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Algorithm and Computer Code for Predicting Detonation Wave Parameters of Aluminized Explosives

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ABSTRACT

In this work, the detonation wave parameters (i.e., the velocity of detonation and the detonation pressure) of aluminized explosives were calculated by the algorithm and computer code (named DETO). DETO is established based on the chemical equilibrium theory of detonation products, the hydrodynamic theory of the detonation process, and the Becker - Kistiakowsky - Wilson (BKW) equation of state. The aluminum content that reacts with detonation products on the detonation wavefront can be customized according to the user's assumptions. Compared to experimental data for several aluminized explosive types, the results calculated by DETO have the same, even higher accuracy than those calculated by other computer codes previously published. Specifically, the mean absolute deviation from experimental data is about 2 % for the velocity of detonation (VOD) and about 8 % for the pressure on the detonation wavefront. In addition, the study also confirmed that about 50 % of Al powders participate in the reaction on the detonation wavefront. The software can help researchers select the composition of explosives with and without aluminum according to the given detonation characteristics.

Keywords: Aluminized explosives; Computer code; Detonation wave; Pressure; VOD

1. INTRODUCTION

To improve the working capacity of explosives, Al powder is often used as an energetic additive[1]. Experimental studies show that the main factors, such as the content, particle size, and morphology of Al powder, affect the explosion properties (i.e., the VOD, the pressure on the detonation wavefront, the heat of explosion, etc.) of aluminized explosives[2-8]. Since Al mainly reacts with detonation products (i.e., CO, CO_2, H_2O, etc.) during the expansion process behind the detonation wavefront, computer codes such as FORTRAN BKW[9], TIGER[10], CEC71[11], CHEETAH[12], EXPLO5[13], LOTUSES[14], etc. can not accurately predict the detonation characteristics of aluminized explosives.

Hobbs & Baer[15] found that the calculation results of VOD of aluminized explosives would be consistent with the experimental data when assuming that 50 % of the Al powder reacted on the detonation wavefront. Unfortunately, they did not provide a specific algorithm, hence could not help readers build their computer codes to verify with previously published data.

Keshavarz[16-19], *et al.* have established a simple formula to determine the VOD of aluminized explosives based on the assumption that the proportion of Al reacting on the detonation wavefront depends on the elemental composition of explosives. Calculation results for many classes of aluminized explosives are consistent with experimental data and results calculated by a computer code using the BKWS equation of state. Jafari[20], *et al.*used the linear regression method to find the empirical formula for determining the pressure on the detonation wavefront of $C_aH_bN_cO_dF_eCl_fAl_g(NH_4NO_3)_h$ explosives. The issue with this method is that only a few individual parameters can be calculated, and the number of applied explosives is limited.

Zhang[21-22], *et al.*adjusted the coefficient *k* in the BKW equation of state to predict the VOD and pressure on the detonation wavefront of non-ideal aluminized explosives. These parameters calculated by this method agree well with the experimental data, with the deviation for the calculated VOD and pressure being less than 7 % and 9 %, respectively. In addition, these authors also calculated the coefficient in the Jones - Wilkins - Lee (JWL) equation of state to predict the air shock wave pressure. They also found that the composite explosives containing 30 % Al would produce the highest air shock wave pressure. Similarly, Li, *et al.*[23] adjusted the coefficients in the BKW equation of state to predict the detonation properties of explosives containing 2,4-dinitroanisole (DNAN), hexogen (RDX), octogen (HMX), and Al. However, these works did not present a method to adjust the coefficients in the BKW equation of state.

Li[24], *et al.* established a system of algebraic equations describing the detonation of explosives containing micrometer Al powder. In which, authors take into the effect of the acceleration of Al powder and the heat exchange between Al powder and detonation products on the VOD. However, the calculation requires using the coefficients in the JWL equation of state together with the assumption about the ratio of the velocity disequilibrium of the Al powder and the detonation product.

