

ACCELERATING DETONATIONS IN COMPOSITION B-3 EXPLOSIVE

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INTRODUCTION

The problem of predicting what will happen when a fragment or projectile strikes cased high explosive munitions is complicated not only by the complexity of the projectile-munition geometry but also by the number of different reactions which can and do occur.

Recourse to the literature on the subject exposes one to such terms as no reaction, burning, deflagration, low order, mild low order, large low order, partial detonation, high order and deflagration to detonation transition.

Examining the literature on explosive sensitivity is about as helpful and introduces a series of tests which regularly produce confused ranking of the "sensitivity" of high explosive systems. (The theory or theories of detonation are not a great deal of help either.)

The major problem is actually one of continual attempts to link all the various modes of chemical reaction and all the means of physical excitation into one simple model which would be useful in explosive applications. The probability of success in such a venture is small at best, but an attempt must be made since studies are going to be made with or without adequate models.

In any attempt to tackle this problem the explosive system should first be examined from a chemical as well as a physical viewpoint, the adiabatic auto ignition temperature and its connotations, the shock sensitivity spectrum, experimental results, effects of geometry, and an attempt to create a limited analytic model.

THE EXPLOSIVE

GENERAL COMMENTS

Explosives in general use vary over a wide range of chemical compositions, but do have several similar characteristics.

They consist of chemical compositions which contain both the fuel and the oxidizer in an "unstable" molecular configuration which when broken allows the various atoms to combine into such products as H_2O , CO , CO_2 , N_2 , etc., with a rapid net production of energy.

The stability of the explosive molecule should and apparently does play an important part in the sensitivity of the explosive.

Analysis of the statistical nature of chemical kinetics shows that some of the molecules are decomposing at any temperature above absolute zero but that the number of molecules decomposing or reacting per second remains "insignificant" up to some critical temperature dependent on the ability of the explosive to dissipate the energy generated by the reacting molecules. Above this temperature the number of molecules involved increases exponentially leading to significant evolution of energy. The dissipative factors involve the heat capacity, the thermal conductivity, the geometry of the explosive, the nature of the confining media, and the temperature of the environment.

(In the presence of air, surface reactions involving the oxygen in the air are, of course, possible.)

In an investigation of the problem of explosive storage and handling, Longwell (ref. 1) measured the adiabatic auto-ignition temperatures of various explosives and developed relations for safe storage times and temperature for various charge geometries.

SHOCK MOLECULAR EFFECTS

When a shock wave strikes a molecule, the molecule absorbs energy and if the energy is high enough, bond rupture occurs. As long as the energy is absorbed into the molecule with no effect from other molecules or their decomposition fragments, the weakest part of the molecule will undergo rupture first. This will be regardless of other factors and certainly is the first effect of the shock wave.

However, once the molecule is disrupted, reactive fragments such as ions and free radicals can collide with the unreacted molecule to cause further bond rupture. Since this latter effect will depend on the spatial features of the molecule, steric factors are important and the bonds disrupted may not necessarily be the weakest in the molecule. In fact they may well be the strongest if the atoms involved are easier to reach by being on the outside of the molecule.

This being the case it is easy to select the bonds that are broken first, i.e., the N-NO₂ and the C-NO₂ (Table I). However, after the initial phase it is probable that the C-H bonds are next ruptured since they occur in both molecules and the hydrogen atoms are on the outside of the molecule.

SHOCK SENSITIVITY SPECTRUM

Energy levels calculated as associated with shock waves in explosives show that for shocks of the order of a few kilobars some chemical reaction is quite probable, but the extent and rate of propagation of the reaction would be strongly dependent on the duration of the pressure pulse as well as its amplitude and thus strongly dependent on the nature of the confinement. Studies by Liddiard et al. (ref. 2) have shown that with proper confinement sustained chemical reaction can be produced in Comp B at pressure amplitudes of the order of 5 to 7 kbars.

This sustained chemical reaction is not to be confused with detonation, which is a chemically supported shock wave, but it can produce burning or deflagration which has often, improperly, been called low order detonation.

Low order detonation--a nonideal detonation--is generally unstable (it is either accelerating or decaying) and is produced when a shock wave with intensity above a given level (dependent on the curvature of the shock front) enters the explosive and either accelerates to full high order detonation or decays to no reaction. The curvature of the wave front during acceleration is strongly dependent on the confinement, the size and shape of the shock producing system, and the physical properties of the explosive.

