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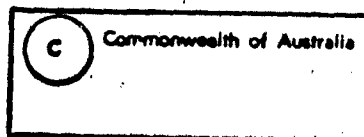
Application of the CPEX Non-Ideal Explosive Model to PBXW-115

D.A. Jones and D.L. Kennedy*

MRL Technical Report
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Abstract

We present a detailed description of the use of the ICI non-ideal detonation code CPEX to model the performance of the composite underwater explosive PBXW-115 (20% RDX, 43% AP, 25% Al and 12% HTPB). We use both the ICI chemical equilibrium code IDEX and Mader's BKW code to first estimate the Chapman-Jouguet parameters for PBXW-115. Two different reaction rate models are assumed for the decomposition of the explosive components and the time constants for each are found by fitting to experimental US data on the variation of detonation velocity with charge diameter. The data is best fitted by a three term reaction rate model which equates hotspot content to some fraction of RDX content, the intermediate scale reaction primarily to the AP decomposition, and the slowest process to the Al reaction. After adjusting some of the reaction time constants because of differences between the US and Australian compositions the model then accurately reproduces the variation of detonation velocity with charge diameter found for Australian PBXW-115.



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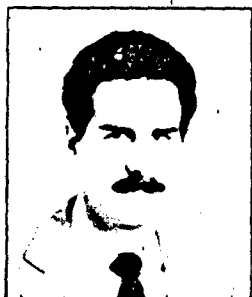
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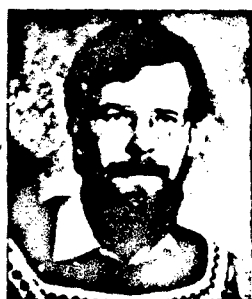
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Application of the CPEX Non-Ideal Explosive Model to PBXW-115

1. Introduction

Several years ago Materials Research Laboratory (MRL) was asked to advise on the choice of a suitable explosive filling for use in Australian naval mines. A range of explosives in current UK or US service, or undergoing qualification, for underwater applications was surveyed and a recommended warhead filling was proposed. In addition, it was recommended that R & D work be initiated on ammonium perchlorate (AP) based polymer bonded explosives (PBXs) because of their reported lower vulnerability and higher performance. PBXW-115, an experimental formulation under active development in the US, was identified as being most suitable because of its projected lower cost compared with other PBX alternatives and its desirable vulnerability characteristics. Another attractive feature was that the binder system was similar to that used in Australia for composite propellant production.

MRL was subsequently tasked by Navy to consider the feasibility of PBXW-115 as a fill for Australian naval mines. Work on this task to date has concentrated mainly on formulation aspects. PBXW-115 is a cast cured explosive with a nominal composition of 20% RDX, 43% AP, 25% Al and 12% HTPB based polyurethane binder. Research has concentrated on the blend of RDX grades, the Al particle size, and both the binder chemistry and mechanical techniques for processing the formulation.

In parallel to these predominantly chemical studies, we have undertaken an investigation into the possibility of modelling the performance of PBXW-115 and related formulations. This is a new area of endeavour for MRL as PBXW-115 is a non-ideal explosive [1] and therefore not amenable to the more usual techniques used for the modelling of military explosives. Mader has defined a non-ideal explosive as one having a C-J pressure, velocity, or expansion isentrope significantly different from those expected from equilibrium, steady state calculations such as those performed by the computer code BKW [2]. Johnson *et al.* [3] have modelled the performance properties of a variety of non-ideal explosives using data obtained from the aquarium test

and have made comparisons with results from BKW calculations assuming varying degrees of reaction at the detonation front. We will consider this approach in more detail in a later section.

All explosives exhibit some form of diameter effect in which the detonation velocity decreases with decreasing charge diameter until a critical diameter is reached and stable detonation cannot be sustained. For ideal explosives the change in velocity with diameter is minimal until very close to the critical diameter, whereas for non-ideal explosives the diameter dependence is very pronounced and the velocity at the critical diameter can be as low as 30% of the value at infinite diameter. Commercial explosives often behave very non ideally and their performance properties depend strongly on charge diameter and confinement. These explosives, like military underwater explosives, contain separate fuel and oxidizer species, often in physically separated phases, and their heterogeneous nature leads to much larger reaction zones and more curved detonation fronts than those in ideal explosives [4].

To model the performance of commercial explosives Kirby and Leiper have developed a small divergent detonation theory for intermolecular explosives [5]. Their model has been developed into the computer code known as CPEX (Commercial Performance of Explosives) and used for a variety of applications [6-8].

