

A New Method for Predicting the Detonation Velocity of Explosives with Micrometer Aluminum Powders

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Abstract: In the present study we carried out a thermodynamic analysis for explosives with micrometer aluminum (Al) powders, and found that the acceleration of Al powders and heat exchange between Al powders and the detonation products may have a significant influence on the detonation velocity. Relying on velocity disequilibrium between the two phases at the C–J plane and heat absorption of inert Al powders in the detonation zone, this paper has introduced a new method to study the detonation velocity

of explosives with micrometer Al additives. The method is a closed system of algebraic equations and the detonation velocity can be solved efficiently by numerical codes. The detonation velocities predicted by the new method are in excellent agreement with experimental data of RDX-, HMX-, NM- and TNT-based aluminized explosives, and the heat exchange has been proved significant on the detonation velocity, while the acceleration of Al powders is of little effect.

Keywords: aluminized explosives • micrometer Al powders • detonation velocity • heat exchange • Al acceleration

1 Introduction

In order to find new explosives with better performances, many new explosives are fabricated by adding aluminum (Al) additives to organic explosives. A good potential of aluminized explosives exists as the combustion enthalpy of Al is nearly five times that of normal high explosives. However, the detonation performances of the aluminized explosives, e.g., detonation velocity, are not comparable with the matrix explosives, and the detonation deficit enlarges [1,2] when the size of Al powders is small or the content of Al becomes large. Furthermore, the protective effect of the oxidation layer covering the Al powders strongly delays the reaction of Al [3–5], therefore Al powders commonly participate in detonation as inert ingredients and much combustion heat is released in post-detonation [6,7]. The detonation deficit and the secondary reaction in post-detonation are the two characteristics of non-ideal aluminized explosives.

Keshavarz et al. [8–10] proposed a series of empirical equations to calculate the detonation velocity of aluminized explosives, and they are useful for many aluminized explosives. Many codes have been introduced to calculate the detonation velocity of the aluminized explosives, e.g., BKW [11], RUBY [12], TIGER [13], CHEETAH [14] KHT [15] and WK [16]. Although much work has been done, application of these models to a wide range of aluminized explosives is still limited, and the deviations are sometimes too large to be tolerated. A large body of analyses of the great differences between the experimental detonation velocities and the calculated results upon the multiphases equilibrium assumption has been accumulated [8,11], and it may generally result from the non-equilibrium within the detonation components of aluminized explosives.

Through the detonation of organic explosives, thermodynamic equilibrium is maintained within mixture of unreacted explosives and detonation products, which is called matrix in brief below. However, the thermodynamic relation between Al powders and the matrix may be more complicated for aluminized explosives. According to the study of Li [17], if the difference of particle velocities increases between Al powders and the matrix, the detonation velocity would be higher. Kapila [18] and Pei [19] et al. believe that the larger the difference of the temperatures between Al powders and the matrix, the higher the detonation velocity. The reaction of Al powders consumes a lot of gas and releases much heat, and the two processes have both negative and positive effects on the detonation velocity, respectively. Through a calculation of detonation zone by the BKW code, Keshavarz [10], Hobbs and Baer [20] et al. found that the temperature of the detonation products corresponding to 50% Al reacted is lower than that corresponding to 100% Al reacted, which benefits from the high reaction heat of Al. However, the detonation velocities upon 50% Al reacted are higher than that of 100% Al reacted, and it was explained that the negative effect dominates.

Based on the analysis above, both the non-equilibrium between Al powders and the matrix and the reaction properties of Al in detonation zone have great influences on the detonation velocity of aluminized explosives. The addition

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of micrometer Al powders (approximately 2–20 micrometers) is popular as the corresponding aluminized explosives exhibit excellent detonation performances and secondary working capabilities [21]. However, researches based on the disequilibrium of phases within the detonation zone are still lacking. By considering the velocity and temperature disequilibrium between inert Al powders and the detonation products at the C–J plane (no more unreacted explosives), this paper proposed a new method to predict the detonation velocities of explosives with micrometer Al powders. The new method was applied for HMX-, RDX-, NM- and TNT-based aluminized explosives and it shows a higher accuracy than other models.

