

Stable detonation velocities for aluminized explosives

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Abstract

Traditional Chapman-Jouguet detonation theory does not explain the observed detonation states achieved by aluminized explosives. As a result, the detonation properties of these explosives have been studied using new and literature experimental data and EXP-6 thermo-chemical potential calculations with the JAGUAR computer program. It has been found that the observed detonation velocity behavior for aluminized explosives can be accurately represented by a reaction zone model in which aluminum, coated with aluminum oxide, is initially non-reactive and in equilibrium with H-C-N-O compounds. The JAGUAR procedures have been modified to represent the aluminum reaction zone behavior and to enable specified temperature differences between the gas and aluminum particles in the initial portion of this reaction zone. The result of this work is that detonation velocities for aluminized explosives which agree closely with experimental data may be readily calculated.

Keywords: Aluminum, Explosives, Eigenvalue detonation, Velocity, Reaction

1. Introduction

The JAGUAR analytical procedures have been augmented to provide accurate calculation of detonation properties of high-blast aluminized explosives¹⁾. These new routines are an extension of the EXP-6 thermochemical equation of state procedures previously developed and optimized for H-C-N-O explosives²⁾. Accurate relationships for the melting curves of aluminum and aluminum oxide are utilized to identify the correct phases present at every calculation point. The individual aluminum and aluminum oxide descriptions have been carefully parameterized to reproduce existing experimental Hugoniot data. This new capability was subsequently utilized to investigate the detonation behavior of aluminized explosives.

2. Chapman-Jouguet calculations

For a large number of aluminized explosives, Chapman-Jouguet (CJ) detonation velocities calculated with JAGUAR and the assumption of little or no aluminum reaction are consistent with recent experimental values to within the accuracy of the data and the analytical procedures utilized³⁾. For most of the explosives studied, the calculated CJ detonation velocities decrease slightly in the

range 0-25 % aluminum reaction, and are substantially lower for 100 % reaction. Comparisons of experimental detonation velocities indicate that even with micron or sub-micron particles, at most a small amount of the aluminum reacts at the detonation front. For sub-micron particles, the inclusion of a realistic fraction of initial aluminum oxide improves the JAGUAR agreement for zero aluminum reaction with the corresponding experimental detonation velocities.

In Table 1 recent experimental detonation velocities⁴⁾⁻⁸⁾ are compared with CJ values calculated with JAGUAR with the assumption of 0 % or 100 % aluminum reaction. Measurements obtained by standard procedures⁹⁾ at Picatinny Arsenal are included for PAX-3 (an HMX based explosive with 20 wt % aluminum), and for PAX-29, PAX-30, and PAX-42, aluminized formulations with Cl-20, HMX, and RDX, respectively. The aluminum particle sizes of the data range from large to sub-micron. For sub-micron particles, the initial aluminum content is assumed to include 13 wt % aluminum oxide. For larger particles the calculated detonation velocities are independent of the particle size. For 35 aluminized explosive detonation velocity experiments with various composi-

Table 1 Detonation velocities of aluminized explosives.