In this report we describe the application of the CPEX code to PBXW-115 using experimental data on the detonation velocity/diameter effect obtained by Forbes *et al.* [1], and also by Bocksteiner *et al.* [9] in a recent MRL field trial. Section 2 describes the theory and basic equations underlying the CPEX code, and Section 3 discusses the problems involved in calculating the equilibrium Chapman-Jouguet state for PBXW-115, which is needed as input for the CPEX code. In Section 4 we describe the results obtained from the application of CPEX to PBXW-115, and in the final section we discuss these results and our approach in relation to other methods which have been used to model the behaviour of non-ideal explosives.

2. CPEX Code Description

The CPEX code is based on the analytical non-ideal detonation theory of Kirby and Lieper [5], which is a further development of the work of Chan [10], and is ultimately based on the small divergent detonation theory of Wood and Kirkwood [11]. The theory is applicable to both unconfined and confined axisymmetric detonations and its application requires the numerical solution of a set of coupled, nonlinear ordinary differential equations between the shock front and the end of the reaction zone.

A detonation wave is a supersonic shock wave travelling through a reactive medium. The high temperature generated by the passage of the shock through the material initiates chemical reaction and energy release. A stable detonation with a unique detonation velocity (the Chapman-Jouguet or C-J velocity) will then develop if the chemical reaction zone can remain coupled to the wave and continuously feed energy to the shock front. Any model of a detonation therefore requires the simultaneous solution of the coupled equations describing

both material flow and chemical reaction. In the CPEX model the material flow equations used are the Euler equations, a set of three coupled partial differential equations describing the conservation of mass, momentum, and energy for an inviscid fluid. These have the general form

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \underline{v}) = 0 \quad (1)$$

$$\frac{\partial (\rho \underline{v})}{\partial t} + \nabla \cdot (\rho \underline{v} \underline{v}) = -\nabla P \quad (2)$$

$$\frac{\partial E}{\partial t} + \nabla \cdot (E \underline{v}) = -\nabla \cdot (P \underline{v}) \quad (3)$$

where ρ is the density, $\underline{v}$ the fluid velocity, and P the pressure. The quantity E is the total energy per unit volume and is defined by

$$E = \rho \epsilon + \frac{1}{2} \rho \underline{v} \cdot \underline{v} \quad (4)$$

where ϵ is the specific internal energy.

The extent of chemical reaction is described by a progress variable λ , which is the fraction of reacted explosive in the material. The equation governing the time evolution of λ has the form

$$\frac{d\lambda}{dt} = R(\rho, P, \lambda) \quad (5)$$

where the exact functional form of R will be specified shortly. Note that the time derivative in equation (5) is a total time derivative following the fluid flow and has the form

$$\frac{d}{dt} = \frac{\partial}{\partial t} + (\underline{v} \cdot \nabla) \quad (6)$$

The CPEX code models steady state detonation in a cylindrical charge for the case of slightly divergent flow. In this case several simplifications can be made. We first rewrite equations (1) to (3) in an axisymmetric cylindrical coordinate system

$$\frac{d\rho}{dt} + \rho(u_x + w_r) + \rho \frac{w}{r} = 0 \quad (7)$$

$$\rho \frac{du}{dt} + P_x = 0 \quad (8)$$

$$\rho \frac{dw}{dt} + P_r = 0 \quad (9)$$

$$\frac{de}{dt} - \frac{P}{\rho^2} \frac{d\rho}{dt} = 0 \quad (10)$$

Here u and w are the axial (x) and radial (r) components of the velocity vector $\underline{v}$ and subscript x or r denotes partial differentiation with respect to x or r .

Using the steady state condition and the assumption of small divergent flow, and considering motion only in the axial direction (at $r = 0$, i.e. along the centreline), equations (7) to (10) and equation (5) can be written in the form

$$u\rho_x + \rho u_x = -2\rho w_r \quad (11)$$

$$\rho u u_x + P_x = 0 \quad (12)$$

$$P_r = 0 \quad (13)$$

$$e_x - \frac{P}{\rho^2} \rho_x = 0 \quad (14)$$

$$\lambda_x = R/u \quad (15)$$

Kirby and Lieper [5] further simplify the above set of equations by using the equation of state in the form $e = e(\rho, P, \lambda)$ to derive the following expression for P_x

$$P_x = c^2 \rho_x + \rho c^2 \sigma \lambda_x \quad (16)$$

where c is the local sound speed and σ is the thermicity, defined by

$$\sigma = \left(\frac{\partial P}{\partial \lambda} \right) / \rho c^2 \quad (17)$$