2 Calculation Method

2.1 Analysis and Estimation of the Key Mechanisms

The detonation zone of aluminized explosives is constructed by a shock front and a following reaction zone. The initial pressure, temperature and particle velocity of Al powders are less than those of the matrix behind the shock front [17] as there is a great difference in the thermodynamic properties between them. Therefore the disequilibrium of pressures, temperatures and velocities between Al powders and the matrix may be kept for a long period throughout the reaction zone.

2.1.1 Research of Pressure Disequilibrium

Petitpas et al. [22] proposed that the time Al particle needed to get a pressure equilibrium in the flow field can be estimated by the following equation:

$$\tau_p \approx \frac{d}{C} \quad (1)$$

where τ_p is time to pressure equilibrium, d and C are the particle diameter and sonic velocity of Al particle, respectively. Huang et al. [23] suggested that C should be turned from 5.4 Km/s to 5.545 Km/s. In the particle diameter range of 0.1–20 μm , the time varies from 0.02 ns to 20 ns, and it is comparable to the length of shock front. So the micrometer Al powders would reach a pressure equilibrium with the matrix rapidly in the detonation zone.

2.1.2 Research of Velocity Disequilibrium

The matrix would drive Al powders in the reaction zone as Al powders have a lower initial velocity behind the front shock. Part of kinetic and internal energy of the matrix is transformed into the kinetic energy of Al powders throughout the acceleration. In the reaction zone, a stronger accel-

eration of Al powders would lead to a lower internal energy of the matrix and weaker detonation properties of explosives. For the mixture of Al powders and matrix, the velocity U^* is defined as the average of the two phases velocities:

$$U^* = Y_1 U_1 + Y_2 U_2 \quad (2)$$

where U is the particle velocity and Y the mass fraction, subscript 1 is for matrix and 2 for Al powders. If there is a velocity disequilibrium between the two phases, the velocity ratio R_u is defined:

$$R_u = U_2 / U_1 \quad (3)$$

Combining Equation (2) and (3), the kinetic energy of Al powders E_k is obtained:

$$E_k = \frac{1}{2} Y_2 \frac{R_u^2}{(Y_1 + Y_2 R_u)} U^{*2} \quad (4)$$

R_u has a minimum, i.e., $R_{u\text{MIN}}$, just behind the shock front, and it roughly equals to the density ratio of ρ_{10}/ρ_{20} , where ρ_{10} and ρ_{20} are the initial density of the matrix explosives and Al powders, respectively. If the two phases reach the same velocity in the reaction zone, the kinetic energy of Al powders would be the largest and the matrix would have a maximum loss in internal energy. Therefore the maximum kinetic energy of Al powders $E_{k\text{MAX}}$ can be computed through Equation (4) when R_u has a maximum of 1:

$$E_{k\text{MAX}} = \frac{1}{2} Y_2 U^{*2} \quad (5)$$

As the original method of this paper is on the assumption of velocity equilibrium, original internal energy of the mixture of matrix and Al powders is the minimum. If there is a velocity disequilibrium between Al powders and matrix, the original internal energy of the mixture needs to be modified. In this paper, it is assumed that the energy consumed to drive Al powders comes from the internal energy of the matrix. Referring to the above analysis, $(E_{k\text{MAX}} - E_k)$ is the extra costing energy for Al powders to achieve the velocity equilibrium and it should be added to the original internal energy of the mixture if the velocity disequilibrium still exists.

2.1.3 Research of Temperature Disequilibrium

In the reaction zone, the hot matrix with a temperature of 3000 K–4000 K would transfer heat to the ambient cold Al powders. Since the specific surface area of Al powders is inversely proportional to its diameter, a smaller size of Al powders results in a higher efficiency of heat absorption [19]. Li proposed a temperature increasing rate for Al powders due to heat convection [17]:

$$\frac{dT_2}{dt} = \frac{6K_1N_u(T_1 - T_2)}{\rho_2 C_{p2} d_2^2} \quad (6)$$

where T_2 is the temperature of Al powders, and T_1 is the temperature of matrix. t is the time, and K_1 is the heat conduction coefficient of detonation products, which is $0.32 \text{ W} \times \text{m}^{-1} \times \text{K}^{-1}$. N_u is the Nusselt number with a value of 46.57. $(T_1 - T_2)$ is the temperature difference, and it is assumed to be a constant of 3000 K during calculation. ρ_2 and C_{p2} are the density and specific heat of Al powders, respectively. The increase of internal energy due to heat conduction can be estimated for Al powders through an integration of Equation (6):

$$\Delta e = \frac{6K_1N_u(T_1 - T_2)T_R}{\rho_2 d_2^2} \quad (7)$$

where Δe is the increase of the internal energy of Al powders due to heat conduction, and T_R is the time length of detonation zone.

