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A simple method to assess detonation temperature without using any experimental data and computer code

Mohammad Hossein Keshavarz *, Hamid Reza Nazari

Department of Chemistry, Malek-ashtar University of Technology, Shahin-shahr P.O. Box 83145/115, Islamic Republic of Iran

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Abstract

Detonation temperature of $C_aH_bN_cO_d$ explosives can be predicted from a, b, c, d and calculated gas phase heat of formation of explosives without using any assumed detonation products and experimental data. Two new correlations are introduced for calculation of detonation temperature of aromatic and non-aromatic explosive compounds so that it is shown here how simply calculated heat of formation by additivity rule and atomic composition are only necessary data for this simple prediction. Calculated detonation temperatures by the introduced correlations for both pure and explosive formulations show good agreement with respect to measured detonation temperatures and complicated computer codes. The average mean absolute error in detonation temperature is within about 7.0%.

Keywords: Detonation temperature; $C_aH_bN_cO_d$ explosives; Gas phase heat of formation; Additivity rule

1. Introduction

Detonation products of high explosives are obtained at high pressures and temperatures simultaneously, which covers a wide range of pressures, ~1–100 GPa, and temperatures, ~1000–5000 K [1]. One of the detonation parameters with least information in the Chapman–Jouguet (C–J) state is detonation temperature, which is measured experimentally from the brightness of the detonation front as it proceeds toward detector. Thermochemical/hydrodynamic computer codes such as BKW [2] and RUBY [3] and latter's offspring TIGER [4], CHEQ [5], and CHEETAH [6] (a C version of TIGER) with an appropriate empirical equation of state such as Becker–Kistiakosky–Wilson (BKW-EOS) [7], the Jacobs–Cowperthwaite–Zwisler (JCZ-EOS) [8,9] and Kihara–Hikita–Tanaka (KHT-EOS) [10] can be used to determine detonation properties. Of different equations of states, the BKW-EOS in spite of its weak theoretical basis is used extensively to calculate detonation properties of high explosives. The BKWC-EOS [6], BKWR-EOS [11] and BKWS-EOS [12] are three different parameterizations of the BKW-EOS. The BKWS-EOS is one of the best equations of states for predicting detonation temperatures. The computation of detonation parameters by computer codes in spite of its complexity usually requires measured condensed heat of formation of the explosive. It should be noted that the accuracy of predictive methods are not necessarily enhanced by greater complexity.

The development of simple reliable methods is attractive to chemist for the expenditure connected with the development and synthesis of a new energetic material. Some new various empirical methods have been recently introduced for simple evaluation or desk calculation of performance parameters such as C–J detonation pressure, detonation velocity and heat of detonation of ideal and less ideal pure or mixture of different classes of explosives [13–19]. These methods can develop systematic and scientific formulations of appropriate futuristic target molecules having desired performance and the other properties. Detonation temperature can be calculated via molar heat capacities of detonation products if the quantities and the nature of the gaseous products as well as heat of detonation are known. A review of existing methods based on this procedure is given elsewhere [20]. The main focus, thereafter, will be on introducing the simplest method for calculating detonation temperature of high explosives without the use of any experimental data of the explosive and detonation products. In the recent work, a new procedure is used to introduce two new correlations for desk cal-

* Corresponding author. Tel.: +98 312 522 5071; fax: +98 312 522 5068.
E-mail addresses: mhkeshavarz@mut-es.ac.ir, mhkir@Yahoo.com (M.H. Keshavarz).

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culation of detonation temperature of aromatic and non-aromatic explosives. The purpose of this work is to correlate and to predict the detonation temperature of $C_aH_bN_cO_d$ explosives, which can be predicted directly from the values of a, b, c, d and gas phase heat of formation of the explosive. Later can be determined by additivity rules related to the molecular structure, e.g. the methods of Benson [21], Yoneda [22], Joback [23], etc., with little loss of accuracy. It is felt that the introduced correlations represent a significant advance in a priori computational method of detonation temperature. Another goal of this work is to provide insight to understanding the molecules, which are responsible for higher detonation temperature and which are not. The calculated detonation temperatures will also be tested with experimental data as well as computed results of BKWR-EOS and BKWS-EOS for well-known pure and mixture of explosives.

