



## A Predictive Method for the Heat of Explosion of Non-ideal Aluminized Explosives

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**Abstract:** The heat of explosion is one of the most important thermodynamic parameters of aluminized explosives. Two improvements in numerical calculations to predict the behaviour of the explosion of non-ideal aluminized explosives were completed in this work. The chemical reaction between aluminum and the C-J detonation products of high energy ingredients was determined and the equation of state for the detonation products of high energy ingredients was revised. The constant  $k$  in the BKW equation was revised to obtain perfect results for predicting the C-J parameters for high energy ingredients. The predicted results show that the heats and temperatures of aluminized explosives become maximized when the mass fraction of aluminum powder is 30%, which is in good agreement with the results obtained by empirical formulae.

**Keywords:** aluminized explosives, heat of explosion, thermodynamic, non-ideal explosives, high energy materials

### Introduction

Since aluminum increases the energy and raises the reaction temperature of explosion, it is a common ingredient in explosives. The heat of explosion is usually defined as the difference between the energies of formation of a material and the energies of formation of the explosion products. Muthurajan *et al.* [1] defined the heat of explosion: ‘Heat of explosion is the quantity of heat released when high energy material undergoes detonation as an explosive (*e.g.*, RDX, HMX, TNT, *etc.*) or deflagration (burning) as a propellant (*e.g.*, a rocket propellant)’. It is one of the most important thermodynamic parameters of

aluminized explosives.

Extensive publications [2-10] are available in the literature on theoretical calculations to predict the detonation behaviour of ideal explosives and the detonation velocity and pressure of aluminized explosives. However, there is a general lack of information in the literature for predicting the heat of explosion for non-ideal aluminized explosives.

Keshavarz introduced a new pathway to predict the detonation pressure of CHNO and CHNOAl explosives through the molecular structure [11] and a simple method for the prediction of the detonation velocity of ideal and non-ideal explosives [12]. Keshavarz proposed an empirical formula for predicting the detonation pressure and velocity of aluminized explosives [13-14]. Eight adjustable parameters in the formula need to be determined empirically. These adjustable parameters still do not reflect the physical behavior of the aluminized explosive. Muthurajan *et al.* presented a computational approach for predicting the heat of explosion of high energy materials which do not contain aluminum powder [15].

The Chapman-Jouguet (C-J) detonation velocity and pressure predicted from existing thermodynamic computer codes were reported in references [16-20]. The reported data showed that the Chapman-Jouguet detonation parameters of non-ideal explosives calculated using existing thermodynamic computer codes were significantly different from experimental results. Some investigators assumed that non-equilibrium effects in the reaction zones may contribute to this confusion, and the measured pressures may be higher than equilibrium calculations predict if the measurement is taken behind the von Neumann spike and in front of the C-J plane. In fact, aluminum powder needs to be excited for several  $\mu\text{s}$  before chemical reaction occurs. Therefore, it is impossible for the aluminum powder to participate in chemical reaction in the reaction zones from high energy ingredients.

The size of aluminum particles added to high explosives is of the order of magnitude of  $10^0$ - $10^1 \mu\text{m}$ . Nanometer aluminum powder has been used in aluminize mixtures in recent years. However, most of the aluminum powder added to aluminized explosives is at present of micrometer size. The length of the C-J reaction zone in high explosives is about  $10^1 \text{ nm}$ , which is three orders of magnitude smaller than the size of the micrometer aluminum particles commonly used in aluminized explosives. Therefore, the aluminum particles cannot participate in the chemical reaction in the C-J detonation zone produced by high energy ingredients [11]. We assumed that Al does not react in the chemical reaction zone and at the C-J point because the aluminum particles examined in this work are of micron order. The C-J pressure and temperature produced by

the HE ingredients in the mixture are the reaction conditions for the aluminum.

The main purpose of the present work was to develop a new approach to predict the heat of explosion, based on a revised equation of state and thermodynamic detonation theory.

## Computational approach

The heat of explosion is dependent on the reaction conditions (loading density, and consequently pressure). Two significant improvements in numerical calculations to predict the behaviour of the explosion of non-ideal aluminized explosives were completed in this work. One is determined by the chemical reaction between the aluminum powder and the C-J detonation products of high energy ingredients. The second is that the equation of state for the detonation products of high energy ingredients is revised.