2.1.4 Reaction Properties of Micrometer Al Powders

Miller et al. [24] suggested that nanoscale Al powders may partially react in the detonation zone, while it may take more time for a larger size to be ignited. For micrometer and larger size, Friedman and Maček [25] proposed that the reaction of Al powders would be delayed until its temperature is high enough to reach the melting point of Al_2O_3 (approximately 2300 K). Lewis [26], Leiper and Cooper [27] et al. recognized that this reaction delay is several microseconds for micrometer Al powders through spectrum tests, which is dozens of times that of the detonation zone (about 100 ns) [28]. As the micrometer Al powders behaves chemically inert in the detonation zone, the reaction heat of the aluminized explosives released at the C–J plane generally comes from the detonation heat of the matrix explosives.

2.2 Governing Equations

Since all the matrix explosives have been transformed into the detonation products at the C–J plane of aluminized explosives, the mixture of Al powders and the detonation products satisfies the following C–J detonation relations based on the pressure equilibrium.

Mass conservation:

$$\rho_{CJ}(U^* - D) + \rho_0 D = 0 \quad (8)$$

where ρ and D represent the density and detonation velocity of the mixture, respectively. U^* is the mean velocity of the two phases, as described above. The subscript *CJ* de-

notes the C–J state and the subscript 0 denotes the initial state.

Momentum conservation:

$$P_{CJ} - P_0 = \rho_0 D U^* \quad (9)$$

where P is the pressure of the mixture.

The original C–J internal energy is obtained based on the velocity equilibrium within all components. To study the effect of velocity disequilibrium at the C–J plane, the original C–J internal energy needs to add $(E_{k\text{MAX}} - E_k)$ as a correction according to the analysis in Section 2.1.2. Therefore the energy conservation of the mixture upon velocity disequilibrium is:

$$e_{CJ} - e_0 = \frac{1}{2} P_{CJ} \left(\frac{1}{\rho_0} - \frac{1}{\rho_{CJ}} \right) + Q + \frac{1}{2} Y_2 U^{*2} \left[1 - \frac{R_u^2}{(Y_1 + Y_2 R_u)} \right] \quad (10)$$

where e is the specific internal energy of the mixture, and Q stands for reaction heat of the mixture released at the C–J plane. As micrometer Al powders keep inert in the detonation zone, Q equals to the detonation heat of the matrix explosives, and Y_1 and Y_2 remain unchangeable.

C–J condition:

$$D = U^* + C_{CJ} \quad (11)$$

where C represents the sonic speed of the mixture. For the mixture, the mass coupling method is applied for the density and the internal energy, while the volumetric coupling method is used for the sonic speed [29]:

$$1/\rho_{CJ} = Y_1/\rho_1 + Y_2/\rho_2 \quad (12)$$

$$e_{CJ} = Y_1 e_1 + Y_2 e_2 \quad (13)$$

$$1/C_{CJ}^2 = \rho \varphi_1 / (\rho_1 C_1^2) + \rho \varphi_2 / (\rho_2 C_2^2) \quad (14)$$

where φ_i represent the volume fraction at the C–J plane.

The equations of states (EOS) are also needed to complete the method. The JWL EOS is applied for the detonation products:

$$P = A \left(1 - \frac{\omega}{R_1 \bar{v}} \right) \exp(-R_1 \bar{v}) + B \left(1 - \frac{\omega}{R_2 \bar{v}} \right) \exp(-R_2 \bar{v}) + \omega e p \quad (15)$$

$$C^2 = (AR_1 \exp(-R_1 \bar{v}) + BR_2 \exp(-R_2 \bar{v}) + c(\omega + 1) \bar{v}^{(-\omega-2)}) \bar{v}^2 / \rho_0 \quad (16)$$

Table 1. The JWL parameters and T_R of HMX, RDX, NM and TNT.