The quantity σ is a measure of the heat release. The system is exothermic if σ is positive and endothermic if σ is negative. Use of equation (16) then results in the following defining set of equations

$$f_x = -\rho(u_x + 2w_r)/u \quad (18)$$

$$u_x = (1 - u^2/c^2) / (\sigma R - 2w_r) \quad (19)$$

$$e_x = \frac{P}{\rho^2} \rho_x \quad (20)$$

$$\lambda_x = R/u \quad (21)$$

The term w_r in equations (18) and (19) represents the radial divergence of the flow. If the flow was completely one-dimensional this term would be zero and the equations would represent the standard Zeldovich, von Neumann, Doering (ZND) model of detonation [12]. In this model the initial disturbance shocks the material to the von Neumann point, which results in an increased value of the density, and considerably higher values of both pressure and temperature. This initiates chemical reaction, which then proceeds at a finite rate until all of the explosive has been converted to detonation products. In the one-dimensional case (i.e. $w_r = 0$), equations (18) to (21) can be used to show that the end of the reaction zone always coincides with the Chapman-Jouget (CJ) point, which is defined as the point at which the sum of the fluid velocity plus the local sound speed is equal to the detonation velocity. This is an important point in the flow because if reaction occurs beyond this point then the energy which is released is unable to contribute to the support of the detonation wave.

For divergent flow the simple ZND picture no longer applies, and some degree of reaction will always occur beyond the CJ point. Equations (18) to (21) (for finite w_r) can be used to show that the reaction must satisfy the following criteria at the CJ point

$$\sigma \lambda_x = 2w_r/u \quad (22)$$

which implies that the rate of chemical energy release is balanced by the energy diminution to the lateral flow expansion. Thus for radially divergent flow there are two sources of energy loss: (a) the energy loss to the radial motion, (b) the fraction of chemical energy released beyond the CJ point. This means that the detonation velocity for a cylindrical charge with a finite diameter will always be less than the planar or CJ value, and will only approach the CJ value as the diameter becomes infinite.

Before equations (18) to (21) can be solved an expression for the radial divergence w_r must be specified. It is easily shown [12] that w_r can be related to the radius of curvature of the detonation front, R_d , by the expression

$$w_r = (D - u(o)) / R_d \quad (23)$$

where D is the detonation velocity and $u(o)$ is the flow velocity at the shock front. The problem thus reduces to the specification of R_d . The developers of the CPEX code surveyed many explosives and found that R_d was inversely proportional to charge diameter d , provided that both R_d and d were scaled by

the critical diameter d_{cr} . There is some scatter in the data, and the proportionality constant depends on whether the explosive is a Group 1 or Group 2 explosive (as defined by Price [13]), but the correlation is sufficiently strong enough to provide the necessary relationship between R_d and d . If more exact experimental data are available for a particular explosive then CPEX has an option to accept this data. We used both methods in our analysis of PBXW-115.

The reaction rate law used by CPEX has the following functional form to allow for the multi-phase, multi-component nature of composite explosives

$$\frac{d\lambda}{dt} = (1 - \lambda) \frac{a_h (P - P_h)^{b_h}}{\tau_h} + \frac{a_l P_l^{b_l}}{\tau_l} + \frac{a_s P_s^{b_s}}{\tau_s} \quad (24)$$

The subscripts h , l , and s refer to the hot spot, matrix (in commercial explosives this is often a liquid phase) and included solid phases within the explosive. The pressure exponents b_i ($i = h, l, s$) are normally set to unity and the a_i are gaussian form functions which switch the reactions on and off as the various phases are ignited and consumed. The a_i depend on λ and the initial formulation of the explosive. The τ_i are characteristic reaction times for each of the phases, and P_h is a hot spot critical pressure. In typical applications of CPEX the a_i and b_i are fixed and the τ_i and P_h are used as adjustable fitting parameters.

The equation of state for a single phase has a simple density dependent polytropic equation of the form

$$e = \frac{P}{\rho} (g - 1)^{-1} \quad (25)$$

$$g = g_0 + g_1 \rho + g_2 \rho^2 \quad (26)$$

The reasoning behind the choice of equations (25) and (26) to describe the equation of state is discussed in detail by Kirby and Leiper [5]. The values of the constants g_i for the explosive products are found by fitting to isentrope data from an ideal thermodynamic code, while the constants for the unreacted phase are obtained by considering the shock state of the explosive and using known Hugoniot data. The unreacted solid state is usually a mixture of ingredients, and in this case the Hugoniots of the components are combined using the method of Afanasenkov *et al.* [14].

Equations (18) to (21) are a coupled set of nonlinear ordinary differential equations which must be solved subject to a mixed set of boundary conditions; at the CJ plane both the CJ condition and equation (22) must be satisfied, and immediately behind the shock front the variables must agree with the unreacted shock state. The detonation velocity now becomes an eigenvalue of the equation set and its value is dependent on the charge diameter, degree of confinement, and on the chemical reaction rate of the explosive.