Expl.	Ref.	Al%	Density kg m ⁻³	p, micron	JAGUAR			JAGUAR	
					D, exptl km s ⁻¹	D, Al inert km s ⁻¹	D, Al km s ⁻¹	% error inert	% error Al
HMX	4	5	1840	150	8.74	8.66	8.53	0.92	2.41
HMX	4	5	1840	50	8.73	8.66	8.53	0.80	2.30
HMX	4	5	1830	20	8.72	8.62	8.49	1.12	2.64
HMX	4	5	1840	0.5	8.66	8.66	8.53	0.00	1.51
HMX	4	15	1890	150	8.66	8.49	8.05	1.96	7.02
HMX	4	15	1880	50	8.61	8.45	8.00	1.86	7.08
HMX	4	15	1870	20	8.55	8.42	7.95	1.56	7.05
HMX	4	15	1870	0.5	8.35	8.37	7.95	0.24	4.83
HMX	4	25	1950	150	8.55	8.35	7.32	2.32	14.39
HMX	4	25	1930	50	8.44	8.28	7.21	1.91	14.57
HMX	4	25	1920	20	8.37	8.24	7.16	1.51	14.46
HMX	4	25	1910	0.5	7.97	8.14	7.11	2.13	10.79
BTNEN	5	15	1965	150	8.38	8.43	7.50	0.54	10.50
BTNEN	5	15	1955	15	8.30	8.38	7.45	0.96	10.27
BTNEN	5	15	1955	7	8.28	8.38	7.45	1.21	10.05
BTNEN	5	15	1914	0.1	8.04	8.16	7.24	1.49	9.91
BTNEN	5	15	1910	0.1	8.07	8.14	7.22	0.87	10.53
BTNEN	5	15	1900	0.1	7.92	8.10	7.18	2.27	9.38
BTNEN	5	15	1830	0.1	7.66	7.81	6.87	1.96	10.35
TNT	6	20	1635	5	6.41	6.38	5.77	0.47	10.12
TNT	6	20	1590	0.1	6.14	6.18	5.65	0.57	8.03
TNT	7	20	1760	0.1-0.2	6.72	6.69	6.12	0.45	9.00
TNT	7	20	1740	0.1-0.2	6.72	6.63	6.06	1.47	9.95
TNT	7	30	1840	0.1-0.2	6.74	6.63	4.92	1.66	27.02
TNT	7	30	1820	0.1-0.2	6.63	6.56	4.85	1.03	26.83
TNT	7	10	1670	0.1-0.2	6.51	6.68	6.52	2.66	0.15
NG	8	15	1743	15	7.94	8.07	7.93	1.61	0.16
NG	8	15	1720	p	7.78	7.97	7.83	2.38	0.64
NG	8	15	1785	0.1	8.13	8.26	8.10	1.59	0.33
PAX-3		18	1866	50	7.96	8.05	7.65	1.13	3.89
PAX-3		20	1878	micron	8.18	8.03	7.59	1.83	7.21
PAX-29		15	1999	micron	8.95	8.79	8.16	1.79	8.83
PAX-29		15	2010	sub-micron	8.77	8.79	8.32	0.23	5.13
PAX-30		15	1909	micron	8.51	8.43	8.09	0.94	4.94
PAX-42		15	1827	micron	8.25	8.14	7.75	1.33	6.06
Average % Error								1.34	8.24

tions included in Table 1, the average absolute deviation between the experimental and calculated CJ values is 1.34 % for 0 % aluminum reaction and 8.24 % for 100 % reaction. In Fig. 1, detonation velocities for PAX-30 calculated with JAGUAR at an initial density of 1909 kg m⁻³ are presented for varying extents of aluminum reaction. It can be seen that the experimental value is in close agreement to the CJ velocity corresponding to no aluminum reaction.

The analyses of cylinder test data indicate that with the use of large particles, such as for Picatinny Arsenal measurements for PAX-3, little or no reaction occurs for more than 10 volume expansions³⁾. However, with smaller aluminum particles there is evidence that substantial aluminum reaction can occur at low values of expansion⁵⁾.

3. Model for aluminized explosives

In order to account for the observed behavior of aluminized explosives, a model is postulated in which the explosive expands through a reaction zone at constant detonation velocity. At the zero aluminum reaction Hugoniot, the other gaseous and solid C-H-N-O products are in equilibrium. For the partially reacted aluminum Hugoniots, the reacted aluminum fraction detonation products (unreacted aluminum and aluminum oxide) are in equilibrium with the other C-H-N-O products. The reasoning behind this construct is that the organic reactions are significantly faster than aluminum decomposition and reaction. For the reaction zone, a standard assumption is adopted, where the necessary Hugoniot and Rayleigh line relationships are satisfied. However, it has been noted that for the aluminized explosives investigated to date, the unreacted

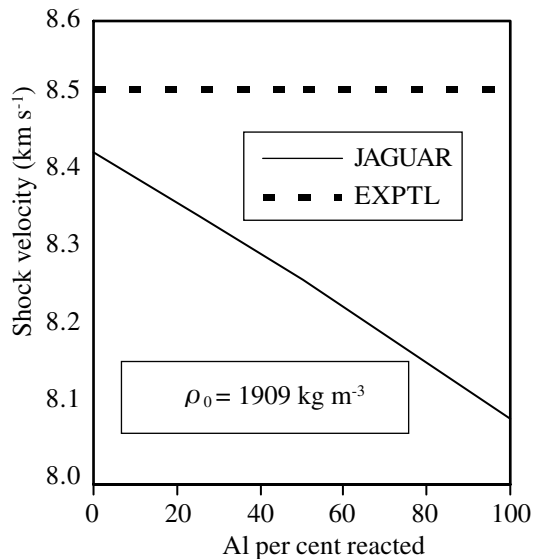


Fig. 1 CJ velocity PAX-30.