### Revised equation of state for detonation products

Like some other reports [21], in the present work, one of parameters,  $k$ , in the BKW equation of state was adjusted slightly. This is because aluminum particles acting as inert material in the reaction zones causes an increase in the solid products of the C-J reaction. The value of  $k$  depends on the fraction of solid products in the C-J reaction and it should be adjusted when the fraction of solid products in the C-J reaction increases. The original value of  $k$  for RDX type explosives in the BKW equations of state was 10.91 and was adjusted to 9.2725 in this work by a series of trial calculation. The original value of  $k$  for TNT type explosives in the BKW equations of state was 12.685 and was adjusted to 10.4017. The revised parameters in the BKW equations of state are listed in Table 1.

**Table 1.** Revised parameters in the BKW equations of state

Parameters	$\alpha$	$\beta$	$k$	$\theta$
RDX type aluminized explosives	0.5	0.16	9.2735	400
TNT type aluminized explosives	0.5	0.09585	10.4017	400

### Determination of the chemical reaction of aluminum

The chemical reactions of aluminum and the detonation products of high energy ingredients have three reaction channels:





The dependence of the specific heat capacity on temperature can be given as follows:

$$C_p(T) = a + bT + cT^2$$

where:  $C_p(T)$  is the specific heat of ingredient  $i$  in a chemical reaction;  $T$  is the instantaneous temperature;  $a$ ,  $b$  and  $c$  are the constants which can be determined by experimental data fitting.

For a chemical reaction, the change of specific heats from reactants to products is

$$\Delta C_p = \sum v_i C_p(t) = \Delta a + \Delta bT + \Delta cT^2 \quad (4)$$

where:  $\Delta C_p$  is the difference between the specific heats of the products and those of the reactants for a chemical reaction;  $v_i$  is the number of moles of ingredient  $i$  which is positive for the products and negative for the reactants;

$$\Delta a = \sum v_i a; \Delta b = \sum v_i b; \Delta c = \sum v_i c. \Delta a = \sum v_i a_i; \Delta b = \sum v_i b_i; \Delta c = \sum v_i c_i.$$

The relationship between  $\Delta H$  and  $\Delta C_p$  is:

$$\Delta H(T) = \int \Delta C_p(T) dT \quad (5)$$

From Eqs. (4) and (5):

$$\Delta H(T) = \Delta H_0 + \Delta aT + \frac{1}{2} \Delta bT^2 + \frac{1}{3} \Delta cT^3 \quad (6)$$

where:  $T_0$  is the initial temperature;  $\Delta H_0$  is the change in enthalpy at the initial temperature  $T_0$ .

$$\Delta H_0 = -(\Delta aT_0 + \Delta bT_0^2 + \Delta cT_0^3) \quad (7)$$

The van't Hoff equation is:

$$\frac{d \ln K}{dT} = \frac{\Delta H(T)}{RT^2} \quad (8)$$

From the van't Hoff equation:

$$\int d \ln K = \int \frac{\Delta H(T)}{RT^2} dT \tag{9}$$

where:  $K$  is the equilibrium constant for a chemical reaction;  $\Delta H(T)$  is the change of enthalpy in a chemical reaction which is a function of the instantaneous temperature  $T$ .

From Eqs. (6) , (7) and (9):

$$\ln K(T) = -\frac{\Delta H_0}{RT} + \frac{\Delta a}{R} \ln T + \frac{1}{2R} \Delta bT + \frac{1}{6R} \Delta cT^2 + I \tag{10}$$

where  $I$  is the integral constant which can be determined for  $K$  at normal temperature.

The data for the change of specific heats with temperature can be found in the reported literature [23]. The correlation between the equilibrium constant and the instantaneous (current) temperature for the three chemical reactions can be obtained by data fitting, as shown in Table 2.

