Some Perspectives on Estimating Detonation Properties of C, H, N, O Compounds

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Abstract: We have explored various aspects of the Kamlet-Jacobs equations for estimating detonation velocities and pressures. While the loading density of the explosive compound is certainly an important determinant of these properties, its effect can sometimes be overridden by other factors, such as the detonation heat release and/or the number of moles of gaseous products. Using a gas phase rather than solid phase enthalpy of formation in obtaining a compound's heat release can produce a significant error in the calculated detonation velocity. However a negative enthalpy of formation is not necessarily incompatible with excellent detonation properties. Additional evidence is presented to support Kamlet and Jacobs' conclusion that, for C, H, N, O explosives, assuming the detonation product composition to be $N_2(g)/H_2O(g)/CO_2(g)/C(s)$ gives overall quite satisfactory results.

Keywords: detonation velocity, detonation pressure, density, enthalpy of formation, detonation product composition, explosives

Detonation Properties

Two key measures of explosive performance are the detonation velocity D and the detonation pressure P. These refer, respectively, to the stable velocity of the shock front that characterizes detonation and the stable pressure that is developed behind the front [1-3]. In general, it is desired that D and P be as high as is compatible with avoiding excessive sensitivity of the compound to unintended stimuli (impact, shock, friction, etc.) [4-6].

Over a period of years, a number of computer codes – e.g. RUBY, TIGER, BKW, CHEETAH, EXPLO5 – have been developed for evaluating detonation velocities and pressures [7-10]. This requires predicting the composition of the

detonation products, which involves the use of an appropriate equation of state.

Some time ago, Kamlet and Jacobs identified four primary determinants of D and P [7]: the number of moles N of gaseous detonation products per gram of the explosive compound, their average molecular mass M_{ave} in g/mol, the heat release $Q = -\Delta H$ for the detonation reaction in cal/g of compound, and the loading density ρ of the compound, in g/cm³. They proposed the empirical relationships,

$$D \text{ (mm/μs)} = 1.01[N^{0.5}M_{ave}^{0.25} Q^{0.25} (1 + 1.30\rho)] \qquad (1)$$
$$P \text{ (kbar)} = 15.58[NM_{ave}^{0.5}Q^{0.5}\rho^2] \qquad (2)$$

and showed that eqs. (1) and (2) reproduce quite well the D and P values given by the RUBY code when N, M_{ave} and Q are taken from the RUBY output [7]. (Note that the loading density is often less than the crystal density of the pure compound [3, 7].)

Eqs. (1) and (2) clearly indicate the importance of the density as a determinant of D and P; it appears to a higher power in each equation than do any of the other quantities. However one or more of the other factors do sometimes override the effects of the density. Consider, for instance, TATB (1,3,5-triamino-2,4,6-trinitrobenzene, **1**) and RDX (1,3,5-trinitro-1,3,5-triazacyclohexane, **2**). At a loading density of 1.895 g/cm³, TATB has D = 7.860 mm/μs, P = 315 kbar, while RDX, at a significantly lower density of 1.80 g/cm³, has D = 8.754 mm/μs, P = 347 kbar [8]. Other examples will be given later.
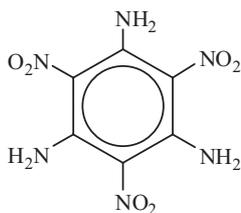
TATB, **1**
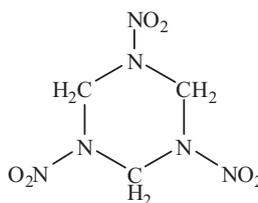
RDX, **2**
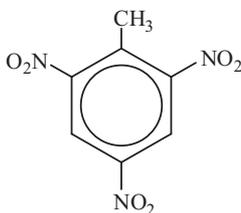
TNT, **3**
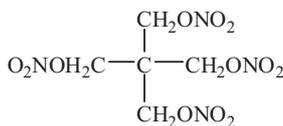
PETN, **4**

Eqs. (1) and (2) are widely used in assessing various proposed compounds as potential explosives [11-16]. For such applications, it is necessary to predict in some manner the product composition. N and M_{ave} then follow immediately, as does Q provided that the enthalpies of formation of the products and of the compound itself are available or can be evaluated. The crystal density of the compound, if not known, must be estimated. In evaluating new compounds, the crystal density – whether known or estimated – is generally used to predict D and P, even though it may be more than the loading density would be.