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This work focuses on developing an algorithm and a computer code to calculate the detonation wave characteristics of composite explosives containing Al powder, based on the chemical equilibrium and detonation theories, with the assumption that Al partial participates in a reaction zone on the detonation wavefront.

2. CALCULATION METHODS

2.1 System of Algebraic Equations describing Detonation Process

The algebraic equations describing the detonation are established based on the mass, momentum, and energy conservation laws[25]:

$$D_{CJ} = V_0\sqrt{\frac{P_{CJ} - P_0}{V_0 - V_{CJ}}} \tag{1}$$

$$U^2 = (P_{CJ} - P_0)(V_0 - V_{CJ}) \tag{2}$$

$$E_{CJ} - E_0 = \frac{1}{2}(P_{CJ} + P_0)(V_0 - V_{CJ}) \tag{3}$$

where, the symbol "CJ" stands for the Chapman-Jouguet point reflecting the state on the detonation wavefront; D_{CJ} - velocity of detonation; P_{CJ}, P_0 - the pressure on the detonation wavefront and the initial pressure of the explosive (i.e., atmospheric pressure); V_{CJ}, V_0 - specific volume of the detonation product on the detonation wavefront and of the initial explosive; U - the velocity of the detonation product; E_0, E_{CJ} - the specific internal energy of the explosive at the point (P_0, V_0) and of the detonation product at C-J point (P_{CJ}, V_{CJ}), respectively, which are functions dependent on pressure and specific volume. Eqn. (3) is also known as the Hugoniot adiabatic equation.

To describe detonation products at high pressure and temperature, the authors use the BKWR equation of state for gases[15] and the Cowan-Ficket equation for solid products (e.g., graphite, Al, Al_2O_3)[9]. These equations can be expressed in the general form:

$$f\left(P_{CJ}, V_{CJ}, T_{CJ}\right) = 0 \tag{4}$$

A detonation occurs when the Chapman-Jouguet hypothesis is accepted (also known as the "condition of contact"):

$$D - U = a_{CJ} \tag{5}$$

where, a_{CJ} is the speed of sound in the detonation product on the detonation wavefront, its value depends on P_{CJ} and V_{CJ}.

Five parameters of the detonation wave (i.e., P_{CJ}, V_{CJ}, T_{CJ}, D_{CJ}, U) are determined by solving the system of algebraic equations (from Eqn. (1) to Eqn. (5)) according to following algorithm:

2.2 Algorithm

To reuse many times throughout the algorithm, the authors build two separate blocks:

Block I. Given the pressure P and temperature T, the equilibrium compositions of the detonation products were calculated according to the principle of minimum Gibbs free energy[26]. Assume that each detonation product has the corresponding mole number X_i. When the pressure P and the temperature T are known, the chemical equilibrium occurs when the Gibbs free energy of the detonation product composition $g(X_1, X_2, \ldots, X_i, ..)$ reaches the minimum value. Thus, determining the chemical equilibrium compositions of the detonation products $X_1, X_2, \ldots, X_i, \ldots$ is an optimization problem to find the minimum of the Gibbs free energy function with the constraint that the material balance equations for each chemical element in the explosives are:

$$\sum_{i=1}^{NT} \alpha_{i,k} X_i - b_k = 0 \qquad (k = 1, ..., M) \tag{6}$$

where, M - the total number of chemical elements in the system; b_k - the mole number of kth constituent in the explosive mixture; $\alpha_{i,k}$ - the mole number of the kth element in the ith detonation product.

Because the aluminum does not burn completely on the detonation wavefront, the algorithm allows fixing the Al content that has not participated in the reaction (i.e, the contents of Al and Al_2O_3 in the detonation product are fixed). Then, calculate the total internal energy E_{CJ} and specific volume V_{CJ} of the detonation product. This calculation must use the BKWR equations of state and Cowan-Fickett equations.

