Study on the Detonation Parameters of Aluminized Explosives Based on a Disequilibrium Multiphase Model

Hongbo PEI [*], Jianxin NIE, Qingjie JIAO

State Key Laboratory of Explosion Science and Technology, Beijing Institute of Technology, Beijing 100081, China
[*]*E-mail: hongbo2751@sina.com*

Abstract: Detonation models are usually based on the classical Euler equations of gas dynamics under the assumption of thermodynamic equilibrium. However reported data show the Chapman-Jouguet (CJ) detonation parameters of non-ideal explosives based on thermodynamic equilibrium codes are significantly different from experimental results. Based on the conventional CJ model, a new multiphase flow model, not in thermal equilibrium, was considered in this study. This approach was applied to compute the velocity of detonation for several aluminized explosives. The predictions are better than the CJ equilibrium model and are in excellent agreement with experimental data. All of the deviations for the velocity of detonation (VOD) are less than 4%.

Keywords: non-ideal explosives, velocity of detonation, detonation pressure, relaxation timescale

1 Introduction

The use of aluminum (Al) particles in high explosives is well known to increase their ballistics, blast and underwater efficiencies [1-6]. The mechanism of detonation in high explosives (HE) containing Al particles has been the object of numerous studies, both theoretical and experimental [7-15]. Most researchers believe that combustion of micrometer sized Al particles occurs mainly behind the reaction front (during the expansion of the detonation products), so that the particles do not participate in the reaction zone, but rather act as inert ingredients [16-21].

    The velocity of detonation (VOD) is the only detonation parameter that can

be measured easily and accurately. However reported data show that the CJ detonation parameters of aluminized explosives calculated from thermodynamic equilibrium codes are significantly different from experimental results, whether Al is regarded as an inert or reactive ingredient [11-13, 15]. Detonation models such as CJ and ZND are usually based on the conventional Euler equations of gas dynamics, under the assumption of temperature equilibrium among the various constituents. However theoretical analysis shows that temperature equilibrium is invalid for explosives containing micro Al particles at the CJ plane [13, 18, 21]. A temperature non-equilibrium model was proposed by Kapila *et al.* [22]. Shock jump conditions for mechanical equilibrium mixtures were given by Petitpas *et al.* [21] and Saurel *et al.* [23], allowing closure of the two-phase flow model. This new modelling approach offers new options for detonation modelling.

A new multiphase flow model, not in thermal equilibrium, was considered in this study. This approach was applied to compute the velocity of detonation and detonation pressure for several aluminized explosives. The aim was to compute the detonation pressure and the VOD of aluminized explosives using a multiphase model involving as few parameters as possible. In this approach, pressure disequilibrium and velocity disequilibrium was omitted but temperature disequilibrium was considered.
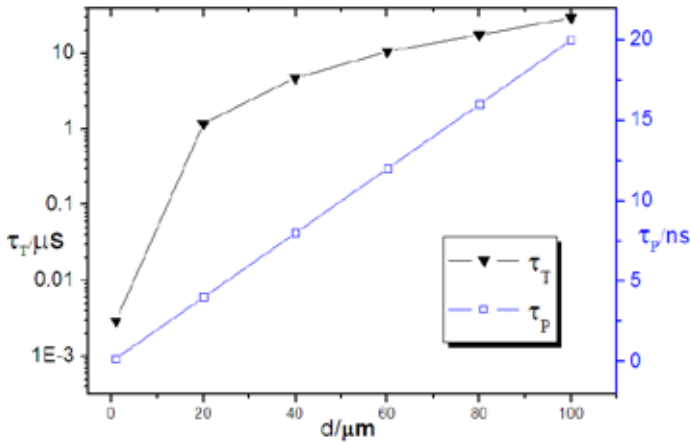
2   Pressure and Thermal Relaxation Timescales

The pressure and thermal relaxation timescales can be examined using the following relations respectively [21]:

$$\tau_p \propto \frac{d}{c} \tag{1}$$

$$\tau_t \approx \frac{\rho C_v}{K} (\frac{d}{2})^2 \tag{2}$$

where d and c are the particle diameter and particle velocity of sound, respectively. The variables C_v, K, and ρ represent the specific heat, thermal conductivity, and density, respectively. The pressure relaxation timescale for Al particle varies between a few nanoseconds and 20 ns in the diameter range of 0.1-100 μm. The temperature relaxation timescale remains larger than 0.1 μs when the particle size is larger than 2 μm, and strongly increases with the particle diameter. The threshold diameter for temperature equilibration in the reaction zone is 1 μm for Al. The assumption of mechanical equilibrium and temperature disequilibrium is clearly valid for applications where the diameter of the Al particles is greater

than a few μm (Figure 1).

