

# JAGUAR CALCULATIONS OF DETONATION PROPERTIES FOR ALUMINIZED EXPLOSIVES

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## ABSTRACT

In this study relationships have been incorporated into JAGUAR for aluminum and aluminum oxide in the solid and liquid phases. Revised calculation procedures for detonation properties (JAGUAR/Al) based on the minimization of the Gibbs free energy of the coexisting gas and condensed phases have been implemented. Relationships for the melting curves of aluminum and aluminum oxide are utilized to identify the correct phases present at every calculation point. The procedures enable varying weight fraction of unreacted aluminum to be incorporated in the calculations. JWLB thermodynamic equation of state parameters can be established for each explosive formulation. Explosive compositions can be identified with JAGUAR/Al which result in optimum detonation energies. This approach is illustrated for the addition of aluminum to an HMX based explosive system based on PAX2. The resulting explosive composition which includes aluminum is PAX-3.

## INTRODUCTION

The goal of this study is the development of an advanced EXP-6 based thermochemical equation of state and analytical procedures for the calculation of the detonation properties of high-blast explosives. The JAGUAR procedures for H-C-N-O explosives have been extended to aluminized compositions. Since aluminum systems are known to exhibit kinetic effects inhibiting complete reaction of the metal, the model allows specified amounts of inert aluminum to be included with the explosive products.

JAGUAR is an efficient and accurate computer program [1] which uses NLQPEB advanced variable metric optimization routines [2] to determine equilibrium compositions with optimally parameterized JCZ3 relationships. Input options include the calculation of C-J points, isentropes, and Hugoniot curves of explosives. The JAGUAR procedures enable the accurate calculation of the detonation properties of explosives for wide ranges of temperatures and pressures, including overdriven conditions [3,4]. The JAGUAR program incorporates the ability to automatically generate parameters of the JWLB equation of Baker [5] from the calculated thermodynamic properties for the principal isentrope.

## ALUMINUM AND ALUMINUM OXIDE PROPERTIES

Aluminum can react with oxygen present in the explosive to form aluminum oxide through the reaction



Since both aluminum and aluminum oxide melt at elevated temperatures, relationships for heat capacities at low pressures and for molar volumes as functions of temperature and pressure are required for both species in the solid and liquid phases. In this study polynomial relationships for heat capacities and molar volumes of aluminum and aluminum oxide from BKWC [6] were tested and augmented with the recommended JANAF values [7]. For liquid aluminum, the JANAF heat capacity is constant at 7.589 cal/g mole°K for temperatures above 720°K. For aluminum oxide liquid, the JANAF heat capacity is constant at 46 cal/g mole°K for the range 1350°–4000°K.

In order to test the application of the derived functions for heat capacities and volumes of solid and liquid aluminum and aluminum oxide, melting pressures as functions of the temperature of the solid were determined through the relationship

$$\mu^l(T, P) = \mu^s(T, P) \quad (2)$$

where  $\mu$  is the chemical potential. It was found that this procedure did not result in a realistic melting curve for aluminum. Therefore, experimental melting points [8] for this element for pressures to 60 kilobars were utilized to develop the following relationship:

$$\ln P(\text{kbar}) = 9.15831 - \frac{6611.32}{T} \quad (3)$$

Equation (3) is utilized in this study to extrapolate the melting curve of aluminum to elevated pressures.

For aluminum oxide a realistic melting curve resulted with the derived thermodynamic property relationships for the liquid and solid through the application of Equation (2), and the low pressure limit is in close agreement with the experimental value of 2327°K. If the calculated chemical potential for aluminum oxide solid is lower at a specified temperature and pressure, properties for the solid are utilized for this component; otherwise liquid properties are used at this condition. The melting curves developed in this study enable the correct phase of the species to be identified for each point calculation.

