An Improved Simple Method for the Calculation of the Detonation Performance of CHNOFCl, Aluminized and Ammonium Nitrate Explosives

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Abstract: An improved simple method is presented for calculation of the detonation velocity of CHNO and CHNOFCl explosives, as well as non-ideal explosives containing aluminum (Al) and ammonium nitrate (AN) additives. In contrast to the available complex computer codes, where the estimated detonation velocities of non-ideal explosives for equilibrium and steady state calculations show significant differences from the measured data, this simple method gives more reliable results. Suitable decomposition paths are suggested in which the partial interaction of Al with the gaseous products and the decomposition of AN are assumed for composite explosives containing Al/AN additives. The predicted detonation velocities using the new method are good compared to those from one of the well-known empirical methods and from computer codes using full and partial equilibrium of Al/AN.

Keywords: decomposition reaction, detonation velocity, ideal explosive, non-ideal explosive, safety

1   Introduction

The reliable prediction of the performance and thermochemical properties of a new energetic material from its molecular structure is highly desirable for chemists and the chemical industry. Suitable predictive methods should be used prior to actual synthesis and formulation of new energetic compounds because they can reduce the costs associated with synthesis and testing, as well as the evaluation of the materials [1-4]. The synthesis and assessment of energetic materials are difficult and dangerous processes [5]. Hence it is necessary to develop theoretical methods for assessing new energetic materials.

The detonation velocity is one of the important performance parameters, which can be used for an assessment of the effectiveness of energetic compounds [1, 3, 4]. Since detonation velocity can be measured to within a few percent, at various charge diameters, the measured data can be extrapolated to an infinite diameter for comparison with steady state calculations [6, 7]. Thermochemical equilibrium codes such as CHEETAH [8] and Explo5 [9], with different equations of states such as the exponential-6 potential [10], Becker-Kistiakosky-Wilson (BKW-EOS) [11] and its three different parameterizations [8, 11, 12], *i.e.* the BKWC-EOS, BKWS-EOS and BKWR-EOS, as well as empirical methods [3] and related computer codes such as LOTUSES [13] and EDPHT [14], can be used to determine the detonation velocity.

Performance can be described for an ideal explosive by steady-state detonation calculations using the appropriate equations of state or appropriate empirical methods [11]. By contrast, a non-ideal explosive has significantly different detonation properties to those predicted by well-known computer codes or empirical methods [11, 12]. Aluminum (Al) and ammonium nitrate (AN) have wide applications in the explosives industry [15-19]. Explosives containing these compounds show non-ideal behaviour [11, 12]. Diffusion may influence the experimental determination of the detonation properties and physical separation of the fuel and oxidizer in non-ideal explosives results in an extended chemical reaction zone [11, 12]. Non-ideal explosives have Chapman-Jouguet (C-J) detonation pressure/velocity significantly different from that expected from a thermochemical equilibrium code for steady state calculations [8, 11, 12], although some of the new thermochemical codes, which include the kinetics of slow reactions, overcome this difficulty. A high degree of inhomogeneity and secondary reactions occurring in the detonation products expanding behind the detonation zone, are two important characteristics for the non-ideal behaviour of Al/AN composite explosives [11].

Several methods have been developed recently to predict the detonation

velocity and pressure of CHNOFCl and aluminized explosives, through the molecular structure of the explosive component [20-27] and the heat of detonation [27, 28]. For those methods that are based on molecular structure [20-26], they are rather limited because deviations of these correlations may be large for some energetic compounds containing unusual new molecular fragments, and they cannot be used for those explosives containing a positive oxygen balance [20-26]. The purpose of the present work is to improve previous studies based on heats of detonation for the prediction of detonation velocities of ideal and non-ideal explosives containing the general formula CHNOFCl as well as Al/AN composite explosives at any loading density only from appropriate decomposition reactions. It is shown here how the detonation velocity of pure and mixed ideal and non-ideal CHNOFCl(Al/AN) explosives can be predicted using suitable detonation products. Briefly, the new model is an extension of the model presented in [28] which cannot be used for AN containing explosives.

2   Managing Non-ideal Behaviour of Al/AN Explosives by Computer Codes

Since Al particles do not fully participate in the reaction zone, thermodynamic calculations of detonation velocities are carried out by assuming a certain degree of Al oxidation. Combustion of Al raises the temperature, which can increase the rate of Al burning until it is completely burned near the C-J plane. In contrast to Al, decomposition of AN lowers the temperature and determines how much AN is decomposed near the C-J plane.

For computer codes, partial equilibrium rather than a complex reacting mechanism can be used for non-ideal explosives. This is realized by specifying the amount of reacted Al/AN through the inclusion of inert Al atoms in the product species database of computer codes in the form of solid, liquid or gaseous aluminum. This situation can prevent Al reacting with oxygen or other reactive species. The other pathway for preventing the oxidation of Al is to decrease the amount of condensed carbon, which can increase the number of gaseous products, *e.g.* CO and CO_2. It should be mentioned that the high-temperature oxidation of Al produces a hot, fuel rich gaseous phase and more solid carbon because of the large negative heat of formation of Al_2O_3. For complete equilibrium, more condensed Al_2O_3 is produced which forces oxygen to react with Al rather than carbon. Zhang and Chang [29] adjusted the parameter *k* in the BKW-EOS rather than use the assumption of full and partial equilibrium of Al powder in the reaction zones, to obtain the detonation pressure/velocity of aluminized explosives.

Either complete reaction or no reaction of AN with the rest of the reaction products can be assumed, which produces large differences between the observed and calculated performances. For the computation of the detonation velocity by a computer code, it can be assumed that some of the AN molecules can be decomposed and the rest remain intact, *e.g.* the experimental detonation velocities of Amatex and Amatol may be reproduced by a BKW computer code, if 50% and 19% of AN decompose, respectively [11]. Since the Amatex has higher detonation temperatures, more AN decomposition occurs at the higher temperatures.