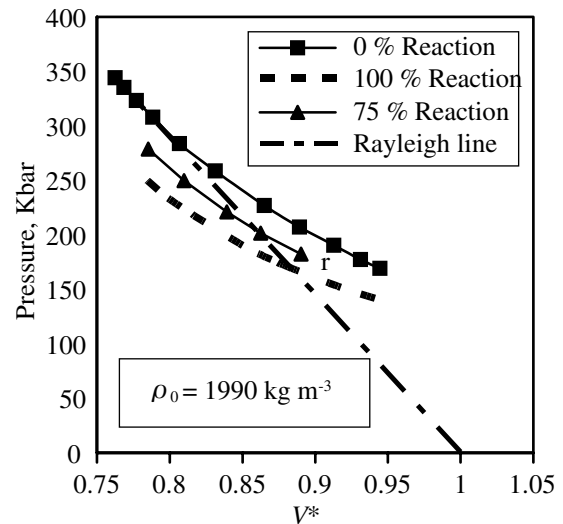


Fig. 2 Hugoniot curves BTNEN 85/AI 15.

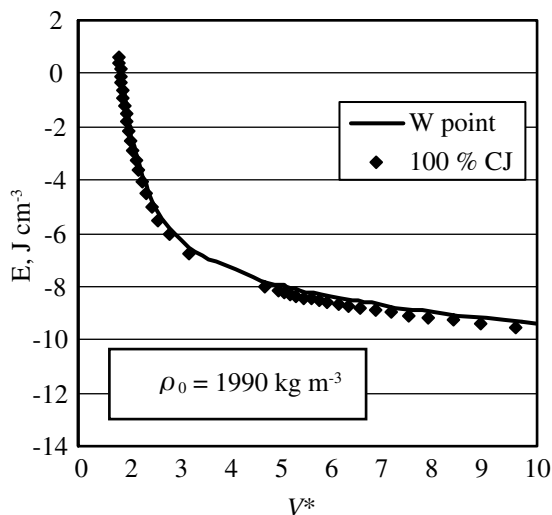


Fig. 3 Energy, BTNEN/AI 85/15.

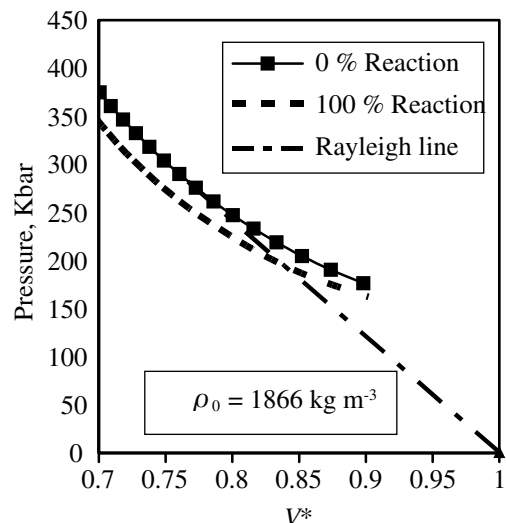


Fig. 4 Hugoniot curves PAX-3.

aluminum Hugoniot curve actually lies above the reacted aluminum Hugoniot. For this reason, the minimum detonation velocity solution (and minimum entropy solution) occurs with the Rayleigh line intersecting the zero aluminum reaction Hugoniot at the tangency point. The associated detonation velocity is the velocity that would be measured in experiment. This type of detonation is known in the literature as an eigenvalue detonation¹⁰. The eigenvalue detonation velocity, which is consistent with the measured detonation velocity, is determined by the tangency of the Rayleigh line to the unreacted Hugoniot curve.

