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An empirical method for predicting detonation pressure of CHNOFCl explosives

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Abstract

This paper describes a new method for prediction of the Chapman–Jouguet detonation pressures of CHNOFCl explosives using the heat of detonation, Q_{det}, the number of moles of gaseous products of detonation per gram of explosive, α, and the average molecular weight of gaseous products, M. The equation has the form: $P_{\mathrm{CJ}} = 15.88\alpha(MQ_{\mathrm{det}})^{1/2}\rho_0^2 - 11.17$, where P_{CJ} is the Chapman–Jouguet detonation pressure and ρ_0 the loading density. Calculated P_{CJ} by this procedure show good result with respect to measured detonation pressure for any pure or mixture of ideal and some of less ideal CHNOFCl explosives at $\rho_0 > 0.8\,\mathrm{g/cm^3}$.

Keywords: CHNOFCl explosives; Detonation pressure; Initial density; Heat of detonation

1. Introduction

Manufacture, development and testing of new explosive is so costly in time and money, thus theoretical simple methods can help to eliminate any poor candidate due to performance problem. The Chapman–Jouguet (C–J) detonation pressure, as well as the heat of detonation and detonation velocity, is a quantity used to assess a candidate's detonation performance. For condensed phase explosives, there is a continuing need for reliable prediction of the C–J detonation pressure through the means of Chapman–Jouguet thermodynamic detonation theory.

A sophisticated computational network, e.g. TIGER computer code [1], as well as an equation of state for detonation products are usually used for determination of time-independent state of chemical equilibrium which is defined with the Chapman–Jouguet hypothesis. Some of well-known equations of state, as representative examples, are the Becker–Kistiakosky–Wilson equation of state (BKW-EOS) [2], the Jacobs–Cowperthwaite–Zwisler equation of state (JCZ-EOS) [3,4], Kihara–Hikita–Tanaka equation of state (KHT-EOS) [5]. Among these examples the JCZ-EOS has the strongest theoretical basis so that the total pressure can be described by the sum of volume dependent term and a term which is function of both the volume and the temperature. Kamlet and Jaccobs [6], Kamlet and Ablard [7], Kamlet and Dickinson [8] and Kamlet and Hurwitz [9] in an effect to investigate the formidable appearance of the data of many computations for a wide variety of CHNO explosives, introduced a simple method for calculation of detonation properties. They assumed that the reaction products could be represented by N_2, H_2O and CO_2 (but not CO) as well as condensed carbon. Two correlations have also recently introduced for determination of the C–J detonation pressure of ideal pure CHNO explosives [10] on the basis of two parameters, namely the combustion temperature and the number of moles of gaseous products per molecular weight of explosive.

The purpose of this work is to show a new correlation for predicting the detonation pressure of ideal and some of less ideal CHNOFCl explosives. This work assumes a more reliable new decomposition reaction, which contains major detonation gaseous products, namely CO, H_2O, CO_2, N_2, H_2, O_2, HF and HCl as well as the solid carbon in the form of graphite for very oxygen lean explosive such as TNT. The calculated heats of detonation using the assumed product sets will be applied to some ideal CHNO explosives for showing the reliability of the predicted values against experiment as compared to Kamlet's method. We will also investigate the interrelationships between the detonation pres-

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sure of large classes of ideal and less ideal explosives over a wide range of loading densities using the predicted heats of detonation and the other fundamental detonation parameters such as density and the number of moles of gaseous products. The heats of detonation, based on the assumed decomposition reactions, are correlated with C–J detonation pressure at initial density of the explosive. The new procedure presented herein show that this method to predict C–J detonation pressure of CHNOFCl explosives is a very simple computational tool to be used for quick calculation and screening of notional energetic materials with about the same reliability as one might attach to the more complex computer output.

