

A simple approach for determining detonation velocity of high explosive at any loading density

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Abstract

A simple empirical relationship is introduced between detonation velocity at any loading density and chemical composition of high explosive as well as its gas phase heat of formation, which is calculated by group additivity rules. The present work may be applied to any explosive that contains the elements of carbon, hydrogen, nitrogen and oxygen with no difficulties. The new correlation can easily be applied for determining detonation velocity of explosives with loading densities less than 1 g/cm^3 as well as greater than 1 g/cm^3 . Calculated detonation velocities by this procedure for both pure and explosive formulations show good agreement with respect to measured detonation velocity over a wide range of loading density.

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1. Introduction

The prediction of the performance of new high explosives from a given molecular structure and known or estimated crystal density eliminate easily any poor candidate. The performance of new energetic materials should be evaluated prior to their actual synthesis because it reduces the costs associated with synthesis, test and evaluation of the materials. Due to the difficulty of synthesis and the instability of energetic material, few experimental studies have been done. The detonation parameters such as velocity, pressure and energy have been regarded as the principal measures of the performance of detonating explosives for many years.

Although reliable experimental data are always preferred over values obtained by computer codes or estimation procedures, all too often reliable data are not available in the field of energetic materials. The detonation wave has the feature of attaining the final state of maximum density and temperature simultaneously. Detonation parameters can

usually calculated on the basis of Chapman–Jouguet (C–J) theory. All of the C–J state parameters can be determined either by the use of computer codes, or estimates based on the chemical composition and/or structure, and thermochemical properties, or by simple experiment. The parameters such as detonation velocity, pressure and temperature can be calculated by a computer code, e.g. TIGER [1], when the heat of formation and the density of the explosive substance are known and the equation of state is assumed. Many of equations of state have been developed to describe shock and detonation performance of condensed matter [2]. Some of the well-known equations of state for gaseous detonation products are Becker–Kistiakosky–Wilson (BKW) [3], the Jacobs–Cowperthwaite–Zwisler (JCZ) [4,5], Kihara–Hikita–Tanaka (KHT) [6], Exp-6 [7] and Lennard–Jones–Devonshire (LJD) [8]. Some empirical methods have been introduced for determination of the C–J detonation pressure of ideal and non-ideal pure or mixed explosives of different classes [9–15]. In efforts to develop prediction capabilities for the detonation performance of explosives, numerous studies have also been performed that attempt to relate chemical structure and either theoretical maximum density or loading density with detonation

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velocities [9,20–29]. To compare with steady-state calculations, detonation velocities are measured at various charge diameters and extrapolated to an “infinite diameter”. In contrast to detonation velocity, which can typically be measured to within a few percent, the detonation pressure is not easy to determine accurately. Non-equilibrium effects in reaction zones may contribute to large uncertainty for determining detonation pressures by various indirect methods, which span a range of 10–20% [30]. The measured pressures may be higher than equilibrium calculations if in this situation the measurement is taken behind the von Neumann spike and in front of C–J plane. The brightness of the detonation front can be used to measure detonation temperatures using detectors, temperatures are those of a blackbody of equivalent photographic brightness, with absolute accuracies estimated to be ± 100 K for liquid explosives and ± 200 K for solid explosives [31].

There is a continuing need in the field of energetic materials for reliable predictions of detonation parameters. Knowledge of the detonation velocity is important because it is the easiest C–J state parameter to measure accurately. A number of useful equations relate the detonation velocity to the other C–J state parameters [32]. The purpose of this work was to correlate detonation velocity with the explosive’s elemental composition, loading density and gas phase heat of formation which can be determined by the additivity rules of a group estimation method related to the molecular structure, e.g., the methods of Benson et al. [33], Yoneda [34], Joback [35], etc. This work shows useful (predictive) applications to solid explosive mixtures. The procedure has been tested on some well-known mixtures of explosives. It should be noted that the results predicted by the new simple method are comparable with outputs of complex computer codes and that accuracy is not necessarily enhanced by greater complexity. Since the values of solid or liquid heat of formation are rarely known experimentally for new explosives of interest, the present method for estimating detonation velocity at any loading density without using experimental data is of significant value. The most important aspect of the present work is that easily calculated gas phase heat of formation of a CHNO explosive can be used to determine its performance. The present work also shows to what extent detonation velocity can be easily determined at loading density above 1 g/cm^3 as well as below 1 g/cm^3 .