Our objective in this paper is to address certain aspects of assigning the values of N, M_{ave} and Q. We will also look at the relative roles of these quantities and the density ρ in determining the magnitudes of D and P. (For other discussions related to the calculation of detonation properties, see Sikder *et al.* [17] and Klapötke [18].)

Product Composition

The composition of the products of a detonation process is a key issue. Even if the explosive compound is composed only of the atoms C, H, N and O (as is very often the case), the products can conceivably include the gases CO_2, CO, N_2, H_2O, H_2, O_2, NH_3, CH_4 and NO, as well as solid carbon [8]. Furthermore, the product composition may vary considerably depending upon the loading density of the explosive compound, as is shown in Table 1.

Table 1.   Dependence of BKW-computed detonation product compositions upon loading density ρ (g/cm³).[a] All products are gaseous except for carbon

Compound	ρ	Moles of product per mole of compound									
		N_2	H_2O	CO_2	CO	H_2	O_2	NH_3	CH_4	NO	C(s)
RDX, **2**, $C_3H_6N_6O_6$	1.80	3.00	3.00	1.49	0.022	---	---	---	---	---	1.49
	1.0	2.98	2.80	0.67	1.855	0.111	---	0.029	0.021	---	0.45
PETN, **4**, $C_5H_8N_4O_{12}$	1.77	2.00	4.00	3.89	0.223	---	---	---	---	---	0.89
	0.50	1.93	3.73	2.81	2.188	0.167	0.072	0.001	---	0.134	0.0
TNT, **3**, $C_7H_5N_3O_6$	1.64	1.50	2.50	1.66	0.188	---	---	0.001	---	---	5.15
	0.732	1.49	1.76	0.69	2.865	0.707	---	0.020	---	---	3.45

a   Data are from reference 8.

One route to arriving at a reasonable product composition is by means of an appropriate equation of state, such as the Becker-Kistiakowsky-Wilson [7, 8].

Another approach, much easier to implement, comes from an observation by Kamlet and Jacobs [7], based upon output from the RUBY code. They noted that the predicted detonation product compositions of C, H, N, O explosives follow a definite pattern. We will further substantiate their findings, using more recent and more extensive data and we will compare the resulting D and P to experimental values.

In Table 2 are the detonation product compositions of a series of C, H, N, O explosives, as produced by the BKW code [8]. These correspond to relatively high loading densities, usually (but not always) similar to the crystal densities of the compounds. The striking feature of Table 2 is the consistency of the product compositions. For each compound, regardless of its chemical type, all or nearly all of the nitrogen goes to form N_2, the hydrogen to H_2O and the remaining oxygen to CO_2. Oxygens go to H_2O before CO_2. Unused carbon is present as the solid. To a good approximation, therefore, the product compositions are $N_2(g)/H_2O(g)/CO_2(g)/$ C(s). This is not the case, however, for lower loading densities, as can be seen in Table 1. In particular, the amount of CO increases markedly and CO_2 decreases.

Table 2. BKW-computed detonation product compositions at high loading densities ρ (g/cm^3).[a] All products are gaseous except for carbon

