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Prediction of Detonation Pressure and Velocity of Explosives with Micrometer Aluminum Powders

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Abstract: The data reported shows that the Chapman-Jouguet (CJ) detonation parameters of non-ideal explosives calculated from existing thermodynamic computer codes are significantly different from experimental results. We use CJ detonation theory to present a new approach predicting detonation pressure and velocity of aluminized explosives by thermodynamic detonation theory. There is no need to use the assumption of full and partial equilibrium of aluminum powder in reaction zones in the new approach. In this work the best agreement with experimental data was obtained by adjusting the parameter *k* in the Becker–Kistiakosky–Wilson equations of state (BKW-EOS). The detonation pressure and velocity values calculated by the present method agree well with the experimental results. All of the deviations for the calculated pressures of aluminized explosives are less than 9% and those for the detonation velocities are less than 7%.

Keywords: aluminized explosives, detonation pressure, non-ideal explosives, detonation velocity

Introduction

The Chapman-Jouguet (CJ) detonation velocity and pressure predicted from existing thermodynamic computer codes have been reported in the references [1-12], which use empirical equations of state such as Becker-Kistiakosky-Wilson (BKW-EOS) [13], or Kihara-Hikita-Tanaka (KHT-EOS) [14].

The data reported showed that the (CJ) detonation parameters of non-ideal explosives calculated from existing thermodynamic computer codes are significantly different from experimental results. Some investigators assumed that non-equilibrium effects in the reaction zones may contribute to this confusion and that measured pressures may be higher than equilibrium calculations if the measurement is taken behind the von Neumann spike and in front of the CJ plane.

The mean size of aluminum particles used in mixed explosives is around 10^1 μm. In fact, aluminum powder needs to be excited for several μs before it participates in chemical reaction. But the reaction time of reaction zones is about 10^{-1} μs. Therefore, it is impossible for aluminum powder, whose mean size is 10^1 μm, to participate in chemical reaction of reaction zones from high energy ingredients.

Leonard I. Stiel et al. [15-17] compared the experimental detonation values for a number of explosives with CJ velocities by JAGUAR procedures; this indicated that little aluminum reaction occurs at the detonation front, while the other gaseous and carbon products are in chemical equilibrium. Aluminum particles are able to achieve ignition temperature by the thermal effect of the reaction zones.

The prediction of detonation pressure has traditionally been accomplished by means of CJ thermodynamic detonation theory. This theory assumes that thermodynamic equilibrium is reached instantaneously. Combustion of aluminum particles in explosives is assumed to occur behind the reaction front, during the expansion of the gaseous detonation products. Aluminum particles in this case do not participate in the reaction zone, but act as inert ingredients [1, 12].

The calculation of detonation parameters based on thermodynamic theory reflects the detonation mechanism in aluminized explosives, which has advantages over the other approaches. The main purpose of the present work is to develop a new approach predicting the CJ pressure and velocity of non-ideal aluminized explosives based on thermodynamic theory. The predicted detonation pressures and velocities for non-ideal aluminized explosives in the present method are compared with experimental data as well as computed results obtained by the empirical formula, and the new method gives the best results. Also, the calculated results show good agreement with the measured data as compared to estimated results using the empirical formula. There is no need to use the assumption of full and partial equilibrium of aluminum powder in reaction zones in the new approach.

Theory and Computational Approach

CJ detonation theory assumes that thermodynamic equilibrium of the detonation products is reached instantaneously [18]. The detonation performance of aluminized explosives cannot be described by the CJ theory which assumes energy release to be instantaneous. The majority of researchers believe that for the case of powerful aluminized HE, aluminum behaves as an inert additive in the reaction zone and is oxidized only in expanding detonation products [19].