In Fig. 2, Hugoniot curves (P versus $V^* = v/v_R$) are presented for BTNEN at an initial density of 1990 kg m^{-3} for varying fractions of reacted aluminum. For zero aluminum reaction, the initial point is at $P = 334 \text{ Kbar}$, $T = 3247 \text{ K}$, and $v = 3.87 \times 10^{-4} \text{ m}^3 \text{ kg}^{-1}$. The calculated detonation velocity for zero reaction (8.53 Km s^{-1}) is attained on the Hugoniot curve for 100% reaction at $P = 170 \text{ Kbar}$, $T = 4901 \text{ K}$, and $v = 4.44 \times 10^{-4} \text{ m}^3 \text{ kg}^{-1}$. The points of intersection of the Rayleigh line with the Hugoniot curves

are designated as “W-points”, since they are weak intersections of the curves. The W-point conditions for 100% aluminum reaction compare with those at the CJ point for 100% reaction: $P = 249 \text{ Kbar}$, $v = 3.95 \times 10^{-4} \text{ m}^3 \text{ kg}^{-1}$, $T = 4745 \text{ K}$. Since the entropies at the W-point and 100% reaction C-J point are very similar, as shown in Fig. 3 almost identical energies on the isentropic expansion curve result from either starting point, even though the CJ point is never achieved.

In Fig. 4, Hugoniot curves are presented for PAX-3 at an initial density of 1866 kg m^{-3} for 0 and 100% of reacted aluminum. At this density with 50 micron particles, the detonation velocity measured at Picatinny Arsenal is 7.96 Km s^{-1} . For zero aluminum reaction, the initial detonation point is at $P = 294 \text{ Kbar}$, $T = 2941 \text{ K}$. The calculated eigenvalue detonation velocity for zero aluminum reaction (8.05 Km s^{-1}) is attained on the Hugoniot curve for 100% reaction at $P = 195 \text{ Kbar}$, $T = 3543 \text{ K}$. The W-point conditions compare with those of the never achieved 100% aluminum reaction CJ point for which the calculated detona-

tion velocity is 7.66 Km s^{-1} ; $P = 265 \text{ Kbar}$, $T = 3578 \text{ K}$.

New JAGUAR procedures were developed to enable the determination of the reaction zone conditions for aluminized explosives. At a specified initial density, the W-Point is established as the point on the 100 % reaction Hugoniot curve with the eigenvalue detonation velocity established for zero reaction. The detonation velocity at each Hugoniot point is calculated as:

$$D = \sqrt{\frac{v_R(P - P_R)}{1 - \frac{v}{v_R}}} \quad (1)$$

where P_R and v_R are the pressure and specific volume at the reference state.

4. Effect of melting behavior of aluminum particles

The melting behavior of aluminum and aluminum oxide has been examined for an explanation of the reaction zone behavior of aluminized explosives. For BTNEN with three per cent aluminum oxide content, at the initial zero reaction point the temperature and pressure are 3251 K and 333 Kbar, and the unreacted aluminum is liquid and the aluminum oxide coating solid at these conditions. The thermal conductivity of aluminum oxide, which is considerably lower than aluminum, decreases strongly with temperature¹¹⁾. Therefore, the aluminum oxide layer may serve to insulate the aluminum core to a lower temperature than the gas and to suppress the melting and reaction of the particles. As the pressure decreases in the reaction zone, aluminum and aluminum oxide will melt and therefore reaction of the aluminum core may occur almost instantaneously.

The JAGUAR procedures were modified to enable a temperature difference between the gas and aluminum particle cores. All thermodynamic properties for aluminum are

calculated at its specified temperature. Estimated curves for the temperature and pressure variation for BTNEN in the reaction zone from 0 % to 100 % aluminum reaction are shown in Figs. 5 and 6. The temperature of aluminum at the zero reaction point was selected so that it is solid and close to its melting point (2550 K) at 343 Kbar. Calculations were then performed by the W-Point procedures for varying fractions of aluminum reaction to determine the corresponding states with the zero-point detonation velocity, $D = 8.49 \text{ Km s}^{-1}$. The aluminum temperature was assumed to become equal to the gas temperature at 50% conversion, and to vary linearly for intermediate fractional conversions. It can be seen from Fig. 5 that the gas temperature increases in the reaction zone because of the aluminum reaction. These calculations indicate that aluminum oxide is liquid for most of the reaction zone.