Compound [b]	ρ	Moles of product per mole of compound									
		N_2	H_2O	CO_2	CO	H_2	O_2	NH_3	CH_4	NO	C(s)
HMX, $C_4H_8N_8O_8$	1.90	4.00	4.00	2.00	0.008	---	---	---	---	---	2.0
RDX, **2**, $C_3H_6N_6O_6$	1.80	3.00	3.00	1.49	0.022	---	---	---	---	---	1.49
PETN, **4**, $C_5H_8N_4O_{12}$	1.77	2.00	4.00	3.89	0.223	---	---	---	---	---	0.89
Nitroguanidine, $CH_4N_4O_2$	1.629	2.0	2.00	---	---	---	---	---	---	---	1.0
TATB, **1**, $C_6H_6N_6O_6$	1.895	3.00	3.00	1.50	0.006	---	---	---	---	---	4.5
Tetryl, $C_7H_5N_5O_8$	1.70	2.50	2.50	2.66	0.173	---	---	---	---	---	4.16
DATB, $C_6H_5N_5O_6$	1.788	2.50	2.50	1.73	0.055	---	---	---	---	---	4.22
TNT, **3**, $C_7H_5N_3O_6$	1.64	1.50	2.50	1.66	0.188	---	---	0.001	---	---	5.15

a Data are from reference 8.
b Compound names: HMX, 1,3,5,7-tetranitro-1,3,5,7-tetraazacyclooctane; Tetryl, 2,4,6-trinitrophenylme-thylnitramine; DATB, 1,3-diamino-2,4,6-trinitrobenzene.

Table 3.   Comparison of experimental and calculated detonation velocities and pressures at given loading densities. The calculated values are based upon a $N_2(g)/H_2O(g)/CO_2(g)/C(s)$ product composition. Units: D, mm/µs; P, kbar; N, moles/g; M_{ave}, g/mol; Q, cal/g

Compound[a]	D(exp)[b]	P(exp)[b]	ρ(exp)[b]	N	M_{ave}	Q[c]	D(calc)	P(calc)
ε-CL-20, $C_6H_6N_{12}O_{12}$	9.380[d]	---	2.04[d]	0.03081	31.12	1567	9.62	441
HMX, $C_4H_8N_8O_8$	9.100	393	1.90	0.03376	27.22	1498	9.15	383
FOX-7, $C_2H_4N_4O_4$	8.869[e]	---	1.89[e]	0.03377	27.21	1200	8.63	340
RDX, **2**, $C_3H_6N_6O_6$	8.754	347	1.80	0.03377	27.21	1501	8.81	345
PETN, **4**, $C_5H_8N_4O_{12}$	8.300	335	1.77	0.03164	30.41	1514	8.69	331
Nitroguanidine, $CH_4N_4O_2$	7.980	---	1.629	0.03842	23.02	912	7.43	230
TATB, **1**, $C_6H_6N_6O_6$	7.860	315	1.895	0.02906	27.21	1149	7.93	287
Tetryl, $C_7H_5N_5O_8$	7.560	---	1.70	0.02699	30.46	1438	7.71	254
DATB, $C_6H_5N_5O_6$	7.520	259	1.788	0.02777	28.45	1175	7.57	253
Picric acid, $C_6H_3N_3O_7$	7.350[e]	---	1.7[e]	0.02510	33.05	1280	7.37	232
Picramide, $C_6H_4N_4O_6$	7.300[e]	---	1.72[e]	0.02630	30.01	1243	7.37	234
TNB, $C_6H_3N_3O_6$	7.300[e]	---	1.71[e]	0.02464	32.01	1358	7.38	234
HNS, $C_{14}H_6N_6O_{12}$	7.130	---	1.74	0.02333	32.00	1362	7.27	230
TNT, **3**, $C_7H_5N_3O_6$	6.950	190	1.64	0.02532	28.53	1295	6.98	204

a   Compound names: CL-20, hexanitrohexaazaisowurtzitane; HMX, 1,3,5,7-tetranitro-1,3,5,7-tetraa-zacyclooctane; FOX-7, 1,1-diamino-2,2-dinitroethene; Tetryl, 2,4,6-trinitrophenylmethylnitramine; DATB, 1,3-diamino-2,4,6-trinitrobenzene; picric acid, 2,4,6-trinitrophenol; picramide, 2,4,6-trinitroanili-ne; TNB, 1,3,5-trinitrobenzene; HNS, hexanitrostilbene.
b   Experimental D, P and ρ are from reference 8 unless otherwise indicated.
c   Experimental solid phase ΔH_f are from reference 23 except for picramide, which is from reference 3. Experimental gas phase ΔH_f of products are from reference 19.
d   Reference 17.
e   Reference 3.