Explosive	$\rho/g \times cm^{-3}$	$D/km \times s^{-1}$	A/GPa	B/GPa	c/GPa	R_1	R_2	ω	$T_R[28]/ns$
HMX[32]	1.725	8.587	681.4	10.10	1.60	4.3	1.25	0.3	100
RDX[33]	1.650	8.190	640.0	17.60	1.98	4.5	1.35	0.3	100
NM[18]	1.128	6.290	209.25	5.69	0.77	4.4	1.20	0.3	60
TNT[34]	1.580	6.836	371.2	3.231	1.045	4.15	0.95	0.3	280

where A , B , R_1 , R_2 , c and ω are the JWL constants, and $\bar{v} = \rho_0/\rho_1$ is the density ratio.

The micrometer Al powders are regarded as pure substance of Al since the content of surface oxidation layer is small. The Murnaghan EOS for Al [30] is:

$$P = m(\bar{v}^{-n} - 1) \quad (17)$$

where m is 18.17 GPa and n is 4.352. Since the isentropic compression line of Al is almost identical to its shock compression line below 50 GPa, the sonic velocity of Al can be derived from Equation (17):

$$C^2 = \frac{mn}{\rho_0} \bar{v}^{(1-n)} \quad (18)$$

According to the analysis of heat transfers in the detonation zone, the internal energy of Al is modified:

$$e - e_0 = \frac{P\bar{v} - mn(1 - \bar{v})}{(n-1)\rho_0} + \frac{6K_1 N_u (T_1 - T_2) T_R}{\rho_2 d_2^2} \quad (19)$$

and the values of variables in Equation (19) are mentioned in Section 2.1.3.

The new method is a closed system of algebraic equations from Equation (8) to (19), which contains 12 variables: D , ρ_1 , ρ_2 , φ_1 , φ_2 , C_1 , C_2 , P_{CJ} , e_1 , e_2 , e_{CJ} , U^* . The numerical codes are helpful for the efficient solution of D . In the process of finding a root, an initial solution is assumed, and then the numerical codes begin to search for a root within a certain radius of the initial solution. When the errors are smaller than the set values, the calculation stops and the results come out. In this paper, the absolute values of the set errors are less than $1E-6$ under the basic units of cm-g- μ s.

2.3 Initial Conditions

For the solution of the algebraic equation system, R_u , T_R and Q are needed as initial conditions. R_u can be adjusted artificially, T_R refers to the experimental data of matrix explosives [28], and the value of Q can be obtained through the detonation heat of matrix explosives.

For the matrix explosive $C_4H_8N_8O_8$ with a density of ρ_{10} , J.I. OPJEHKO [31] give a reliable calculation method for the detonation heat:

$$Q_{\rho_{10}} = Q_{\max} \left[1 - (0.528 - 0.165\rho_{10})(1.4 - \alpha)^{1.4} \left(1 - \left(\frac{b}{a+c} \right)^{(3.73-2.28\rho_{10})/(1.4-\alpha)^2} \right) \right] \quad (20)$$

where $Q_{\rho_{10}}$ is the detonation heat in $J \times g^{-1}$, ρ_{10} is in g/cm^3 . In Equation (20), α is a non-dimensional coefficient, and the definition is:

$$\alpha = \frac{d}{2a + b/2} \quad (21)$$

Q_{\max} is the theoretical maximum detonation heat:

$$Q_{\max} = \frac{128.8b + 196.5(d - b/2) + 4.18\Delta H}{M} \quad (22)$$

where Q_{\max} is in $J \times g^{-1}$, ΔH is the enthalpy of formation of explosive in $kJ \times mol^{-1}$, and M is the molecular weight of explosive in $kg \times mol^{-1}$. If the density of matrix component keeps ρ_{10} in the aluminized explosive, it is easy to get Q from Equation (20) to (22):

$$Q = Y_1 Q_{\rho_{10}} \quad (23)$$

3 Calculation Results

The new method is applied to compute the detonation velocities of HMX-, RDX-, NM- and TNT- based explosives with micrometer Al additives, and the calculated results are compared with those of other models and measured values. The JWL parameters [18,32–34] and T_R [28] of the matrix explosives are listed in Table 1.