As in another report [20], in this present work, one of the parameters, *k*, in the BKW equations of state was adjusted slightly. This is because the value of *k* depends on the fractions of solid products in the CJ reaction and it should be adjusted when they increase. Aluminum particles of aluminized explosives act as inert material in reaction zones which means there is an increase of solid products in the CJ reaction. The original value of *k* for RDX type explosives in the BKW-EOS is 10.91 and was adjusted to 9.2725 in this work. The original value of *k* for TNT type explosives in the BKW-EOS is 12.685 and was adjusted to10.4017.

Table 1. Revised parameters in the BKW equations of state

Parameters	α	β	k	θ
RDX type explosives	0.5	0.16	9.2735	400
TNT type explosives	0.5	0.09585	10.4017	400

The logic for the computation is shown in Figure1.

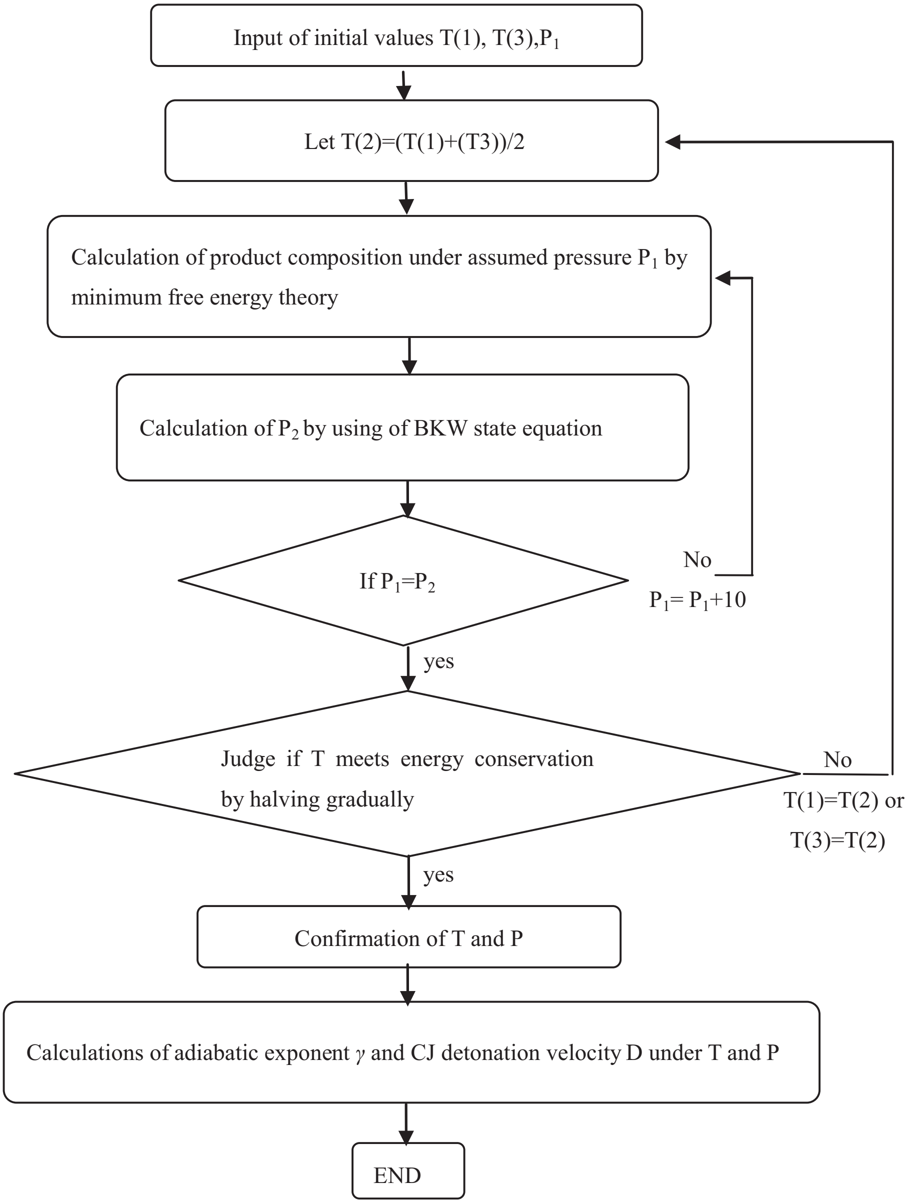

Figure 1. Logic for computation of CJ detonation pressure and velocity of aluminized explosives by thermodynamic detonation theory.