### GIBBS FREE ENERGY MINIMIZATION

Previously, JAGUAR chemical equilibrium calculations for the distribution of explosive products were performed by the minimization of the Helmholtz free energy at constant  $T$  and mixture total volume  $V$ . In addition to the mole numbers of the components, this procedure requires an additional parameter and constraints for a single carbon phase involving the ratios of the solid volume to the total volume. This procedure was considered to be inconvenient for extension to multiple condensed phases. Therefore, in this study revised procedures (JAGUAR/Al) have been developed for the minimization of the Gibbs free energy of the composite system at fixed  $T$  and  $P$ . The revised objective function for multiple condensed phases is:

$$\text{Min } G(T, P) = \sum_{i=1}^m n_i \mu_i + \sum_{j=m+1}^p n_j \mu_j \quad (4)$$

where  $\mu_i$  is the chemical potential of the  $m$  gaseous products and  $\mu_j$  the chemical potential for the liquid and solid carbon and aluminum components. The optimization variables are the

number of moles  $n_i$  of each of the  $p$  species of the system. The material balance constraints are

$$g(k) = \sum_{i=1}^p a_{ki} n_i - b_k \quad k = 1, K, m \quad (5)$$

where  $a_{ki}$  is the number of atoms of element  $k$  present in a molecule of species  $i$ , and  $b_k$  is the number of moles of element  $k$  in 100 grams of the explosive.

For gaseous components, the chemical potential is calculated from the JCZ3 equation of state. For solid or liquid products the residual chemical potentials are calculated from the relationships for molar volumes of the condensed components.

### JAGUAR OPTIONS FOR ALUMINIZED EXPLOSIVES

The input options which have been implemented for the revised JAGUAR/Al procedures include the calculation of properties at  $T$ ,  $P$  points, Hugoniot curves, C-J properties, and for the principal and alternate isentropes. A default freeze temperature of 2200°K has been found to be most suitable for the JCZ3 equation of state with optimized parameters.

In JAGUAR/Al procedures have been implemented to establish the JWLb parameters of aluminized explosives from the calculated thermodynamic properties for the principal isentrope. The FIT option utilizes the RNLQ variable metric optimization routines to parameterize the following relationships for each explosive:

$$\lambda = \sum_i (A_{\lambda i} V^* + B_{\lambda i}) e^{-R_{\lambda i} V^*} + \omega \quad (6)$$

$$P_s = \sum_i A_i e^{(-R_i V^*)} + C V^{*-(\omega+1)} \quad (7)$$

where  $\lambda$  is the Gruneisen parameter,  $V^*$  the relative expansion volume, and  $P_s$  the isentrope pressure. Numerical procedures are utilized to obtain values of  $\lambda$  along the principal isentrope from the relationship

$$\lambda = \frac{T}{V} \left( \frac{\partial V}{\partial T} \right)_s \approx \frac{T}{V} \left( \frac{\Delta V}{\Delta T} \right)_s \quad (8)$$

If overdriven points are included isoline calculations are performed at 110 points for pressures from 500 to 0.005 kbar.

For the parameterization of the Gruneisen parameter relationship, Equation (6), the  $A_{\lambda i}$  values are constrained to be positive, the value of  $\lambda$  is constrained to be between maximum and minimum values (0.2 and 0.5), and the following additional constraint is employed to insure that the Gruneisen parameter is positive at  $V^*=0$ :

$$\sum_i B_{\lambda i} + \omega \geq 0 \quad (9)$$

For the isentropic  $P$ - $V^*$  relationship, Equation (7), the  $A_i$ ,  $R_i$ , and  $C$  variables are constrained to be positive, and the C-J pressure and detonation velocity resulting from the JWLb relationship are constrained to be equal to the calculated values. The detonation energies at  $V^* \approx 7$  and at 5 bar pressure are also constrained so that the JWLb and JAGUAR values are equal.