**Table 2.** Correlation between the equilibrium constants and temperature

Reaction formula	Temperature range	Correlation between K and T
Al+1.125CO <sub>2</sub> → 0.5Al <sub>2</sub> O <sub>3</sub> +0.75CO+0.375C	298-2400 K	ln K <sub>p</sub> = 25.0764/T - 3.6790e - 004lnT + 0.1889
	2400-2800 K	ln K <sub>p</sub> = 20.3359/T + 8.144e - 004lnT + 0.1900
	>2800 K	ln K <sub>p</sub> = 60.1298/T + 0.0027e + 0.1727
Al+1.5CO → 0.5Al <sub>2</sub> O <sub>3</sub> +1.5C	298-2400 K	ln K <sub>p</sub> = -48.0051/T + 8.3774e - 004lnT + 0.2840
	2400-2800 K	ln K <sub>p</sub> = -52.7457/T + 0.0020lnT + 0.2851
	>2800 K	ln K <sub>p</sub> = -12.951/T + 0.0039lnT + 0.2677
Al+1.5H <sub>2</sub> O → 0.5Al <sub>2</sub> O <sub>3</sub> +1.5H <sub>2</sub>	298-2400 K	ln K <sub>p</sub> = 57.4704/T + 9.2795e - 004lnT + 0.1649
	2400-2800 K	ln K <sub>p</sub> = 52.7298/T + 0.0021lnT + 0.1660
	>2800 K	ln K <sub>p</sub> = 92.5238/T + 0.0040lnT + 0.1486

The calculated results of the equilibrium constants for the three chemical reactions showed that the equilibrium constant is highest for the reaction of aluminum and H<sub>2</sub>O, that for the reaction of aluminum and CO<sub>2</sub> is medium and that for the reaction of aluminum and CO is the lowest.

Based on the detonation products calculated for the reaction zone of high energy ingredients, the initial ingredients for the three chemical reactions of aluminum and the detonation products are obtained. Suppose that 'x' is the number of moles of CO<sub>2</sub> in the reactants of reaction 1, 'y' is the number of moles of C in the products for reaction 2 and 'z' is the number of moles of H<sub>2</sub> in the products for reaction 3. The numbers of moles of the initial ingredients in the

three chemical reactions and those at the equilibrium state can be confirmed through calculation, as shown in Table 3.

**Table 3.** Ingredients of the three reactions

Ingredients	Al	CO <sub>2</sub>	CO	C	H <sub>2</sub> O	H <sub>2</sub>
Initial state	a	b	c	d	e	f
Balance state	a-1/1.125x- 2/3y-2/3z	b-x	c+ 0.75/1.125x-y	d+ 0.375/1.125x+y	e-z	f+z

Based on the definition of the equilibrium constants:

$$K^{\ominus} = \Pi \left( \frac{p_B}{P^{\ominus}} \right)^{v_B} = \Pi \left( \frac{n_B}{\sum n_B} \times \frac{p}{P^{\ominus}} \right)^{v_B} = \left( \frac{p/P^{\ominus}}{\sum n_B} \right)^{\sum v_B} \Pi n_B^{v_B} \quad (11)$$

where  $K^{\ominus}$  is the equilibrium constant;  $p$  is the full pressure of the gaseous products;  $p_i$  is the fractional pressure of species  $i$ ;  $p_i = p \left( \frac{n_i}{\sum n_i} \right)$ ;  $P^{\ominus}$  is the standard atmosphere (10<sup>5</sup> Pa);  $\sum v_i$  is the summation of numbers of moles of reactants in every reaction equation;  $v_i > 0$  for products and  $v_i < 0$  for reactants. For example, reaction 3 (Eq. (3)),  $\sum v_i = 1.5 + 0.5 - 1 - 1.5 = -0.5$ .

$\sum n_B$  is the summation of the number of moles of all the gaseous products including reactions 1, 2 and 3, which can be expressed by  $x$ ,  $y$  and  $z$ .  $K^{\ominus}_1$ ,  $K^{\ominus}_2$ ,  $K^{\ominus}_3$  and  $p/P^{\ominus}$  are known. Therefore, the three non-linear equations including  $x$ ,  $y$ , and  $z$  can be obtained. The values of  $x$ ,  $y$  and  $z$  can be found by numerical calculation of the three non-linear equations. By placing the calculated values of  $x$ ,  $y$ , and  $z$  into the formulae in Table 3, the final ingredients in the products can be obtained.

From the mole number of every ingredient in the reactions between aluminum and the detonation products from high energy ingredients, the heat produced by these reactions can be calculated by use of following equation:

$$Q = -[H(T_p) - H(T_{CJ})] = \int_{T_{CJ}}^{T_p} \sum n_i C_{p_i}(t) dt \quad (12)$$

where  $H(T_{CJ})$  is the summation of the enthalpy of every ingredient at the C-J temperature:

$$H(T_{CJ}) = \sum n_i H_i(T_{CJ}) \quad (13)$$

where:  $n_i$  is the mole number of ingredient  $i$ ;  $H_i(T_{CJ})$  is the enthalpy of ingredient  $i$  at the C-J temperature;  $T_p$  is the parameter to be found. By the use of the iteration method, the solution of Eq. (7) can be obtained until  $T_p$  meets the required calculation precision.