3.1 HMX-based Aluminized Explosives

The Al powders used in production of the HMX-based Aluminized explosives [35] is in average size of 13 μ m. There are 5% (mass fraction) inert binders in the aluminized explosive, and its influence on Q can be neglected due to the small content. The molecular formula of HMX is $C_4H_8N_8O_8$, and the enthalpy of formation is 74.822 kJ/mol. The density of the matrix explosives is assumed to remain unchanged and equals to the density of H0 in various HMX-based Aluminized explosives for calculation convenience, so Q could

Table 2. Calculated detonation velocities of HMX containing Al powders (13 μm).

Formula NO.	Mass percent		$\rho/\text{g} \times \text{cm}^{-3}$	$Q/\text{J} \times \text{g}^{-1}$	$D_{\text{exp}}[35]/\text{km} \times \text{s}^{-1}$	$D_{\text{this paper}}/\text{km} \times \text{s}^{-1}$	R_u	error* %
	HMX	Al						
H0	100	0	1.721	5195.7	8.584	8.673	—	1.041
H1	90	10	1.781	4676.2	8.452	8.518	1	0.781
						8.525	0.820	0.864
						8.531	0.639**	0.935
H2	80	20	1.844	4156.6	8.313	8.365	1	0.626
						8.377	0.820	0.770
						8.389	0.639**	0.914
H3	70	30	1.905	3637.0	8.141	8.169	1	0.344
						8.185	0.820	0.540
						8.201	0.639**	0.737
H4	60	40	1.971	3117.4	7.969	7.951	1	−0.226
						7.969	0.820	0
						7.988	0.639**	0.238
H5	50	50	2.029	2597.9	7.621	7.635	1	0.184
						7.653	0.820	0.420
						7.674	0.639**	0.695

Note: * $\text{error} = (D_{\text{new}} - D_{\text{exp}}) \times 100 / D_{\text{exp}}$; **The value of $R_{u\text{MIN}}$

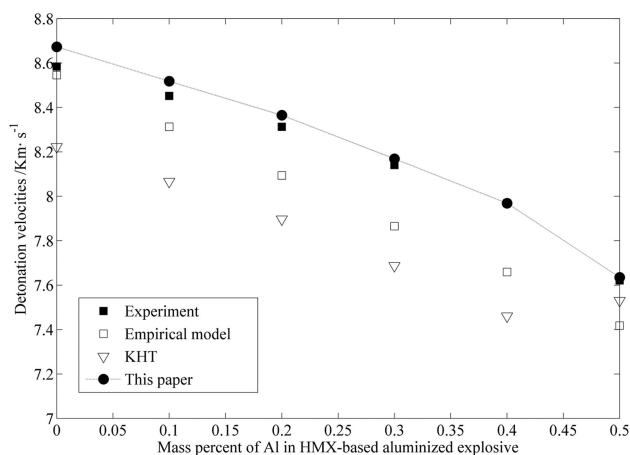
be computed according to Equation (20) to (23). The calculation results of Q and the detonation velocities of HMX-based aluminized explosive are shown in Table 2.

As shown in Table 2, Q declines as the content of Al powders increases, therefore the energy used to support propagation of the detonation wave is less and the detonation velocity decreases. The results in Table 2 also reveal that the computed detonation velocities reach a better agreement with the experimental values generally under the condition of $R_u = 1$, indicating that the Al powders can be accelerated to get a velocity equilibrium rapidly in the reaction zone. However, as the change in the kinetic energy of Al powders is two orders of magnitude smaller than the internal energy of the mixture, the differences between the detonation velocities corresponding to various R_u is less than 0.5% for H1~H5 samples. Therefore, the velocity disequilibrium within the two phases has a little impact on the detonation velocity of HMX-based aluminized explosives. The detonation velocities of the new method upon the optimal R_u , which equals to 1, are compared with that of other models in Figure 1. It can be concluded from Figure 1 that the new method has a higher degree of precision than KHT model and empirical model [36].

