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Determination of performance of non-ideal aluminized explosives

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Abstract

Non-ideal explosives can have Chapman–Jouguet (C–J) detonation pressure significantly different from those expected from existing thermodynamic computer codes, which usually allows finding the parameters of ideal detonation of individual high explosives with good accuracy. A simple method is introduced by which detonation pressure of non-ideal aluminized explosives with general formula $C_aH_bN_cO_dAl_e$ can be predicted only from *a*, *b*, *c*, *d* and *e* at any loading density without using any assumed detonation products and experimental data. Calculated detonation pressures show good agreement with experimental values with respect to computed results obtained by complicated computer code. It is shown here how loading density and atomic composition can be integrated into an empirical formula for predicting detonation pressure of proposed aluminized explosives.

Keywords: Non-ideal explosives; Detonation pressure; $C_aH_bN_cO_dAl_e$ explosives; Elemental composition; Loading density

1. Introduction

Aluminum powder is widely used in rocket propellants, fuel–air and aluminized explosives because it is a combustible high-energy material. Since aluminum increases the energy and raises the flame temperature in rocket propellants, it is common ingredient in solid propellants. Aluminum is also incorporated in explosives to raise reaction temperature, increase bubble energies in under water weapons, enhance air blast and create incendiary effect. It increases the heat of detonation and acts as intermediate sensitive agent. Some investigations try to explain the role of aluminum powder in the detonation process of aluminized explosives [1–8].

The necessity of predicting the detonation characteristics of high explosives simulates the development of theoretical methods to calculate detonation parameters. Prediction of detonation pressure has traditionally been accomplished through the means of Chapman–Jouguet (C–J) thermodynamic detonation theory. This theory assumes that thermodynamic equilibrium is reached instantaneously. Existing thermodynamic computer codes, such as BKW [9] and RUBY [10] and latter's offspring TIGER [11], CHEQ [12], and CHEETAH [13] (a C version of TIGER), allow to find detonation parameters of individual explosives with good accuracy. They use an appropriate empirical equation of state (EOS) such as Becker–Kistiakosky–Wilson (BKW-EOS) [14], the Jacobs–Cowperthwaite–Zwisler (JCZ-EOS) [15,16] and Kihara–Hikita–Tanaka (KHT-EOS) [17] which were fitted to experimental data of specific explosives. By assuming all of the chemical equations for all possible species in the reaction product gases and solving theses with thermochemical analogues, one can estimate the isentropic expansion having the equilibrium energy and gas quantities along with the Rankine–Hugoniot jump equations. Suitable equation of state can accurately reflect the thermodynamic properties of multicomponent mixtures at several 1000 K and hundreds of kbar to much lower temperatures and pressures obtained during expansion of the reaction products. The BKWC-EOS [13], BKWR-EOS [18] and BKWS-EOS [19] are three different parameterizations of the BKW-EOS which can be used to calculate detonation properties of high explosives. Some new theoretical methods have been recently introduced for simple reliable evaluation or desk calculation of various thermodynamic and detonation performance parameters [20–35] so that the results are comparable with output of complex computer codes.

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Since the large difficulties lie in the uncertainty of degree of chemical reactions completeness occurring in detonation wave, for mixture of high explosives with aluminum, it is not clear what degree aluminum oxidized in the C–J point. The thermodynamic calculations of detonation parameters with computer code are usually carried out by assuming a certain degree of oxidation of aluminum. Combustion of aluminum particles in explosives is assumed that it occurs behind the reaction front, during the expansion of gaseous detonation products. Aluminum particles in this case do not participate in the reaction zone, but act as inert ingredients [19]. Detonation pressure is one of the basic performance properties of an explosive. It should be emphasized that the accuracy of predictive method is not necessarily enhanced by greater complexity. The main focus, thereafter, will be on introducing the simplest procedure for calculating detonation pressure of aluminized explosives as an important class of composite explosives at any loading density without using any experimental data. It is shown here, how detonation pressure of aluminized explosives with formula $C_aH_bN_cO_dAl_e$ can be predicted directly from elemental composition. The present method is remarkable respect to output of complicated computer code because it provides a simple pathway of quick estimation of detonation pressure at given loading density without using experimental condensed heat of formation and assumed detonation products. The calculated detonation pressure will also be tested with experimental data of some well-known aluminized explosives as well as compared with BKWS-EOS output using full and partial, 50% interaction of aluminum with detonation products.