## DETONATION PROPERTIES FOR ALUMINIZED EXPLOSIVES

Calculations of C-J velocities and detonation properties on the principal isentrope were performed by the JAGUAR/Al procedures for an HMX based explosive with varying weight fractions of aluminum. The composition with 64% HMX, 4.8% BDA, 4.8% BDF, 6.4 % CAB, and 20% Al by weight is designated as PAX-3. The compositions of the other components were adjusted proportionately for alternate aluminum weight fractions. All calculations were for 99% TMD for each explosive mixture, and assume that all the aluminum charge is in chemical equilibrium with the reaction products. In Figure 1 the C-J velocity of the explosive is seen to decrease with increasing aluminum weight per cent. The velocity drops substantially at weight fractions higher than 20%. At the C-J condition for each formulation, all of the aluminum charge is reacted to aluminum oxide, which is in the solid phase as established through the equilibrium calculations. The corresponding temperatures are as high as 6000°K for a 30 weight per cent charge.

In Figure 2 calculated values of the detonation energy for the principal adiabat at  $V^*=7.0$  established by the resulting JWL relationships for each formulation are plotted against the weight fraction of aluminum addition. It can be seen that the detonation energy at this condition exhibits a minimum at about 20 weight per cent aluminum charge. A phase transformation of the aluminum oxide formed from solid to liquid was observed in the calculations at low pressures along the adiabat for aluminum additions greater than 20%.

Values of the detonation energy at infinite volume,  $E_o$  as established by the JWL procedures are plotted in Figure 2 against the weight percent aluminum in the formulation. The limiting detonation energy decreases rapidly with aluminum weight fraction for the range 0-20%, and exhibits a slight negative minimum for about 25% aluminum. A comparison of the curves in Figure 2 indicates that at high aluminum weight fractions, large increases in detonation energy are observed for expansion volumes greater than 7.

Calculations were also performed for PAX-3 (20 weight per cent total aluminum), with varying fractions of reacting and inert aluminum. For virtually all cases the unreacted aluminum is identified to be liquid at the C-J and expansion conditions. In Figure 3 the C-J detonation velocity of the explosive is shown to decrease with increasing fraction of metal reacted. The temperature varies from 5227°K for 100% reacted to 3015°K for 100% inert aluminum.

In Figure 4, for 20 weight per cent total aluminum, the calculated detonation energies at  $V^*=7$  are substantially more negative for increasing fraction of reacted metal. Similar behavior is indicated in this figure for the limiting detonation energies  $E_o$  for these systems. A comparison of Figures 3 and 4 indicates that the detonation energy at  $V^*=7$  varies by a larger percentage than the C-J velocity with the fraction of reacting aluminum. Therefore, experimental cylinder velocities and derived detonation energies in conjunction with JAGUAR/Al calculations should provide a sensitive test of the effectiveness of the aluminized explosive formulation.

## DISCUSSION

The JAGUAR/Al procedures developed in this study enable the calculation of detonation properties of aluminized explosives for wide ranges of conditions. Calculations for several systems [9] indicate that optimum performance for a balance of metal pushing

capability and high blast effectiveness results for 20-25% aluminum addition by weight for high energy HMX based compositions. The calculations indicate that for high weight fractions of reacting aluminum, large increases in the detonation energy occur at high expansion volumes. Because of the sensitivity of the calculated detonation energy at 7 volume expansions to the fraction of aluminum reacted, analyses in conjunction with experimental cylinder tests should significantly help to determine the extent of reaction and the corresponding effectiveness of aluminized composition. Ongoing work with PAX-3 includes cylinder expansion testing and detonation velocity measurements as a function of scale.