3.2 RDX-Based Aluminized Explosives

The molecular formula of RDX is $\text{C}_3\text{H}_6\text{N}_6\text{O}_6$, and its enthalpy of formation is 61.446 kJ/mol. The average size of Al additives in RDX-based aluminized explosive [35] is 13 μm and the content of the inert binder is 5%. The calculated detonation velocities of the new method are listed in Table 3.

The relation between the optimal R_u and Al content is more complicated for RDX-based aluminized explosives

**Figure 1.** The relation between detonation velocities and Al content in HMX containing 13 μm Al powders.

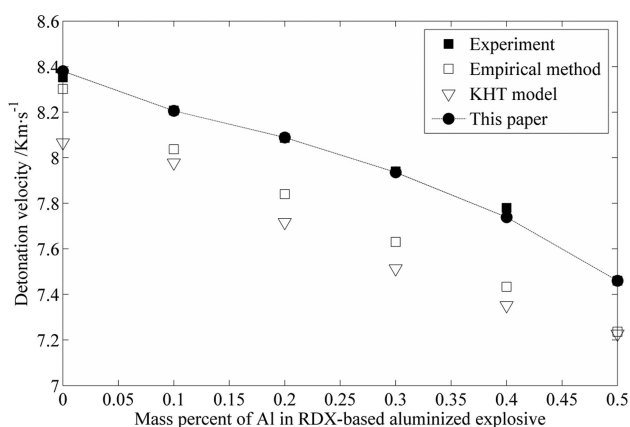
than that of HMX containing 13 μm Al powders. In Table 3, the optimal R_u is 1 when Al content is 10%; When the Al content increases to 20%, the optimal R_u is 0.809; while the optimal R_u equals to $R_{u\text{MIN}}$ if Al content is larger. This phenomenon may result from the weaker detonation performances of RDX when compared to HMX, therefore the detonation products of RDX are not powerful enough to drive Al powders drastically when the content of matrix explosive is small. Under the optimal R_u , the deviation of detonation velocities between the new method and the experimental data is less than 0.527%.

A comparison of detonation velocities with other models and the experimental values is shown in Figure 2. By comparing the results in Figure 2, it is clear that the new

Table 3. Calculated detonation velocities of RDX containing Al powders (13 μm).

Formula NO.	Mass percent		$\rho/\text{g} \times \text{cm}^{-3}$	$Q/\text{J} \times \text{g}^{-1}$	$D_{\text{exp}}[35]/\text{km} \times \text{s}^{-1}$	$D_{\text{this paper}}/\text{km} \times \text{s}^{-1}$	R_u	error* %
	RDX	Al						
R0	100	0	1.667	5181.1	8.353	8.380	–	0.322
R1	90	10	1.720	4663.2	8.207	8.206	1	–0.012
						8.213	0.809	0.073
						8.219	0.617**	0.146
R2	80	20	1.788	4144.9	8.087	8.076	1	–0.136
						8.089	0.809	0.025
						8.101	0.617**	0.173
R3	70	30	1.853	3627.0	7.940	7.902	1	–0.479
						7.919	0.809	–0.264
						7.936	0.617**	–0.050
R4	60	40	1.921	3108.7	7.780	7.699	1	–1.041
						7.719	0.809	–0.784
						7.739	0.617**	–0.527
R5	50	50	1.989	2590.8	7.460	7.440	1	–0.268
						7.460	0.809	0
						7.482	0.617**	0.295

Note: * error = $(D_{\text{new}} - D_{\text{exp}}) \times 100 / D_{\text{exp}}$; **The value of $R_{u\text{MIN}}$

**Figure 2.** The relation between detonation velocities and Al content in RDX containing 13 μm Al powders.

method reaches a better agreement with the measured velocities than the other two models.

3.3 NM-Based Aluminized Explosives

The molecular formula of liquid NM [37] is CH_3NO_2 , and the enthalpy of formation is -113.278 kJ/mol . Al powders in an average size of $5 \mu\text{m}$ and 3% PMMA gelation are added during the preparation of NM. The calculated detonation velocities of NM-based aluminized explosive are shown in Table 4, and the calculation results of different models are shown in Figure 3.