2. Estimation of detonation velocity

The effectiveness of an explosive depends on the amount of energy available in it and the rate of release of available energy when detonation occurs. Detonation velocity and pressure are two performance parameters, which may be used to measure the effectiveness of different explosives. Though detonation parameters may be measured experimentally or calculated from theory, theoretical calculations are more convenient and useful in comparing the relative performance

of one explosive with another. The calculation of the performance of energetic materials by the usual thermochemical methods is highly tedious, often requiring intricate balancing of chemical equations. Fairly accurate predictions by simple empirical methods are highly desired for calculating the various parameters of energetic compounds.

Of the different empirical methods for calculation of detonation velocity [9,20–29], the well-known method of Kamlet and coworkers [9,16,17] can determine detonation velocity of C–H–N–O explosives at loading density above 1.0 g/cm^3 within about few percent. An interesting and useful test is a direct comparison of experimental with the calculated detonation velocity versus loading density using one of the best empirical relationships proposed by Kamlet and coworkers. Kamlet and Jacobs [9] originally found that estimates of detonation velocity, corresponding surprisingly well with RUBY predictions [36], are possible for C–H–N–O explosives using the following empirical relation:

$$D \text{ (km/s)} = A(NM^{1/2}Q^{1/2})^{1/2}(1 + B\rho_0) \quad (1)$$

where A and B are constants, N is the number of moles of gaseous products of detonation per gram of explosive, M is the average molecular weight of the gas found from the chemical reaction equations with an assumed equilibrium composition, Q is the heat of detonation in calories per gram of explosive and ρ_0 is loading density. The equilibrium composition of the product gases must be determined for evaluating the heat of formation of the detonation products. They assumed that all of the oxygen available in the explosive is used in the formation of water and carbon dioxide, and none of oxygen is used in the formation of carbon monoxide. The heat of detonation can be determined from the heats of formation of the explosive and the products of detonation. They also assumed that most often C–H–N–O explosives generally have crystal densities of $1.7\text{--}1.9 \text{ g/cm}^3$, and that they are most often used at high fractions of theoretical maximum density. Kamlet and Hurwitz found Eq. (1), with $A = 1.01$ and $B = 1.30$, predicts experimental values of detonation velocities (in $\text{mm}/\mu\text{s}$ or km/s) for 24 C–H–N–O explosives to within $\pm 3\%$ at loading density above 1 g/cm^3 . The Kamlet et al. method is appealing because it requires as input only the heat of formation of the explosive and simple gas phase products. Though the heat of formation is the most effective parameter for the prediction of the characteristics of blast wave pressure and energy of underwater explosion in which the total energy released into the surrounding media is a dominant factor, initial density of the explosive is effective for prediction of detonation pressure and velocity at theoretical maximum density. Heat of formation of energetic materials is an important property to evaluate their instabilities and performances, which can be determined experimentally or estimated for some classes of explosives [37–40].

From an examination of detonation velocity of explosives, it can be inferred that detonation velocity depends on three principal parameters:

- (1) The composition of explosive and its oxygen balance, since it is reasonable to assume that all the chemical bonds present in the reacting molecules are broken, resulting in the formation of monatomic species, which subsequently recombine to stable products. It is, therefore, possible to represent detonation velocity of an explosive as a function of its composition. This concept formed the basis of an approach proposed earlier by some authors, e.g. by Stine [27] and Rothstein and Petersen [18,19], for defining and evaluating in a fairly simple and straightforward manner detonation velocity at theoretical maximum density or initial high explosive density near its crystalline value.
- (2) The heat content of the explosive, since the heat of detonation depends on the heat of formation of the explosive per unit weight and greater energy content leads to greater release of energy upon detonation and higher detonation temperatures.
- (3) Loading density, since experiments reveal a linear relationship between detonation velocity and loading density [41,42].

Application of an empirical correlation approach to explosives comprised of C, H, N and O has resulted in a relationship between detonation velocity, chemical composition, and somewhat surprisingly, heat of formation of the explosive in the gas phase as calculated from additivity rules. The first step in developing this correlation is to express detonation velocity as function of the above mentioned basic param-

eters, as follows:

$$D \text{ (km/s)} = U + \left(\frac{Va + Wb + Xc + Yd + Z\Delta H_f(\text{g})}{\text{MW}} \right) \rho_0 \quad (2)$$

