

# Simple determination of performance of explosives without using any experimental data

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## Abstract

A simple procedure is introduced by which detonation pressure of  $C_aH_bN_cO_d$  explosives can be predicted from  $a$ ,  $b$ ,  $c$ ,  $d$  and calculated gas phase heat of formation of explosives at any loading density without using any assumed detonation products and experimental data. It is shown here that the loading density, simply calculated heat of formation by additivity rule and atomic composition can be integrated into an empirical formula for predicting the detonation pressure of proposed explosives. Calculated detonation pressures by the introduced method for both pure and explosive formulations show good agreement with respect to measured detonation pressure over a wide range of loading density. The deviations are within about experimental errors.

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## 1. Introduction

The importance of a prediction tool for searching of new explosives with a given performance, sensitivity and physical properties increases with greater relevance for synthesis, performance and vulnerability. The expenditure connected with the development and synthesis of a new, high-energetic material necessitates the development of theoretical methods, which help the chemist in decision as to whether it is worth the effort to attempt a new and complex synthesis. The advantages of a computation or calculated approach for determining of new-energetic compound are, of course, that it can be applied to suggested target molecules prior to undertaking syntheses. Simply calculation approaches play an important role in the study of energetic molecules, since they permit both existing and proposed systems to be analyzed and evaluated. The expenditure connected with the development and synthesis of new-energetic materials also necessitates the

development of theoretical methods as well as various empirical methods complemented the computer output for desk calculations of factors detonation performance along with structure-sensitive relationships of C–H–N–O explosives.

One of the basic performance properties of an explosive is detonation pressure, which is a function of energy produced by its decomposition. The detonation products of condensed explosives of practical interest are usually produced at high pressure and a temperature of several thousand degrees [1]. The application of the hydrodynamic theory for calculating the detonation properties requires knowledge of the equation of state of the system. Explosives that yield only gaseous products can be modelled by a single form of the equation of state. Thermochemical/hydrodynamic computer codes such as BKW [2], RUBY [3], latter's offspring TIGER [4], CHEQ [5], and CHEETAH [6] (a C version of TIGER), by assuming all of the chemical equations for all possible species in the reaction product gases and solving these with thermochemical analogues, can estimate the isentropic expansion having the equilibrium energy and gas quantities along with the Rankine–Hugoniot jump equations. An appropriate equation of state can accurately reflect the thermodynamic

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properties of multi-component mixtures at several thousand Kelvin and hundreds of kbar, as well as at much lower temperatures and pressures obtained during expansion of the reaction products. There are several forms of empirical equation of states such as Becker–Kistiakosky–Wilson (BKW-EOS) [7], the Jacobs–Cowperthwaite–Zwisler (JCZ-EOS) [8,9] and Kihara–Hikita–Tanaka (KHT-EOS) [10], which were fitted to experimental data for specific explosives at specific densities.

Some empirical methods have been introduced for determination of the Chapman–Jouguet (C–J) detonation pressure of ideal pure or mixture of  $C_aH_bN_cO_d$  explosives [11–16] so that all of them require at least an estimate of detonation products. The Kamlet and coworkers method [11–13] can be applied for the explosives with loading density above 1 g/cc. Their method also needs the measured condensed heat of formation of the explosive. New correlations [14–16] have been recently introduced, by assuming reliable decomposition products, to determine detonation pressure of pure and mixture of explosives at any loading density via the calculated combustion temperature based on computed heat of formation by PM3 procedure or experimental crystalline heat of formation. Since the calculation of the combustion temperature requires the optimization of heat capacities of detonation products, it takes much more time for determining detonation pressure.