2. Procedure for determining of detonation temperature

The detonation pressure and temperature are not well-resolved measurements in contrast to detonation velocity [12]. The measurements of detonation temperature are usually done by the brightness of the detonation front interacting with a detector with absolute accuracies estimated to be ±100 K for liquid explosives and ±200 K for solid explosives. Since any voids or density discontinuities can lead to measurements of the brightness of the shocked air or shocked detonation products rather than the C–J detonation products, density discontinuities free system such as a liquid or a single crystal is to be useful for measurement of the detonation temperature. The C–J detonation temperature of nitromethane is better known than for any other explosives because it is transparent. Measured its C–J detonation temperature results lie between 3300 and 3500 K [24]. Experimental data for detonation temperatures are scarce because difficulty of measurement of detonation temperature. A blackbody of equivalence photographic brightness with the absolute accuracy of about 200 K is usually used for reporting detonation temperatures. Since it is not known whether the detonation products radiate like a blackbody, the relationship between these numbers and the actual detonation temperature is unknown.

Predicting of the detonation temperature of a new high explosive from a given molecular structure without using experimental measurement is very important to chemist because the calculated detonation temperature as well as the other detonation parameters of a notional explosive 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 detonation temperature can be obtained by assuming that heat of detonation of the explosive is entirely used to the products. Molar heat capacities of detonation products at or near detonation temperature as well as experimental condensed heat of formation of the explosive would be needed in this situation [25]. It can be assumed that the energy released is completely transferred to detonation products during a very short time because decomposition reaction of explosive in detonation is very fast. 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 temperature of an explosive as a function of its composition. It was recently shown that linear combination of elemental compositions of explosive and estimated gas phase heat of formation with some adjustable parameters can be used to derive two reliable correlations for obtaining heats of detonation of aromatic and non-aromatic explosives [18]. Crystal effects can also be excluded for determining the detonation temperature in this manner [13,14] because crystalline heat of formation can correlate with gas phase heat of formation for some classes of explosives [26]. Since so very approximately it can be stated that detonation temperature is proportional to heat of detonation [27], the results indicated that the following general equation is suitable for $C_aH_bN_cO_d$ explosive with six adjustable parameters A–F in it:

$$T_{\mathrm{d}}(\mathrm{K}^{-1}) = \mathrm{A} + \mathrm{B}a' + \mathrm{C}b' + \mathrm{D}c' + \mathrm{E}d' + \mathrm{F}\Delta\mathrm{H}_f^{\circ\prime}(\mathrm{g}) \quad (1)$$

where a', b', c', d' and $\Delta\mathrm{H}_f^{\circ}(\mathrm{g})$ are a, b, c, d and gas phase heat of formation of explosive divided by molecular weight of explosive respectively. Agreement with measurement has been secured in that the adjustable constants in introduced correlation consistent with experimental results. To obtain reliable correlations for determining of detonation temperature, experimental detonation temperatures were used to optimize the correlations. The measured values of TNT, TETRYL, HMX, NG, NM, PETN, RDX and TNM were used for obtaining adjustable parameters. The method of Kamlet and Hurwitz [28] can be used to find coefficients A–F in Eq. (1). The results show that two following correlations (2) and (3) can be obtained for aromatic and non-aromatic explosives, respectively:

$$T_{\mathrm{d}}/1000 = -75.8 + 950.8a' + 12.3b' + 1114.9c' + 1324.5d' + 1.2\Delta\mathrm{H}_f^{\circ\prime}(\mathrm{g}) \quad (2)$$

Table 1
Parameters used in calculations

Explosive[a]	a'	b'	c'	d	$\Delta\mathrm{H}_f^{\circ\prime}$(kcal/g)[b]
ABH	0.02746	0.00686	0.01602	0.02746	0.05481
DATB	0.02469	0.02058	0.02058	0.02469	0.05802
DIPM	0.02643	0.01322	0.01762	0.02643	0.04912
HNAB	0.02655	0.00885	0.01770	0.02655	0.05066
HNS	0.03111	0.01333	0.01333	0.02667	0.06600
NONA	0.02835	0.00787	0.01417	0.02835	0.09276
PA	0.02620	0.01310	0.01310	0.03057	−0.17031
TATB	0.02326	0.02326	0.02326	0.02326	0.07519
TETRYL	0.02439	0.01742	0.01742	0.02787	0.03233
TNT	0.03084	0.02203	0.01322	0.02643	−0.01894
HNB	0.01724	0.00000	0.01724	0.03448	0.10460
DEGN	0.02041	0.04082	0.01020	0.03571	−0.66327
HMX	0.01351	0.02703	0.02703	0.02703	0.15203
NG	0.01322	0.02203	0.01322	0.03965	−0.56828
NM	0.01639	0.04918	0.01639	0.03279	−0.29344
NQ	0.00962	0.03846	0.03846	0.01923	0.48462
PETN	0.01582	0.02532	0.01266	0.03797	−0.55063
RDX	0.01351	0.02703	0.02703	0.02703	0.17027
TNM	0.00510	0.00000	0.02041	0.04082	−0.14133

[a] See Appendix A for glossary of compound names.
[b] Gas phase heat of formation was calculated by Joback additive group procedure [23].