Results and Discussion

The data reported shows that for non-ideal explosives, detonation velocities are significantly different from those predicted by equilibrium, one-dimensional and steady-state calculations. In the present work the calculated CJ detonation pressure and velocity agree well with experimental results if the parameters in the BKW equations of state are adjusted (see Table 2).

Table 2. Comparison of detonation parameters predicated by the new approach for aluminized composite explosives with thermodynamic detonation theory and measured values

Explosives	Parameters	Exp. [21]	Ref. [21]	New	% Dev new
H-6	P_{CJ} (GPa)	-	22.5	23.317	-
	D_{CJ} (km/s)	7.194	7.235	7.639	6.18
	T_{CJ} (K)	-	-	3577	-
HBX-1	P_{CJ} (GPa)	-	22.9	24.429	-
	D_{CJ} (km/s)	7.224	7.270	7.487	3.64
	T_{CJ} (K)	-	-	3502	-
HBX-3	P_{CJ} (GPa)	-	19.5	19.453	-
	D_{CJ} (km/s)	6.917	6.853	7.389	6.82
	T_{CJ} (K)	-	-	3506	-
Alex 20	P_{CJ} (GPa)	23	25.2	25.936	2.92
	D_{CJ} (km/s)	7.53	7.496	7.4128	1.56
	T_{CJ} (K)	-	-	3558	-
Alex 32	P_{CJ} (GPa)	21.5	21.3	23.211	8.97
	D_{CJ} (km/s)	7.3	7.066	7.300	0.01
	T_{CJ} (K)	-	-	3555	-
Tritonal	P_{CJ} (GPa)	-	19.1	18.259	-
	D_{CJ} (km/s)	6.475	6.583	6.294	2.79
	T_{CJ} (K)	-	-	2607	-
Torpex	P_{CJ} (GPa)	-	25.9	27.114	-
	D_{CJ} (km/s)	7.495	7.492	7.289	2.75
	T_{CJ} (K)	-	-	3501	-
Destex	P_{CJ} (GPa)	-	17.5	17.469	-
	D_{CJ} (km/s)	6.65	6.439	6.303	5.22
	T_{CJ} (K)	-	-	2607	-

Note: $\% \text{ Dev new} = \frac{\text{Exp} - \text{New}}{\text{Exp}} \times 100\%$

According to the comparisons in this table, the results agree well with the experimental results. It is worth mentioning that there are two groups of factors, temperature and heat. One group is the CJ detonation parameters, the other is the temperature and heat of the final product. These all produce better results, which will be introduced in another paper. The parameters in Table 2 are the parameters of Chapman-Jouguet detonation.

Table 2 shows that the values of the detonation pressure and velocity calculated by the new approach agree well with the experimental results. All of the deviations for the calculated detonation pressure are less than 9% and those for the calculated detonation velocity are less than 7%.

The detonation pressure depends on the loading density of the explosives [22]:

$$p = p_{\max}\left(\frac{\rho_0}{\rho_{\max}}\right)^2 \tag{1}$$

where p is the detonation pressure (GPa) under the loading density ρ_0(g/cm^3) and $p_{\max}$ is the maximum detonation pressure (GPa) under the theoretical density $\rho_{\max}$(g/cm^3).