2. Detonation behavior of non-ideal aluminized explosives

The advantages of theoretical computation or calculated approach for determining of various detonation parameters of a new explosive are of course that it can be applied to suggested target compounds. Simply, calculation approaches play an important role in the study of energetic molecules because they permit both existing and proposed systems to be analyzed and evaluated. Predicting of the performance of new energetic materials from a given molecular structure without using experimental measurement is very important to scientist because the calculated detonation properties are recognized to be cost-effective, environmentally-desirable and time-saving.

Pressure and temperature are the most important thermodynamic characteristics of a shock-compressed material. They can also furnish information on physicochemical conversions in the course of shocked compression. Non-ideal explosives have significantly different detonation properties than predicted by equilibrium, one-dimensional and steady state calculations so that physical separation of the fuel and oxidizer in such explosives results in extended chemical reaction zones. They are often poorly modeled by the C–J theory because the C–J assumption of instantaneous thermodynamic equilibrium breaks down. The high degree of inhomogenity and the secondary exothermic reactions occurring in the detonation products expanding behind the detonation zone are two characteristics of non-ideal explosives. Diffusion may play a major role in experimentally determined detonation properties and the amount of reacted material may be a function of reaction zone length. Aluminized composite explosives can be classified as non-ideal explosives.

To predict detonation properties for non-ideal explosives by using thermodynamic computer code, as a simple approximation, partial equilibrium can be used rather than a complex reacting mechanism. Since it is not clear what degree of aluminum oxidized in the C–J point for mixture of high explosives with aluminum, thermodynamic calculations of detonation parameters are carried out by assuming a certain degree of oxidation of aluminum. However, inert aluminum atoms were included in the product species database that could only form solid, liquid or gaseous aluminum. Thus, preventing reaction of aluminum with oxygen or other reactive species occurs. Partial equilibrium is invoked by specifying the amount of the initial aluminum that is assumed to react. Prevention of aluminum from forming such product as Al_2O_3 in combination with composite explosives such as RDX causes an increase in the number of gaseous products. If complete equilibrium is assumed, more condensed Al_2O_3 is produced. Since the higher temperature is a result of the large negative heat of formation of Al_2O_3, complete equilibrium force oxygen to react with aluminum rather than carbon which produce a hot, fuel-rich gas phase and more solid carbon. However, reaction temperature and prolongation of the reaction time can be raised to increase explosive performance by adding aluminum to explosives.

Combustion of aluminum gives the products that lower the particle density of detonation products because the product molecules from burning of aluminum are Al_2O_3. Since the energy from the thermal to intermolecular potential can be shifted by increasing particle density, the burning of aluminum raises the temperature which would increase the rate of aluminum burning until is burned near the C–J plane.

3. Detonation pressure of non-ideal explosives

Detonation pressure increases with the higher gas yield. The pressure associated with the state of complete reaction is the important parameter that has been regarded as one of the principal measures of performance of detonating explosive for many years. To calculate detonation parameters of condensed phase explosives, the determination of the time-independent state of chemical equilibrium, which is defined in accordance with the C–J condition had historically special attention. It is reasonable to expect the calculated and experimental C–J pressures to differ by 10–20% because the non-steady-state nature of the detonation wave.

Experiments for determining the performance of most explosives reveal that detonation pressure is roughly proportional to square of loading density [36,37]. Recent works have shown that elemental composition of an explosive rather than using assumed composition of detonation products as well as additional parameters can be correlated to detonation parameters [26–29,38]. One can express detonation pressure of non-ideal aluminized explosives as a function of basic parameters, namely the elemental composition, oxygen balance, heat of formation and initial den-

Table 1
Comparison of detonation pressure (in kbar) of the new correlation, Eq. (2), and BKWS-EOS (using full and partial, 50%, interaction of aluminum with detonation products) [19] and measured values