Figure 1. Temperature and pressure relaxation timescales.

3   The Multiphase Model

A simplified version of the Petitpas *et al*. model [21], in the absence of heat transfer, so that the metallic particles evolve freely without heat exchange with the high explosives and the detonation products, was proposed by Baudin *et al.* [13]. A single irreversible reaction is considered, as follows:

$$HE + Al(inert) \rightarrow Detonation \ Products \ (DP) + Al(inert) \qquad (3)$$
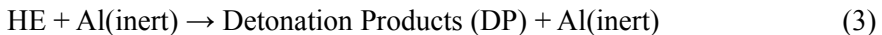
In the CJ plane (one dimensional), the approximate shock jump relations have been determined by Saurel *et al*. [23]:

$$Y_k^* = Y_k^0$$
$$\rho^*(u^* - D) = \rho_0(u_0 - D)$$
$$p^* - p_0 = \rho_0(u_0 - D)(u^* - u_0)$$
$$e_k^* - e_k^0 = \frac{p^* - p_0}{2}(v_k^0 - v_k^*)$$
$$\frac{1}{\rho} = \sum_k \frac{Y_k}{\rho_k}, v = \sum_k Y_k v_k, e = \sum_k Y_k e_k$$

$$(4)$$

The variables Y_k, ρ_k, e_k and v_k represent the mass fraction, density, internal energy and specific volume of different phases respectively, whilst p, u, D, ρ, and v represent the pressure, velocity of the particles, velocity of detonation, density and specific volume for the mixture, respectively. The symbol * denotes the shocked state and the symbol ^{0} denotes the initial state. These equations represent conservation of mass, momentum and total energy conservation. Another two equations (equation of state and CJ conditions) are needed to calculate the detonation parameters.

In the CJ plane, the following relationship exists:

$$D = u^* + c^* \tag{5}$$

The velocity of sound in the mixture was calculated with the help of Wood's relationship [24]:

$$\frac{1}{\rho c^2} = \sum_k \frac{\alpha_k}{\rho_k c_k^2}, \quad \alpha_k = \frac{\rho Y_k}{\rho_k} \tag{6}$$

The variables c_k, and α_k represent the sound and volume fractions of the different phases, whilst c represents the velocity of sound in the mixture.

The JWL equation of state (EOS) was used for the HE detonation products:

$$
\begin{aligned}
p_s &= A\exp(-R_1\frac{\rho}{\rho_0}) + B\exp(-R_2\frac{\rho}{\rho_0}) + C(\frac{\rho}{\rho_0})^{-(\omega+1)} \\
e_s &= \frac{A}{R_1}\exp(-R_1\frac{\rho}{\rho_0}) + \frac{B}{R_1}\exp(-R_2\frac{\rho}{\rho_0}) + \frac{C}{\omega}(\frac{\rho}{\rho_0})^{-\omega}
\end{aligned}
\tag{7}
$$

where A, B, C, R_1, R_2, and ω are constants, and are determined by the cylinder test. The JWL EOS parameters for the different HE [25] used in this paper are listed in Table 1.

Table 1.   The JWL EOS parameters of various HEs

HE	ρ, [kg/m³]	D, [km/s]	A, [GPa]	B, [GPa]	C, [GPa]	R_1	R_2	ω
NM*	1128	6290	209.25	5.69	0.77	4.40	1.2	0.3
HMX	1891	9110	778.28	7.07	0.64	4.20	1.0	0.3
RDX	1601	8193	609.77	12.95	1.04	4.5	1.4	0.25

*NM: nitromethane

The Murnagham EOS [26] was used for Al:

$$p = a[(\frac{\rho}{\rho_0})^n - 1]$$
$$e = e_0 + \frac{p - p_0}{(n-1)\rho_0} + C_v \Delta T$$