Table 2
Comparison of detonation temperature of the new correlations, BKWR-EOS and BKWS-EOS with measured values [12]

Explosive[a]	ρ_0 (g/cc)	T_{exp} (K)	$T_{BKWS\text{-}EOS}$ (K)	$T_{BKWR\text{-}EOS}$ (K)	T_d (K)	%Dev BKWS-EOS[b]	%Dev BKWR-EOS[b]	%Dev new[b]
ABH	1.64		4710	3960	4689			
DATB	1.80		3550	2860	3643			
	1.78		3690	2870	3643			
DIPM	1.76		4040	3310	4207			
HNAB	1.60		4620	3900	4509			
HNS	1.60		4150	3580	4209			
	1.70		4120	3500	4209			
NONA	1.70		4510	3780	4707			
PA	1.76		4010	3280	4161			
	1.71		4030	3330	4161			
	1.60		4080	3420	4161			
TATB	1.88		3250	2550	3418			
	1.85		3260	2580	3418			
TETRYL	1.73		4210	3460	3987			
	1.71		4220	3480	3987			
	1.68		4240	3520	3987			
	1.61	4200	4270	3590	3987	−1.67	14.52	5.07
	1.40	4130	4350	3750	3987	−5.33	9.20	3.46
	1.36		4360	3780	3987			
	1.20	4300	4380	3840	3987	−1.86	10.70	7.28
	1.00	4390	4340	3840	3987	1.14	12.53	9.18
TNT	1.64		3720	3210	3511			
	1.45		3780	3330	3511			
	1.36		3790	3380	3511			
	1.00	3400	3750	3410	3511	−10.29	−0.29	−3.26
	0.80		3610	3330	3511			
HNB	1.97		5640	4360	5613			
DEGN	1.38		3690	3240	4412			
HMX	1.89		4070	3090	4162			
	1.60	4300	4270	3470	4162	0.70	19.30	3.21
	1.40		4380	3680	4162			
	1.20		4450	3830	4162			
	1.00		4480	3900	4162			
	0.75		4440	4000	4162			
NG	1.60	4260	4550	3750	3656	−6.81	11.97	14.18
NM	1.13	3430	3580	3220	3371	−4.37	6.12	1.72
NQ	1.78		2740	2090	2882			
	1.72		2760	2130	2882			
	1.62		2790	2210	2882			
	1.55		2830	2260	2882			
PETN	1.76		4280	3330	4161			
	1.70		4320	3400	4161			
	1.60	4400	4390	3520	4161	0.23	20.0	5.43
	1.45		4490	3710	4161			
	1.23		4600	3940	4161			
	0.99		4640	4150	4161			
	0.88		4640	4240	4161			
	0.48		4560	4460	4161			
	0.30		4450	4470	4161			
	0.25		4400	4460	4161			
RDX	1.80		4140	3220	4184			
	1.77		4160	3260	4184			
	1.72		4200	3330	4184			
	1.66	4320	4230	3400	4184	2.08	21.30	3.15

Table 2 (*Continued*)

Explosive[a]	ρ_0 (g/cc)	T_{exp} (K)	$T_{BKWS\text{-}EOS}$ (K)	$T_{BKWR\text{-}EOS}$ (K)	T_d (K)	%Dev BKWS-EOS[b]	%Dev BKWR-EOS[b]	%Dev new[b]
	1.60		4280	3480	4184			
	1.46		4360	3630	4184			
	1.40	4610	4390	3690	4184	4.77	19.96	9.24
	1.29		4430	3780	4184			
	1.20	4610	4460	3840	4184	3.25	16.70	9.24
	1.10		4480	3890	4184			
	1.00	4600	4490	3920	4184	2.39	14.78	9.04
	0.95		4490	3920	4184			
	0.70		4450	4060	4184			
	0.56		4450	4180	4184			
TNM	1.64	2800	2860	2180	3178	−2.14	22.14	−13.50
COMP B-3	1.72		4000	3260	3918			
CYCLOTOL-78/22	1.76		4070	3240	4308			
CYCLOTOL-77/23	1.74		4070	3260	4032			
CYCLOTOL-75/25	1.76		4050	3240	4019			
CYCLOTOL-75/25	1.62		4130	3400	4019			
CYCLOTOL-70/30	1.73		4040	3270	3985			
CYCLOTOL-65/35	1.72		4030	3270	3952			
CYCLOTOL-60/40	1.74		3990	3240	3918			
CYCLOTOL-60/40	1.72		4000	3260	3918			
CYCLOTOL-50/50	1.63		4000	3340	3851			
OCTOL-78/22	1.82		4020	3160	3984			
OCTOL-76/23	1.81		4020	3170	3974			
OCTOL-75/25	1.81		4010	3170	3965			
OCTOL-60/40	1.80		3950	3160	3859			
PENTOLITE	01.64		4030	3360	3785			

