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DETONATION E.O.S. PATTERNS FOR SEVERAL EXPLOSIVES\*

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#### ABSTRACT

The available overdriven shockwave data for a number of exoplosives have been analyzed and compared. The data follows neither a constant gamma pattern nor the JWL EOS that fits expansion data to high accuracy. Modifications of the JWL function are proposed to correct for discrepancies and also to allow for the appropriate volume dependence of the Grüneisen constant indicated by previous and more recent work. The deviations from the JWL form of the equation of state appear directly above the CJ point for 9404 and PETN while Pentolite and TNT agree with this form over a portion of the Hugoniot. The comparisons with other experiments and a theoretical EOS indicate nonequilibrium behavior.

#### INTRODUCTION

The gamma  $\left[\Gamma = (V/P) (\partial P/\partial V)_{S}\right]$  law form [1] of explosive equation of state (EOS) was considered adequate until the middle of the sixties. Large expansion experiments on detonated sperical charges showed that this form needed to be modified. This resulted in the inclusion of a term of the form exp(-RV). It was noted that this term was undesirable at high pressure, since it tended to depress the value of the adiabatic gamma  $(\Gamma)$  above the CJ point [3]. This violated the constant  $\Gamma$  approximation that had been so useful. This contention was supported by high pressure shock wave measurements on composition-B from England [4]. Nevertheless the need for the exponential term in an equation of state constrained by the CJ hypothesis was established. Further work with more accurate data from cylinder expansions required the addition of a second exponential to further increase the slope of the isentrope [5]. More recently, shock-wave measurements [6] over a larger range of pressures, that indicate a failure of the  $\Gamma$  law form, have demanded a closer look at the high pressure form.

#### DATA ANALYSIS AND EOS CORRECTIONS

The 1970 shockwave data [6] were analyzed with the best molybdenum EOS available at that time. Better data are now available and a new Hugoniot fit was used in a reanalysis [7] of the data. In addition, a reflected Hugoniot approximation used before was replaced with a self-consistent simple elastic-plastic model for the EOS. The Hugoniot function used is a quadratic of D over  $U_p$  with coefficients  $C_0 = 5.1135$  km/s,  $S_1 = 1.24922$ ,  $S_2 = -1.41008E-3$  s/km. This analysis slightly reduced the particle velocities within the uncertainty of the data and increases the slope of the  $U_g-U_p$  curve.

The data was compared to the Hugoniot predicted by the JWL EOS. For 9404 [8] the computed shock speeds fall significantly below the measured ones if the 37.0 GPa. CJ pressure is used in the determination of the constants. The experimental adiabatic  $\Gamma$  may be calculated from an isentrope determined with the Grüneisen equation and the Hugoniot curve as a reference line. This yields,

$$P_{s} = P_{H} + k \left[ E_{CJ} - E_{H} + \int_{V}^{VCJ} P_{s} dV \right]$$

with the constant  $k=\gamma/V$  and  $\gamma$  the Grüneisen constant. This function is integrated numerically from the CJ point to yield the isentrope consistent with the Hugoniot and the value of k. The result is a value of  $\Gamma_{exp}$  that is considerably larger than that predicted by the CJ slope ( $\Gamma_{CJ} = \rho_{c} D^2 / P_{CJ}$ ) and consistent with the behavior described below.

In order to determine the coefficients for a useful overdriven detonation product EOS the CJ pressure may have to be modified to be consistent with the higher value of  $\Gamma$ . This worked well for PETN [8], but is not sufficient in other cases as we shall see. It has also been shown before that the value of  $\gamma$  rises from its gas phase value of about .3 to .65 or .7 for PETN [9] and HNB [10]. Recent calculations on PETN [9] and 9404 yield similar results except that the presence of a graphite to diamond transitions and a possible phase separation of a nitrogen rich phase increases this value to as much a .9 in the transition regions. Additional corrections are therefore needed.

We introduce the variable volume dependent  $\gamma$  by adding a fourth term to the JWL isentrope, so that:

$$P_{s} = A_{e}^{(-R_{1}V)} + Be^{(-R_{2}V)} + C/V^{\omega+1} + f$$

where  $f = aV^2/(1+bV^2)^2$ . This leads to the standard JWL EOS form in which  $\omega$  is now replaced by  $\gamma$ , which is defined by:

$$\gamma = \omega [C + aV^{\omega+2}/(1+bV^2)^2]/[C + aw^{\omega}/\{2b(1+bV^2)\}]$$

To improve the energy independent part of the EOS we proceed as follows:

First, we check if the data allows us to change  $P_{CJ}$  to match the Hugoniot.