In typical applications of CPEX the equations of state of both reactants and products are known and the ideal CJ parameters are obtained from a chemical

equilibrium code such as BKW or the ICI IDEX code. The reaction rate parameters τ_i and P_h are then estimated by using CPEX to obtain a fit to experimental data on the variation of detonation velocity with charge diameter, and then CPEX can be used to predict the explosive performance for a variety of confinements [7], as well as the effect of charge diameter and porosity on initiation behaviour [6], and also to make comparisons with other theoretical approaches for predicting the performance of condensed explosives [8].

3. Calculation of Equilibrium Chapman-Jouguet State

Before running CPEX on a particular explosive formulation an estimate must be made of the CJ velocity and ideal CJ gamma for the given explosive. This can be done using any chemical equilibrium detonation code and we have used both Mader's BKW code and the ICI IDEX code to estimate these parameters for PBXW-115.

The BKW code employs the Becker-Kistiakowsky-Wilson (BKW) equation of state to calculate the detonation properties of explosives [15]. Steady-state time-independent behaviour is assumed and the detonation products are considered to be in instantaneous chemical equilibrium. For an explosive consisting of a mixture of chemical compounds the necessary input data are the fraction by weight, elemental composition, and heat of formation of each compound. The code requires the entropy of the product species to be expressed as a polynomial function of temperature and then the detonation parameters are calculated by iteratively minimizing the free energy once an initial guess of the product composition has been made.

The MRL version of BKW is run through a user interface package known as USERBKW [16]. This is an interactive FORTRAN program which prepares an input data file for BKW by asking a series of questions about the explosive and its products. USERBKW also maintains three database files, BKWCMP, BKWGAS and BKWSOL. BKWCMP contains information on standard explosive components while BKWGAS and BKWSOL contain information on gaseous and solid detonation products. It was necessary to update BKWCMP by the addition of the elemental composition, heat of formation, density, and formula weight for AP, while BKWGAS required the heat of formation, entropy constants, and the covolumes for both HCl and Cl₂. These were obtained from standard compilations [17]. For the purposes of the BKW calculation the HTPB binder in PBXW-115 was replaced by an existing plasticizer in the BKWCMP database (C₄₁H₇₆O₆). This should have negligible effect on the calculated CJ parameters.

USERBKW provides three methods for estimating the initial amount of each of the assumed detonation products; explicitly, where the user gives his own estimates, hierarchically, where the user assigns priorities with first priority being given to the product most likely to be formed, and by default. We used both the explicit and hierarchical methods and these gave quite different initial estimates of the equilibrium products. However, when both these estimates

were given to BKW and the free energy minimization procedure was followed the final equilibrium state produced by each estimate was identical, as Table 1 shows. The detonation parameters at a density of 1.80 Mg/m^3 calculated by BKW are also listed in Table 1.

Table 1: Detonation Products for PBXW-115 Calculated by BKW Code

Species	Initial No. of Moles (100 g explosive)		Equilibrium (Final) No. of Moles
	Explicit	Hierarchical	
H_2	0.169×10^2	0.875	0.866
NO	0.000	0.000777	0.000409
CO	0.000	0.174	0.0443
N_2	0.453	0.453	0.453
HCl	0.000	0.340	0.290
Cl_2	0.153	0.0131	0.0382
H_2O	0.000	0.532	0.675
H	0.000	0.017	0.00510
CO_2	0.000	0.0550	0.00158
C(solid)	0.121×10^2	1830	0.964
Al_2O_3	0.60	0.463	0.463

CJ Parameters:

Density = 1.80 Mg/m^3

Gamma = 2.75

Detonation Temperature = 5175 K

Detonation Pressure = 28.8 GPa

Detonation Velocity = 8.05 mm/ μs

The CJ pressure of 28.8 GPa and detonation velocity of 8.05 mm/ μs are both higher than expected. Forbes has measured the CJ pressure of PBXW-115 using the aquarium test method and found a value close to 12.2 GPa. While the analysis of the aquarium test data is based on expressions which are only valid for ideal explosives, so that some error is introduced in calculating CJ pressures for non-ideal explosives, it is thought that this would introduce errors of no more than about 30%, so the value of 28.8 GPa must be viewed with some suspicion.

Forbes has also measured the dependence of the detonation velocity on charge diameter [1], and the extrapolated infinite diameter detonation velocity

from this data is 6.195 mm/ μ s; the value obtained from the MRL detonation velocity/diameter measurements is 5.650 mm/ μ s. These values may underestimate the CJ velocity of PBXW-115 because in both cases the maximum charge radius used was only approximately twice the critical diameter, and this may have prevented some late time reactions from contributing. When considered in conjunction with the discrepancy between the measured and predicted CJ pressure however, the difference between the extrapolated and predicted CJ velocity also casts some doubt on the validity of the CJ state calculated by BKW.

We have also estimated the CJ state of PBXW-115 using the ICI IDEX chemical equilibrium code and the results are shown in Table 2. IDEX uses an intermolecular potential equation of state for fluids and a Murnaghan equation of state for solids.