Using the calculated temperature  $T_p$ , the heat of explosion of the aluminized explosive can be obtained:

$$Q_p = -\sum n_i H_i(T_p) - Q_{ef} \quad (14)$$

where  $Q_{ef}$  is the heat of formation of the aluminized explosive.

### Numerical approach

The logic for the computation is shown in Figure 1. After the C-J pressure and temperature have been obtained, they are used as the initial conditions for calculating the aluminum reaction parameters. The pressure is calculated through the composition and temperature by the BKW equation of state. Then, an assessment is made for the calculated pressure and temperature meeting energy conservation or not. If energy conservation is not met, another temperature value is taken and the calculation is repeated by the iteration method.

### Empirical method for estimating the heat of explosion of mixed explosives [22]

To validate the calculation method and the code used in this work, the previous empirical method was used to estimate the heats of explosion for aluminized explosives. The heats of explosion which were estimated were then used for comparison with the results calculated in this work.

For a mixed explosive consisting of several ingredients, the heat of explosion is estimated generally by using the following approach. Suppose  $Q_{oi}$  to be the heat of explosion for every ingredient in the mixture at the theoretical density. This can be obtained from reported data. The heats of explosion for the mixed explosives at the theoretical density,  $Q_o$ , can be obtained by summation of  $Q_{oi}$  and  $m_i$  (mass fraction of every ingredients) by a weighted method:

$$Q_p = \sum m_i Q_{oi} \quad (15)$$

Because the heat of explosion for oxygen lean explosives increases with the density, the heat of explosion at the density  $\rho$  can be obtained by the following equation:

$$Q_v = Q_o - B(\rho_o - \rho) \quad (16)$$

where:  $\rho_o$  is the theoretical density of the explosive;  $Q_v$  is the heat of explosion for the mixed explosive at the density  $\rho$ ;  $B$  is the revision coefficient for the mixed explosive which is the summation of  $B_i$  (the revision coefficients for every ingredient) and the mass fractions by a weighted method.

$$B = \sum m_i B_i \quad (17)$$

By using the above equation, the heat of explosion for a mixed explosive at any density can be obtained from the heat of explosion ( $Q_{oi}$ ) and the revision coefficients ( $B_i$ ) for every ingredient. The characteristic heats of explosion ( $Q_{oi}$ ) and the revision coefficients ( $B_i$ ) for some explosives are listed in Table 4.