(8)

where: a and n are constants, $a = 18.17$ GPa, $n = 4.352$, and $C_v = 890$ J·kg^{-1}·K^{-1} for Al [26]. It is not necessary to know the value of e_0 because only e-e_0 would be used in the calculation. ΔT is the temperature increase due to heat exchange with the detonation products. The temperature of the Al particles will increase to around 1000 K due to adiabatic shock compression [27]. The temperature of the HE is usually below 4500 K [28], so ΔT was given different values (0, 1000, 2000, 3000 K) in order to evaluate the influence of temperature disequilibrium on the VOD. When $\Delta T = 0$, the condition corresponds to there being no heat exchange between the Al particles and the detonation products, as assumed by Baudin *et al*. [13].

Subsequently, equations containing five variables were obtained:

$$f(p^*, \rho^*, u^*, e^*, D) = 0 \tag{9}$$

where the system of Equations (9) contains Equations (4)-(8). For the Equations (9), it is impossible to obtain an analytical solution, so the FSOLVE function in the MATLAB program was used to solve the equations in this study. In the process of solving the equations, an initial solution was assumed, and the program then begin to search for the solution. When the error was smaller than the set values, the program stopped calculating and exported the results.

4   Results and Discussion

4.1   Application to aluminized HMX

The VODs of HMX-based aluminized explosives have been extensively studied by Gogulya [14]. The reported VODs were measured in cylindrical charges of diameter 40 mm, with several Al particle diameters. The measured VODs are shown in Table 2 and compared to the multiphase model values. The results calculated by Cheetah [29] and reported by Baudin *et al*. [13] are also shown in Table 2. The threshold diameter for temperature equilibration in the reaction

zone is 1 µm for Al. The temperature relaxation timescale for 20 µm Al is greater than 1 µs, much longer than the reaction time of HMX. It may be concluded that the heat exchange for Al particles larger than 20 µm can be neglected. The experimental results have also proved that for aluminized explosives with the same Al content, the VODs for 20, 50 and 150 µm are similar, but the VOD for 0.5 µm is obviously smaller than that for 20 µm.

Table 2.   HMX-Al detonation characteristics

Explosives	Al size [µm]	ρ_0 [kg/m^3]	D_{exp} [m/s]	$D_{Cheetah}$ [m/s]	P^*_{CJ} [GPa]	ΔT [K]	$D_{multiphase}$ [m/s]	P^{**}_{CJ} [GPa]
HMX-Al 95-5	150	1840	8740			0	8930	37.51
	50	1840	8730	8998	33.00	1000	8835	36.51
	20	1830	8720			2000	8741	35.53
	0.5	1840	8660			3000	8648	34.59
HMX-Al 85-15	150	1890	8660			0	8595	32.88
	50	1880	8610	8936	31.04	1000	8350	30.49
	20	1870	8550			2000	8113	28.26
	0.5	1870	8350			3000	7881	26.17
HMX-Al 75-25	150	1950	8550			0	8312	28.91
	50	1930	8440	8904	29.79	1000	7956	25.65
	20	1920	8370			2000	7612	22.70
	0.5	1910	7970			3000	7279	22.02

Note: * calculated by Cheetah; ** calculated by the multiphase model.

These results show that heat exchange has an important influence on the VOD. For HMX-Al 95-5, the calculated VOD for ΔT = 3000 K is smaller (by 3.1%) than that for ΔT = 0 K. For HMX-Al 75-25 the calculated VOD for ΔT = 3000 K is smaller (by 12.4%) than that for ΔT = 0 K. The influence of temperature disequilibrium on the VOD increased with the Al fraction.

Table 3.   Comparison of HMX-Al VODs, predicated and experimental

Explosives	Al size [µm]	D_{exp} [m/s]	$D_{Cheetah}$ [m/s]	Dev-Cheetah [%]	$D_{multiphase}$ [m/s]	Dev-multiphase [%]
HMX-Al 95-5	150	8740	8998	2.9	8930	2.2
HMX-Al 85-15	150	8660	8936	3.2	8595	0.8
HMX-Al 75-25	150	8550	8904	4.1	8312	2.8

Note: %Dev = | (D_{model}-D_{exp})/ D_{exp} | × 100%.