2. Decomposition products and the heat of detonation

Accurate determination of product decomposition species for energetic materials with complex elemental composition remains a major unresolved problem. The equilibrium composition of the products gases, which is necessary for evaluating the heat of formation of the detonation products, can be determined through experimental measurement, thermochemical equilibrium or by suggesting an appropriate detonation reaction. As a first step in our attempt to express the C–J detonation pressure as a function of basic parameters such as the heat of detonation, a more reliable decomposition reaction than Kamlet's method is used. Since for 34 CHNO explosives thermochemical calculations indicates that 94% of gaseous products consist of CO, H_2O, H_2, N_2 and CO_2 [11], we can select a procedure for decomposition so that these products are counted. A good approximation can be obtained on the assumption that all nitrogens go to N_2, fluorines to HF, chlorines to HCl while a portion of the oxygens form H_2O and carbons preferentially will be oxidized to CO rather than CO_2. The following pathways can be written to obtain detonation products:

$$
C_aH_bN_cO_dF_eCl_f
\begin{cases}
\xrightarrow{d \le a} eHF + fHCl + \frac{c}{2}N_2 + dCO + (a-d)C(s) + \left(\frac{b-e-f}{2}\right)H_2 & \text{(1a)} \\[2ex]
\xrightarrow[\frac{b-e-f}{2} \succ d-a]{d \succ a \text{ and}} eHF + fHCl + \frac{c}{2}N_2 + aCO + (d-a)H_2O + \left(\frac{b-e-f}{2} - d + a\right)H_2 & \text{(1b)} \\[2ex]
\xrightarrow[d \le 2a + \frac{b-e-f}{2}]{d \ge a + \frac{b-e-f}{2} \text{ and}} eHF + fHCl + \frac{c}{2}N_2 + \left(\frac{b-e-f}{2}\right)H_2O + \left(2a - d + \frac{b-e-f}{2}\right)CO + \left(d - a - \frac{b-e-f}{2}\right)CO_2 & \text{(1c)} \\[2ex]
\xrightarrow{d \succ 2a + \frac{b-e-f}{2}} eHF + fHCl + \frac{c}{2}N_2 + \left(\frac{b-e-f}{2}\right)H_2O + aCO_2 + \left(\frac{2d-b+e+f}{4} - a\right)O_2 & \text{(1d)}
\end{cases}
\qquad (1)
$$

The heat of detonation, defined as the negative of the enthalpy change of the detonation reaction, can be determined from the heats of formation of reactants and decomposition products of the explosive through the relation:

$$
Q_{\text{det}} \cong -\frac{[\Delta H_f(\text{detonation products}) - \Delta H_f(\text{explosive})]}{\text{formula weight of explosive}} \qquad (2)
$$

where Q_{det} is the heat of detonation.

A positive heat of formation (per unit weight) is favorable for an explosive, since this leads to a greater release of energy upon detonation. If the heat of formation of CHNOFCl explosive is known, then using the standard heats of formation of assumed detonation products will lead to the prediction of the heat of detonation of an explosive. To determine solid-state heat of formation, as well as the experimental method obtained by bomb calorimeter [12], a general scheme aimed for organic solids has been forward and applied to energetic compounds [13,14]. The heat of formation of some CHNO explosives can also be obtained by semiempirical PM3 procedure [15] from calculated heat of formation in its gas phase [16]. The heat of detonation indicates the energy available to do mechanical work and has been used to estimate potential damage of the surroundings [11]. The heat of detonation can be evaluated by the GIPF methodology using quantum mechanical information about a single explosive molecule [11,14].

To show the reliability of the new decomposition procedure, heats of detonation for some well-known ideal CHNO explosives using the new detonation product sets and using Kamlet and Jaccobs [6], Kamlet and Ablard [7], Kamlet and Dickinson [8] and Kamlet and Hurwitz [9] prescription are given in Table 1. As seen, predicted heats of detonation for $H_2O_{(g)}$ using the new decomposition procedure and Kamlet's method have rms deviations from experiment of 0.954 and 1.006 kJ/g, respectively, whereas for $H_2O_{(l)}$ Kamlet's method shows larger deviation from experiment (1.364 kJ/g) as compared to the new method (1.049 kJ/g).