The BKWR equations of state for gaseous detonation products has the form:

$$\frac{pV_g}{RT} = 1 + xe^{\beta x} \tag{7}$$

where, $x = \frac{K}{V_g(T+\theta)^{\alpha}}$; $K = \chi\sum_i n_i k_i$; n_i, k_i represent the mole fraction and covolume of ith constituent in the detonation product, respectively; $\alpha = 0.5$, $\beta = 0.176$, $\chi = 11.8$ and $\theta = 1850$ are the empirical constants; p, V_g, T represent the pressure, gas volume and temperature of the detonation product, respectively.

The Cowan-Fickett equations of state for solid detonation products has the form:

$$p = p_1(V_s) + a(V_s)T_v + b(V_s)T_v^2 \tag{8}$$

where,

$p_1(V_s) = a_0 + a_1\eta + a_2\eta^2 + a_3\eta^3 + a_4\eta^4$;

$a(V_s) = a_5 + a_6\eta$; $b(V_s) = a_7 + a_8\eta^{-1} + a_9\eta^{-2}$; $a_1 \div a_7$ are the empirical constants; $\eta = \rho/\rho_0$ is the compression ratio of solids; ρ, ρ_0 are the density of solid at the present temperature and at the standard temperature, respectively; T_v = T/11605.6 (K).

Block II. (Block I is done). Given the pressure P, the temperature T was determined by solving the Hugoniot equation (3) using the secant method. The parameters on the detonation wavefront are determined according to the Chapman-Jouguet "condition of contact", namely determining the minimum point (P_{min}, D_{min}) of the function $D(P)$. The algorithm for finding the minimum point using an iterative method for finding the minimum of a parabola passing through three points (P_i, D_i) calculated by Eqn. (1):

$$P_{\min} = \frac{1}{2}\frac{P_1^2(D_3 - D_2) + P_2^2(D_1 - D_3) + P_3^2(D_2 - D_1)}{P_1(D_3 - D_2) + P_2(D_1 - D_3) + P_3(D_2 - D_1)} \quad (9)$$

The convergence criterion is that the difference between two of the three values D_1, D_2, D_3 is less than a given deviation.

The algorithm diagram for determining the parameters on the detonation wavefront of aluminized explosives is shown in Fig.1. Based on this algorithm, the authors have established the algorithm and computer code, named DETO, to predict the detonation wave parameters of many conventional explosives as well as aluminized explosives.

3. RESULTS AND DISCUSSIONS

Table 1 presents the calculated results of the velocity of detonation D_{CJ} and the pressure P_{CJ} of four two-component explosives, containing single explosives HMX, RDX, TNETB, TNT, and Al by using the DETO program. Every explosive was mixed with Al in a different mass ratio (values in parentheses). The unreacted Al content on the detonation wavefront is selected as 50%. The results are compared with experimental data (in the column "Exp.") and previously calculated values of the other computer code[15]. In this literature, the calculation used the BKWS equation of state with the assumption that 50% of Al participates in the reaction. For each calculated value by DETO or BKWS, the deviation from the experimental data is determined by the formula:

$$Dev. = \frac{X_{Cal.} - X_{Exp.}}{X_{Exp.}} \quad (10)$$

where: *Dev.* is the deviation between the calculated result and the experiment data; $X_{Cal.}$, $X_{Exp.}$ are the calculated and experimental values, respectively.

As shown in Table 1, both experimental and calculated results confirm that, with increasing aluminum content, the D_{CJ} and the P_{CJ} values both decrease, even though the density increases. The absolute deviations of D_{CJ} values obtained using the DETO code and BKWS code range from 0.2 to 6.0% (with an average of 1.6%) and 0.5 to 11.6% (with an average of 2.9%), respectively. On the other hand, the absolute deviations of P_{CJ} values determined using DETO and BKWS computer codes range from 1.1 to 24.2% (with an average of 7.7%) and 1.0 to 37.4% (with an average of 8.1%), respectively. Thus,