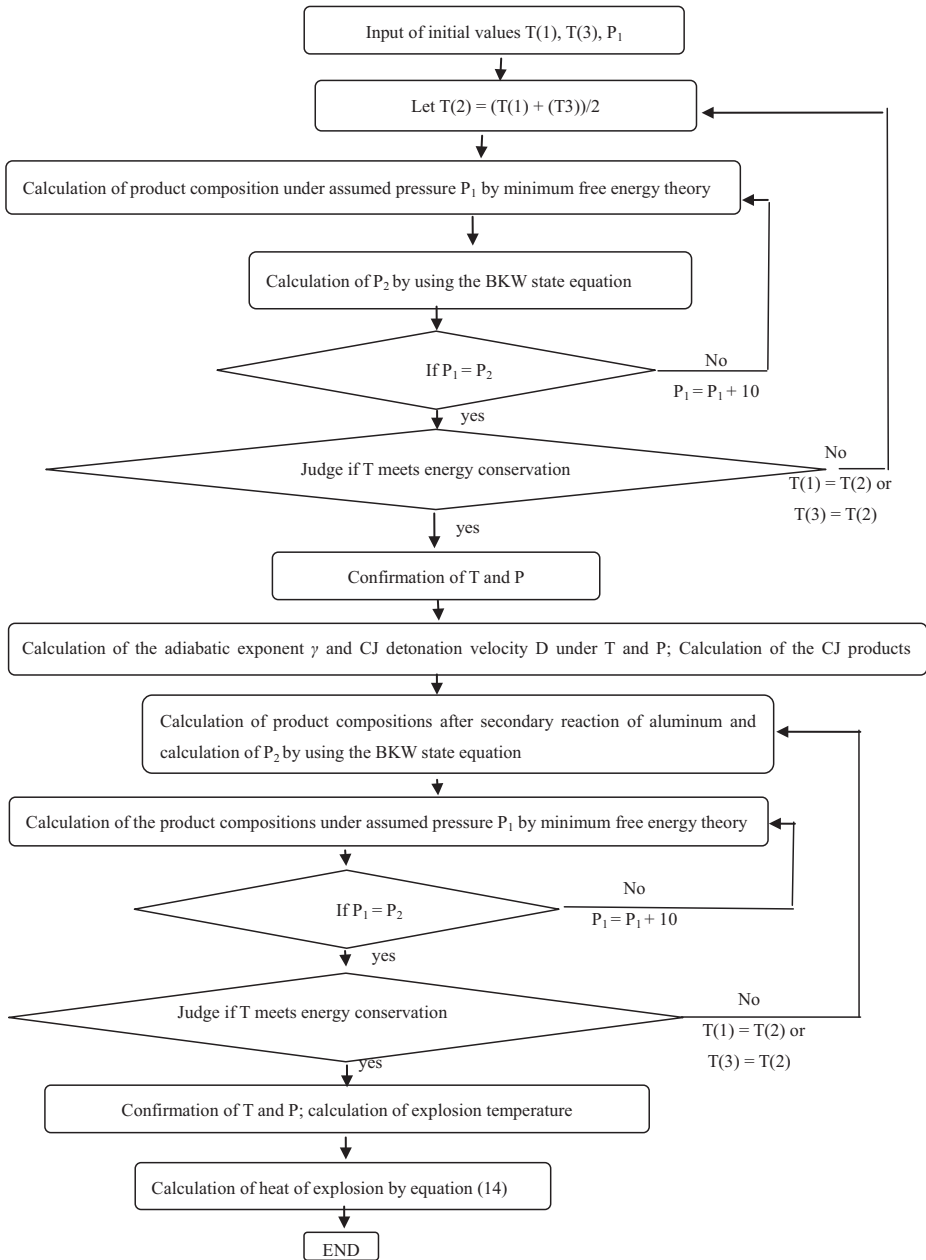
**Table 4.**  $Q_{oi}$  and  $B_i$  for some explosives

Ingredient	$Q_{oi}$ (kJ/kg)	$B_i$ (kJ/(kg·g/cm <sup>3</sup> ))
TNT	4554.4	1340
RDX	5986.0	712
HMX	6040.4	712
Al	11930.1	2093

### Calculation results and comparisons

The heats of explosion for some explosives calculated with the code presented in this work, those estimated with the empirical formulae, and experimental results are listed in Tables 5 and 6. Tables 4 and 5 show that the heats and temperatures of explosion predicted in this work are in good agreement with those obtained by the empirical formulae and experimentally. The heats of explosion for all explosives can be predicted by using the code presented in this work. The empirical formulae and experimental results have their limitations for predicting the heats of explosion, because  $Q_{oi}$  and  $B_i$  can only be found for a limited number of special explosives and experimental determinations are expensive.





**Figure 1.** Logic for the computation of the C-J detonation pressure and velocity of aluminized explosives by thermodynamic detonation theory.

**Table 5.** Comparison of heats of explosion calculated with the new code and those estimated using empirical formulae and measured experimentally for some single explosives

Explosive	Density (g/cm <sup>3</sup> )	Heat of explosion (kJ/mol)			Temperature of explosion (K)	
		Experimental	Empirical	This work	Calculated [25]	This work
TNT	1.50	959 [23]	1080.7	1172.5	2829	2633.5
RDX	1.80	1270 [24]	1330.5	1300.5	2587	2599.8
HMX	1.90	1844 [24]	1788.0	1789.5	2693	2520.8

**Table 6.** Comparison of the heats of explosion calculated with the new code and those estimated using empirical formulae and measured experimentally for some aluminized explosives

Explosive	Density (g/cm <sup>3</sup> )	Heat of explosion (kJ/kg)		Temperature of explosion (K)	
		Empirical	This work	Calculated [25]	This work
H-6	1.71	4488	5357	5138	5230
HBX-1	1.72	4843	5139	4839	4510
HBX-3	1.81	2826	2597	5690	6015
Alex 20	1.80	4528	5199	5166	5122
Alex 32	1.88	3245	3791	5928	6224
Tritonal	1.72	4494	4393	5330	4598
Torpex	1.81	5191	5104	5261	6530
Destex	1.72	4085	4320	4866	4598

The results calculated by the new code presented in this work and listed in Table 7 show that the heats of explosion for aluminized explosives become maximized when the mass fraction of aluminum is 30%, which is in good agreement with the results obtained using the empirical formulae.