It has been shown (ref. 3) that for pressures greater than 21 kbars the growth to detonation is dependent upon peak pressure and is relatively independent of impulse. It is interesting to note that the factor of 3 between the values of critical pressures obtained by Liddiard et al. (ref. 4) and Cosner and Burford (ref. 4) correspond to the factor of 3 between the average bond strengths of the N-NO₂ and the C-H bonds.

The initiation of explosive by shock impact is characterized by several zones or thresholds. At very low shock levels no significant chemical reaction occurs, as the shock level is increased surface reactions will be triggered, and as the shock level is increased still further other effects will begin to predominate.

If the input shock level is above 202 kbars (ref. 3), an almost instantaneous jump to stable detonation is observed with a CJ pressure of 272 kbars. Studies have shown that in the region from 21 to 202 kbars the growth of pressure with distance can be represented by

$$\frac{dP}{dx} = k(P - P_c) \quad (\text{ref. 3}) \quad (1)$$

where $P_c = 21$ kbars and $k = 0.132 \text{ mm}^{-1}$ with P in kilobars and x in millimeters.

Using an assumption based on Adams' (ref. 5) investigation of nonideal detonation, the pressure is directly proportional to the square of the propagation velocity

$$P = \gamma U^2 \quad (\text{ref. 5}) \quad (2)$$

The constant γ in this expression is found to be 3.38 with P in kilobars and U in millimeters/microseconds.

Integration of eq. (1) yields solutions for pressure as a function of distance and these combined with eq. (2) yield shock velocity as a function of distance and input pressure. A table of parameters of interest associated with these solutions is shown in Table II.

Wedge experiments of the type performed by Boyle, Jameson, and Allison (ref. 6) measure directly the shock velocity as a function of distance. Their determination of the pressure is dependent on the assumption that the explosive will return to its initial density upon release of the pressure. This assumption seems highly unjustified in view of the accelerating reaction which is observed. Their velocity-position data are free of these assumptions and could be used for direct comparison. Unfortunately, "for ease of plotting," Boyle, Jameson, and Allison divided their actual distance by the initiation distance to "normalize" the measurements and failed to publish the actual distances. Working from what they have published, the initiation distance is found to be 15 mm with a variation of about 1 mm. A plot of their data compared to our calculated values is shown in Fig. 1.

If a spherically divergent system is presumed, eq. (1) is modified by substituting r for x and introducing a spherical loss term

$$\frac{dP}{dr} = k(P - P_c) - \frac{P}{r} \quad (3a)$$

or

$$\frac{dP}{dr} = P(k - \frac{1}{r}) - kP_c \quad (3b)$$

If eq. (3b) is correct and if the constant k is correct a minimum radius of curvature for any stable detonation becomes

$$r = \frac{1}{k} \quad (4)$$

For Comp B-3 this would be $r = \frac{1}{0.133} = 7.52 \text{ mm}$.

This value is not the limiting radius of a cylinder which would propagate detonation but would be the radius of curvature of the central portion of the detonation wave in the limiting cylinder. Actually since the pressure would not be much above 202 kbar at the limit situation the limiting radius of curvature would be about 8.4 mm. If a hemispherical front is postulated the limiting diameter for full detonation velocity would be 16.8 mm which is equivalent to the d_m^* of ref. 7.

A graph of the pressure required to produce an accelerating detonation as a function of the radius of curvature of the front is shown in Fig. 2. Converging wave fronts (negative radius of curvature) require less pressure than the critical pressure to produce an accelerating front which tends to invert rapidly to a divergent wave front. If during the period of convergence the pressure increases enough over a large enough zone, continued acceleration should occur.

Below and to the left of the positive radius of curvature curve the reaction produced is a decaying detonation. Near the curve, a slight change in radius of curvature through a density change or a void in the explosive could have a large effect on the occurrence of growth to detonation.