The calculation of detonation pressure by a computer code, e.g. BKW [2], TIGER [4], etc., in spite of its complexity usually requires condensed measured heat of formation of the explosive. The main focus, thereafter, will be on introducing the simplest procedure for calculating detonation pressure of the explosive at any loading density without the use of any experimental data of the explosive and detonation products. It should be noted that the accuracy of predictive method is not necessarily enhanced by greater complexity. It is shown here how detonation pressure of  $C_aH_bN_cO_d$  explosives can be predicted directly from the values of  $a$ ,  $b$ ,  $c$ ,  $d$  and gas phase heat of formation of the explosive which can be determined by additivity rules related to the molecular structure, e.g. the methods of Benson et al. [17], Yoneda [18], Joback [19], etc., with little loss of accuracy. The present result is remarkable respect to predictive method of detonation pressure via heat of detonation [11–13,20] because it shows to what extent detonation pressure can be easily determined directly from elemental composition over a wide range of loading density without using experimental condensed heat of formation and assumed detonation products of explosive. Moreover, the introduced correlation does not have complexity of combustion temperature procedure [14–16], which needs to optimize combustion temperature via heat capacities of detonation products at or near the computed combustion temperature. The calculated detonation pressure will also be tested with experimental data of well known pure and mixture of explosives. It is felt that the introduced correlation represents a significant advance in a priori estimation of explosive performance. Another goal of this work, complemented the

computer output for the simplest hand calculations related to C–J pressure, is to provide insight to understanding the molecules which are responsible for higher performance and which are not.

## 2. Simply determining of detonation pressure

Predicting of the performance of new energetic materials from a given molecular structure without using experimental measurement is very important to chemist because the calculated detonation properties of a notional energetic compound are recognized to be cost-effective, environmentally-desirable and time-saving in the decision to whether it is worth the effort to attempt a new or complex synthesis. The pressure associated with the state of complete reaction, the detonation velocity and detonation energy are three important parameters that have been regarded as principal measures of performance of detonating explosive for many years. Chapman and Jouguet introduced a simple explanation of detonation so that as the shock compresses the material, the chemical reaction takes place instantaneously. For thermochemical calculations of condensed phase explosives, the determination of the time-independent state of chemical equilibrium, which is defined in accordance with the Chapman–Jouguet (C–J), had historically special attention. Since the nonsteady-state nature of the detonation wave, it is reasonable to expect the calculated and experimental C–J pressures to differ by 10–20% [2]. The C–J pressure coupled with the adiabatic ( $\gamma$ ) exponent, i.e. the initial pressure–volume slope in the isentropic expansion of detonation products from the C–J state, is considered to be an index of explosive's ability to accelerate metal [21]. Detonation velocity is an important parameter of the explosive material at which the detonation shock wave proceeds through a charge. It can be measured directly with a high accuracy to within a few percent at various charge diameters and extrapolated to an 'infinite diameter' for comparison with steady-state calculations. The energy content of an explosive can be determined from its heat of detonation. Detonation calorimetry allows the experimental evaluation and some theoretical methods, such as a general interaction properties function (GIPF) methodology using quantum mechanical information about a single molecule, can also be used to compute the heat of detonation [22,23]. Experimental or calculated heats of formation [23–25] are essential parameters to evaluate the enthalpy change of detonation reaction.

It is proposed that the detonation performance of a high explosive can most appropriately be expressed as its elemental composition and heat content in gas phase rather than condensed phase. In this paper two bases have been developed for estimating detonation pressure of  $C_aH_bN_cO_d$  explosives at any bulk density of interest. Rothstein and Petersen [26,27] and Stine [28] used elemental composition of the explosive as well as the other parameters to calculate detonation velocity. However, one is possible to represent detonation pressure as a function of elemental composition of the explosive without

using assumed or computed detonation products. The other is simply calculated gas phase heat of formation that shows crystal effects can be excluded for determining the performance in this manner [15]. The complicated computer code and empirical methods are convincing evidence of the utility of them for engineering calculations of detonation properties of explosives. In this regard, a new correlation is introduced for detonation pressure, which has historically been used as indicator of relative explosive ‘effectiveness’. It is emphasized that no precise prediction of gas phase heat of formation was required in order to reproduce the experimental data within the error limits ascribed to that of data. Further, the calculated C–J pressure is insensitive to large variation in the gas phase heat of formation of the unreacted explosive that is significant in view of the uncertainty often associated with different methods of calculation the heats of formation of the explosive in gas phase by additivity rules. This is, in fact, to be expected since for most of subject explosives, the  $|\Delta H_f^\circ(g)|$  of the explosive is small relative to the elemental composition of the  $C_aH_bN_cO_d$  explosive. The following general equation can be assumed for  $C_aH_bN_cO_d$  explosive with six adjustable parameters  $A, B, C, D, E$  and  $F$  in it:

$$P \text{ (kbar)} = F + \left( \frac{Aa + Bb + Cc + Dd + E \Delta H_f^\circ(g)}{MW} \right) \rho_0^2 \quad (1)$$

where  $\rho_0$  is loading density, MW and  $\Delta H_f^\circ(g)$  are molecular weight of explosive and its calculated gas phase heat of formation by additivity rules respectively. This equation shows that pressure is proportional to  $\rho_0^2$  which is adapted to experimentally measured values of detonation pressure [29,30]. Agreement with measurement has been secured in that the adjustable constants in introduced correlation consistent with a vast number of experimental results. The procedure of Kamlet and Hurwitz [31], in determining adjustable parameters, can be used to find coefficients  $A$ – $F$  in Eq. (1). Experimental detonation pressure of six well-known explosives HMX, RDX, TNT, PETN, Tetryl and DATB at different loading densities are used for finding adjustable parameters of relation (1) so that the following equation is derived:

$$P \text{ (kbar)} = -2.6 + \left( \frac{-1026a + 226b + 1031c + 3150d + 30.7 \Delta H_f^\circ(g)}{MW} \right) \rho_0^2 \quad (2)$$

For  $C_aH_bN_cO_d$  explosives, Eq. (2) shows that the relative weight fractions of the four elements present in the unreacted compound is far important than the details of the bonding arrangements within the molecular structure. The equation covers the range from the oxygen lean to oxygen rich explosives. The new correlation requires no prior knowledge of any measured, estimated or calculated physical, chemical or thermochemical properties of explosive and assumed deto-

Table 1  
Parameters used in calculations

Explosive <sup>a</sup>	Chemical formula	Gas phase <sup>b</sup> $\Delta H_f$ (kJ/mol) at 298 K
HMX	C <sub>4</sub> H <sub>8</sub> N <sub>8</sub> O <sub>8</sub>	45.02
RDX	C <sub>3</sub> H <sub>6</sub> N <sub>6</sub> O <sub>6</sub>	37.85
TNT	C <sub>7</sub> H <sub>5</sub> N <sub>3</sub> O <sub>6</sub>	–4.30
PETN	C <sub>5</sub> H <sub>8</sub> N <sub>4</sub> O <sub>12</sub>	–174.3
TETRYL	C <sub>7</sub> H <sub>5</sub> N <sub>5</sub> O <sub>8</sub>	9.28
DATB	C <sub>6</sub> H <sub>5</sub> N <sub>5</sub> O <sub>6</sub>	14.06
NG	C <sub>3</sub> H <sub>5</sub> N <sub>3</sub> O <sub>9</sub>	–129.6
TATB	C <sub>6</sub> H <sub>6</sub> N <sub>6</sub> O <sub>6</sub>	19.4
NM	CH <sub>3</sub> NO <sub>2</sub>	–17.88
COMP B	C <sub>2.03</sub> H <sub>2.64</sub> N <sub>2.18</sub> O <sub>2.67</sub>	10.06
COMP B-3	C <sub>2.04</sub> H <sub>2.50</sub> N <sub>2.15</sub> O <sub>2.68</sub>	9.47
CYCLOTOL-78/22	C <sub>1.73</sub> H <sub>2.59</sub> N <sub>2.40</sub> O <sub>2.69</sub>	12.88
CYCLOTOL-77/23	C <sub>1.75</sub> H <sub>2.59</sub> N <sub>2.38</sub> O <sub>2.69</sub>	12.67
CYCLOTOL-75/25	C <sub>1.78</sub> H <sub>2.58</sub> N <sub>2.36</sub> O <sub>2.69</sub>	12.31
CYCLOTOL-65/35	C <sub>1.96</sub> H <sub>2.53</sub> N <sub>2.22</sub> O <sub>2.68</sub>	10.42
CYCLOTOL-50/50	C <sub>2.22</sub> H <sub>2.45</sub> N <sub>2.01</sub> O <sub>2.67</sub>	7.54
OCTOL-76/23	C <sub>1.76</sub> H <sub>2.58</sub> N <sub>2.37</sub> O <sub>2.69</sub>	11.15
OCTOL-60/40	C <sub>2.04</sub> H <sub>2.50</sub> N <sub>2.15</sub> O <sub>2.68</sub>	8.36
PENTOLITE-50/50	C <sub>2.17</sub> H <sub>2.11</sub> N <sub>1.17</sub> O <sub>2.84</sub>	–23.0