Table 1
Predicted and experimental heats of detonation for ideal CHNO explosives

Explosive[a]	$Q_{det}[H_2O_{(g)}]$ (kJ/g)[b]			$Q_{det}[H_2O_{(l)}]$ (kJ/g)[b]		
	Experimental[c]	Predicted[d]	Kamlet[d]	Experimental[c]	Predicted[d]	Kamlet[d]
HMX	5.732 [12]	5.017 (0.715)	6.180 (−0.448)	6.192 [19]	5.611 (0.581)	6.774 (−0.582)
RDX	5.941 [12]	5.038 (0.903)	6.201 (−0.260)	6.318 [19]	5.636 (0.682)	6.799 (−0.481)
TNT	4.268 [12]	2.644 (1.624)	5.418 (−1.150)	4.561 [19]	2.644 (1.917)	5.904 (−1.343)
PETN	5.732 [12]	5.791 (−0.059)	6.335 (−0.603)	6.318 [19]	6.351 (−0.033)	6.891 (−0.573)
TETRYL	4.561 [12]	3.607 (0.954)	5.941 (−1.380)	4.770 [19]	3.761 (1.009)	6.326 (−1.556)
DATB	3.807 [12]	2.322 (1.485)	4.912 (−1.105)	4.100 [12]	2.322 (1.778)	5.368 (−1.268)
NQ	2.732 [19]	2.498 (0.234)	3.761 (−1.029)	3.071 [19]	2.920 (0.151)	4.607 (−1.536)
TATB	–	1.975	4.502	3.063 [19]	1.975 (1.088)	5.012 (−1.949)
NM	4.301 [12]	3.925 (0.377)	5.703 (−1.402)	4.820 [19]	4.644 (0.176)	6.786 (−1.966)
rms deviation (kJ/g)		0.954	1.006		1.049	1.364

[a] See Appendix A for glossary of compound names and chemical formulas.
[b] Heat of formation for pure CHNO and FEFO explosives were obtained from [12] and the other values from [18].
[c] References are given in brackets.
[d] Difference of the new and Kamlet predictions from experiment are given in parentheses.

The results indicate that the inclusion of the other gaseous products, even for ideal CHNO explosives as compared to Kamlet's method, are important.

3. The new C–J detonation pressure correlation

Experiments show that the C–J detonation pressure is roughly proportional to the loading density squared [17]. One of the most important properties of an explosive is the solid-state density, which determines the performance of the explosive. To express the C–J detonation pressure as a function of the basic parameters, namely the heat of detonation as well as the number moles of gaseous products and loading density, plotting of the experimental C–J detonation pressure versus various combinations of mentioned parameters are studied. The decomposition reactions and some other parameters are given in Table 2. As shown

Table 2
Parameters used in calculations

Explosive[a]	Reaction products	M	Q_{det}[b] (J/g)	Q_{det}[b,c] (cal/g)	α
HMX	$4CO + 4N_2 + 4H_2O$	24.67	5017	1199	0.0405
RDX	$3CO + 3N_2 + 3H_2O$	24.67	5038	1204	0.0405
TNT	$C_{(s)} + 6CO + 1.5N_2 + 2.5H_2$	21.50	2644	632	0.0441
PETN	$3CO_2 + 2CO + 2N_2 + 4H_2O$	28.73	5791	1384	0.0348
TETRYL	$7CO + 2.5N_2 + 1.5H_2 + H_2O$	23.92	3607	862	0.0418
DATB	$6CO + 2.5N_2 + 2.5H_2$	22.09	2322	555	0.0453
NG	$3CO_2 + 1.5N_2 + 2.5H_2O + 0.25O_2$	31.31	6230	1489	0.0319
TNM	$CO_2 + 2N_2 + 3O_2$	32.67	2284	546	0.0306
NQ	$CO + H_2O + 2N_2 + H_2$	20.80	2498	597	0.0481
TATB	$6CO + 3N_2 + 3H_2$	21.50	1975	472	0.0465
NM	$CO + 0.5N_2 + 0.5H_2 + H_2O$	20.33	3925	938	0.0492
FEFO	$2CO + 2N_2 + 2H_2O + 3CO_2 + 2HF$	29.09	5263	1258	0.0344
TFNA	$5CO + 2N_2 + H_2O + H_2 + 3HF$	23.00	3096	740	0.0435
TFENA	$2CO + N_2 + 3HF$	24.00	2448	585	0.0417
Composition B	$6.851CO + 3.825N_2 + 2.449H_2O + 1.926H_2$	23.05	3950	944	0.0434
Cyclotol	$5.045CO + 3.438N_2 + 2.708H_2O + 1.0225H_2$	23.61	4343	1038	0.0424
Octol	$6.835CO + 4.6075N_2 + 3.595H_2O + 1.417H_2$	23.58	4305	1029	0.0424
50/50 NM/CCl_4	$1.375CO + 0.46N_2 + 0.355H_2O + 0.055CO_2 + 2.05HCl$	31.44	2222	531	0.0318
65/35 RDX/TFNA	$3.7CO + 2.65N_2 + 2.3H_2O + 0.35H_2 + 1.05HF$	23.97	4259	1018	0.0417
PBX-9010	$0.342CO + 3N_2 + 2.5763H_2O + 0.6354HF + 0.212HCl$	25.05	4548	1087	0.0399
90.54/9.46 HMX/Exon	$4.63CO + 4N_2 + 3.37H_2O + 0.4732H_2 + 0.4696HF + 0.313HCl$	24.45	4569	1092	0.0409
PBX-9502	$0.27C(s) + 6CO + 2.798H_2 + 3N_2 + 0.3662HF + 0.123HCl$	21.93	1958	468	0.0451
90.1/9.9 RDX/Exon	$3.544CO + 2.456H_2O + 0.408H_2 + 3N_2 + 0.408HF + 0.272HCl$	24.42	4422	1057	0.0410