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Table I

Average Bond Dissociation Energies

C=C	146 kcal/mole	(ref. 8)
C-H	98.7 kcal/mole	(ref. 8)
C-C	86.6 kcal/mole	(ref. 8)
C-N	72.8 kcal/mole	(ref. 8)
C-NO ₂	48 kcal/mole	(calcd. from ref. 9)
N-NO ₂	32 kcal/mole	(calcd. from ref. 9)

Table II

Pressure Distribution and Propagating Velocity for Accelerating Shock

mm x	kbars $\Delta P = (P_o - P_c)e^{kx}$	kbars $P = \Delta P + P_c$	mm/ μ sec $U = \sqrt{P/\gamma}$	Distance to go to detonation, mm 70 - x
70	181	202	7.78	0
65	93.5	114	5.86	5
60	48.3	69.3	4.56	10
55	25.0	46.0	3.71	15
50	12.9	33.9	3.19	20
45	6.68	27.7	2.88	25
40	3.45	24.5	2.71	30
35	1.78	22.8	2.61	35
30	0.92	21.9	2.56	40
25	0.48	21.5	2.54	45
20	0.25	21.3	2.52	50
15	0.13	21.1	2.52	55
10	0.07	21.1	2.51	60
5	0.03	21.0	2.51	65
0	0.02	21.0	2.51	70

$k = 0.132$

$\gamma = 3.34$

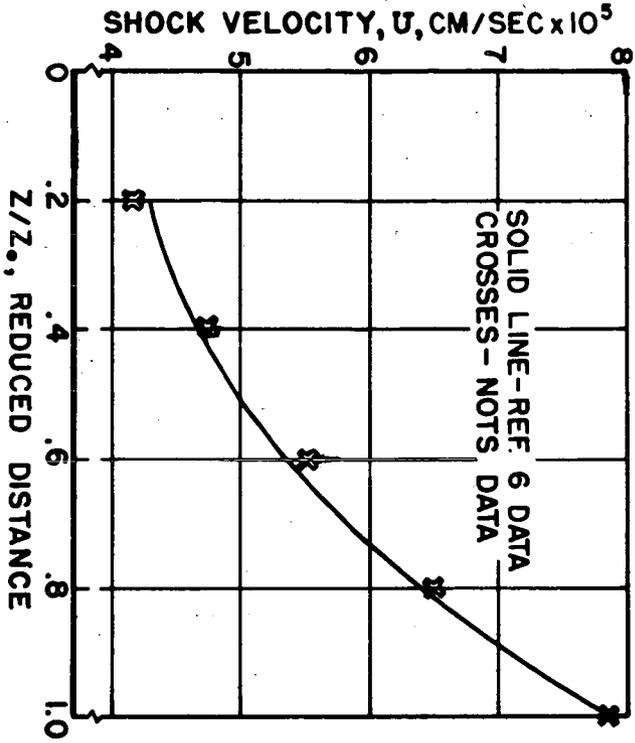


Fig. 1. Shock velocity, U, versus reduced distance Z/Z₀.

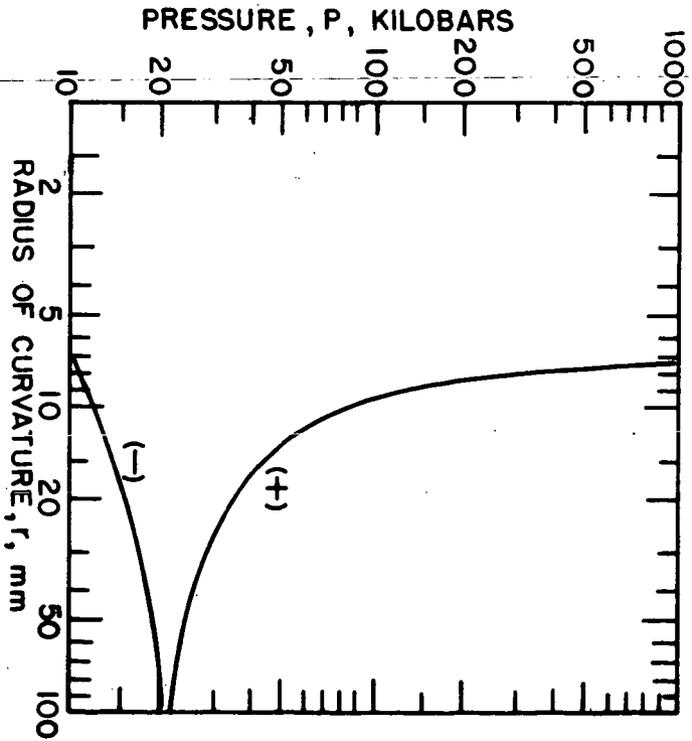


Fig. 2. Shock pressure required to produce an accelerating detonation in Composition B-3 as a function of radius of curvature.