where a , b , c , and d are stoichiometric coefficients for an explosive of general formula $C_aH_bN_cO_d$, MW is the molecular weight of the explosive, $\Delta H_f(\text{g})$ is the gas phase heat of formation calculated from additivity rules, and U , V , W , X , Y , and Z are values to be adjusted to obtain the best fit to experimental detonation velocity data. This equation provides the basis for a simple procedure for estimation of detonation velocity, which requires as input information only the elemental composition, loading density, and heat of formation of the explosive in the gas phase as calculated from an additivity method such as Benson et al. [33], Yoneda [34], Joback [35], etc. To find the constants of Eq. (2), experimental detonation velocity of six well-known explosives HMX, RDX, TNT, PETN, Tetryl and DATB at different loading densities was used, giving the following equation:

$$D \text{ (km/s)} = 1.90 + \left(\frac{-2.97a + 9.32b + 27.68c + 98.9d + 1.22\Delta H_f(\text{g})}{\text{MW}} \right) \rho_0 \quad (3)$$

Table 1
Parameters used in calculations

Explosive ^a	Chemical formula	ΔH_f (kcal/mol), condensed phase ^b	ΔH_f (kcal/mol), gas phase ^c
PETN	$C_5H_8N_4O_{12}$	-128.7	-174.3
RDX	$C_3H_6N_6O_6$	14.71	37.85
HMX	$C_4H_8N_8O_8$	17.93	45.02
TNT	$C_7H_5N_3O_6$	-15.0	-4.30
NQ	$CH_4N_4O_2$	-22.1	50.4
TETRYL	$C_7H_5N_5O_8$	4.67	9.28
DATB	$C_6H_5N_5O_6$	-23.6	14.06
NG	$C_3H_5N_3O_9$	-88.6	-129.6
TATB	$C_6H_6N_6O_6$	-36.85	19.4
NM	CH_3NO_2	-27.03	-17.88
PA	$C_6H_3N_3O_7$	-51.3	-39.04
DEGN	$C_4H_8N_2O_7$	-99.4	-130.16
COMP B	$C_{2.03}H_{2.64}N_{2.18}O_{2.67}$	1.00	10.06
COMP B-3	$C_{2.04}H_{2.50}N_{2.15}O_{2.68}$	1.33	9.47
CYCLOTOL-78/22	$C_{1.73}H_{2.59}N_{2.40}O_{2.69}$	3.71	12.88
CYCLOTOL-77/23	$C_{1.75}H_{2.59}N_{2.38}O_{2.69}$	3.58	12.67
CYCLOTOL-75/25	$C_{1.78}H_{2.58}N_{2.36}O_{2.69}$	3.32	12.31
CYCLOTOL-70/30	$C_{1.87}H_{2.56}N_{2.29}O_{2.68}$	2.66	11.36
CYCLOTOL-65/35	$C_{1.96}H_{2.53}N_{2.22}O_{2.68}$	1.99	10.42
CYCLOTOL-60/40	$C_{2.04}H_{2.50}N_{2.15}O_{2.68}$	1.33	9.47
CYCLOTOL-50/50	$C_{2.22}H_{2.45}N_{2.01}O_{2.67}$	0.01	7.54
OCTOL-76/23	$C_{1.76}H_{2.58}N_{2.37}O_{2.69}$	3.05	11.15
OCTOL-75/25	$C_{1.78}H_{2.58}N_{2.36}O_{2.69}$	2.89	10.93
OCTOL-60/40	$C_{2.04}H_{2.50}N_{2.15}O_{2.68}$	0.99	8.36
PENTOLITE-50/50	$C_{2.17}H_{2.11}N_{1.17}O_{2.84}$	-19.6	-23.0

^a See Appendix A for glossary of compound names.

^b Heat of formation of pure explosives were obtained from [39].

^c Heat of formation calculated by Joback additive group procedure [31].

Table 2
Comparison of detonation velocity of the new correlation and Kamlet and coworkers method with measured values [43]