Second, we may replace the energy independent part of the Grüneisen function to describe the high pressure region. The data indicates that this should be a polynomial which includes a term of the form  $A_0/(a_0 - V)$  that allows for a rapid change in slope near the point where the EOS forms are joined.

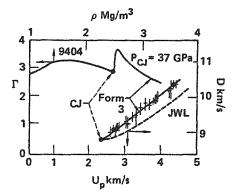
Third, we may apply a correction to the JWL form. A useful correction term is:

$$\delta P = R_3^2 A_3 [\ln 2 \cosh(V - V_c) / R_3 - (V - V_c) / R_3] ,$$

where A<sub>3</sub>, R<sub>3</sub> and V<sub>c</sub> are constants.

#### EOS CHARACTERISTICS AND HYDRO CALCULATIONS

We have used the third option (or form) to fit the data. The corrections for 9404 and PETN must be applied directly above the CJ point. This results in a sharp change in the value of  $\Gamma$  near this point. Our re-evaluation of the PETN data [8] has reduced the probable value of  $P_{CJ}$  sufficiently to make the correction term small, as opposed to the behavior of 9404 shown in Fig. 1. It is also clear from Fig. 1 that the correction term reproduces the data accurately.



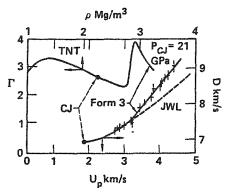
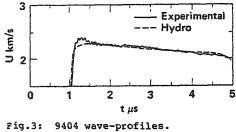


Fig. 2: As Fig. 1 but for TNT.

Fig. 1: Γ vs. ρ - upper curve, p vs. Up-lower curves and data, for 9404.

In contrast to 9404 and PETN, the correction to the JWL form for TNT (Fig. 2) and 50/50 Pentolite do not occur right at the CJ point but at smaller volumes. The best fits for these explosives cause an even higher  $\Gamma$  excursion than was needed for 9404. The reason for this behavior is far from clear. Comparisons with theory and further experimental work may clarify the picture.



The equation for 9404 was used to reproduce an experimental velocity guage wave profile [11] (see Fig. 3). The wave profile calculation reproduces the Taylor wave well, but it is about 3 percent low near the front. Here a structure reminiscent 5 of a broad von Neuman spike is noticeable. The Beta burn formulation used in these calculations cannot reproduce such features.

The effect of detonation wave buildup time is illustrated in Fig. 4a, where a couple of one-dimensional hydro code calculations are compared to the results of a plate acceleration experiment [12]. Erickson and coworkers used the 4 inch LLNL gun to initiate a 17 mm piece of 9404 with a copper plate moving at 1.27 km/s. The measured velocity profile is that of a .5 mm copper plate that is accelerated by the detonated 9404. The calculation predicts a somewhat higher average shock speed, but accurately predicts the initial three acceleration pulses. Further improvement is obtained by increasing the time over which the detonation wave builds up to full pressure. Both the decrease in average wave velocity and the improved agreement during the later stages of the acceleration indicate that burn conditions are important in this experiment.

The sensitivity of these calculations to the equation of state is illustrated in Fig. 4b. Here we compare the empirical EOS of 9404 and a theoretical EOS with the same plate velocity data. The theoretical EOS is an equilibrium calculation of the product species that uses a statistical mechanics approach to compute the pressure and energy of the mixture of product species. The interaction potentials are determined with the corresponding states principle and indclude a dipole interaction for water. The agreement of Hugoniot calcu- lations of individual product

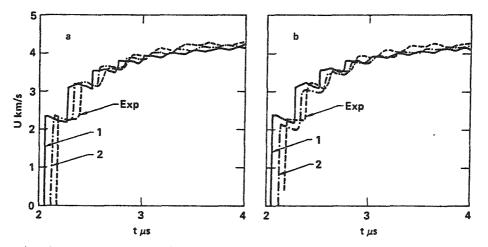


Fig. 4: Plate acceleration profiles <u>a</u>: 1-rapid build-up to detonation, 2 - 2.5 mm build-up. <u>b</u>: 1 -  $P_{CJ}$  = 37.0 GPa, Empirical EOS. 2 -  $P_{CJ}$  = 34.0 GPa theoretical EOS.

species with experiment is good and has been discussed before [10]. This theoretical EOS for 9404 closely reproduces the experimental JWL expansion isentrope below the CJ point. The lower (34.0 GPa) CJ pressure predicted by theory clearly shows up as a lower initial acceleration of the plate. The last part of the velocity profile, however, shows slghtly better agreement with the data than the empirical equation.

The overall behavior of the empirical EOS and its differences with the theoretical equilibrium EOS imply a lack of complete equilibrium in the experiments that go into the empirical form. Further work to close the gap between theory and experiment is clearly needed.

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