3   Method of Evaluation

On the basis of the different categories of explosives (CHNO, CHNOFCl, and composite explosives containing Al/AN) the new model will be compared with the different presently available methods. One of the best empirical methods, *i.e.* Kamlet-Jacobs (K-J) [30], has been used as a general method for all three categories. For Al/AN composite explosives, the calculated detonation velocity will also be compared with the outputs of the BKWS-EOS using full and partial equilibrium of Al/AN. Moreover, the method of Zhang and Chang [29] will be used as a further comparison in the case of aluminized explosives. In addition, the method of [28], which is a precise method for CHNO, CHNOFCl, and aluminized explosives, will be used for a comparison of the calculated detonation velocities.

The mean absolute percentage error, MAPE, will be used as a statistical parameter for evaluating the results of the new method. It also enables a relative comparison among the various methods. MAPE provides an easy and intuitive way of judging the extent of errors and this is its biggest advantage [31, 32]. MAPE is defined as $(1/n)\Sigma(|D_{Calc.}-D_{Exp.}|/D_{Exp.})\times100$, where $D_{Calc.}$ and $D_{Exp.}$ are calculated and experimental detonation velocities, respectively, and n is the number of datapoints.

4   Results and Discussion

For the detonation of different classes of CHNO and CHNOFCl energetic compounds, it was found that the detonation velocity depends on the kind and number of moles of gaseous products as well as the heat of detonation (Q_d) and the loading density (ρ_0) [30, 33]. Thus, selection of suitable decomposition paths can help to find the appropriate composition of the detonation products. Q_d can
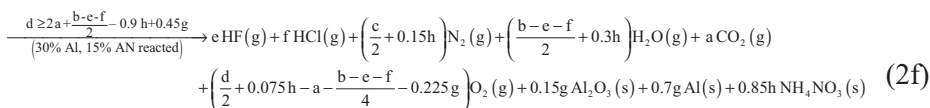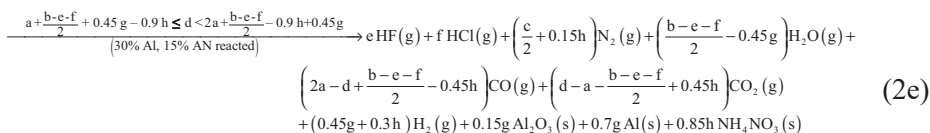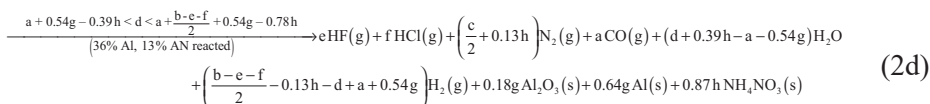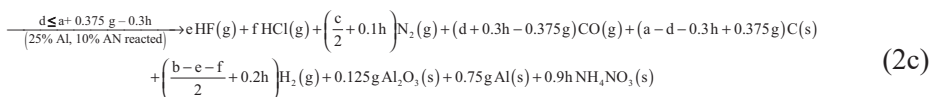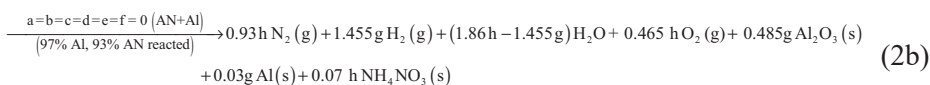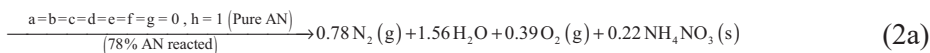
be determined from the heats of formation of the reactants and decomposition products as in [30]:

$$Q_d \cong -\frac{\left[\sum_i \Delta_f H^\theta (\text{Products})_i - \Delta_f H^\theta(c) \right]}{\text{formula weight of explosive}} \qquad (1)$$

where $\Delta_f H^\theta$(Products) and $\Delta_f H^\theta$(c) are the heats of formation of the ith product and the condensed phase heat of formation of the explosive, respectively. The measured detonation velocities reveal that the detonation velocity may be roughly proportional to ρ_0 [11, 30, 33].

A reliable estimate of the equilibrium composition of the products for the decomposition of energetic materials remains a major unresolved problem. Different methods can be used for this purpose, such as experimental measurement, thermochemical equilibrium or by suggesting appropriate decomposition paths. It was found that inclusion of the gaseous products CO, H_2O, H_2, N_2, HCl, HF and CO_2 in the form of four decomposition paths for CHNOFCl explosives gives more reliable Q_d, detonation velocity and pressure as compared to experimental data [33, 34]. It was found that the four decomposition paths can be extended for non-ideal aluminized explosives with the general formula CHNOFClAl, and gives a more reliable detonation pressure [27] and velocity [28] as compared to the outputs of complex computer codes. Due to the importance of using AN in commercial explosives [15, 16], the study on various detonation products and their interactions with Al, as well as partial decomposition of AN, shows that it is possible to improve the predictive power of recent studies [27, 28] for a wide range of CHNOFClAl(AN) explosives. A study of the heats of detonation and available experimental data of detonation velocities, which were collected from the open literature, showed that the decomposition paths in previous studies [27, 28, 30, 33, 34] can be extended for different CHNOFCl and non-ideal Al/AN explosives with the general formula $C_aH_bN_cO_dF_eCl_fAl_g(NH_4NO_3)_h$. Equation 2 shows the appropriate decomposition paths in which the percent participation of Al and AN in these reactions depends on the oxygen content of the other ingredients. Part of the Al will react with the oxygen rich detonation products to form Al_2O_3. Meanwhile, part of the AN decomposes to produce N_2, H_2O and O_2, so that oxygen molecules can react with oxygen deficient detonation products. Furthermore, it was also assumed that all nitrogen atoms go to N_2, fluorines to HF, chlorines to HCl, while a portion of the oxygen atoms form H_2O, carbon atoms being preferentially oxidized to CO rather than CO_2. The decomposition paths of Equation 2 can be used to predict Q_d, the number of moles of gaseous products per