[a] See Appendix A for glossary of compound names and chemical formulas.
[b] Heat of formation for pure CHNO and FEFO explosives were obtained from [12] and the other values from [18].
[c] To use Eq. (3) for obtaining P_{CJ} in kbar, the unit of Q_{det} is cal/g.

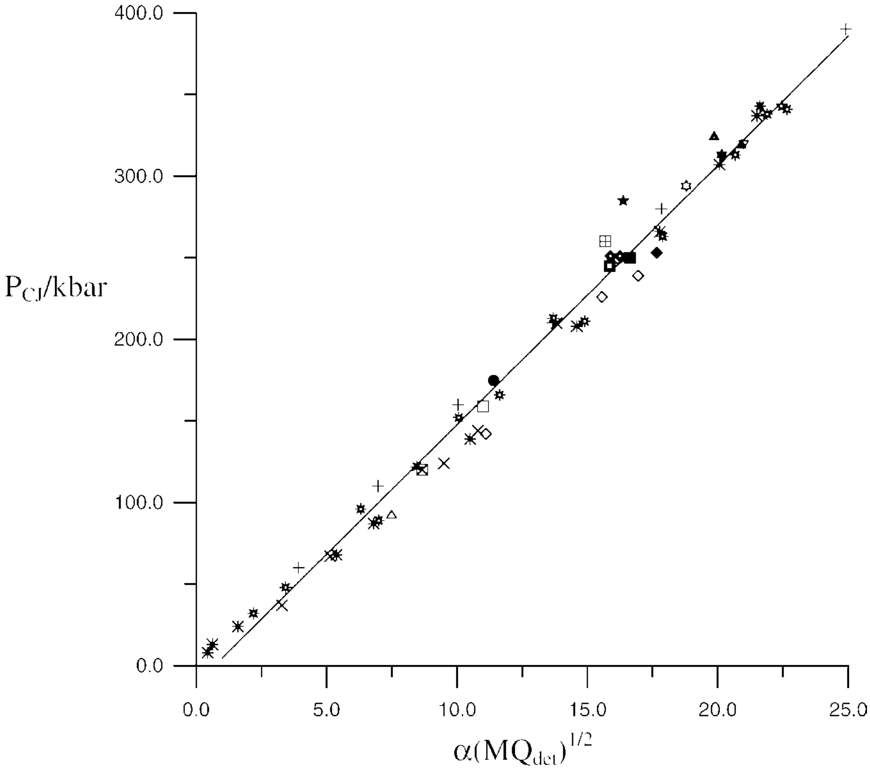

Fig. 1. The experimental C–J detonation pressure vs. $\alpha(MQ_{det})^{1/2}\rho_0^2$. The points are: (◆) NG; (◇) TETRYL; (×) TNT; (◈) DATB; (*) PETN; (✲) RDX; (☒) NM; (+) HMX; (⊞) TATB; (◘) NQ; (☐) TNM; (■) FEFO; (○) TFNA; (●) TFENA; (✡) Composition B; (✱) Cyclotol; (✳) Octol; (▲) PBX-9010; (★) PBX-9502; (△) NM/CCl_4; (▲) RDX/TFNA; (▽) RDX/Exon; (☆) HMX/Exon.