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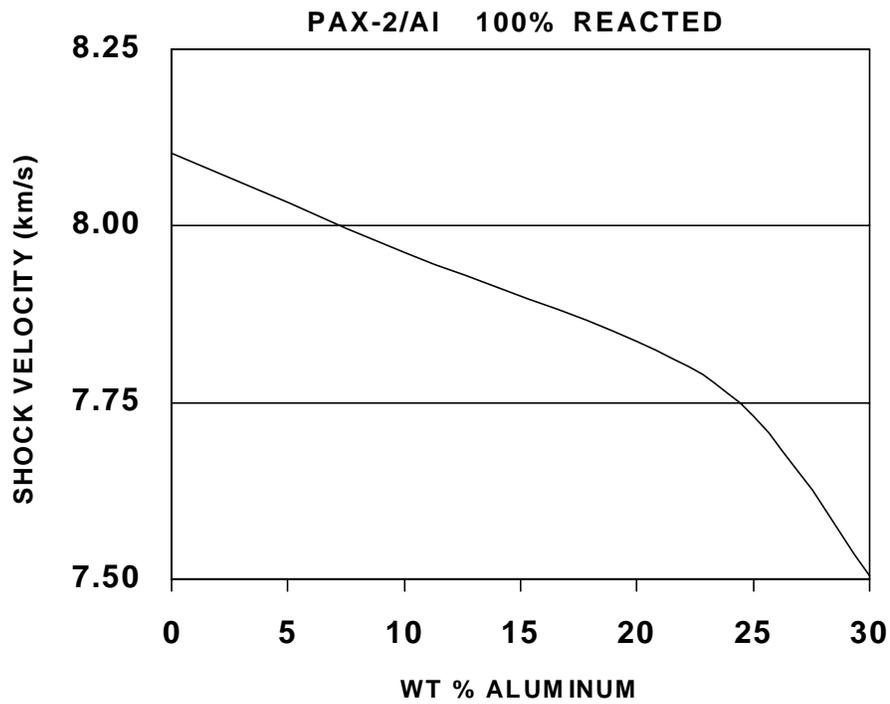


Figure 1. JAGUAR/Al calculation of Chapman-Jouguet detonation velocity versus weight percent aluminum addition to PAX-2.

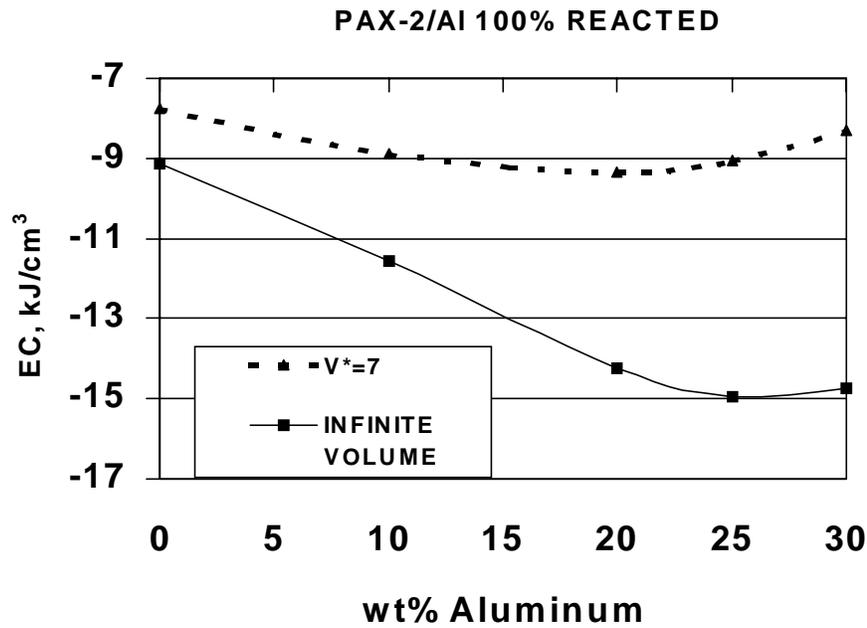


Figure 2. JAGUAR/Al calculation of detonation energy versus weight percent aluminum addition to PAX-2.