gram of explosive (α) and the average molecular weight of the gaseous products ($\overline{Mw_g}$). Since the detonation velocity of an energetic compound depends on α, $\overline{Mw_g}$ and Q_d, the decomposition paths of Equation 2 can control these parameters to obtain a reliable correlation for the calculation of the detonation velocity of ideal and non-ideal explosives. A list of the energetic materials, as well as their compositions, may be found in Appendix A.

$$\frac{a=b=c=d=e=f=g=0 ,\; h=1 \;(\text{Pure AN})}{(78\% \text{ AN reacted})} \rightarrow 0.78\,N_2\,(g) +1.56\,H_2O +0.39\,O_2\,(g) + 0.22\,NH_4NO_3\,(s) \tag{2a}$$

$$\frac{a=b=c=d=e=f=0 \;(\text{AN+Al})}{(97\% \text{ Al, } 93\% \text{ AN reacted})} \rightarrow 0.93h\,N_2\,(g) +1.455g\,H_2\,(g) +(1.86h-1.455g)\,H_2O+ 0.465\,h\,O_2\,(g)+ 0.485g\,Al_2O_3\,(s)$$
$$+0.03g\,Al\,(s)+ 0.07\,h\,NH_4NO_3\,(s) \tag{2b}$$

$$\frac{d \leq a+ 0.375\,g - 0.3h}{(25\% \text{ Al, } 10\% \text{ AN reacted})} \rightarrow e\,HF\,(g)+ f\,HCl\,(g) +\left(\frac{c}{2}+0.1h\right)N_2\,(g)+(d+0.3h-0.375g)\,CO\,(g)+(a-d-0.3h+0.375g)\,C\,(s)$$
$$+\left(\frac{b-e-f}{2}+0.2h\right)H_2\,(g)+0.125g\,Al_2O_3\,(s)+0.75g\,Al\,(s)+0.9h\,NH_4NO_3\,(s) \tag{2c}$$

$$\frac{a + 0.54g - 0.39h < d < a+\frac{b-e-f}{2}+0.54g - 0.78h}{(36\% \text{ Al, } 13\% \text{ AN reacted})} \rightarrow e\,HF\,(g)+ f\,HCl\,(g) +\left(\frac{c}{2}+0.13h\right)N_2\,(g)+a\,CO\,(g)+(d+0.39h-a-0.54g)\,H_2O$$
$$+\left(\frac{b-e-f}{2}-0.13h-d+a+0.54g\right)H_2\,(g)+0.18g\,Al_2O_3\,(s)+0.64g\,Al\,(s)+0.87h\,NH_4NO_3\,(s) \tag{2d}$$

$$\frac{a+\frac{b-e-f}{2}+0.45\,g-0.9\,h \leq d < 2a+\frac{b-e-f}{2}-0.9h+0.45g}{(30\% \text{ Al, } 15\% \text{ AN reacted})} \rightarrow e\,HF\,(g)+ f\,HCl\,(g) +\left(\frac{c}{2}+0.15h\right)N_2\,(g)+\left(\frac{b-e-f}{2}-0.45g\right)H_2O\,(g)+$$
$$\left(2a-d+\frac{b-e-f}{2}-0.45h\right)CO\,(g)+\left(d-a-\frac{b-e-f}{2}+0.45h\right)CO_2\,(g)$$
$$+(0.45g+0.3h)\,H_2\,(g)+0.15g\,Al_2O_3\,(s)+0.7g\,Al\,(s)+0.85h\,NH_4NO_3\,(s) \tag{2e}$$

$$\frac{d \geq 2a+\frac{b-e-f}{2}-0.9h+0.45g}{(30\% \text{ Al, } 15\% \text{ AN reacted})} \rightarrow e\,HF\,(g)+ f\,HCl\,(g) +\left(\frac{c}{2}+0.15h\right)N_2\,(g)+\left(\frac{b-e-f}{2}+0.3h\right)H_2O\,(g)+ a\,CO_2\,(g)$$
$$+\left(\frac{d}{2}+0.075h-a-\frac{b-e-f}{4}-0.225g\right)O_2\,(g)+0.15g\,Al_2O_3\,(s)+0.7g\,Al\,(s)+0.85h\,NH_4NO_3\,(s) \tag{2f}$$

A study of various combinations of Q_d, α, $\overline{Mw_g}$ and ρ_0 has confirmed that the suggested function in related studies [28, 33], *i.e.* $\alpha^{0.5}\,(\overline{Mw_g}\,Q_d)^{0.25}\,\rho_0$, has a suitable form for deriving a new correlation for various $C_aH_bN_cO_dF_eCl_fAl_g(NH_4NO_3)_h$ explosives. Figure 1 shows that there is a linear relationship between the measured detonation velocities at different ρ_0 versus $\alpha^{0.5}\,(\overline{Mw_g}\,Q_d)^{0.25}\,\rho_0$ for various explosives in the form of Equation 3.