Kiciński *et al.* measured the heats of explosion of RDX-based compositions in four different atmospheres (argon, nitrogen, air and argon/oxygen mixture) by calorimetry. Charges of phlegmatized RDX containing 30% aluminum powder were fired in a calorimetric bomb of volume 5.6 dm<sup>3</sup>. The influences of inert and reactive additives, and the atmosphere filling the bomb, on the heat output was examined. A comparison of the heat of explosion calculated in this work with that measured in nitrogen is listed in Table 8 and shows that the measured value [26] is lower, because energy loss in the measurement is inevitable. But

energy loss was not considered in the calculation. Moreover, the explosive sample charged in the calorimetric bomb measurement [26] was too small (charge mass 20 g) to reach detonation and the released energy was consequently lower. It is noteworthy that our previous research found that the effect of the aluminum reaction in aluminized explosives is dependent upon the charge scale. If the scale is too small, aluminum particles cannot react completely. Consequently, the experimental results for aluminized explosives on a small scale should not be used to evaluate the heat of detonation or explosion.

**Table 7.** Calculated heats and temperatures of explosion for aluminized explosives

Explosives (mass fraction)	Density (g/cm <sup>3</sup> )	Heat of explosion (kJ/kg)		Temperature of explosion (K)
		This work	Empirical	
RDX/Al(90/10)	1.68	5064	6069	3600
RDX/Al(80/20)	1.73	8434	7904	4972
RDX/Al(70/30)	1.79	10331	9611	5447
RDX/Al(60/40)	1.84	8808	8204	4017
RDX/Al(50/50)	1.89	7299	6673	2316
HMX/Al(90/10)	1.76	5194	5118	3504
HMX/Al(80/20)	1.82	8506	8932	4879
HMX/Al(70/30)	1.86	10418	9643	5362
HMX/Al(60/40)	1.94	8840	8201	3938
TNT/Al(89.4/10.6)	1.72	2906	2777	2829
TNT/Al(78.3/21.7)	1.80	5772	5826	4472
TNT/Al(67.8/32.2)	1.89	6835	6698	5075

**Table 8.** Comparison of the heat of explosion calculated with that measured in nitrogen

Mixture	Density (kg·m <sup>-3</sup> )	Explosion heat (J·g <sup>-1</sup> )	
		measured in nitrogen [26]	calculated in this work
RDX/wax (CH <sub>2</sub> )n/ Al=65.8/4.2/30	1860	7337	8607

Our new approach for predicting the heat of explosion for aluminized explosives is based on the physical and chemical mechanism, which is superior to the empirical method.

## Conclusions

(1) This work presents a new code for predicting the heat and temperature of explosion for aluminized explosives. The new approach is based on the least free energy theory, successive approximation methods and assessment of the reactions between aluminum and the detonation products from high energy ingredients.

(2) Aluminum powder added to high energy explosives (ingredients) impacts on the state of detonation in the C-J reaction zones. Therefore, the equation of state calculating the C-J detonation parameters (BKW equation) should be revised. The constant in the BKW equation has been revised to obtain perfect results for predicting the C-J parameters from high energy ingredients and the heat and temperature from reactions of aluminum powder with the detonation products.

(3) The predicted results show that the heats and temperatures of aluminized explosives become maximized when the mass fraction of aluminum powder is 30%, which is in good agreement with the results obtained using the empirical formulae.

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## References

- [1] Muthurajan H., Sivabalan R., Saravanan N.P., Talawar M.B., Computer Code to Predict the Heat of Explosion of High Energy Materials, *J. Hazard. Mater.*, **2009**, *161*, 714-717.
- [2] Zhang Q., Xiang C., Liang H., Prediction of the Explosion Effect of Aluminized Explosives, *Sci. China-Phys. Mech. Astron.*, **2013**, *56*, 1004-1009.
- [3] Zhang Q., Chang Y., Prediction of Detonation Pressure and Velocity of Explosives with Micrometer Aluminum Powders, *Cent. Eur. J. Energ. Mater.*, **2012**, *9*, 279-292.
- [4] Maranda A., Research on the Process of Detonation of Explosive Mixtures of the Oxidizer Fuel Type Containing Aluminum Powder, *Propellants Explos. Pyrotech.*, **1990**, *15*, 161-165.
- [5] Maranda A., Cudziło S., Explosive Mixtures Detonating at Low Velocity, *Propellants Explos. Pyrotech.*, **2001**, *26*, 165-167.
- [6] Cudziło S., Maranda A., Nowaczewski J., Trzciński W., Shock Initiation Studies