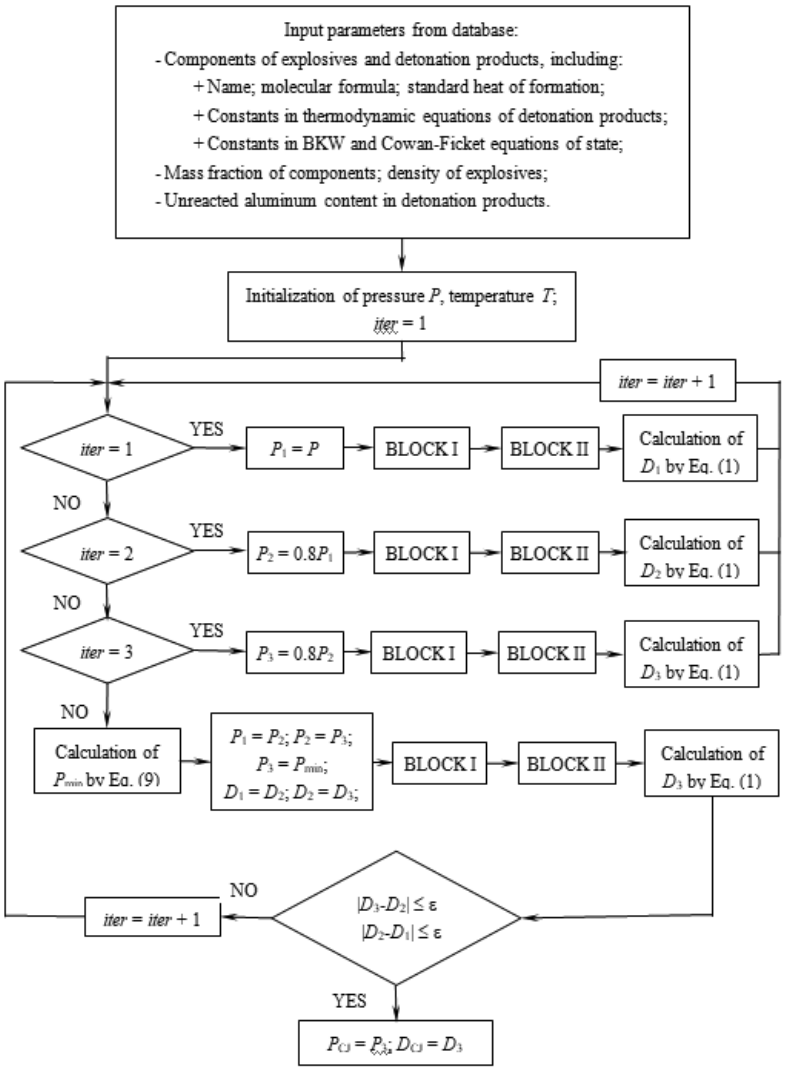

Figure 1. Algorithm diagram for determining detonation wave parameters of aluminized explosives.

Table 1. Comparison of D_{CJ} and P_{CJ} values of some aluminized two-component explosives calculated by DETO with experimental and calculated data in the literature[15]