$$D = 5.468\,\alpha^{0.5}\,(\overline{Mw_g}\,Q_d)^{0.25}\,\rho_0 + 2.045 \tag{3}$$

where D, Q_d and ρ_0 are the detonation velocity (in $km \cdot s^{-1}$), the heat of detonation (in $kJ \cdot g^{-1}$), and the initial density (in $g \cdot cm^{-3}$), respectively. Six examples of the calculation of the detonation velocity, one for each reaction path, are solved in Appendix B.
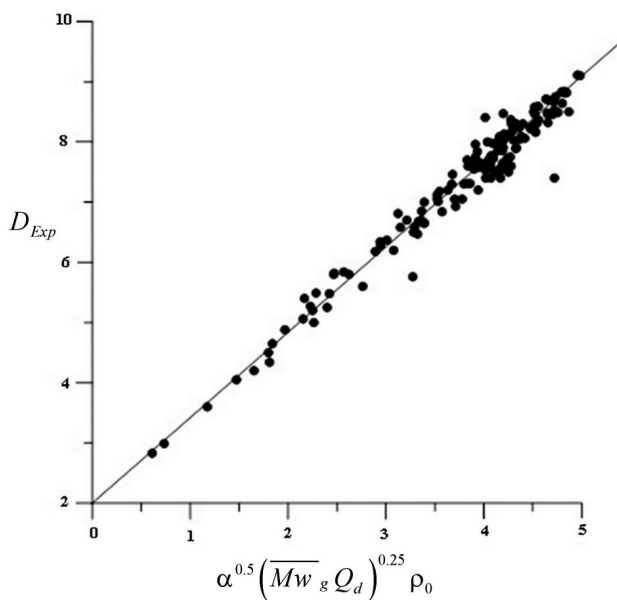

Figure 1. The measured detonation velocity versus $\alpha^{0.5} (\overline{Mw}_g Q_d)^{0.25} \rho_0$ for various explosives.

The amounts of reacted AN and Al in each path of Equation 2 were determined on the basis of experimental detonation velocities, by maximizing the value of the coefficient of determination (R^2). The value of R^2 for Equation 3 was 0.973, which is a reasonable value. The thermodynamic principle of Equation 3 is the same as our previous model [28], but the new model contains AN explosives, which cannot be treated by its predecessor, so this model can be viewed as an extension of the model of [28]. For CHNO, CHNOFCl, aluminized explosives, and explosives containing AN, the calculated detonation velocities are given in Tables 1-3, respectively. In Table 1, the calculated detonation velocities for CHNO explosives are compared with the K-J method [30] and the method of [28]. As seen in Table 1, the MAPE value for the new method is lower than that for both of the other two methods. For CHNO explosives at $\rho_0 < 1.0$ $g \cdot cm^{-3}$, e.g. PETN, the deviations of the K-J method [30] are high. Thus, as compared to the K-J equation [30] for CHNO explosives, Equation 3 has the advantage

that it can give reliable predictions for loading densities less than 1.0 g·cm^{-3}.

It is important to check the reliability of Equation 3 on the basis of the decomposition paths of Equation 2 for CHNOFCl explosives as compared to the K-J equation [30] and the method of [28]. As seen in Table 2, the new method gives good predictions of D for CHNOFCl explosives because the MAPE of Equation 3 is better than that for the K-J method [30] and the method of [28], similar to Table 1.

In contrast to the K-J equation [30] which is restricted to ideal explosives, the new method can also be used for non-ideal explosives. The predicted detonation velocities for non-ideal explosives containing Al and AN, as shown in Table 3, are compared with the computed results of the BKWS-EOS using full and partial equilibrium of Al/AN, the method of Zhang and Chang [29] and the method of [28] for aluminized explosives. For partial equilibrium, only 50% of Al/AN is assumed to interact with the combustion products. The predicted results from the new method show very good agreement with experimental data, compared to the results of the thermochemical equilibrium code for non-ideal Al/AN explosives. The K-J method [30] cannot be applied for these classes of explosives due to their non-ideal behaviour. However, the decomposition paths of Equation 2 can assume the extent of reaction of Al with the detonation products or the decomposition of AN. Moreover, in contrast to the other two methods which can be used for aluminized explosives, *i.e.* the method of Zhang and Chang [29] and the method of [28], the new model has lower MAPE values, which means that the new model can be proposed as an effective modification of our previous models.

Table 1.   Detonation velocities (km·s^{-1}) of CHNO explosives

Explosive	ρ_0 [g·cm^{-3}]	D_{Exp} [km·s^{-1}]	Ref.	D_{New} (%Dev)	D_{K-J} (%Dev)	Ref. [28] (%Dev)
ABH	1.78	7.60	[11]	7.99 (5.18)	7.69 (1.18)	8.04 (5.79)
	1.64	7.20	[12]	7.53 (4.52)	7.27 (0.97)	7.57 (5.14)
BTF	1.86	8.49	[12]	8.66 (2.03)	8.37 (-1.41)	8.72 (2.71)
	1.76	8.26	[12]	8.31 (0.56)	8.05 (-2.54)	8.36 (1.21)
DATB	1.80	7.60	[12]	7.65 (0.63)	7.60 (0.00)	7.69 (1.18)
	1.79	7.52	[11]	7.62 (1.28)	7.57 (0.66)	7.65 (1.73)
DEGN	1.38	6.76	[12]	6.93 (2.54)	7.06 (4.44)	6.96 (3.00)
DIPAM	1.79	7.50	[11]	7.81 (4.20)	7.62 (1.60)	7.86 (4.80)
	1.76	7.40	[12]	7.70 (4.10)	7.53 (1.76)	7.74 (4.59)
Explosive D	1.55	6.85	[12]	6.72 (-1.84)	6.80 (-0.73)	6.75 (-1.46)
	1.48	6.70	[11]	6.51 (-2.80)	6.60 (-1.49)	6.54 (-2.39)
HMX	1.89	9.11	[12]	8.98 (-1.41)	9.12 (0.22)	9.04 (-0.77)