[a] See Appendix A for glossary of compound names.
[b] $\%\text{Dev} = \frac{\text{measured}-\text{predicted}}{\text{measured}} \times 100$.

$$T_d/1000 = 149.0 - 1513.9a' - 196.5b' - 2066.1c' - 2346.2d' + 1.2\Delta H_f^{\circ\prime}(g) \quad (3)$$

These equations provide the simplest empirical procedure for estimation of detonation temperature of pure explosives, which require as input information only the elemental composition and heat of formation of the explosive in the gas phase as calculated from an additivity method such as Benson [21], Yoneda [22], Joback [23], etc. The calculated gas phase heats of formation of explosives by additivity rule and the other necessary data are shown in Table 1 for the oxygen lean as well as oxygen-rich pure explosives. As an example, TNT according to Joback method [23] has two =CH– and four $=C<$ ring increments as well as one $-CH_3$ and three $-NO_2$ increments, which gives $\Delta H_f^{\circ\prime}(g) = -4.3$ kcal/mol. Thus, as mentioned in Table 1, TNT with molecular formula $C_7H_5N_3O_6$ gives $a' = 0.03084$, $b' = 0.02203$, $c' = 0.01322$, $d' = 0.02643$ and $\Delta H_f^{\circ\prime}(g) = -0.01894$ kcal/g. If the Benson method [21] was used, the value −7.69 kcal/mol is obtained, which gives $T_d = 3497$ K. This confirms that the contribution of $\left|\Delta H_f^{\circ\prime}(g)\right|$ of the explosive is small relative to the elemental composition of the $C_aH_bN_cO_d$ explosive. Thus, as seen in Eqs. (2) and (3) rough estimate of gas phase heat of formation of explosive is sufficient for calculation of detonation temperature.

It is possible to use data on the pure explosives for estimating detonation temperature of their mixtures. Explosives can be used in mixed compositions so as to optimize their performance. To use Eqs. (3) and (4) for mixture of explosives, an equation is required which relate detonation temperature of mixed explosive to pure components. We can assume that the components contribute individually to detonation temperature of mixture [15]. We have found that the following equation is the simplest way to give acceptable results:

$$T_{d,mix} = \sum_j x_j T_{d,j} \quad (4)$$

where x_j is the mole fraction of the jth component in the mixture of explosives.

Calculated detonation temperatures for underoxidized and overoxidized pure as well as mixed explosives are given in Table 2 and compared with corresponding measured values and computed results by complicated BKWR-EOS and BKWS-EOS. As seen, the introduced simple hand calculated empirical correlations for determining detonation temperatures

show surprisingly very good agreement with experimental values, which may be taken as appropriate validation test of the new method with pure and mixed $C_aH_bN_cO_d$ explosives. It is worthwhile to note that by considering large percent deviations generally attributed to experimental measurements of detonation temperature, the agreement between calculated and measured values are also satisfactory. As seen from Table 2, the mean absolute error in detonation temperature for BKWS-EOS, BKWR-EOS and new method are 3.6, 13.8 and 7.0% respectively.

3. Conclusions

The expenditure connected with the development and synthesis of a new energetic material also necessitates the development of theoretical methods as well as various empirical methods complemented the computer output for desk calculations. The complicated computer codes and empirical procedures are convincing evidence of the utility of them for engineering calculations of detonation properties of explosives. There is some uncertainty for determination of radiation in measurement of detonation temperature because it is not known how much it is absorbed from detonation products by the shocked and partially decomposed explosive between the detector and the end of the reaction zone. The explosive with high oxygen content like tetranitromethane produces the products with lots of free oxygen. The observed temperature in this case is higher than one would be obtain for an ideal gas equation of state [2]. The simplest empirical correlations are introduced for desk calculations of detonation temperature of pure and mixed $C_aH_bN_cO_d$ explosives through gas phase heat of formation calculated by group additivity rule and atomic composition of either pure mixed explosive. There is no need to assume detonation products that is usually done by complicated computer codes. Given the chemical formula of a real or hypothetical pure or mixture of explosives, one can estimate detonation temperature that is consistent with large uncertainty of detonation temperature. Since the new method permits a simple calculation of detonation temperature of explosives without using any experimental data, it can be used to any new proposed explosives or any mixtures of explosives in order to obtain specified detonation temperature. 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 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 gas phase heat of formation and elemental composition of the explosive correlate quite well with the values of detonation temperatures. Though the measured condensed heat of formation is an important factor to consider in designing new energetic materials, there is no need to use it in the present method. However, the introduced correlations require no prior knowledge of any measured properties of explosive and assumed detonation products other than simply calculated gas phase heat of formation by additivity rule.