Name[a]	ρ_0 (g/cc)	P_{exp}	P_{new}	%Dev new	$P_{BKWS\text{-}EOS}$, full	%Dev BKWS-EOS full	$P_{BKWS\text{-}EOS}$, partial	Percent deviation BKWS-EOS partial
RDX/Al (90/10)	1.68	246 [19]	245	0.5	264	−7.3	257	−4.5
RDX/Al (80/20)	1.73	227 [19]	230	−1.3	244	−7.5	237	−4.4
RDX/Al (70/30)	1.79	210 [19]	217	−3.4	205	2.4	212	−1.0
RDX/Al (60/40)	1.84	211 [19]	203	3.9	156	26.1	174	17.5
RDX/Al (50/50)	1.89	190 [19]	189	0.6	120	36.8	119	37.4
HMX/Al (90/10)	1.76	–	257	–	291	–	285	–
HMX/Al (80/20)	1.82	–	244	–	271	–	268	–
HMX/Al (70/30)	1.86	–	228	–	224	–	235	–
HMX/Al (60/40)	1.94	–	220	–	180	–	204	–
TNETB/Al (90/10)	1.75	262 [19]	258	1.6	269	−2.7	258	1.5
TNETB/Al (80/20)	1.82	248 [19]	247	0.4	256	−3.2	244	1.6
TNETB/Al (70/30)	1.88	227 [19]	234	−3.0	219	3.5	219	3.5
TNT/Al (89.4/10.6)	1.72	–	192	–	203	–	200	–
TNT/Al (78.3/21.7)	1.8	189 [19]	187	1.2	183	3.2	187	1.1
TNT/Al (67.8/32.2)	1.89	–	185	–	144	–	168	–
H-6	1.75	–	224	–	215	–	216	–
HBX-1	1.71	220 [19]	218	0.8	211	4.1	209	5
HBX-3	1.84	–	205	–	152	–	173	–
Alex-20	1.801	230 [43]	228	0.7	–	–	–	–
Alex-32	1.88	215 [43]	216	−0.3	–	–	–	–
PBXN-1	1.77	245 [43]	245	0.1	–	–	–	–
Destex	1.68	175 [43]	178	−1.8	–	–	–	–

[a] See Appendix A for glossary of compound name.

sity of mixture. Various combinations of mentioned parameters are studied and optimized with experimental data. The study of various aluminized composite explosives has shown surprisingly that only elemental composition is sufficient for reliable prediction of detonation pressures at specified loading density. The results showed that for 100 g mixture of high explosive with aluminum, the following simple equation can provide the suitable pathway for predicting detonation pressure:

$$P\,(\text{kbar}) = \sum_{i=1}^{5} z_i n_i + z_6 \rho_0^2 \tag{1}$$

where z_i is adjustable parameters, ρ_0 loading density and n_i the number of moles of carbon, hydrogen, nitrogen, oxygen and aluminum. To obtain adjustable parameters, experimental data of aluminized explosives, which are listed in Table 1, were used. It should be mentioned that reported detonation pressures are rare because they are measured by various indirect hydrodynamic methods and their exact interpretation is also uncertain [39]. Adjustable parameters can be determined by using the procedure of Kamlet and Hurwitz [40]. However, agreement with measurement has been secured in that the adjustable constants in introduced correlation consistent with experimental data. The correlation for aluminized explosives with general formula $C_aH_bN_cO_dAl_e$ can be given as follows (R-squared value or the coefficient of determination [41] = 0.972):

$$P\,(\text{kbar}) = -35.531a + 41.422b - 14.770c + 44.004d - 21.320e + 43.950\rho_0^2 \tag{2}$$

The necessary data for calculations are given in Table 1. Since detonation pressure increases with an increase in the amount of gaseous products which depends on oxygen content of explosive, positive and negative signs appear for correlation coefficients of elements in Eq. (2). Calculated detonation pressures of aluminized explosives are also given in Table 1 and compared with the results from the BKWS-EOS using full and partial equilibrium. Only 50% of aluminum is assumed to interact with combustion products in the case of partial equilibrium. As seen in Table 1, the new hand calculated detonation pressures show surprisingly very good agreement with experimental data as compared to the computed results of complicated computer program. Comparison of the calculated results with experimental data may be taken as appropriate validation test of the introduced simple correlation for use with aluminized explosives. Though measured data of detonation pressures are rare in open literature, predicted detonation pressures of Eq. (2) are consistent with reported values from different sources, e.g. calculated detonation pressure for tritonal 80/20 at loading density 1.77 g/cc is 184 kbar which is close to the measured data of 189 kbar [42]. However, there are some calculated values for aluminized explosives as well as the computed values of Hobbs and Baer [19] in Table 1 where their measured data have not been reported.

Eq. (2) shows that the number of moles of the five elements present in 100 g aluminized explosives is far important than the details of the bonding arrangements within the molecular structure. New correlation covers the range from the oxygen lean to oxygen rich explosives. It requires no prior knowledge of any measured, estimated or calculated physical, chemical or thermochemical properties of explosive and assumed detonation

products. It is worthwhile to note by considering large percent deviations generally attributed to experimental measurements of detonation pressure, up to 20% [42], the agreement between calculated and measured pressures is also satisfactory.