Explosives	Parameters	Exp.	BKWS		DETO	
			Value	Dev., %	Value	Dev., %
HMX/Al (90/10) ρ_0 = 1.76 g/cm^3	D_{CJ} (km/s)	8.3	8.41	1.3	8.41	1.3
	P_{CJ} (GPa)	-	28.5	-	29.3	-
HMX/Al (80/20) ρ_0 = 1.82 g/cm^3	D_{CJ} (km/s)	8.3	8.22	-1.0	8.28	-0.2
	P_{CJ} (GPa)	-	26.8	-	27.7	-
HMX/Al (70/30) ρ_0 = 1.86 g/cm^3	D_{CJ} (km/s)	8.0	7.82	-2.3	7.87	-1.6
	P_{CJ} (GPa)	-	23.5	-	24.4	-
HMX/Al (60/40) ρ_0 = 1.94 g/cm^3	D_{CJ} (km/s)	7.7	7.46	-3.1	7.67	-0.4
	P_{CJ} (GPa)	-	20.4	-	21.8	-
RDX/Al (90/10) ρ_0 = 1.68 g/cm^3	D_{CJ} (km/s)	8.03	8.08	0.6	8.10	0.9
	P_{CJ} (GPa)	24.6	25.7	4.5	26.5	7.7
RDX/Al (80/20) ρ_0 = 1.73 g/cm^3	D_{CJ} (km/s)	7.77	7.81	0.5	7.88	1.4
	P_{CJ} (GPa)	22.7	23.7	4.4	24.6	8.4
RDX/Al (70/30) ρ_0 = 1.79 g/cm^3	D_{CJ} (km/s)	7.58	7.49	-1.2	7.55	-0.4
	P_{CJ} (GPa)	21.0	21.2	1.0	22.3	6.2
RDX/Al (60/40) ρ_0 = 1.84 g/cm^3	D_{CJ} (km/s)	7.2	6.93	-3.8	7.14	-0.8
	P_{CJ} (GPa)	21.1	17.4	-17.5	19.0	-10.0
RDX/Al (50/50) ρ_0 = 1.89 g/cm^3	D_{CJ} (km/s)	6.81	6.02	-11.6	6.58	-3.4
	P_{CJ} (GPa)	19.0	11.9	-37.4	14.4	-24.2
TNETB/Al (90/10) ρ_0 = 1.75 g/cm^3	D_{CJ} (km/s)	8.12	7.91	-2.6	8.02	-1.2
	P_{CJ} (GPa)	26.2	25.8	-1.5	26.5	1.1
TNETB/Al (80/20) ρ_0 = 1.82 g/cm^3	D_{CJ} (km/s)	7.99	7.73	-3.3	7.90	-1.1
	P_{CJ} (GPa)	24.8	24.4	-1.6	26.1	5.2
TNETB/Al (70/30) ρ_0 = 1.88 g/cm^3	D_{CJ} (km/s)	7.84	7.43	-5.2	7.66	-2.3
	P_{CJ} (GPa)	22.7	21.9	-3.5	23.8	4.8
TNT/Al (89.4/10.6) ρ_0 = 1.72 g/cm^3	D_{CJ} (km/s)	7.05	7.12	1.0	7.10	0.7
	P_{CJ} (GPa)	-	2.00	-	19.91	-
TNT/Al (78.3/21.7) ρ_0 = 1.80 g/cm^3	D_{CJ} (km/s)	7.05	6.94	-1.6	6.94	-1.6
	P_{CJ} (GPa)	18.9	18.7	-1.1	18.6	-1.6
TNT/Al (67.8/32.2) ρ_0 = 1.89 g/cm^3	D_{CJ} (km/s)	7.05	6.71	-4.8	6.63	-6.0
	P_{CJ} (GPa)	-	16.8	-	16.8	-

both results calculated according to DETO as well as BKWS are similar to the experimental data, especially the detonation velocity values. It can be predicted that for aluminized explosives, about 50% of Al powders participate in the reaction on the detonation wavefront. This content can vary depending on the size, and morphology of the Al particles. In addition, the calculation results according to the DETO code are more accurate than those of the BKWS code.

Table 2 presents the detonation velocity and pressure on the detonation wavefront of several common aluminized explosives using the DETO computer program with the assumption that 50% of Al participates in the reaction on the detonation wavefront.

The composition of these explosives contains high explosive, Al powder, and several non-explosive organic substances. The calculated results are compared to the

Table 2. Comparison of D_{CJ} and P_{CJ} values of several common aluminized explosives calculated by DETO with experimental and calculated data in the literature[9]