in Fig. 1, the measured C–J detonation pressure versus $\alpha(MQ_{det})^{1/2}\rho_0^2$ shows linear correlation of the form:

$$P_{CJ} = 15.88\alpha(MQ_{det})^{1/2}\rho_0^2 - 11.17 \tag{3}$$

where P_{CJ} is the C–J detonation pressure (kbar), α the number of moles of gaseous products of detonation per gram of explosive, M the average molecular weight of gaseous products and ρ_0 loading density. The necessary parameters are given in Table 2, as seen, it contains a number of plastic bonded compositions, PBXs, that are less ideal compositions. The PBX-explosives formed from energetic solids and binder ingredient, which are representative of today's state-of-the-art military explosives. In this plot, the explosives are reasonable close to the least square lines and exhibit R^2-correlation coefficient of 0.988. Eq. (3) follows experimental observation that the measured detonation pressure is proportional to ρ_0^2. The explosives in Table 2 cover a wide range in oxygen balance and are considered to be representative of the entire class of CHNOFCl explosives. It is often to use data on the pure constituents to estimate the C–J detonation pressure of a mixture. To calculate the heat of detonation for an explosive formulation, the heat of formation of the mixture can be calculated from their percentage concentrations in the mixture.

4. Conclusions

One of the fundamental goals in the filed of the energetic materials is to develop methods for predicting the performance of new energetic materials before synthesis. However, the main intent in this work was to investigate the likelihood of a generalized simple method for CHNOFCl explosives of somewhat more practical importance to the explosive user. A convenient estimate of reliable decomposition of the explosive is obtained if it is assumed that the explosive reacts to form products composed of HF, HCl, CO, N_2, H_2O, H_2 and CO_2 as determined by the oxygen balance of the unreacted explosive. We assumed that α, M and Q_{det} are constants for each CHNOFCl explosives, the same as in the Kamlet's method. Since high percentage errors generally attributed to experimental measurements of the C–J detonation pressure, up to ±20% [18], comparison of calculated results with experimental data listed in Table 3 may be taken as appropriate validation tests of the new method for use in CHNOFCl explosives. As seen in Table 3, good agreement is obtained between measured and calculated values of the detonation pressure over the wide range of initial density of explosive defined by experiment, namely $>0.8\ g/cm^3$. Of the explosives considered here, nitroglycerine is an example of overoxidized explosive.

In brief, calculation of the C–J detonation pressure by this procedure show good result with respect to measured

Table 3
Comparison between the calculated C–J detonation pressure of Eq. (3), using the predicted heats of detonation of Eq. (2) with the assumed product sets of Eq. (1), and the measured values for different explosives

Explosive	ρ_0 (g/cm^3)	P_{CJ} (kbar)		Deviation (%)
		Experimental[a]	Calculated	
HMX	1	110	99.53	9.52
	1.2	160	148.24	7.35
	1.4	210	205.80	2.00
	1.6	280	272.22	2.78
	1.89	390	384.26	1.47
RDX	0.95	96	88.97	7.32
	1	89	99.79	−12.13
	1.1	122	123.09	−0.90
	1.2	152	148.62	2.23
	1.29	166	173.48	−4.51
	1.4	213	206.32	3.14
	1.46	211	225.36	−6.80
	1.6	263	272.89	−3.76
	1.72	313	317.10	−1.31
	1.77	338	336.46	0.45
	1.8	341	348.35	−2.15
TNT	0.8	37	41.03	−10.89
	1	67	70.39	−5.06
	1.36	124	139.69	−12.65
	1.45	144	160.31	−11.33
	1.64	210	208.20	0.86
PETN	0.88	68	74.20	−9.12
	0.99	87	96.88	−11.35
	1.23	139	155.61	−11.95
	1.45	208	220.61	−6.06
	1.6	266	271.05	−1.90
	1.7	307	307.43	−0.14
	1.76	337	330.31	1.98
Tetryl	1.36	142	165.17	−16.32
	1.61	226	235.96	−4.41
	1.68	239	257.91	−7.91
DATB	1.78	251	241.07	3.96
	1.8	251	246.77	1.68
NG	1.6	253	269.20	−6.40
TNM	1.64	159	163.47	−2.81
NQ	1.72	245	240.58	1.80
TATB	1.83	260	237.90	8.50
NM	1.13	120	126.52	−5.43
FEFO	1.59	250	252.87	−1.15
TFNA	1.692	249	246.78	0.89
TFENA	1.523	174	170.76	1.86
50/50 NM/CCL$_4$	1.35	92	107.79	−17.16
65/35 RDX/TFNA	1.754	324	307.07	5.23
PBX-9010	1.781	319	320.62	−0.51
90.54/9.46 HMX/Exon	1.833	343	345.38	−0.69
PBX-9502	1.894	285	248.83	12.69
90.1/9.1 RDX/Exon	1.786	320	322.16	−0.68
Composition B	1.713	294	287.12	2.34
Cyclotol	1.743	313	308.79	1.35
Octol	1.809	343	332.04	3.19