For mixed explosives there is

$$p_{\max} = \sum\left(p_{e\max i}\frac{\alpha_{evi}}{\rho_{e\max i}}\right)\rho_{\max} \tag{2}$$

where $p_{\max}$ is the detonation pressure for the mixed explosives; $p_{e\max i}$ is the theoretical detonation pressure for the species i in the mixtures; α_{evi} is the volume fraction of the species i; $\alpha_{evi} = \frac{g_{ei}}{\rho_{e\max i}}\rho_{\max}$, gei is the mass fraction of the species i in the mixtures; $\rho_{e\max i}$ is the theoretical density of the species i in the mixtures. From Eqs. (1) and (2), there is

$$p = \sum\left(p_{e\max i}\frac{g_{ei}}{\rho_{e\max i}}\right)\left(\frac{1}{\rho_{\max}}\right)\rho_0^2. \tag{3}$$

This is an empirical formula for predicting detonation pressure for mixed explosives. By using Eq. (3), the detonation pressure of the aluminized explosives can be obtained when $p_{e\max i}$ is known; the latter is called the empirical value in this work. The detonation velocity for the mixed explosives can be estimated by a similar pathway to the detonation pressure. A comparison of the values calculated by the new approach with thermodynamic detonation theory in this work with the experimental data [7], as well as the empirical values estimated by Eq. (3) is shown in Table 3.

Table 3. Comparison of the values calculated in the new approach with thermodynamic detonation theory in this work with experimental data [7] as well as the empirical values estimated by Eq. (3)

Explosives	Density g/cm^3	Parameters	Exp. [11]	Emp. in Eq. (3)	New
DX/Al(90/10)	1.68	P (GPa)	24.6	26.298	25.903
		D (km/s)	-	7.869	7.724
		T (K)	-	-	2694
RDX/Al(80/20)	1.73	P (GPa)	22.7	23.933	23.584
		D (km/s)	-	7.706	7.697
		T (K)	-	-	2453
RDX/Al(70/30)	1.79	P (GPa)	21.0	21.619	21.312
		D (km/s)	-	7.554	7.612
		T (K)	-	-	2217
RDX/Al(60/40)	1.84	P (GPa)	21.1	18.855	18.596
		D (km/s)	-	7.348	7.535
		T (K)	-	-	1934
RDX/Al(50/50)	1.89	P (GPa)	19.0	15.940	15.730
		D (km/s)	-	7.123	7.454
		T (K)	-	-	1636
HMX/Al(90/10)	1.76	P (GPa)	-	29.450	29.184
		D (km/s)	-	8.136	8.058
		T (K)	-	-	2620
HMX/Al(80/20)	1.82	P (GPa)	-	27.139	26.893
		D (km/s)	-	7.990	7.987
		T (K)	-	-	2414
HMX/Al(70/30)	1.86	P (GPa)	-	24.020	23.803
		D (km/s)	-	7.760	7.932
		T (K)	-	-	2137
HMX/Al(60/40)	1.94	P (GPa)	-	21.670	21.473
		D (km/s)	-	7.629	7.785
		T (K)	-	-	1928

TNT/ Al(89.4/10.6)	1.72	P (GPa)	-	18.356	18.553
		D (km/s)	-	6.808	6.232
		T (K)	-	-	2437
TNT/ Al(78.3/21.7)	1.8	P (GPa)	18.9	16.818	16.998
		D (km/s)	-	6.797	6.160
		T (K)	-	-	2233
TNT/ Al(67.8/32.2)	1.89	P (GPa)	-	15.342	15.507
		D (km/s)	-	6.805	6.045
		T (K)	-	-	2037

Table 3 shows that the values calculated by the new approach proposed in this work agree well with the experimental data as well as the empirical values calculated by Eq. (3). The values of the calculated detonation pressures in the new approach proposed in this work are closer to the experimental results than the empirical values.

Conclusion

A new computer approach using the thermodynamic detonation theory has been introduced for the calculation of detonation pressure and velocity of aluminized explosives. There is no need to assume full and partial equilibrium of aluminum powder in reaction zones in the new approach. In this work the closest agreement to the experimental data was obtained by adjusting the parameter *k* in the BKW equations of state. The detonation pressure and velocity calculated in the present method agree well with the experimental results. All of the deviations for the calculated pressures are less than 9% and those for the detonation velocities are less than 7%.

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