Explosives	Parameters	Exp.	BKW (RDX TYPE)		DETO	
			Value	Dev., %	Value	Dev., %
Alex 20 (ρ_0 = 1.801 g/cm^3) RDX/TNT/Al/Wax (44/32.2/19.8/4)	D_{CJ} (km/s)	7.53	7.50	-0.4	7.62	1.2
	P_{CJ} (GPa)	23.0	25.2	9.6	22.9	-0.4
Alex 32 (ρ_0 = 1.88 g/cm^3) RDX/TNT/Al/Wax (37.4/27.8/30.8/4)	D_{CJ} (km/s)	7.30	7.07	-3.2	7.48	2.5
	P_{CJ} (GPa)	21.5	21.3	-0.9	21.1	-1.9
HBX-1 (ρ_0 = 1.72 g/cm^3) RDX/TNT/Al/Wax (40/38/17/5)	D_{CJ} (km/s)	7.22	7.27	0.7	7.32	1.4
	P_{CJ} (GPa)	-	22.9	-	20.8	-
HBX-3 (ρ_0 = 1.81 g/cm^3) RDX/TNT/Al/Wax (31/29/35/5)	D_{CJ} (km/s)	6.92	6.85	-1.0	6.94	0.3
	P_{CJ} (GPa)	-	19.5	-	17.4	-
H6 (ρ_0 = 1.71 g/cm^3) RDX/TNT/Al/Wax (45/30/20/5)	D_{CJ} (km/s)	7.19	7.24	0.7	7.21	0.3
	P_{CJ} (GPa)	-	22.5	-	20.0	-
Torpex (ρ_0 = 1.81 g/cm^3) RDX/TNT/Al (42/40/18)	D_{CJ} (km/s)	7.50	7.49	-0.1	7.73	3.1
	P_{CJ} (GPa)	-	25.9	-	24.2	-
PBXN-1 (ρ_0 = 1.77 g/cm^3) RDX/Al/Nylon (68/20/12)	D_{CJ} (km/s)	7.93	7.69	-3.0	7.71	-2.8
	P_{CJ} (GPa)	24.5	25.4	3.7	23.0	-6.1
Destex (ρ_0 = 1.68 g/cm^3) TNT/Al/Wax/Graphite (74.766/18.691/4.672/1.869)	D_{CJ} (km/s)	6.65	6.44	-3.2	6.42	-3.5
	P_{CJ} (GPa)	17.5	17.4	-0.6	15.4	-12.0

experimental data (in the column "Exp.") and the calculated values according to the BKW computer code published in the literature[9]. It should be noted that the calculation by the BKW code uses the BKW equation of state (RDX Type).

Similar to two-component explosives, the D_{CJ} and P_{CJ} values calculated by DETO and BKW (type RDX) are also in good agreement with the experimental data. The absolute deviations of D_{CJ}, determined by using DETO, range from 0.3 to 3.6 % (with an average of 1.9 %), while that using the BKW (RDX Type) is in the range of 0.1 to 3.2 % (with an average of 1.5%). For the P_{CJ} values, the calculated absolute deviations of DETO vary from 0.4 to 12.0 % (with an average of 5.1 %), and that of BKW (RDX Type) is in the range of 0.6 to 9.6 % (with an average of 3.7 %). Therefore, the BKW (RDX Type) computer program is slightly more accurate than the DETO program. However, it should be noted that the calculation conditions of BKW (RDX type) and DETO may be different because the literature[9] did not indicate the Al content participating in the reaction on the detonation wavefront.

4. CONCLUSION

To predict the parameters on the detonation wavefront of aluminized explosives, a reasonable and feasible approach is the combination of the method of determining the balanced compositions of detonation products based on the principle of minimum Gibbs free energy and the assumption that only partially Al participates in the reaction.

To solve the system of algebraic equations describing the detonation process, the authors have established an algorithm, in which the Chapman-Jouguet hypothesis is expressed as finding the minimum point of the VOD function depending on pressure. The calculated detonation wave parameters of several aluminized explosives using the DETO computer program are in good agreement with the experimental data. Besides that, the calculated results of DETO have the same and even higher accuracy than those calculated by other computer codes previously published.

In addition, for aluminized explosives in this study, it can be predicted that about 50 % of Al powders participate in the reaction on the detonation wavefront.

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CONTRIBUTORS

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