Table 2: Detonation Products for PBXW-115 Calculated by IDEX Code

Species	Mole Numbers (100 g explosive)
CH ₄	0.1556
CO	0.3436
CO ₂	0.00673
H ₂	0.2775
NH ₃	0.4661
H ₂ O	0.2681
HCl	0.2591
N ₂	0.2197
NO	0.8538×10^{-3}
O ₂	0.2524×10^{-5}
Cl ₂	0.05340
C (Graphite)	1.0×10^{-12}
C (Diamond)	0.6338
Al ₂ O ₃	0.4632
Al	1.0×10^{-12}

CJ Parameters:

Detonation Pressure = 22.518 GPa
 Detonation Velocity = 6660.81 m/s
 Detonation Temperature = 5297 K
 Density = 1.7900 g/cm³
 Gamma = 2.5268

The calculated CJ pressure of 22.5 GPa is still considerably higher than the experimental value, but also significantly lower than the value calculated by BKW, while the CJ velocity of 6.66 mm/ μ s is now much closer to the value obtained from the extrapolation of the experimental detonation velocity/diameter data.

A comparison of the equilibrium compositions predicted by the two codes shows considerable differences, with the only clear point of agreement being complete conversion of all Al into 0.463 moles of Al_2O_3 per 100 g of explosive. While both codes show appreciable amounts of carbon present in the equilibrium composition, BKW has predicted that this will be in the graphite form, while IDEX has predicted that most carbon will be present in the diamond form.

We have used both estimates of the CJ state as input to the CPEX code calculations described in the next section.

4: Application to PBXW-115

As described in Section 2, the reaction rate model used in CPEX involves three distinct stages, each with a characteristic reaction time. In the initial ignition phase the shock front compresses the explosive and produces hot spots. The hot spots then initiate a fast reaction in the matrix (or liquid phase), and this is followed by a slower reaction of the solid phase as the matrix is depleted. CPEX was developed for commercial explosives and these typically contain a large fraction of voidage, of the order of 15% to 30% in many cases. These voids are important as they are considered to be the sites at which the hot spots are formed as the initiating shock compresses the explosive. In PBXW-115, however, great care is exercised in processing to ensure that the voidage is minimized. Compositions recently produced at MRL for example contain voidage levels of less than 2%.

In order to apply CPEX to PBXW-115 it is first necessary to identify each of the three stages in the reaction rate model with a corresponding process in the explosive decomposition. Two possibilities are immediately apparent: one is to ascribe the hot spot formation to the voidage, as in commercial explosives, and then to attribute the fast reaction to the RDX decomposition and the slower reaction to the AP and Al decomposition. The other possibility is to assume negligible voidage and equate the hot spot content to some fraction of the RDX content, the intermediate scale reaction primarily to the AP decomposition and the slowest process to the Al reaction. We performed calculations for both schemes and the results are described in this section.

The first results we describe are those in which we considered the RDX component to correspond to the fast reacting liquid phase, while the AP, Al and binder together constituted the slower burning solid phase. We used a density of 1.80 Mg/m^3 for RDX and 1.93 Mg/m^3 for the combined AP, Al and binder; the PBXW-115 had a density of 1.79 Mg/m^3 (this is the density of the PBXW-115 used by Fortes *et al.* [1]). This led to approximately 6% voidage, which is certainly higher than would occur in practice. These calculations are not intended to produce exact numbers; they are used primarily to illustrate the capabilities of the CPEX code and explore its applicability to PBXW-115 and similar underwater explosives. Several of the input parameters are specified only approximately, but with sufficient precision so that confidence can be placed in the general trends shown by the results.

The input information required to run CPEX is shown in Table 3. The ideal detonation velocity and CJ gamma were obtained from the BKW results described in the previous section, and the heat of reaction was estimated from the standard relationship between detonation velocity, gamma, and heat of reaction. The Hugoniot parameters for RDX were taken from the Lawrence Livermore compilation [18], while the Hugoniot parameters for the solid phase were combined using the method of Afanasenkov *et al.* [14] from the parameters for AP [19], Al [20] and binder [21]. The hot spot reaction time and critical pressure and liquid and solid reaction times were estimated by fitting to the experimental data of Forbes *et al.* describing the variation of detonation velocity with charge diameter for unconfined charges.

Table 3: Input Data for CPEX Code: hot spot content equated to initial voidage, CJ parameters from BKW code, and detonation velocity measurements from Forbes *et al.* [1].