Name	ρ_0 (g/cm ³)	D_{exp} (km/s)	D_{Kamlet} (km/s)	D_{new} (km/s)	%Dev Kamlet	%Dev new
PETN	0.25	2.83	3.49	2.80	23.22	-0.88
	0.50	2.99	3.66	2.99	22.35	-0.13
	0.48	3.6	4.27	3.64	18.72	1.04
	0.88	5.06	5.64	5.09	11.51	0.50
	0.99	5.48	6.02	5.48	9.83	0.07
	1.23	6.37	6.84	6.35	7.38	-0.27
	1.45	7.18	7.59	7.15	5.75	-0.43
	1.6	7.75	8.11	7.69	4.59	-0.75
	1.7	8.07	8.45	8.05	4.68	-0.20
	1.76	8.27	8.65	8.27	4.63	0.01
RDX	0.56	4.05	4.55	4.05	12.24	0.03
	0.70	4.65	5.02	4.59	8.06	-1.31
	0.95	5.80	5.88	5.55	1.37	-4.32
	1.10	6.18	6.39	6.13	3.44	-0.88
	1.20	6.77	6.73	6.51	-0.52	-3.84
	1.29	7.00	7.04	6.86	0.60	-2.06
	1.40	7.46	7.42	7.28	-0.56	-2.44
	1.46	7.60	7.62	7.51	0.31	-1.20
	1.60	8.13	8.10	8.05	-0.34	-1.03
	1.66	8.24	8.31	8.28	0.82	0.45
	1.72	8.46	8.51	8.51	0.62	0.56
	1.77	8.70	8.68	8.70	-0.19	0.00
	1.80	8.75	8.79	8.81	0.42	0.74
HMX	0.75	4.88	5.19	4.76	6.36	-2.37
	1.0	5.8	6.04	5.72	4.22	-1.40
	1.2	6.85	6.73	6.48	-1.78	-5.36
	1.4	7.3	7.41	7.25	1.53	-0.73
	1.6	7.91	8.09	8.01	2.33	1.27
NQ	1.89	9.11	9.09	9.12	-0.27	0.09
	1.55	7.65	7.16	7.93	-6.39	3.65
	1.62	7.93	7.38	8.20	-6.97	3.42
	1.78	8.59	7.87	8.82	-8.36	2.72
TNT	1.55	7.65	7.16	7.93	-6.39	3.65
	0.8	4.34	4.55	4.36	4.75	0.38
	1	5	5.13	4.97	2.51	-0.59
	1.36	6.2	6.17	6.08	-0.51	-2.00
	1.45	6.5	6.43	6.35	-1.09	-2.28
TETRYL	1.64	6.93	6.98	6.94	0.72	0.08
	1.36	6.68	6.63	6.48	-0.82	-2.98
	1.61	7.58	7.40	7.32	-2.33	-3.39
	1.68	7.5	7.62	7.56	1.61	0.79
	1.71	7.85	7.71	7.66	-1.73	-2.42
DATB	1.73	7.72	7.78	7.73	0.73	0.10
	1.78	7.6	7.54	7.60	-0.76	-0.03
	NG	1.6	7.7	8.17	7.91	-6.1
TATB	1.83	7.58	7.61	7.73	0.40	1.92
NM	1.13	6.28	6.38	6.13	1.61	-2.32
PA	1.60	7.1	7.07	7.05	-0.37	-0.65
	1.71	7.26	7.40	7.41	1.96	2.05
	1.76	7.57	7.55	7.57	-0.24	-0.01
DEGN	1.38	6.76	7.06	6.48	4.38	-4.09
HNS	1.70	6.8	7.16	7.10	5.32	4.48
COMP B	1.72	7.92	8.02	8.00	1.23	0.95
COMP B-3	1.72	7.89	8.00	7.98	1.34	1.11
CYCLOTOL-78/22	1.76	8.31	8.37	8.36	0.68	0.63
CYCLOTOL-77/23	1.74	8.25	8.29	8.28	0.46	0.31
CYCLOTOL-75/25	1.76	8.3	8.33	8.32	0.39	0.23
CYCLOTOL-70/30	1.62	7.95	7.87	7.81	-0.99	-1.78
	1.73	8.06	8.17	8.15	1.31	1.07
	1.72	8.04	8.07	8.04	0.35	0.04
CYCLOTOL-65/35	1.74	8.09	8.07	8.05	-0.27	-0.52
CYCLOTOL-60/40	1.72	7.9	8.00	7.98	1.32	0.98

Table 2 (Continued)

Name	ρ_0 (g/cm ³)	D_{exp} (km/s)	D_{Kamlet} (km/s)	D_{new} (km/s)	%Dev Kamlet	%Dev new
CYCLOTOL-50/50	1.63	7.66	7.59	7.53	−0.92	−1.66
OCTOL-76/23	1.81	8.45	8.50	8.49	0.63	0.49
OCTOL-75/25	1.81	8.48	8.49	8.47	0.07	−0.07
OCTOL-60/40	1.80	8.16	8.26	8.23	1.17	0.92
PENTOLITE-50/50	1.71	7.75	7.77	7.57	0.27	−2.34
	1.70	7.53	7.74	7.54	2.79	0.07
	1.68	7.65	7.68	7.47	0.35	−2.37
	1.64	7.53	7.55	7.34	0.29	−2.57