These calculations are consistent with observed experimental data. For BTNEN with 15 weight per cent aluminum, the cylinder velocity data of Gogulya et al⁵⁾ with 150 micron particles are considerably lower than the values for 15 micron for this system at an initial density of 1990 kg m^{-3} . JAGUAR calculations indicate that virtually no aluminum reaction occurs at early time expansions for the data with 150 micron particles³⁾. Some reaction may occur with these large particles at higher expansions. With large particles the products may expand unreacted from the initial point because of insufficient time for melting and aluminum reaction. For BTNEN with micron aluminum particles, the equilibration time is sufficiently small that aluminum reaction can occur at least partially in the reaction zone. The aluminum reaction then proceeds to completion at early times along the expansion curve. Measured brightness experiments by Gogulya et al⁵⁾ indicated that the temperatures of aluminized BTNEN explosives with micron or sub-micron particles are somewhat higher than for pure BTNEN after a short time behind the detonation front.

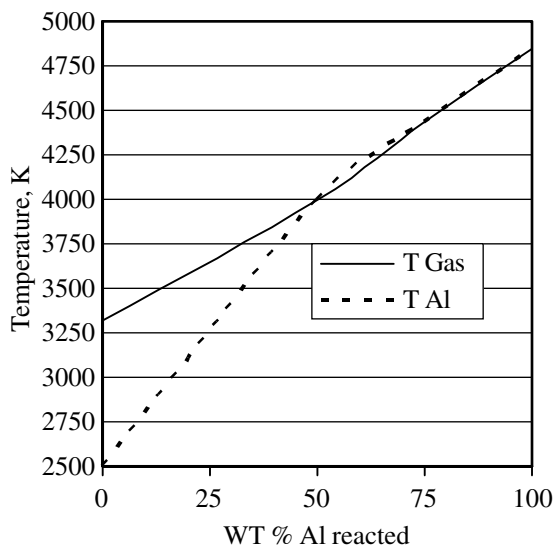


Fig. 5 BTNEN reach zone temperature.

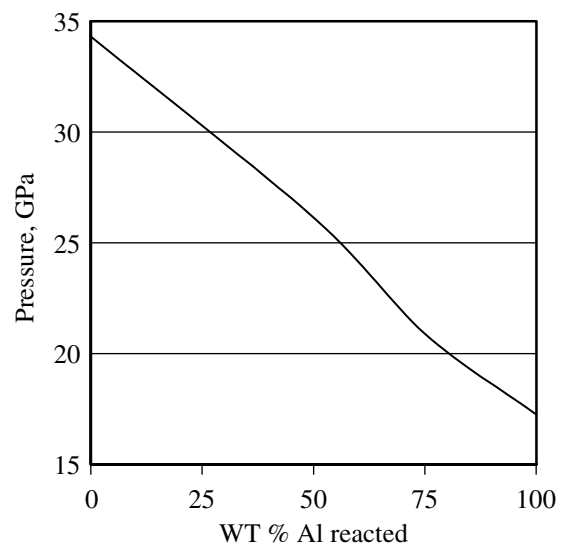


Fig. 6 BTNEN reaction zone pressure.

5. Conclusions

It appears that for most explosives with all aluminum particle sizes (large, micron and sub-micron), appreciable aluminum reaction does not occur at the reaction zone front, which establishes the detonation velocity for the reaction zone. The organic detonation products are considered to reach chemical equilibrium at the reaction zone front. This initial state appears to control the stable detonation velocity, producing the zero aluminum reaction detonation velocity observed in the time frame of experimental measurements. This is consistent with an eigenvalue detonation theory model, where the minimum detonation velocity solution occurs with the Rayleigh line intersecting the zero aluminum reaction Hugoniot at the tangency point. There is evidence that for some explosives such as BTNEN, which has a favorable oxygen balance, significant aluminum reaction is attained in a short time after the initial point. This is in contrast to explosives incorporating large aluminum particles where the gaseous products expand to low pressures before significant aluminum reaction takes place. The stable detonation velocity corresponds to the eigenvalue detonation solution for zero aluminum reaction, regardless of the extent of aluminum reaction achieved in the reaction zone.

An important factor for the behavior of aluminized explosives appears to be the variation of the melting conditions for aluminum and aluminum oxide until complete aluminum reaction. The reaction may not occur appreciably until the temperature and pressure conditions enable both aluminum and aluminum oxide to be in the liquid phase.

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