In brief, this study has led to some simple empirical correlations that can be used for calculations of detonation temperature. It is only based upon the atomic composition of either a pure or mixed explosives and simply calculated gas phase heat of formation by additivity rule, with the same reliability as one might attach to the more complex computer output.

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Appendix A. Glossary of compound names

ABH Azobis(2,2′,4,4′,6,6′-hexanitrobisphenyl) ($C_{24}H_6N_{14}O_{24}$)
COMP B-3 60/40 RDX/TNT ($C_{2.04}H_{2.50}N_{2.15}O_{2.68}$)
CYCLOTOL-78/22 78/22 RDX/TNT ($C_{1.73}H_{2.59}N_{2.40}O_{2.69}$)
CYCLOTOL-77/23 77/23 RDX/TNT ($C_{1.75}H_{2.59}N_{2.38}O_{2.69}$)
CYCLOTOL-75/25 75/25 RDX/TNT ($C_{1.78}H_{2.58}N_{2.36}O_{2.69}$)
CYCLOTOL-70/30 70/30 RDX/TNT ($C_{1.87}H_{2.56}N_{2.29}O_{2.68}$)
CYCLOTOL-65/35 65/35 RDX/TNT ($C_{1.96}H_{2.53}N_{2.22}O_{2.68}$)
CYCLOTOL-60/40 60/40 RDX/TNT ($C_{2.04}H_{2.50}N_{2.15}O_{2.68}$)
CYCLOTOL-50/50 50/50 RDX/TNT ($C_{2.22}H_{2.45}N_{2.01}O_{2.67}$)
DATB 1,3-Diamino-2,4,6-trinitrobenzene ($C_6H_5N_5O_6$)
DEGN Diethyleneglycol dinitrate ($C_4H_8N_2O_7$)
DIPM Dipiramide ($C_{12}H_6N_8O_{12}$)
HMX Cyclotetramethylenetetranitramine ($C_4H_8N_8O_8$)
HNAB 2,2′,4,4′,6,6′-Hexanitroazobenzene ($C_{12}H_4N_8O_{12}$)
HNB Hexanitrobenzene ($C_6N_6O_{12}$)
HNS 2,2′,4,4′,6,6′-Hexanitrostilbene ($C_{14}H_6N_6O_{12}$)
NG Nitroglycerine ($C_3H_5N_3O_9$)
NM Nitromethane (CH_3NO_2)
NONA 2,2′,2″,4,4′,4″,6,6′,6″-Nonanitroterphenyl ($C_{18}H_5N_9O_{18}$)
NQ Nitroguanidine ($CH_4N_4O_2$)
OCTOL-78/22 77.6/22.4 HMX/TNT ($C_{1.74}H_{2.59}N_{2.39}O_{2.69}$)
OCTOL-76/23 76.3/23.7 HMX/TNT ($C_{1.76}H_{2.58}N_{2.37}O_{2.69}$)
OCTOL-75/25 75/25 HMX/TNT ($C_{1.78}H_{2.58}N_{2.36}O_{2.69}$)
OCTOL-60/40 60/40 HMX/TNT ($C_{2.04}H_{2.50}N_{2.15}O_{2.68}$)
PA Picric acid ($C_6H_3N_3O_7$)
PENTOLITE 50/50 TNT/PETN ($C_{2.33}H_{2.37}N_{1.29}O_{3.22}$)
PETN Pentaerythritol tetranitrate ($C_5H_8N_4O_{12}$)
RDX Cyclomethylene trinitramine ($C_3H_6N_6O_6$)
TATB 1,3,5-Triamino-2,4,6-trinitrobenzene ($C_6H_6N_6O_6$)
TETRYL *N*-Methyl-*N*-nitro-2,4,6-trinitroaniline ($C_7H_5N_5O_8$)
TNM Tetranitromethane ($C_1N_4O_8$)
TNT 2,4,6-Trinitrotoluene ($C_7H_5N_3O_6$)

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