Explosive porous density	g/cm ³	1.7900
Ideal detonation velocity	km/s	8.0100
Heat of reaction	MJ/kg	6.3280
Ideal Effective Energy	MJ/kg	0.0000
Gamma (ideal) - expanded gas		1.3000
Gamma CJ - ideal CJ		3.1750
Density liquid ingredients	g/cm ³	1.6000
Hugoniot intercept - liquid	km/s	2.7800
Hugoniot slope - liquid		1.9000
Density solid ingredients	g/cm ³	1.9290
Hugoniot intercept - solid	km/s	2.7670
Hugoniot slope - solid		1.9150
Mass fraction of liquid		0.2000
Hot spot reaction time	μs	6.0000
Hot spot critical pressure	GPa	5.0000
Liquid reaction time	μs	9.0000
Solid reaction time	μs	100.0000
Liquid hot spot factor		1.0000
Solid hot spot factor		0.2500
Kinetic model flag (default = 0)		0.0000

Figure 1 shows the detonation velocity - inverse diameter relationship for unconfined PBXW-115 predicted by CPEX using the parameter values in Table 3. The lower branch of the curve represents an unstable set of solutions to the divergent flow theory. It corresponds to sets of conditions which can just maintain a steady detonation in the absence of perturbations, but which would either decay to failure or lead to detonation at the high value in the presence of any random fluctuations. The upper branch of the curve is a reasonable fit to the experimental data. The predicted critical diameter is 34.5 mm, which is very close to the experimental value of 37.1 ± 1.6 mm [1].

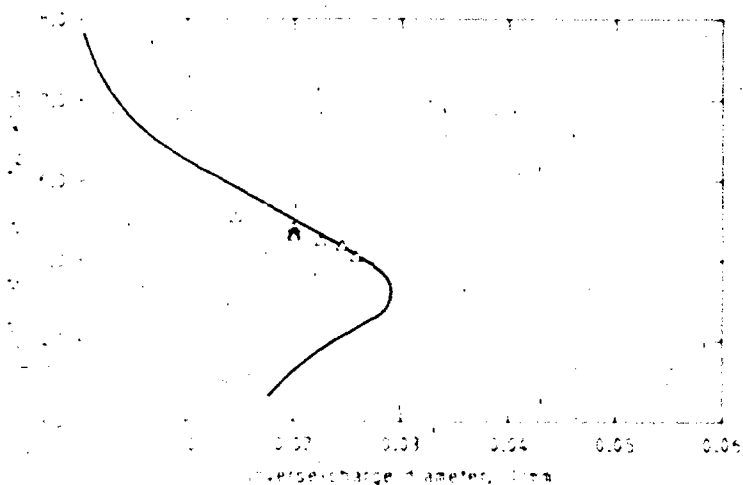


Figure 1. Detonation velocity versus inverse charge diameter for unconfined PBXW-115. The triangles are experimental data from Forbes et al. [1], the solid line is the CPEX fit using the data in Table 3.

Forbes et al. have also measured the detonation velocity - diameter effect for charges confined in 2.5 mm and 5.0 mm brass tubes. They found that the critical diameter for 5 mm thick brass confined charges was about one half that of the unconfined critical diameter. Since the difference between the critical diameters of 2.5 and 5.0 mm brass confined charges was so small they expected that only slightly smaller critical diameters would be obtained if brass confinement greater than 5.0 mm was used. Figure 2 shows the CPEX prediction for the detonation velocity - diameter effect for charges confined in brass tubes. The CPEX calculation assumes an effectively infinite degree of confinement, and approximate shock transit time calculations show that 5 mm thick brass confinement provides sufficient impedance to prevent the rarefactions from effecting the reaction zone. The agreement is not quite as good in this case; CPEX predicts a critical diameter of 22 mm, while the experimental value is approximately 17 mm.

As discussed in Section 2, when considering two-dimensional divergent detonations some concepts from the one-dimensional hydrodynamic theory of detonation require modification. One of these is the concept of the CJ point. In one-dimensional theory the CJ point is defined as the point in the flow at which the sum of the particle velocity and local sound velocity is equal to the detonation velocity. At this point the rate of reaction is zero, and the reaction zone can be defined as the distance between the shock front and the CJ point. In two-dimensional flow the CJ point must satisfy two conditions; the first is the one-dimensional condition defined above, the second is due to the divergence of the flow and requires that the reaction satisfy a criterion such that the rate of chemical energy release is balanced by the energy diminution due to lateral flow expansion (i.e. equation (22)). Thus the reaction rate will always have a finite value at the CJ point in divergent flow and the identification of the reaction zone will be less precise. This effect is illustrated in Figure 3, which shows the extent of reaction at the CJ point as a function of the inverse diameter. At a diameter of 41 mm for example this plot shows that only 25% reaction has occurred by the CJ point. As the diameter increases the flow becomes more one-dimensional and we find the extent of reaction tending to 1.0 at the CJ point as the diameter becomes infinitely large.