<sup>a</sup> See Appendix A for glossary of compound names.

<sup>b</sup> Gas phase heat of formation calculated by Joback additive group procedure [19].

nation products other than simply calculated gas phase heat of formation by additivity rule.

It is possible to use data on the pure explosives for estimating detonation pressure of their mixtures. The value of C–J pressure of a mixture explosives, by using Eq. (2), can be calculated by weighted-average values of  $\Delta H_f^\circ(g)$ .

$$\Delta H_{f,\text{mix}}^\circ = \sum n_i \Delta H_{f,i}^\circ(g) \quad (3)$$

where  $n_i$  and  $\Delta H_{f,i}^\circ(g)$  are the number of moles and gas phase heat of formation of  $i$ th component respectively.

The calculated heat of formation of some pure and mixed explosives in gas phase by additivity rule is shown in Table 1. Calculated detonation pressures for under-oxidized and over-oxidized explosive are given in Table 2 and compared with corresponding measured values. As seen, the introduced simple, hand-calculated empirical correlation for determining detonation pressures show surprisingly very good agreement with experimental values at loading density which may be taken as appropriate validation tests of the new method with  $C_aH_bN_cO_d$  explosives. It is worthwhile to note that the present method by considering large percent deviations generally attributed to experimental measurements of detonation pressure, up to 20 percent [2], the agreement between calculated and measured pressures is also satisfactory.

Among various  $C_aH_bN_cO_d$  explosives, PETN can be prepared in high purity and pressed into manageable charges over a wide range of density that make it an ideal explosive for testing theoretical models [32,33]. The results in Table 2 are fairly consistent with complex statistical mechanical theory approaches [21] for PETN over a wide range of loading densities.

Table 2  
Comparison of detonation pressure of the new correlation with measured values [35]

Name	$\rho_0$ (g/cc)	$P_{\text{exp}}$ (kbar)	$P_{\text{cal}}$ (kbar)	% Dev new <sup>a</sup>
HMX	0.75	60	59.1	-1.4
	1.0	110	107.2	-2.6
	1.2	160	155.5	-2.8
	1.4	210	212.6	1.2
	1.6	280	278.4	-0.6
	1.89	390	389.5	-0.1
RDX	0.56	32	32.0	0.0
	0.70	48	51.5	7.2
	0.95	96	97.0	1.0
	1.10	122	130.9	7.3
	1.20	152	156.3	2.8
	1.29	166	181.0	9.0
	1.40	213	213.7	0.3
	1.46	211	232.6	10.2
	1.60	263	279.9	6.4
	1.72	313	323.8	3.5
	1.77	338	343.1	1.5
1.80	341	354.9	4.1	
TNT	0.8	37	41.9	13.2
	1	67	66.9	-0.1
	1.36	124	126.0	1.6
	1.45	144	143.5	-0.3
	1.64	210	184.4	-12.2
PETN	0.48	24	21.6	-10.0
	0.88	68	78.7	15.8
	0.99	87	100.3	15.3
	1.23	139	156.3	12.5
	1.45	208	218.2	4.9
	1.6	266	266.3	0.1
	1.7	307	301.0	-2.0
	1.76	337	322.8	-4.2
TETRYL	1.36	142	155.6	9.6
	1.68	226	219.1	-3.0
	1.71	239	238.8	-0.1
DATB	1.78	251	253.0	-2.3
NG	1.6	253	284.7	12.5
TATB	1.83	260	287.6	-8.7
NM	1.13	125	131.4	-6.8
COMP B	1.72	295	276.8	-6.2
COMP B-3	1.72	287	275.2	-4.1
CYCLOTOL-78/22	1.76	317	311.3	-1.8
CYCLOTOL-77/23	1.74	313	303.1	-3.2
CYCLOTOL-75/25	1.76	316	307.7	-2.6
	1.62	265	260.3	-1.8
CYCLOTOL-65/35	1.72	292	281.6	-3.6
CYCLOTOL-50/50	1.63	231	236.3	2.3
OCTOL-76/23	1.81	338	325.8	-3.6
OCTOL-60/40	1.80	320	300.9	-6.0
PENTOLITE-50/50	1.68	251	238.2	-5.1