Explosive	ρ_0 [g·cm^{-3}]	D_{Exp} [km·s^{-1}]	Ref.	D_{New} (%Dev)	D_{K-J} (%Dev)	Ref. [28] (%Dev)
HMX	1.60	7.91	[12]	7.92 (0.09)	8.09 (2.28)	7.96 (0.63)
	1.40	7.30	[12]	7.18 (-1.60)	7.41 (1.51)	7.22 (-1.10)
	1.20	6.58	[12]	6.45 (-1.99)	6.73 (2.28)	6.47 (-1.67)
	1.00	5.80	[12]	5.72 (-1.47)	6.04 (4.14)	5.73 (-1.21)
	0.75	4.88	[12]	4.80 (-1.69)	5.19 (6.35)	4.79 (-1.84)
HNAB	1.60	7.31	[12]	7.41 (1.41)	7.20 (-1.50)	7.45 (1.92)
HNS	1.74	7.13	[11]	7.69 (7.80)	7.47 (4.83)	7.66 (7.49)
	1.70	7.00	[12]	7.56 (7.95)	7.36 (5.07)	7.53 (7.63)
	1.60	6.80	[12]	7.23 (6.36)	7.06 (3.78)	7.21 (6.01)
NG	1.59	7.58	[11]	7.89 (4.07)	8.13 (7.31)	7.90 (4.23)
	1.60	7.70	[12]	7.93 (2.92)	8.17 (6.08)	7.94 (3.09)
NM	1.13	6.28	[11]	6.14 (-2.28)	6.38(1.59)	6.16 (-1.93)
	1.13	6.35	[12]	6.14 (-3.36)	6.38 (0.47)	6.16 (-3.01)
NONA	1.78	7.56	[11]	7.98 (5.56)	7.70 (1.81)	7.94 (5.03)
	1.70	7.40	[12]	7.71 (4.23)	7.46 (0.75)	7.67 (3.65)
NQ	1.63	7.98	[12]	7.29 (-8.64)	7.40 (-7.27)	8.05 (0.88)
PETN	1.77	8.30	[11]	8.56 (3.16)	8.69 (4.70)	8.58 (3.37)
	1.76	8.27	[12]	8.53 (3.08)	8.66 (4.67)	8.55 (3.34)
	1.70	8.07	[12]	8.30 (2.90)	8.45 (4.71)	8.32 (3.10)
	1.67	7.98	[11]	8.19 (2.68)	8.35 (4.64)	8.21 (2.88)
	1.60	7.75	[12]	7.94 (2.40)	8.11 (4.65)	7.95 (2.58)
	1.45	7.18	[12]	7.38 (2.84)	7.60 (5.85)	7.39 (2.92)
	1.23	6.37	[12]	6.57 (3.20)	6.84 (7.38)	6.58 (3.30)
	0.99	5.48	[12]	5.69 (3.84)	6.02 (9.85)	5.68 (3.69)
	0.88	5.06	[12]	5.29 (4.45)	5.64 (11.5)	5.27 (4.21)
	0.48	3.6	[12]	3.81 (5.90)	4.28 (18.9)	3.79 (5.28)
	0.30	2.99	[12]	3.15 (5.35)	3.66 (22.4)	3.12 (4.35)
	0.25	2.83	[12]	2.97 (4.80)	3.49 (23.3)	2.93 (3.53)
Picric Acid	1.76	7.57	[12]	7.69 (1.58)	7.55 (-0.24)	7.73 (2.16)
	1.71	7.26	[12]	7.53 (3.71)	7.40 (1.96)	7.57 (4.28)
	1.60	7.10	[12]	7.18 (1.08)	7.07 (-0.37)	7.21 (1.58)
RDX	1.80	8.75	[11]	8.67 (-0.95)	8.79 (0.46)	8.71 (-0.46)
	1.77	8.70	[12]	8.56 (-1.65)	8.68 (-0.23)	8.60 (-1.15)
	1.72	8.46	[12]	8.37 (-1.04)	8.51 (0.59)	8.42 (-0.47)
	1.66	8.24	[12]	8.15 (-1.07)	8.31 (0.85)	8.19 (-0.61)
	1.60	8.13	[12]	7.93 (-2.45)	8.10 (-0.37)	7.97 (-1.97)
	1.46	7.60	[12]	7.42 (-2.42)	7.62 (0.26)	7.45 (-1.97)
	1.40	7.46	[12]	7.20 (-3.55)	7.42 (-0.54)	7.22 (-3.22)
	1.29	7.00	[12]	6.79 (-2.99)	7.04 (0.57)	6.81 (-2.71)
	1.10	6.18	[12]	6.09 (-1.43)	6.39 (3.40)	6.1 (-1.29)