The condensed and gas phase heats of formation of some pure and mixed explosives are shown in Table 1. Detonation velocities estimated by this method for underoxidized and overoxidized explosives are given in Table 2 and compared with values calculated from the method of Kamlet and coworkers as well as measured values. As indicated in Table 2, the newly calculated detonation velocities, in contrast to the method of Kamlet and coworkers, shows surprisingly good agreement with experimental values at loading densities below 1 g/cm³. In some explosives such as NQ, the new method can also predict a better result than the method of Kamlet and coworkers at loading density above 1 g/cm³. Comparison of calculated results with experimental data listed in Table 2 may be taken as appropriate validation of the new simple method for use with C–H–N–O explosives. It is worthwhile to note that the present method is very simple and at the same time, gives results that are comparable to those from other more complex methods involving the equation of state of the products. Large errors in predictions from the method Kamlet and coworkers are observed at initial density less than 1 g/cm³. In contrast, the new equation determines detonation velocity to within about few percent at any loading density. Considering that errors of a few percent can generally be attributed to experimental measurements of detonation velocity, the agreement between calculated and measured velocities is very good.

As with the condensed phase heat of formation, the gas phase heat of formation of an explosive mixture can be calculated from the heat of formation of individual components and their percent concentrations in the mixture. The method can be applied to both pure and mixed explosives, and compared against results predicted using the method of Kamlet and coworkers and against experimental values.

The explosives in Table 2 cover a wide range in oxygen balance and are considered to be representative of the entire class of C–H–N–O explosives. Of explosives given in Table 2, NG has more than enough oxygen in its structure to oxidize fully the fuel elements of the molecule; on the other hand, TNT is very oxygen deficient because some carbon is not been oxidized. The other explosives in Table 2 have oxygen content between NG and TNT.

3. Conclusions

The objective of this study was to develop a simple method of estimating for comparison of the detonation velocities of experimental high explosives that contain carbon, hydrogen, oxygen and nitrogen. The velocity at which the detonation shock wave proceeds through a charge is an important parameter of the explosive material. The results of this work are remarkable because the necessary data for this method is readily calculated and the predicted results are of about the same reliability as one could expect from a more complex computer code. There is also no need to assume specified detonation products, as with the method of Kamlet and coworkers.

Good agreement between predictions from the new estimation method and experimental demonstrated for a vast number of explosive formulations. This correlation gives good detonation velocity for different C–H–N–O explosives at any loading density. It is important to stress that the present correlation operates in a predictive mode. This method is suitable for determination of detonation velocity at any loading density and does not require knowledge of solid or liquid heat of formation, parameters not known for many new explosives.

In summary, a new method for calculating detonation velocity over wide range of loading densities has been developed. Unlike conventional methods which require experimental solid or liquid heat of formation, the new method uses gas phase heat of formation calculated by group additivity rules. The new method is simple in form, easy to use, and appears to give accurate detonation velocities at any loading density.

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Appendix A. Glossary of compound names

DATB 1,3-diamino-2,4,6-trinitrobenzene
 TATB 1,3,5-triamino-2,4,6-trinitrobenzene
 TETRYL *N*-methyl-*N*-nitro-2,4,6-trinitroaniline

TNT	2,4,6-trinitrotoluene
NG	nitroglycerine
NM	nitromethane
PETN	pentaerythritol tetranitrate
RDX	cyclotrimethylene trinitramine
HMX	cyclotetramethylene tetranitramine
NQ	nitroguanidine
PA	picric acid
DEGN	diethyleneglycol dinitrate
COMP B	63/36 RDX/TNT
COMP B-3	60/40 RDX/TNT
CYCLOTOL-78/22	78/22 RDX/TNT
CYCLOTOL-77/23	77/23 RDX/TNT
CYCLOTOL-75/25	75/25 RDX/TNT
CYCLOTOL-70/30	70/30 RDX/TNT
CYCLOTOL-65/35	65/35 RDX/TNT
CYCLOTOL-60/40	60/40 RDX/TNT
CYCLOTOL-50/50	50/50 RDX/TNT
OCTOL-78/22	77.6/22.4 HMX/TNT
OCTOL-76/23	76.3/23.7 HMX/TNT
OCTOL-75/25	75/25 HMX/TNT
OCTOL-60/40	60/40 HMX/TNT
PENTOLITE	50/50 PETN/TNT

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