It can be drawn from Table 4 that the optimal R_u always equals to $R_{u\text{MIN}}$ and the deviations between the test velocities and the calculated values are $-1.804\% \sim 0.206\%$. It can also be deduced that the detonation products of NM are too weak to drive the Al powders to get a high velocity. In Figure 3, when compared with the experimental data, the deviation of the new method is the smallest, while the empirical model and Cheetah code have larger errors.

Table 4. Calculated detonation velocities of NM containing Al powders (5 μm).

Formula NO.	Mass percent		$\rho/\text{g} \times \text{cm}^{-3}$	$Q/\text{J} \times \text{g}^{-1}$	$D_{\text{exp}}[37]/\text{km} \times \text{s}^{-1}$	$D_{\text{this paper}}/\text{km} \times \text{s}^{-1}$	R_u	error* %
	NM	Al						
N0	100	0	1.140	4206.8	6.290	6.220	–	–1.11
N1	80	20	1.281	3365.4	6.097	5.958	1	–2.280
						5.974	0.711	–2.017
						5.987	0.422**	–1.804
N2	60	40	1.485	2524.1	5.762	5.725	1	–0.642
						5.747	0.711	–0.260
						5.774	0.422**	0.208

Note: * error = $(D_{\text{new}} - D_{\text{exp}}) \times 100 / D_{\text{exp}}$; **The value of $R_{u\text{MIN}}$

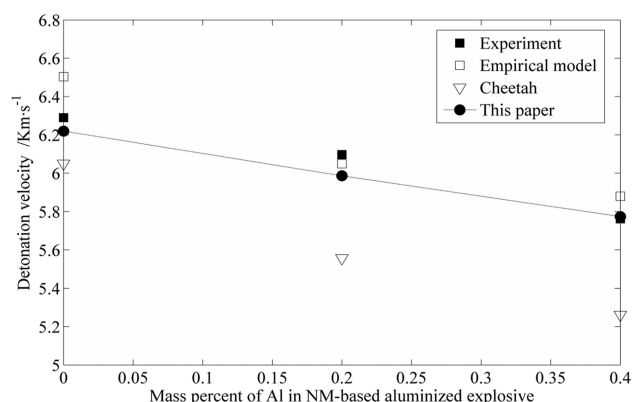


Figure 3. The relation between detonation velocities and Al content in NM containing 5 μm Al powders.

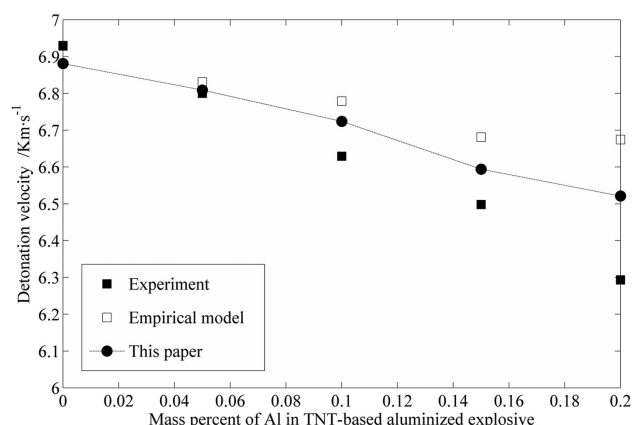


Figure 4. The relation between detonation velocities and Al content in TNT containing 2.38 μm Al powders.

3.4 TNT-Based Aluminized Explosives

The molecular formula of TNT [38] is $\text{C}_7\text{H}_5\text{N}_3\text{O}_6$, the enthalpy of formation is -74.404 kJ/mol, and the Al additives have a average size of 2.38 μm . The calculated detonation velocities of the TNT-based aluminized explosives are shown in Table 5, and the computed detonation velocities of different models are shown in Figure 4.