Kamlet and Jacobs demonstrated that when the $N_2/H_2O/CO_2/C(s)$ product composition is assumed and the resulting N, M_{ave} and Q are inserted into eq.

(2), the detonation pressures obtained are in close agreement with those coming from the RUBY code [7]. This suggests that the $N_2/H_2O/CO_2/C(s)$ assumption is a satisfactory way of dealing with the problem of the product composition.

We have now tested this approach and eqs. (1) and (2) against experimental detonation velocities and pressures. N, M_{ave} and Q were calculated on the basis of the assumed $N_2/H_2O/CO_2/C(s)$ product composition. Experimental enthalpies of formation were utilized in determining Q. Introducing these N, M_{ave} and Q, plus the respective loading densities, into eqs. (1) and (2) yields the D and P in Table 3. They are overall in quite good agreement with the available experimental data. The average absolute errors in D and P are 0.15 mm/μs (1.9%) and 11 kbar (3.8%), respectively. Since the enthalpies of formation of the products are known accurately [19], Tables 2 and 3 reinforce Kamlet and Jacobs' conclusion that, with eqs. (1) and (2) and the $N_2/H_2O/CO_2/C(s)$ assumption, only the density and the enthalpy of formation of a given C, H, N, O compound are needed to obtain a reasonable estimate of its detonation velocity and pressure.

Enthalpies of Formation of C, H, N, O Compounds

If the enthalpy of formation of a proposed explosive is not known experimentally, a number of different procedures are available for obtaining it computationally at an acceptable level of accuracy. For discussions of some of these, see Rice *et al.* [20] and Politzer *et al.* [21].

However these methods usually give gas phase values, whereas what is needed in the context of detonation is typically the solid state enthalpy of formation; this requires subtracting the enthalpy of sublimation:

$$\Delta H_f(\text{solid}) = \Delta H_f(\text{gas}) - \Delta H_{sub} \tag{3}$$

Enthalpies of sublimation can be estimated from the features of the electrostatic potentials on the molecular surfaces of the compounds [20-23]. These features can be computed using, for example, the Wave Function Analysis-Surface Analysis Suite [24]. Nevertheless, many studies have used the gas phase enthalpy of formation of a compound to obtain Q and then D and P via eqs. (1) and (2). Since ΔH_{sub} is always positive, neglecting it will lead to Q, D and P being overestimated.

How serious is the resulting error? Table 4 shows the effects of using gas phase rather than solid phase enthalpies of formation for five of the compounds in Table 3. $N_2/H_2O/CO_2/C(s)$ product compositions are again assumed, and the

densities are the same as in Table 3. The average differences are 0.15 mm/μs for D and 10 kbar for P, with the values based upon $\Delta H_f(gas)$ always being larger. What is most significant, however, is that the root-mean-square errors relative to the experimental D and P are greater, especially for D: 0.29 mm/μs and 14 kbar. This follows from the fact that D is already overestimated in Table 3 for most of the compounds. It is evidently important to use solid state enthalpies of formation in predicting the detonation velocities of C, H, N, O compounds.

Table 4. Comparison of experimental detonation velocities and pressures with those calculated using gas phase and solid phase enthalpies of formation for the explosive compounds. The $N_2(g)/H_2O(g)/CO_2(g)/C(s)$ product composition was assumed. Values of ρ, N and M_{ave} are as in Table 3. Units: D, mm/μs; P, kbar; ΔH_f, kcal/mol; Q, cal/g

Compound[a]	Experimental[b]		Solid phase ΔH_f				Gas phase ΔH_f			
	D	P	$\Delta H_f{}^c$	Q^d	D	P	$\Delta H_f{}^c$	Q^d	D	P
RDX, **2**	8.754	347	18.9	1501	8.81	345	45.8	1622	8.99	358
PETN, **4**	8.300	335	-128.7	1514	8.69	331	-92.4	1629	8.85	344
TNB	7.300	---	-8.9	1358	7.38	234	14.9	1470	7.53	244
HNS	7.130	---	16.2	1362	7.27	230	56.98	1452	7.39	237
TNT, **3**	6.950	190	-15.1	1295	6.98	204	5.75	1386	7.10	211

a   For names of TNB and HNS, see Table 3.
b   Experimental D and P are from reference 8 except for TNB (reference 3).
c   Experimental solid and gas phase ΔH_f are from reference 23.
d   Experimental gas phase ΔH_f are from reference 19.