Explosive	ρ_0 [g·cm^{-3}]	D_{Exp} [km·s^{-1}]	Ref.	D_{New} (%Dev)	D_{K-J} (%Dev)	Ref. [28] (%Dev)
RDX	0.70	4.65	[12]	4.62 (-0.64)	5.02 (7.96)	4.61 (-0.86)
	0.56	4.05	[12]	4.11 (1.36)	4.55 (12.3)	4.09 (0.99)
TACOT	1.85	7.25	[12]	7.87 (8.52)	7.44 (2.66)	7.91 (9.13)
TATB	1.90	7.86	[11]	7.76 (-1.26)	7.82 (-0.51)	7.79 (-0.89)
	1.88	7.76	[12]	7.70 (-0.76)	7.78 (0.26)	7.75 (-0.13)
	1.85	7.66	[12]	7.61 (-0.64)	7.69 (0.39)	7.65 (-0.13)
	1.83	7.58	[12]	7.55 (-0.39)	7.63 (0.66)	7.59 (0.13)
Tetryl	1.73	7.72	[12]	7.94 (2.83)	7.78 (0.78)	7.98 (3.37)
	1.71	7.85	[12]	7.87 (0.26)	7.71 (-1.78)	7.92 (0.89)
	1.70	7.56	[11]	7.84 (3.65)	7.68 (1.59)	7.88 (4.23)
	1.68	7.50	[12]	7.77 (3.57)	7.62 (1.60)	7.81 (4.13)
	1.61	7.58	[12]	7.53 (-0.67)	7.40 (-2.37)	7.57 (-0.13)
	1.36	6.68	[12]	6.68 (0.00)	6.63 (-0.75)	6.70 (0.30)
	1.20	6.34	[12]	6.13 (-3.27)	6.13 (-3.31)	6.15 (-3.00)
TNM	1.64	6.36	[12]	6.67 (4.85)	6.40 (0.56)	6.68 (5.05)
TNT	1.64	6.93	[12]	7.20 (3.94)	6.97 (0.58)	7.25 (4.62)
	1.45	6.50	[12]	6.61 (1.62)	6.42 (-1.23)	6.64 (2.15)
	1.36	6.20	[12]	6.32 (1.97)	6.16 (-0.65)	6.35 (2.42)
	1.06	5.25	[11]	5.38 (2.45)	5.30 (0.95)	5.4 (2.86)
	1.00	5.00	[12]	5.19 (3.80)	5.12 (2.40)	5.2 (4.00)
	0.80	4.34	[12]	4.56 (5.09)	4.54 (4.61)	4.56 (5.07)
	0.73	4.20	[11]	4.34 (3.36)	4.35 (3.57)	4.34 (3.33)
Liquid TNT	1.45	6.58	[11]	6.63 (0.78)	6.43 (-2.28)	6.65 (1.06)
TNTAB	1.74	8.58	[12]	8.33 (-2.91)	8.25 (-3.85)	8.38 (-2.33)
COMP A-3	1.64	8.47	[12]	7.88 (-6.94)	7.86 (-7.20)	7.88 (-6.97)
COMP B	1.72	7.92	[12]	8.08 (2.04)	7.98 (0.76)	8.12 (2.53)
COMP C-3	1.60	7.63	[12]	7.56 (-0.93)	7.57 (-0.79)	7.60 (-0.39)
COMP C-4	1.66	8.37	[12]	7.99 (-4.55)	7.98 (-4.66)	8.04 (-3.94)
Cyclotol-50/50	1.63	7.66	[12]	7.66 (0.00)	7.59 (-0.91)	7.71 (0.65)
Cyclotol-60/40	1.74	8.09	[12]	8.14 (0.57)	8.07 (-0.25)	8.18 (1.11)
	1.72	7.89	[12]	8.07 (2.23)	8.00 (1.27)	8.11 (2.79)
Cyclotol-65/35	1.72	8.04	[12]	8.11 (0.85)	8.07 (0.37)	8.16 (1.49)
Cyclotol-70/30	1.73	8.06	[12]	8.19 (1.57)	8.17 (1.36)	8.24 (2.23)
Cyclotol-75/25	1.76	8.30	[12]	8.34 (0.43)	8.33 (0.36)	8.53 (2.77)
	1.62	7.95	[12]	7.84 (-1.45)	7.87 (-1.01)	8.14 (2.39)
Cyclotol-77/23	1.74	8.25	[12]	8.28 (0.37)	8.29 (0.48)	8.33 (0.97)
Cyclotol-78/22	1.76	8.31	[12]	8.36 (0.58)	8.37 (0.72)	8.41 (1.20)
EDC-11	1.78	8.21	[11]	8.30 (1.10)	8.24 (0.37)	8.35 (1.71)
EDC-24	1.78	8.71	[11]	8.50 (-2.41)	8.49 (-2.53)	8.83 (1.38)
LX-14	1.84	8.83	[12]	8.71 (-1.40)	8.75 (-0.91)	8.77 (-0.68)

Explosive	ρ_0 [g·cm^{-3}]	D_{Exp} [km·s^{-1}]	Ref.	D_{New} (%Dev)	D_{K-J} (%Dev)	Ref. [28] (%Dev)
MEN-II	1.02	5.49	[12]	5.22 (-4.91)	5.57 (1.46)	5.22 (-4.92)
Octol-76/23	1.81	8.45	[12]	8.52 (0.82)	8.51 (0.71)	8.57 (1.42)
Octol-75/25	1.81	8.48	[12]	8.51 (0.32)	8.49 (0.12)	8.56 (0.94)
Octol-60/40	1.80	8.16	[12]	8.34 (2.25)	8.26 (1.23)	8.40 (2.94)
PBX-9007	1.64	8.09	[12]	7.83 (-3.21)	7.79 (-3.71)	7.88 (-2.60)
PBX-9011	1.77	8.50	[12]	8.31 (-2.22)	8.31 (-2.24)	8.36 (-1.65)
PBX-9205	1.67	8.17	[12]	8.00 (-2.07)	7.98 (-2.33)	8.05 (-1.47)
PBX-9501	1.84	8.83	[12]	8.74 (-1.01)	8.80 (-0.34)	8.80 (-0.34)
PBXC-116	1.65	7.96	[11]	7.86 (-1.22)	7.54 (-5.28)	7.52 (-5.53)
PBXC-119	1.64	8.07	[11]	8.14 (0.91)	7.92 (-1.86)	7.95 (-1.49)
Pentolite-50/50	1.71	7.75	[12]	7.91 (2.11)	7.84 (1.16)	8.03 (3.61)
	1.68	7.65	[12]	7.81 (2.10)	7.75 (1.31)	7.92 (3.53)
	1.64	7.53	[12]	7.67 (1.90)	7.62 (1.20)	7.78 (3.32)
Toluene/Nitromethane (14.5/85.5)	1.09	5.84	[11]	5.49 (-6.00)	5.79 (0.86)	5.62(-3.77)
MAPE				**2.62**	**2.93**	**2.66**