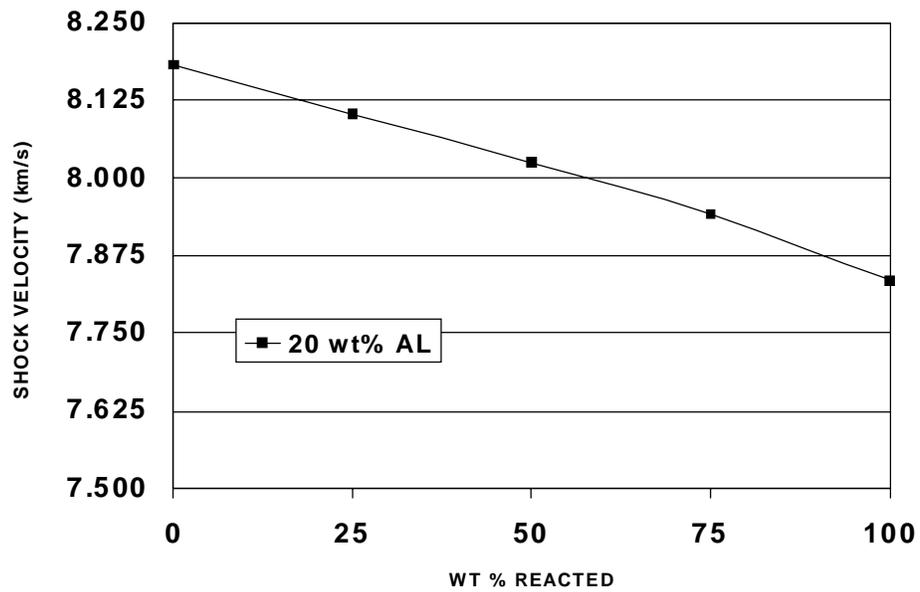


Figure 3. JAGUAR/Al calculation of Chapman-Jouguet detonation velocity versus weight percent aluminum reacted for to PAX-3.

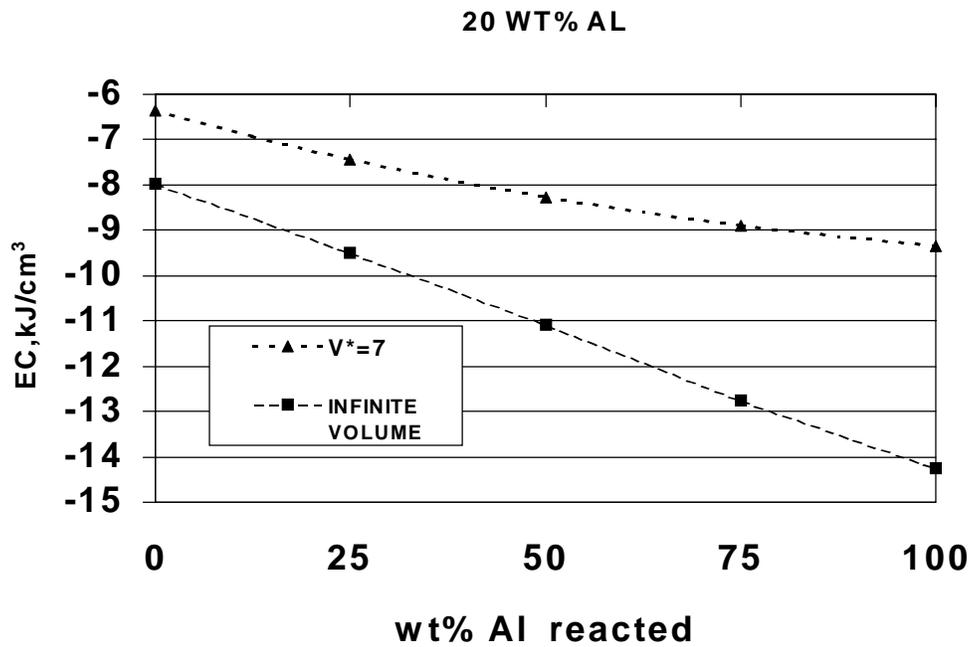


Figure 4. JAGUAR/Al calculation of detonation energy versus weight percent aluminum reacted for to PAX-3.