Relative Roles of ρ, N, M_{ave} and Q in Determining Detonation Velocities and Pressures

In designing potential explosive compounds, a major objective is to achieve as high a crystal density as possible. The importance of the density in determining detonation velocity and pressure can be seen from its presence in eqs. (1) and (2) to a higher power than any of the other quantities. Nevertheless, ρ is by no means the sole arbiter of relative detonation performance. TATB (**1**) and RDX (**2**) were cited earlier as an example; RDX has superior detonation properties even though TATB has a distinctly higher density. This is shown in Table 3, which also provides the reason: TATB is lower in both N and especially in Q. The network of N-H---O-N inter- and intramolecular hydrogen bonding in crystalline TATB [25] is a stabilizing influence that diminishes Q, the heat release associated with detonation.

FOX-7, $(H_2N)_2C=C(NO_2)_2$, also has extensive N-H---O-N inter- and intramolecular hydrogen bonding in the crystal lattice [26], with a negative effect upon Q. This is why FOX-7 has approximately the same D as RDX despite being nearly 0.1 g/cm³ more dense and having the same N and M_{ave} (Table 3).

An example of the role that N can play with respect to detonation properties is provided by nitroguanidine. It has the lowest ρ, M_{ave} and Q of any of the fourteen compounds in Table 3, yet its detonation velocity and pressure are comparable or superior to those of many of them. This is because nitroguanidine has by far the highest value of N, 0.03842 moles/g, well above the next highest, 0.03377 moles/g.

Discussion

It has been demonstrated that crystal density, while a very significant factor in detonation performance, is not as dominant on a relative basis as might be inferred from eqs. (1) and (2). This is because the densities of compounds of interest tend to cover a smaller range than do N, M_{ave} and Q. For the fourteen compounds in Table 3, the ratios of the maximum to the minimum values of each of these quantities is: ρ, 1.25; N, 1.65; M_{ave}, 1.44; Q, 1.72. Thus the density is notably less variable than the others, and its contributions to detonation velocity and pressure do not differentiate between different C, H, N, O explosive compounds as much as might be expected.

In addition to a large crystal density, another property that is commonly invoked as being very desirable is a strongly positive enthalpy of formation, in order to increase Q. This is one of the primary reasons for the interest in high-nitrogen compounds as explosives [27-30]. Indeed, a large enthalpy of formation is very beneficial, as is shown by CL-20; it has the most positive enthalpy of formation (90.2 kcal/mol [23]) and the highest detonation velocity and pressure of any compound in Table 3. On the other hand, nine of the compounds in Table 3 actually have *negative* enthalpies of formation, and yet some of them have quite good detonation properties. Two examples are PETN (ΔH_f = -128.7 kcal/mol) and FOX-7 (ΔH_f = -32.0 kcal/mol) [23], which are in the neighborhood of RDX in detonation velocity and pressure (Table 3).

Quite noteworthy in this respect is the nitrate ester **5** that has recently been prepared [31] and studied computationally [32]. Its experimental density is 1.917 g/cm³, similar to the 1.90 g/cm³ of HMX (Table 3), but its solid state enthalpy of formation is a very negative -88.7 kcal/mol [31], in contrast to the 24.5 kcal/mol of HMX [23]. Nevertheless, the detonation velocity and pressure of **5**, estimated with the CHEETAH code [9], are 9.1 mm/μs and 40 kbar [31],

very much like those of HMX (Table 3). The detonation properties of **5** are accordingly predicted to be second only to those of CL-20 in Table 3.