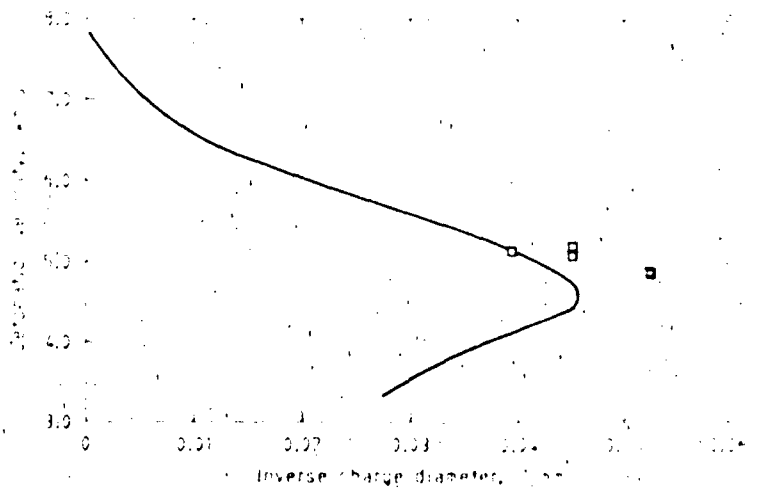


Figure 2: Detonation velocity versus inverse charge diameter for PBXW-115 confined in brass. The squares are experimental data from Forbes et al. [1], the solid line is the CPEX fit using the data in Table 3.

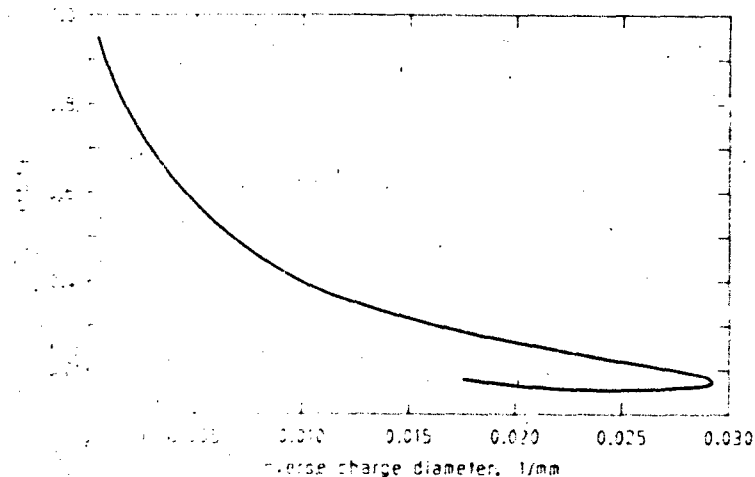


Figure 3: Extent of reaction at the CJ point versus inverse charge diameter for unconfined PBXW-115 calculated by CPEX using the input data in Table 3.

The CJ distance is defined as the distance between the shock front and the CJ point and Figure 4 shows a plot of CJ distance against inverse diameter. At infinite diameter this is equal to the ideal one-dimensional reaction zone length and Figure 4 indicates that this is approximately 70 mm. As the diameter decreases the CJ distance decreases as well because more of the reaction energy is contributing to driving the lateral divergence. Figure 4 indicates CJ distances of approximately 1 mm to 13 mm in the diameter range 40 mm to 70 mm. Forbes *et al.* have used measurements of the radius of curvature of the detonation front and used the original Wood-Kirkwood theory to estimate reaction zone lengths of 2 to 4 mm for this diameter range. The latter estimates of CJ distances differ from those of CPEX due to the effects of several assumptions made in the original Wood-Kirkwood theory. These included a simplified geometry of the reaction zone, an artificial pressure profile, density ratios behind the shock and at the sonic plane appropriate to a particular liquid explosive, and the assumption that reaction is complete at the sonic plane. The infinite diameter reaction zone length of 70 mm is large mainly because the reaction is much slower than those for the common ideal military explosives.

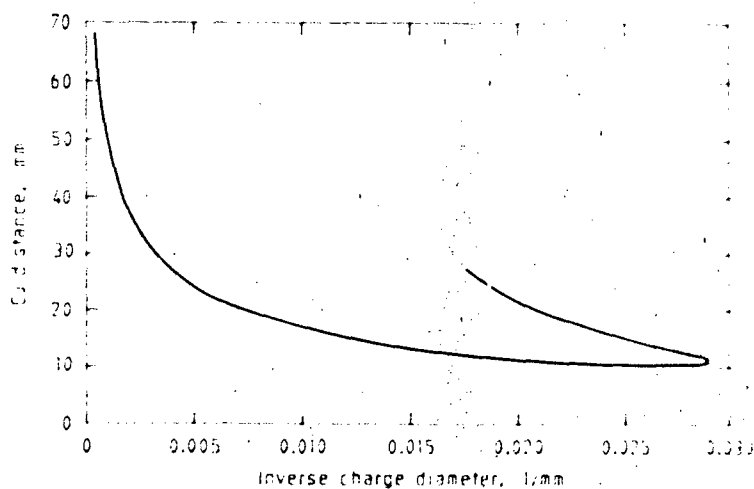


Figure 4: Distance between shock front and CJ point versus inverse charge diameter for unconfined PBXW-115 calculated by CPEX using the input data in Table 3.