Here only the VOD for 150 μm Al, measured by Gogulya [14], was compared with the calculated results (ΔT = 0) in Table 3. It can be seen that although the Al is assumed to be inert, the calculated VOD still agrees well with the experimental value. Cheetah assumes that all Al has reacted in the reaction zone, so the VOD slightly decreases with the Al fraction. The multiphase model also suggests a method for quantitatively evaluating the influence of temperature disequilibrium of the Al particles on the VOD.

4.2 Application to aluminized RDX

Trzcinski *et al*. [9] experimentally studied the detonation characteristics of Al-enriched RDX compositions. For unconfined cylindrical charges, they measured the detonation velocity versus the Al content in commercial grade, phlegmatized RDX (RDXph), which contains 94% RDX and 6% wax. The charge diameters were varied in the range 15-50 mm. The average particle size of Al used in the experiments was around 10 μm. The calculated VODs with the multiphase model in this paper is compared with the experimental results and the results calculated by Cheetah [13] in Table 4.

Table 4 shows that the VODs for RDXph-Al calculated by Cheetah is always higher than the experimental value, and the deviation increased with the Al content in the explosives. Although the VODs for RDXph-Al calculated by the multiphase model is always smaller than the experimental value, it is closer to the experimental results than that obtained with Cheetah. The largest deviation for the multiphase model was 3.68%, smaller than that calculated by Cheetah (7.65%).

Table 4.   RDX-Al detonation characteristics

Explosives	ρ_0 [kg/m³]	D_{exp} [m/s]	D_{model} [m/s]	Dev [%]	P_{CJ} [GPa]	Model
RDXph RDX-Wax 94-6	1630	8300	8240	0.72	26.49	Cheetah
			8346	0.55	28.51	Multiphase*
RDXph-Al 81-15	1730	8020	8167	1.83	24.91	Cheetah
			7934	1.07	23.83	Multiphase
RDXph-Al 70-30	1820	7775	8006	2.97	22.61	Cheetah
			7643	1.69	19.45	Multiphase
RDXph-Al 55-45	1930	7495	7866	4.95	20.38	Cheetah
			7431	0.85	18.26	Multiphase
RDXph-Al 40-60	2020	6880	7407	7.65	16.09	Cheetah
			6627	3.68	16.01	Multiphase

Note**:** * in the multiphase model, ΔT = 0.

4.3 Application to aluminized nitromethane

Baudin [15] experimentally studied the detonation characteristics of NM based aluminized explosives. The NM used in these experiments contained 3% binder by weight. The size and the content of the Al powders were varied to study their effect on detonation. They also calculated the VODs with Cheetah assuming Al behaves as both an inert ingredient and a reactive ingredient. The experimental results show that the VODs for nano-Al is smaller than those for micro Al at the same Al content. The calculated VODs for micro Al with the multiphase model are compared with the experimental values in Table 5.

Table 5.   NM-Al detonation characteristics

Explosives	ρ_0 [kg/m³]	D_{exp} [m/s]	$D_{Cheetah}$ [m/s]	Dev-Cheetah [%]	$D_{multiphase}$ [m/s]	Dev-Multiphase# [%]
NM	1140	6290	6050	3.81	6212	1.40
NM-Al 80-20	1281	6097	5557*	8.86	5853	4.00
			6066**	0.51		
NM-Al 60-40	1485	5762	5262*	8.68	5707	0.95
			5409**	6.13		

Note: *Al inert ingredient, **Al reactive ingredient, # In the multiphase model, ΔT = 0.

Table 5 shows that the multiphase model provides more accurate predictions for VOD than the values calculated by Cheetah.

5   Conclusions

Based on the conventional CJ model, a new multiphase flow disequilibrium model was considered. In this model, Al is assumed to be an inert ingredient. Pressure disequilibrium and velocity disequilibrium were omitted but not temperature disequilibrium, and were considered at the CJ plane. This model was applied for computing the velocity of detonation and detonation pressure for several aluminized explosives. The predictions were better than the CJ model and gave excellent agreement with experimental values. All of the deviations for the VODs were less than 4%. The model was also proposed as an approach for quantitatively evaluating the influence of temperature disequilibrium on detonation characteristic. Although the model is only applied to aluminized explosives in this paper, it may also be used for explosives containing other inert particles.

Acknowledgements

6   References

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