5
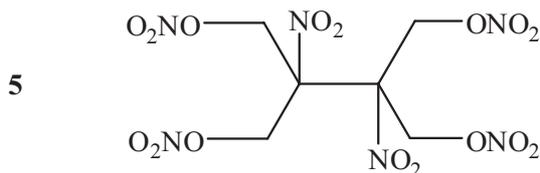
These reported results can be understood by looking at the detonation heat release Q of **5**. Using the experimental ΔH_f and assuming an $N_2/H_2O/CO_2/C(s)$ product composition, we obtain Q = 1682 cal/deg, which exceeds all of those in Table 3, including that of CL-20. This very large Q reflects the fact that, according to the $N_2/H_2O/CO_2/C(s)$ product distribution, **5** is expected to produce 6 moles of CO_2, more than any compound in Table 3; CO_2 has a much more negative enthalpy of formation (-94.05 kcal/mol) than do gaseous H_2O (-57.8 kcal/mol) and N_2 (0 kcal/mol) [19]. Thus, having a negative enthalpy of formation is not incompatible with excellent detonation performance.

It was pointed out earlier, and shown in Table 1, that the products of detonation vary with the loading density. The primary effect is that as ρ decreases, the CO/CO_2 ratio increases. This means of course that N, M_{ave} and Q will change in value. It may therefore seem surprising that the detonation velocities of some explosives (e.g. RDX, PETN, TATB, Tetryl, DATB and TNT) have been expressed as linear functions of density alone over considerable ranges of ρ [33]:

$$D \approx a + b\rho \tag{4}$$

In terms of eq. (1), this implies that the product $N^{0.5}M_{ave}^{0.25}Q^{0.25}$ is roughly constant over that range of ρ, and also suggests, from eq. (2), that

$$P \approx c\rho^2 \tag{5}$$

The fact that the product $N^{0.5}M_{ave}^{0.25}Q^{0.25}$ remains approximately the same can be understood by noting that as the ratio CO/CO_2 becomes larger, more moles of gaseous products are formed (Table 1), since each CO_2 can yield 2 CO. Thus N increases. However M_{ave} and Q both become smaller, the former because CO has a lower molecular mass than CO_2 and the latter because the enthalpy of formation of CO is less negative (-26.42 kcal/mol) than that of CO_2 (-94.05 kcal/mole) [19]. Since N appears to a higher power in eqs. (1) and (2) than do M_{ave} and Q, the

changes somewhat balance and the product $N^{0.5}M_{ave}^{0.25}Q^{0.25}$ is roughly constant. Thus the assumption of the $N_2/H_2O/CO_2/C(s)$ product composition may be reasonably effective even at relatively low loading densities.

Finally, we would like to return to the issue of sensitivity. We have pointed out that the relatively strong inter- and intramolecular interactions in TATB and FOX-7 lead to more compact and stable lattice and/or molecular structures that increase crystal density but decrease Q, so that detonation performance is less than might be anticipated on the basis of the density. On the other hand, these interactions appear to have beneficial consequences for sensitivity [4]. TATB and FOX-7 are both relatively insensitive [34]. One factor may be the diminished amount of available free space in the crystal lattices of these compounds; there is evidence that this lessens sensitivity [35].

Summary

We wish to emphasize the following:
(1) Crystal density is certainly an important determinant of detonation properties, but its relative effect can sometimes be overridden by the other factors appearing in eqs. (1) and (2).
(2) Comparisons with experimental data have provided additional support for Kamlet and Jacobs' approach to predicting detonation velocities and pressures [7], which utilizes eqs. (1) and (2), an assumed $N_2/H_2O/CO_2/C(s)$ product composition and known or estimated values of the compound's density and solid state enthalpy of formation.
(3) The use of a gas phase rather than solid phase enthalpy of formation for the compound may produce a significant additional error in the calculated detonation velocity.
(4) A negative enthalpy of formation does not necessarily preclude a compound's having excellent detonation properties.

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