4. Conclusions

A new simple theoretical approach complemented the computer output is introduced for desk calculation detonation pressure of $C_aH_bN_cO_dAl_e$ explosives only from atomic composition. There is no need to use heat of formation of composite explosive as well as using full and partial oxidation of aluminum that is usually required by computer code. Given the chemical formula of an aluminized composite explosive, one can estimate reliable detonation pressure as a function of square loading density that is consistent with uncertainty of detonation pressure. The motivation in this work is to purpose a simple correlation which can be used for determining detonation pressure of aluminized explosives, formed from the elements C, H, N, O and Al. As seen in Table 1, excellent agreement is obtained between measured and calculated values of detonation pressure for some aluminized explosives such as RDX/Al over a wide percentage of aluminum. Since the necessary data for this method is only elemental composition without using any experimental data of explosives and detonation products, the results of this work are remarkable. Although 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 properties as detonation pressure, there is no need to use it in the present method.

In brief, a relatively accurate method of estimating detonation pressure for aluminized explosives is introduced which is only based upon the atomic composition and square of loading density of explosive.

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Appendix A

Glossary of compound names

1. Alex-20: 44/32.2/19.8/4 RDX/TNT/Al/wax ($C_{1.783}H_{2.469}N_{1.613}O_{2.039}Al_{0.7335}$)
2. Alex-32: 37.4/27.8/30.8/4 RDX/TNT/Al/wax ($C_{1.647}H_{2.093}N_{1.365}O_{1.744}Al_{1.142}$)
3. Destex: 74.766/18.691/4.672/1.869 TNT/Al/wax/graphite ($C_{2.791}H_{2.3121}N_{0.987}O_{1.975}Al_{0.6930}$)
4. H-6: 45/30/20/5/0.5 RDX/TNT/Al/D-2 wax/$CaCl_2$ ($C_{1.89}H_{2.59}N_{1.61}O_{2.01}Al_{0.74}Ca_{0.005}Cl_{0.009}$)
5. HBX-1: 40/38/17/5/0.5 RDX/TNT/Al/D-2 wax/$CaCl_2$ ($C_{2.06}H_{2.62}N_{1.57}O_{2.07}Al_{0.63}Ca_{0.005}Cl_{0.009}$)
6. HBX-3: 31/29/35/5/0.5 RDX/TNT/Al/D-2 wax/$CaCl_2$ ($C_{1.66}H_{2.18}N_{1.21}O_{1.60}Al_{1.29}Ca_{0.005}Cl_{0.009}$)
7. HMX/Al (90/10): $C_{1.216}H_{2.43}N_{2.43}O_{2.43}Al_{0.371}$
8. HMX/Al (80/20): $C_{1.081}H_{2.161}N_{2.161}O_{2.161}Al_{0.741}$
9. HMX/Al (70/30): $C_{0.945}H_{1.89}N_{1.89}O_{1.89}Al_{1.11}$
10. HMX/Al (60/40): $C_{0.81}H_{1.62}N_{1.62}O_{1.62}Al_{1.483}$
11. PBXN-1: 68/20/12 RDX/Al/nylon ($C_{1.498}H_{2.863}N_{1.971}O_{1.791}Al_{0.742}$)
12. RDX/Al (90/10): $C_{1.215}H_{2.43}N_{2.43}O_{2.43}Al_{0.371}$
13. RDX/Al (80/20): $C_{1.081}H_{2.161}N_{2.161}O_{2.161}Al_{0.741}$
14. RDX/Al (70/30): $C_{0.945}H_{1.89}N_{1.89}O_{1.89}Al_{1.11}$
15. RDX/Al (60/40): $C_{0.81}H_{1.62}N_{1.62}O_{1.62}Al_{1.483}$
16. RDX/Al (50/50): $C_{0.675}H_{1.35}N_{1.35}O_{1.35}Al_{1.853}$
17. TNETB/Al (90/10): $C_{1.399}H_{1.399}N_{1.399}O_{3.264}Al_{0.371}$ (TNETB = 2,2,2-trinitroethyl-4,4,4-trinitrobutyrate)
18. TNETB/Al (80/20): $C_{1.244}H_{1.244}N_{1.244}O_{2.902}Al_{0.715}$
19. TNETB/Al (70/30): $C_{1.088}H_{1.088}N_{1.088}O_{2.539}Al_{1.11}$
20. TNT/Al (89.4/10.6): $C_{2.756}H_{1.969}N_{1.181}O_{2.362}Al_{0.393}$
21. TNT/Al (78.3/21.7): $C_{2.414}H_{1.724}N_{1.034}O_{2.069}Al_{0.804}$
22. TNT/Al (67.8/32.2): $C_{2.090}H_{1.493}N_{1.896}O_{1.791}Al_{1.193}$
23. Tritonal 80/20: 80/20 TNT/Al ($C_{2.465}H_{1.76}N_{1.06}O_{2.11}Al_{0.741}$)

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