Table 2.   Detonation velocities (km·s^{-1}) of CHNOFCl explosives

Explosive	ρ_0 [g·cm^{-3}]	D_{Exp} [km·s^{-1}]	Ref.	D_{New} (%Dev)	D_{K-J} (%Dev)	Ref. [28] (%Dev)
FEFO	1.59	7.50	[12]	7.73 (3.06)	7.40 (-1.38)	7.76 (3.46)
LX-04	1.86	8.46	[12]	8.57 (1.33)	8.17 (-3.43)	8.65 (2.25)
	1.87	8.53	[11]	8.61 (0.91)	8.18 (-4.10)	8.66 (1.52)
LX-07	1.87	8.64	[11]	8.72 (0.92)	8.51 (-1.50)	8.79 (1.74)
LX-09	1.84	8.81	[12]	8.76 (-0.60)	8.83 (0.23)	8.81 (0.00)
	1.84	8.84	[11]	8.76 (-0.94)	8.74 (-1.13)	8.81 (-0.34)
LX-10	1.86	8.82	[11]	8.78 (-0.48)	8.75 (-0.79)	8.87 (0.57)
LX-11	1.87	8.32	[12]	8.49 (2.08)	7.85 (-5.65)	8.57 (3.00)
LX-15	1.58	6.84	[12]	7.01 (2.51)	6.64 (-2.92)	7.06 (3.22)
LX-17	1.91	7.63	[12]	7.69 (0.76)	7.52 (-1.44)	7.76 (1.70)
NM/UP (60/40)	1.30	6.70	[11]	6.72 (0.29)	7.83 (16.79)	6.76 (0.90)
PBX-9010	1.78	8.36	[11]	8.37 (0.16)	8.34 (-0.28)	8.46 (1.16)
PBX-9407	1.60	7.91	[11]	7.81 (-1.21)	7.93 (0.25)	7.9 (-0.13)
PBX-9502	1.89	7.71	[11]	7.66 (-0.67)	7.61 (-1.30)	7.76 (0.65)
PBX-9503	1.90	7.72	[12]	7.74 (0.24)	7.82 (1.30)	7.98 (3.37)
PF	1.83	7.50	[11]	7.94 (5.85)	7.36 (-1.87)	8.0 (6.67)
RDX/Exon (90.1/9.9)	1.79	8.40	[11]	7.62 (-9.32)	7.57 (-9.92)	8.47 (0.79)
TFENA	1.52	6.65	[11]	6.63 (-0.33)	-	6.78 (1.95)
TFET	1.79	7.40	[11]	7.82 (5.66)	6.86 (-7.24)	7.89 (6.62)
MAPE				**1.97**	**3.42**	**2.09**

Table 3. Detonation velocities (km·s⁻¹) of composite explosives containing Al/AN

Explosive	ρ_0 [g·cm⁻³]	D_{Exp} [km·s⁻¹]	Ref.	D_{New} (%Dev)	$D_{K\text{-}J}$ (%Dev)	BKW, full (%Dev)	BKW, partial (%Dev)	Ref. [29] (%Dev)	Ref. [28] (%Dev)
ALEX20	1.80	7.53	[11]	7.53 (0.05)	8.02(6.46)	7.50 (-0.45)	-	7.41(-1.55)	7.58(0.68)
ALEX32	1.88	7.30	[11]	7.27(-0.40)	8.20(12.31)	7.07 (-3.21)	-	7.30(0.00)	7.32(0.27)
AMATEX-20	1.61	7.01	[11]	6.88(-1.86)	7.17 (2.32)	7.97(13.71)	6.84(-2.41)	-	-
AMATEX-40	1.66	7.55	[11]	6.16(-18.42)	6.31(-16.31)	8.05(6.69)	7.53(-0.20)	-	-
AMATOL80/20	1.60	5.20	[12]	4.32(-16.85)	-	8.46(62.69)	5.65(8.65)	-	-
	1.50	5.10	[35]	4.18(-18.01)	-	-	-	-	-
AMATOL60/40	1.60	6.20	[36]	4.97(-19.78)	8.11(30.75)	-	-	-	-
	1.60	5.76	[12]	4.97(-13.65)	8.11(40.74)	8.05(39.76)	6.24(8.33)	-	-
	1.60	6.40	[36]	5.26(-17.89)	4.29(-32.94)	-	-	-	-
AMATOL50/50	1.55	6.43	[35]	5.15(-19.83)	4.20(-34.66)	-	-	-	-
	1.55	6.23	[35]	5.15(-17.26)	4.20(-32.56)	-	-	-	-
AMATOL40/60	1.60	6.55	[36]	5.64(-13.89)	5.56(-15.08)	-	-	-	-
AN	1.30	5.27	[7]	5.00(-5.19)	-	5.30(0.57)	-	-	-
	1.05	4.50	[11]	4.43(-1.57)	-	5.30(17.78)	-	-	-
AN/Al(90/10)	1.05	5.60	[11]	5.11(-8.83)	-	5.45(-2.68)	-	-	-
AN/Al(80/20)	1.05	5.80	[11]	5.13(-11.50)	-	5.37(-7.41)	-	-	-
AN/Al(70/30)	1.05	5.40	[11]	4.99(-7.61)	-	5.09(-5.74)	-	-	-
ANFO 6/94	0.88	5.50	[11]	5.10(-7.28)	5.41(-1.72)	5.44(-1.09)	-	-	-
Destex	1.68	6.65	[11]	6.68(0.45)	6.77(1.80)	6.44(-3.17)	-	6.30(-5.26)	6.49(-2.36)
HBX-1	1.71	7.31	[12]	7.27(-0.50)	7.61(4.16)	7.18(-1.78)	7.38(0.96)	7.49(2.42)	7.31(0.02)
	1.75	7.22	[36]	7.40(2.41)	7.74(7.13)	-	-	7.49(3.67)	7.44(2.96)