$$^a \text{ \%Dev new} = \frac{P_{\text{cal}} - P_{\text{exp}}}{P_{\text{exp}}} \times 100.$$

### 3. Conclusions

Simplest empirical method complemented the computer output is introduced for desk calculation C–J pressure of  $C_aH_bN_cO_d$  explosives through gas phase heat of formation

calculated by group additivity rule and atomic composition of either pure mixed explosives. There is no need to assume detonation products that is usually done by previous methods [11–16,20]. Detonation pressures determined by various indirect methods span a range of 10–20%, which non-equilibrium effects in reaction zones may contribute to this large uncertainty [34]. Given the chemical formula of a real or hypothetical pure or mixture of explosives, one can estimate detonation pressure to within about  $\pm 20\%$  as a function of square loading density that is consistent with large uncertainty of detonation pressure. This method permits a simple calculation of detonation pressure of explosives where even their condensed heat of formation is relatively uncertain. The motivation in this work is to propose a simple correlation which can be used for determining the C–J pressure of explosives of arbitrary density, formed from the elements C, H, N and O. As indicated in Table 2 excellent agreement is obtained between measured and calculated values of detonation pressure for some explosives such as RDX over a wide range of loading densities. Since the necessary data for this method is readily hand calculated with about the same reliance on their answers as one could attach to the more complex computer code as well as the other empirical methods [11–16,20] without using any experimental data of explosives and detonation products, the results of this work are remarkable. An important result is that the values of  $\Delta H_f(g)$ , which can be determined by additivity rules, as well as elemental composition of the explosive correlate quite well with the values of detonation pressure. Though the solid or liquid heat of formation is an important factor to consider in designing new energetic materials or evaluating existing ones that can enter into the calculation of such key explosive and propellant properties as detonation velocity, detonation pressure and specific impulse, there is no need to use it in the present method.

In brief, a relatively accurate method of estimating detonation pressure for  $C_aH_bN_cO_d$  explosives is introduced which is only based upon the atomic composition of either a pure or mixed explosives, simply calculated gas phase heat of formation by additivity rule and square of loading density of explosive.

### Appendix A. Glossary of compound names

DATB	1,3-diamino-2,4,6-trinitrobenzene
TATB	1,3,5-triamino-2,4,6-trinitrobenzene
TETRYL	<i>N</i> -methyl- <i>N</i> -nitro-2,4,6-trinitroaniline
TNT	2,4,6-trinitrotoluene
NG	nitroglycerine
NM	nitromethane
PETN	pentaerythritol tetranitrate
RDX	cyclotrimethylene trinitramine
HMX	cyclotetramethylene tetranitramine
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-65/35 65/35 RDX/TNT  
 CYCLOTOL-50/50 50/50 RDX/TNT  
 OCTOL-76/23 76.3/23.7 HMX/TNT  
 OCTOL-60/40 60/40 HMX/TNT  
 PENTOLITE 50/50 PETN/TNT

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