The results in Table 5 show that the optimal R_u always equals to 1 and it proves that the detonation products of TNT have a strong ability of driving Al powders. However, the computed value is not accurate for T4 sample, for the calculation error is significantly higher than that of other samples. The great underestimation of the heat exchange in the reaction zone may be the reason for the overestimation of the detonation velocity of T4. Through a conductivity detection of the detonation of TNT-based aluminized explosives, Zhou et al.[38] found that the detonation zone in-

creases rapidly if Al content increases, and their tests show that the detonation zone of T4 is about 1.7 times that of T0. Therefore Al powders should have absorbed more heat in a longer detonation zone than the heat estimated under the circumstance of constant detonation zone. However, the results of conductivity can only be referenced qualitatively and there is no reliable correlation between the length of the detonation zone and Al content. At $R_u=1$, the detonation velocities of TNT-based aluminized explosives of two methods are compared in Figure 4. As shown in Figure 4, although the deviations of the new method to the test data increase when Al content is more than 10%, the new method is more accurate than the empirical method.

Table 5. Calculated detonation velocities of TNT containing Al powders (2.38 μm).

Formula NO.	Mass percent		$\rho/\text{g} \times \text{cm}^{-3}$	$Q/\text{J} \times \text{g}^{-1}$	$D_{\text{exp}}[38]/\text{km} \times \text{s}^{-1}$	$D_{\text{this paper}}/\text{km} \times \text{s}^{-1}$	R_u	error* %
	TNT	Al						
T0	100	0	1.61	3883.2	6.930	6.881	–	-0.712
T1	95	5	1.63	3689.3	6.800	6.809	1	0.132
						6.812	0.800	0.176
						6.814	0.600**	0.206
T2	90	10	1.66	3494.9	6.629	6.724	1	1.433
						6.730	0.800	1.524
						6.738	0.600**	1.644
T3	85	15	1.68	3300.9	6.498	6.594	1	1.477
						6.602	0.800	1.600
						6.610	0.600**	1.724
T4	80	20	1.72	3106.6	6.293	6.526	1	3.703
						6.536	0.800	3.861
						6.545	0.600**	4.004

Note: * error = $(D_{\text{new}} - D_{\text{exp}}) \times 100 / D_{\text{exp}}$; **The value of $R_{u\text{MIN}}$

4 Conclusion and Discussion

Through a thermodynamic analysis for the detonation of explosives with micrometer Al additives, the acceleration of Al powders and the heat exchanges between Al powders and the matrix are recognized to have important influences on the detonation performances. By considering the velocity-disequilibrium within Al powders and detonation products at the C–J plane and the heat absorption of inert Al powders in the detonation zone, this paper proposed a new method to predict the detonation velocity of explosives with micrometer Al powders. This method is a closed algebraic equation system containing 12 variables including the detonation velocity D . The detonation heat, length of detonation zone and the velocity ratio of Al powders to detonation products are the initial conditions. D could be solved accurately with the help of the numerical code.

The new method was applied to four kinds of aluminized explosives and the results show that the differences of the detonation velocities corresponding to different R_u are less than 0.5%. It is explained that the change of kinetic energy of Al powders is generally two orders of magnitude smaller than the internal energy of the mixture composed by the micrometer Al powders and detonation products. During calculation, all the increased kinetic energy of Al powders due to acceleration is assumed to come from the internal energy of the matrix, and it would overestimate the influence of acceleration process on detonation velocities as the kinetic energy of matrix may also have contributions. Therefore the acceleration of Al powders has little influence on the detonation velocity, and R_u can be set to 1 for calculation convenience.

Compared with the experimental data, the deviations of HMX-based aluminized explosives are $-0.226\% \sim 0.781\%$, the deviations of RDX-based aluminized explosives are less than 0.527%, and those for NM-based aluminized explosives are $-1.804\% \sim 0.206\%$. For TNT-based aluminized explosives, the deviations are 0.132%–1.477% when Al content is less than 20%. However, the computed detonation velocity is 4% higher than the measured value if Al content is 20%. It may be attributed to the fact that the detonation zone of TNT would increase rapidly as the content of Al increases. Since the heat exchange should be stronger in a longer detonation zone, the new method that relying on the constant assumption of detonation zone overestimates the detonation velocity and the error becomes more obvious with a larger content of Al. Therefore the heat absorption of Al powders within the detonation zone has an important effect on the detonation velocity of explosive with micrometer Al powders. Furthermore, the compared results proved that the new method is of higher precision than the empirical method, KHT and Cheetah models.

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