HBX-3	1.84	7.12	[12]	6.92(-2.84)	7.96(11.80)	6.27(-11.94)	6.91(-2.95)	7.39(3.78)	6.75(-5.20)
	1.85	7.53	[19]	6.94(-7.78)	7.99(6.10)	6.27(-16.73)	6.91(-8.23)	7.39(-1.86)	6.78(-10.01)
HMX/Al(90/10)	1.76	8.30	[12]	8.16(-1.73)	8.64(4.10)	8.32(0.24)	8.41(1.33)	8.06(-2.89)	8.21(-1.08)
HMX/Al(80/20)	1.82	8.30	[12]	7.99(-3.69)	8.85(6.58)	7.93(-4.46)	8.22(-0.96)	7.99(-3.73)	8.06(-2.89)
HMX/Al(70/30)	1.86	8.00	[12]	7.65(-4.33)	8.98(12.28)	7.27(-9.13)	7.82(-2.25)	7.93(-0.85)	7.75(-3.13)
HMX/Al(60/40)	1.94	7.70	[12]	7.37(-4.28)	9.26(20.26)	6.86(-10.91)	7.46(-3.12)	7.79(1.17)	7.52(-2.34)
MINOL-2	1.68	5.82	[12]	5.24(-9.95)	4.47(-23.18)	7.23(24.23)	6.30(8.25)	-	-
PBX C-117	1.75	7.70	[11]	7.48(-2.86)	7.83(1.69)	7.68(-0.26)	-	-	7.51(-2.47)
PBXC-9	1.98	8.50	[11]	8.79(3.42)	9.68(13.88)	8.46(-0.47)	-	-	8.89(4.59)
RDX/Al(90/10)	1.68	8.03	[12]	7.88(-1.81)	8.38(4.36)	8.02(-0.12)	8.08(0.62)	7.72(-3.86)	7.94(-1.12)
RDX/Al(80/20)	1.73	7.77	[12]	7.71(-0.84)	8.55(10.04)	7.60(-2.19)	7.81(0.51)	7.70(-0.90)	7.77(0.00)
RDX/Al(70/30)	1.79	7.58	[12]	7.45(-1.74)	8.75(15.44)	7.03(-7.26)	7.49(-1.19)	7.61(0.40)	7.54(-0.53)
RDX/Al(60/40)	1.84	7.20	[12]	7.10(-1.44)	8.92(23.89)	6.42(-10.83)	6.93(-3.75)	7.54(4.72)	7.23(0.42)
RDX/Al(50/50)	1.89	6.81	[12]	6.57(-3.56)	9.09(33.48)	5.78(-15.12)	6.02(-11.60)	6.23(-11.63)	6.85(0.59)
TNT/Al(89.4/10.6)	1.72	7.05	[12]	7.23(2.51)	7.21(2.27)	7.02(-0.43)	7.12(0.99)	6.23(-11.60)	7.15(1.42)
TNT/Al(78.3/21.7)	1.80	7.05	[12]	7.12(0.98)	7.44(5.53)	6.59(-6.52)	6.94(-1.56)	6.16(-12.62)	6.98(-0.99)
TNT/Al(67.8/32.2)	1.89	7.05	[12]	6.92(-1.78)	7.70(9.22)	5.94(-15.74)	6.71(-4.82)	6.04(-14.26)	6.79(-3.76)
TNTEB/Al(90/10)	1.75	8.12	[12]	7.98(-1.74)	8.49(4.56)	7.85(-3.33)	7.91(-2.59)	-	8.02(-1.23)
TNTEB/Al(80/20)	1.82	7.99	[12]	7.82(-2.17)	8.73(9.26)	7.53(-5.76)	7.73(-3.25)	-	7.87(-1.5)
TNTEB/Al(70/30)	1.88	7.84	[12]	7.51(-4.18)	8.93(13.90)	6.99(-10.84)	7.43(-5.23)	-	7.61(-2.93)
Torpex	1.81	7.49	[37]	7.78(3.87)	8.17(9.08)	7.49(0.03)	-	7.29(-2.67)	7.82(4.44)
Tritonal	1.72	6.47	[37]	6.94(7.30)	7.21(11.44)	6.58(1.75)	-	6.29(-2.78)	6.81(5.26)
MAPE (Data Points)				**6.47 (43)**	**10.17 (36)**	**9.03 (36)**	**3.64 (23)**	**4.31 (21)**	**2.39 (26)**

5   Conclusions

The performance of an explosive is determined to some extent by the detonation velocity. A simple approach has been introduced for the desk calculation of the detonation velocity of ideal and non-ideal explosives. It requires no prior knowledge of measured or calculated properties except $\Delta_f H^0(c)$ at a specified ρ_0. The decomposition paths of Equation 2 provide suitable products, which can give a reliable prediction of the detonation velocity. For ideal CHNO explosives, the new method can give good results for $\rho_0 < 1.0$ g·cm^{-3} as compared to the K-J method [30]. The new approach can be easily used for CHNOFCl explosives by considering related products in Equation 2. For composite explosives containing Al/AN additives, partial interaction of Al with the gaseous products and decomposition of AN have been assumed. Also in different classes of CHNO, CHNOFCl, and aluminized explosives, the new model has been compared with our previous model, *i.e.* [28]. Equations 2 and 3 provide good predictions of the detonation velocity for various pure and mixed explosives within a few percent deviation.

Appendix A and Appendix B are available as S.I. at http://www.wydawnictwa.ipo.waw.pl/CEJEM/contents/2016/vol-13-number-2.html

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