616}H_{4.44}N_{2.26}O_{3.53}$
8. AN: ammonium nitrate ($H_4N_2O_3$)
9. 90/10 AN/Al: $H_{4.5}N_{2.25}O_{3.37}Al_{0.37}$
10. 80/20 AN/Al: $H_4N_2O_3Al_{0.74}$
11. 70/30 AN/Al: $H_{3.5}N_{1.75}O_{2.62}Al_{1.11}$
12. ANFO-6/94: $C_{0.43}H_{5.54}N_{2.35}O_{3.53}$
13. BTF: benzotris[1,2,5]oxadiazole,1,4,7-trioxide($C_6N_6O_6$)
14. CL-20: hexanitrohexaazaisowurtzitane ($C_6H_6N_{12}O_{12}$)
15. COMP B: 63/36/1 RDX/TNT/wax ($C_{2.03}H_{2.64}N_{2.18}O_{2.67}$)
16. COMP B-3: 60/40 RDX/TNT ($C_{2.04}H_{2.50}N_{2.15}O_{2.68}$)

17. COMP C-3: 77/4/10/5/1/3 RDX/TNT/DNT/MNT/NC/TETRYL ($C_{1.90}H_{2.83}N_{2.34}O_{2.60}$)
18. CYCLOTOL-78/22: 78/22 RDX/TNT ($C_{1.73}H_{2.59}N_{2.40}O_{2.69}$)
19. CYCLOTOL-77/23: 77/23 RDX/TNT ($C_{1.75}H_{2.59}N_{2.38}O_{2.69}$)
20. CYCLOTOL-75/25: 75/25 RDX/TNT ($C_{1.78}H_{2.58}N_{2.36}O_{2.69}$)
21. CYCLOTOL-70/30: 70/30 RDX/TNT ($C_{1.87}H_{2.56}N_{2.29}O_{2.68}$)
22. CYCLOTOL-65/35: 65/35 RDX/TNT ($C_{1.96}H_{2.53}N_{2.22}O_{2.68}$)
23. CYCLOTOL-60/40: 60/40 RDX/TNT ($C_{2.04}H_{2.50}N_{2.15}O_{2.68}$)
24. CYCLOTOL-50/50: 50/50 RDX/TNT ($C_{2.22}H_{2.45}N_{2.01}O_{2.67}$)
25. DATB: 1,3-diamino-2,4,6-trinitrobenzene ($C_6H_5N_5O_6$)
26. DEGN: diethyleneglycol dinitrate ($C_4H_8N_2O_7$)
27. Destex: $C_{2.791}H_{2.3121}N_{0.987}O_{1.975}Al_{0.6930}$
28. DIPM: dipiramide ($C_{12}H_6N_8O_{12}$)
29. EXP D: ammonium picrate ($C_6H_6N_4O_7$)
30. H-6: $C_{1.888}H_{2.589}N_{1.611}O_{2.00}Al_{0.7415}$
31. HBX-1: $C_{2.068}H_{2.83}N_{1.586}O_{2.085}Al_{0.63}$
32. HBX-3: $C_{1.669}H_{2.1887}N_{1.220}O_{1.603}Al_{1.2977}$
33. HMX: cyclotetramethylenetetranitramine ($C_4H_8N_8O_8$)
34. HMX/Al(90/10): $C_{1.216}H_{2.432}N_{2.432}O_{2.432}Al_{0.371}$
35. HMX/Al(80/20): $C_{1.08}H_{2.16}N_{2.16}O_{2.16}Al_{0.715}$
36. HMX/Al(70/30): $C_{0.944}H_{1.888}N_{1.888}O_{1.888}Al_{1.11}$
37. HMX/Al(60/40):$C_{0.812}H_{1.624}N_{1.624}O_{1.624}Al_{1.483}$
38. 75/25 HMX/hydrazine nitrate: $C_{1.01}H_{3.34}N_{2.81}O_{2.81}$
39. HNAB: 2,2′,4,4′,6,6′-hexanitroazobenzene ($C_{12}H_4N_8O_{12}$)
40. HNB: hexanitrobenzene ($C_6N_6O_{12}$)
41. HNS: 2,2′,4,4′,6,6′-hexanitrostilbene ($C_{14}H_6N_6O_{12}$)
42. 70/30 Hydrazine/hydrazine nitrate: $H_{10.33}N_{5.32}O_{0.946}$
43. 21/79 Hydrazine/hydrazine nitrate: $H_{6.78}N_{3.81}O_{2.50}$
44. Hydrazine nitrate: $H_{5.26}N_{3.16}O_{3.16}$
45. LX-14: 95.5/4.5 HMX/estane 5702-F1 ($C_{1.52}H_{2.92}N_{2.59}O_{2.66}$)