- of Ammonium Nitrate Explosives, *Combust. Flame*, **1995**, *102*, 64-72.
- [7] Keshavarz M.H., Prediction of Heats of Sublimation of Nitroaromatic Compounds via Their Molecular Structure, *J. Hazard. Mater.*, **2008**, *151*, 499-506.
- [8] Mader C.L., Recent Advances in Numerical Modeling of Detonations, *Propellants Explos. Pyrotech.*, **1986**, *11*, 163-166.
- [9] Mader C.L., Kershner J.D., *Three-Dimensional Hydrodynamic Hot-Spot Model. LA-UR-85-742, CONF-850706-6, 1985.*
- [10] Kazandjian L., Danel J.-F., A Discussion of the Kamlet-Jacobs Formula for the Detonation Pressure, *Propellants Explos. Pyrotech.*, **2006**, *31*, 20-24.
- [11] Keshavarz M.H., Simple Correlation for Predicting Detonation Velocity of Ideal and Non-ideal Explosives, *J. Hazard. Mater.*, **2009**, *166*, 762-769.
- [12] Keshavarz M.H., Prediction of Detonation Performance of CHNO and CHNOAL Explosives through Molecular Structure, *J. Hazard. Mater.*, **2009**, *166*, 1296-1301.
- [13] Keshavarz M.H., Mofrad R.T., Poor K.E., Shokrollahi A., Zali A., Yousefi M.H., Determination of Performance of Non-ideal Aluminized Explosives, *J. Hazard. Mater. A137*, **2006**, 83-87.
- [14] Keshavarz M.H., Motamedoshariati H., Moghayadnia R., Nazari H.R., Azarniamehraban J., A New Computer Code to Evaluate Detonation Performance of High Explosives and Their Thermochemical Properties, Part I, *J. Hazard. Mater.*, **2009**, *172*, 1218-1228.
- [15] Muthurajan H., Sivabalan R., Saravanan N.P., Talawar M.B., Computer Code to Predict the Heat of Explosion of High Energy Materials, *J. Hazard. Mater.*, **2009**, *161*, 714-717
- [16] Baroody E.E., Peters S.T., Heats of Explosion, Detonation and Reaction Products: Their Estimation and Relation to the First Law of Thermodynamics, *The 1990 Jannaf Propulsion Meeting*, **1990**, *1*, 345-354.
- [17] Keshavarz M.H., Prediction of Detonation Performance of CHNO and CHNOAL Explosives through Molecular Structure, *J. Hazard. Mater.*, **2009**, *166*, 1296-1301.
- [18] Mader C.L., *Numerical Modeling of Explosives and Propellants*, 2<sup>nd</sup> ed., CRC Press, New York, **1998**.
- [19] Politzer P., Lane P., Concha M.C., in: *Energetic Materials – Part I: Theoretical and Computational Chemistry*, (P. Politzer, J.S. Murray, Eds.), Elsevier, Amsterdam, **2003**, pp. 247-277.
- [20] Rice B.M., Hare J., Predicting Heats of Detonation Using Quantum Mechanical Calculations, *Thermochim. Acta*, **2002**, *384*, 377-391.
- [21] Fried L.E., Souers P.C., BKWC: An Empirical BKW Parameterization Based on Cylinder Test Data, *Propellants Explos. Pyrotech.*, **1996**, *21*, 215-233.
- [22] Yu T.C., Yin M.C., Empirical Method Estimating Heat of Explosion for Mixed Explosives (in Chinese), *Chin. J. Expl. Prop.*, **1984**, *7*, 50-55.
- [23] Zhang B., Zhao H., Jiang H., Li J., Yun S., Zhang S., *Explosion and Effects* (in Chinese), Defence Industry Press, Beijing, **1979**.
- [24] Meyer R., *Explosives*, 2<sup>nd</sup> ed., Verlag Chemie, Germany, **1981**.
- [25] Mader C.L., *Numerical Modeling of Explosive and Propellants*, University of

California Press, Berkeley, **1979**.

- [26] Kiciński W., Trzciński W.A., Calorimetry Studies of Explosion Heat of Non-ideal Explosives, *J. Therm. Anal. Calorim.*, **2009**, *96*, 623-630.