[a] Measured P_{CJ} for pure CHNO explosives were taken from [20], of FEFO from [12] and the other values from [18].

detonation pressure for any CHNOFCl ideal or less some ideal explosives at $\rho_0 > 0.8\,\text{g/cm}^3$. One of the application of this work is that it is possible on the basis of the heat of formation to estimate quite well the performance of many explosives by a simple method.

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Appendix A. Glossary of compound names and molecular formulas

1. DATB: $C_6H_5N_5O_6$; 1,3-diamino-2,4,6-trinitrobenzene
2. TATB: $C_6H_6N_6O_6$; 1,3,5-triamino-2,4,6-trinitrobenzene
3. TETRYL: $C_7H_5N_5O_8$; *N*-methyl-*N*-nitro-2,4,6-trinitroaniline
4. TNT: $C_7H_5N_3O_6$; 2,4,6-trinitrotoluene
5. NG: $C_3H_5N_3O_9$; nitroglycerine
6. NM: CH_3NO_2; nitromethane
7. PETN: $C_5H_8N_4O_{12}$; pentaerythritol tetranitrate
8. RDX: $C_3H_6N_6O_6$; cyclotrimethylene trinitramine
9. HMX: $C_4H_8N_8O_8$; cyclotetra methylenetetranitramine
10. NQ: $CH_4N_4O_2$; nitroguanidine
11. TNM: CN_4O_8; tetranitromethane
12. FEFO: $C_5H_6N_4O_{10}F_2$; 1,1′-[methylene-bis(oxy)]bis-[2-fluoro-2,2-dinitroethane]
13. TFNA: $C_5H_7N_4O_6F_3$; 1,1,1-trifluoro-3,5,5-trinitro-3-azahexane
14. TFENA: $C_2H_3N_2O_2F_3$; 2,2,2-trifluoro-ethylnitramine
15. Octol: $C_{6.835}H_{10.025}N_{9.215}O_{10.43}$; 76.3/23.7 HMX/TNT
16. Cyclotol: $C_{5.045}H_{7.461}N_{6.876}O_{7.753}$; 77/23 RDX/TNT
17. Composition B: $C_{6.851}H_{8.750}N_{7.650}O_{9.3}$; 64/36 RD/TNT
18. PBX-9010: $C_{3.42}H_6N_6O_6F_{0.6354}Cl_{0.212}$; 90/10 RDX/Kel-F
19. PBX-9502: $C_{6.27}H_{6.085}N_6O_6F_{0.3662}Cl_{0.123}$; 95/5 TATB/Kel-F
20. 50/50 NM/CCl$_4$: $C_{1.43}H_{2.76}N_{0.92}O_{1.84}Cl_{2.05}$
21. 65/35 RDX/TFNA: $C_{3.7}H_{6.35}N_{5.3}O_6F_{1.05}$
22. 90.1/9.9 RDX/Exon: $C_{3.544}H_{6.408}N_6O_6F_{0.408}Cl_{0.272}$
23. 90.54/9.46 HMX/Exon: $C_{4.63}H_{8.469}N_8O_8F_{0.4696}Cl_{0.313}$

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