46. NG: nitroglycerine ($C_3H_5N_3O_9$)
47. MEN-II: 72.2/23.4/4.4 nitromethane/methanol/ethylene diamine ($C_{2.06}H_{7.06}N_{1.33}O_{3.10}$)
48. NONA: 2,2′,2″,4,4′,4″,6,6′,6″-nonanitroterphenyl ($C_{18}H_5N_9O_{18}$)
49. NQ: nitroguanidine ($CH_4N_4O_2$)
50. OCTOL-78/22: 77.6/22.4 HMX/TNT ($C_{1.74}H_{2.59}N_{2.39}O_{2.69}$)
51. OCTOL-76/23: 76.3/23.7 HMX/TNT ($C_{1.76}H_{2.58}N_{2.37}O_{2.69}$)
52. OCTOL-75/25: 75/25 HMX/TNT ($C_{1.78}H_{2.58}N_{2.36}O_{2.69}$)
53. OCTOL-60/40: 60/40 HMX/TNT ($C_{2.04}H_{2.50}N_{2.15}O_{2.68}$)
54. PA: picric acid ($C_6H_3N_3O_7$)
55. PBX-9011: 90/10 HMX/estane ($C_{1.73}H_{3.18}N_{2.45}O_{2.61}$)
56. PBX-9501: 95/2.5/2.5 HMX/estane/EDNPA-F ($C_{1.47}H_{2.86}N_{2.60}O_{2.69}$)
57. PBXC-117: $C_{1.65}H_{3.1378}N_{1.946}O_{2.048}Al_{0.6303}$
58. PBXN-1: $C_{1.498}H_{2.863}N_{1.971}O_{1.791}Al_{0.742}$
59. PENTOLITE: 50/50 TNT/PETN ($C_{2.33}H_{2.37}N_{1.29}O_{3.22}$)
60. PETN: pentaerythritol tetranitrate ($C_5H_8N_4O_{12}$)
61. RDX: cyclomethylene trinitramine ($C_3H_6N_6O_6$)
62. RDX/Al(90/10): $C_{1.215}H_{2.43}N_{2.43}O_{2.43}Al_{0.371}$
63. RDX/Al(80/20): $C_{1.081}H_{2.161}N_{2.161}O_{2.161}Al_{0.715}$
64. RDX/Al(70/30): $C_{0.945}H_{1.89}N_{1.89}O_{1.89}Al_{1.11}$
65. RDX/Al(60/40): $C_{0.81}H_{1.62}N_{1.62}O_{1.62}Al_{1.483}$
66. RDX/Al(50/50): $C_{0.675}H_{1.35}N_{1.35}O_{1.35}Al_{1.853}$
67. TACOT: 2,4,8,10-tetranitro-5H-benzotriazolo[2,1,*a*]-benzotriazol-6-ium, hydroxide, inner salt ($C_{12}H_4N_8O_8$)
68. TATB: 1,3,5-triamino-2,4,6-trinitrobenzene($C_6H_6N_6O_6$)
69. TETRYL: N-methyl-N-nitro-2,4,6-trinitroaniline ($C_7H_5N_5O_8$)
70. TNETB/Al(90/10): $C_{1.399}H_{1.399}N_{1.399}O_{3.264}Al_{0.371}$
71. TNETB/Al(80/20): $C_{1.244}H_{1.244}N_{1.244}O_{2.902}Al_{0.715}$
72. TNETB/Al(70/30): $C_{1.088}H_{1.088}N_{1.088}O_{2.539}Al_{1.11}$
73. TNM: tetranitromethane (CN_4O_8)
74. TNT: 2,4,6-trinitrotoluene ($C_7H_5N_3O_6$)
75. TNTAB: trinitrotriazidobenzene ($C_6N_{12}O_6$)
76. TNT/Al(89.4/10.6): $C_{2.756}H_{1.969}N_{1.181}O_{2.362}Al_{0.393}$
77. TNT/Al(78.3/21.7): $C_{2.414}H_{1.724}N_{1.034}O_{2.069}Al_{0.804}$
78. TNT/Al(67.8/32.2): $C_{2.090}H_{1.493}N_{1.896}O_{1.791}Al_{1.193}$
79. Torpex: $C_{1.8}H_{2.015}N_{1.663}O_{2.191}Al_{0.6674}$
80. Tritonal: $C_{2.465}H_{1.76}N_{1.06}O_{2.11}Al_{0.741}$

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