Because of the very low level of voidage in PBXW-115 a more likely approach is to assume that hot spots form at RDX sites in the matrix, and thus to equate the hot spots term in the reaction rate law with some fraction of the RDX content of the explosive. We have found improved agreement with the NSWG data by considering a model in which half of the RDX is used to form hot spots and the remaining RDX and all of the AP and binder react on the intermediate time scale, with the Al alone reacting on the slowest time scale. We have also used the CJ parameters obtained from the IDEX code for this particular calculation, and a complete list of the input data for the CPEX run is shown in Table 4.

Table 4: Input data for CPEX Code: hot spot fraction equated to 50% initial RDX content. CJ parameters from ICI IDEX Code. Detonation velocity measurements from Forbes et al. [1].

Explosive porous density	g/cm ³	1.7900
Ideal detonation velocity	km/s	6.3350
Heat of reaction	MJ/kg	8.2000
Ideal Effective Energy	MJ/kg	4.6740
Gamma Ideal - expanded gas		1.3410
Gamma CJ - ideal CJ		1.6490
Density liquid ingredients	g/cm ³	1.6870
Hugoniot intercept - liquid	km/s	2.4610
Hugoniot slope - liquid		1.6000
Density solid ingredients	g/cm ³	2.7000
Hugoniot intercept - solid	km/s	5.3500
Hugoniot slope - solid		1.3400
Mass fraction of liquid		0.7500
Hot spot reaction time	μs	34.2000
Hot spot critical pressure	GPa	3.5000
Liquid reaction time	μs	380.0000
Solid reaction time	μs	100.0000
Liquid hot spot factor		0.1450
Solid hot spot factor		0.0000
Kinetic model flag (default = 0)		1.0000
Hot spot pressure exponent		2.0000
Liquid pressure exponent		1.0000
Solid pressure exponent		1.0000

Figure 5 shows the predicted detonation velocity as a function of inverse diameter for the input data in Table 4. This shows a much better fit to the experimental data (cf. Fig. 1) and predicts a critical diameter of 38.5 mm, which is within the experimental value of 37.1 ± 1.6 mm. Figure 6 shows CJ distance versus inverse diameter.

Bocksteiner et al. [9] have recently performed a series of detonation velocity measurements on cylinders of Australian PBXW-115 with diameters in the range 40 mm to 200 mm. The results (along with a CPEX fit to the data) are shown in Figure 7. The critical value for the Australian made explosive was found to be approximately 80 mm, which is about twice the value for the US composition. Hence both the US and Australian measurements covered a range of approximately one to two critical diameters for their respective formulations, and within this range the detonation velocities are very similar. Figure 8 shows both sets of data as a function of diameter d , where d has been divided by the appropriate critical diameter d_{cr} for each explosive. For a given value of scaled diameter the two sets of results differ by no more than a few percent.

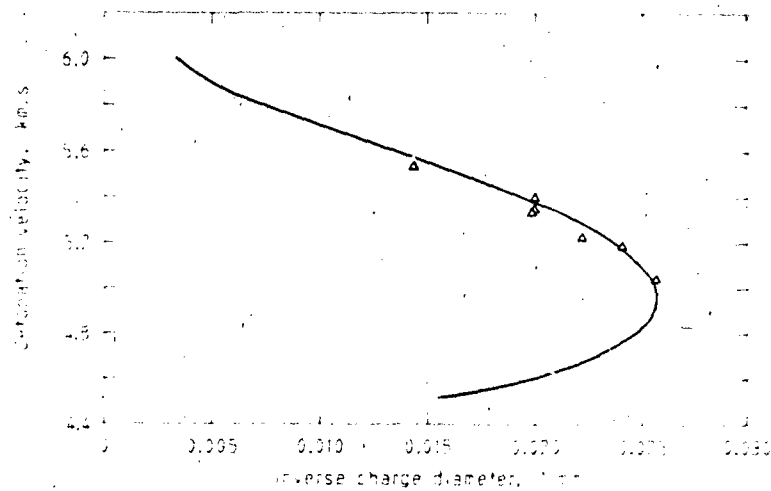


Figure 5: Detonation velocity versus inverse charge diameter for unconfined PBXW-115. The triangles are the experimental data from Forbes et al. [1], the solid line is the CPEX fit using the data in Table 4.

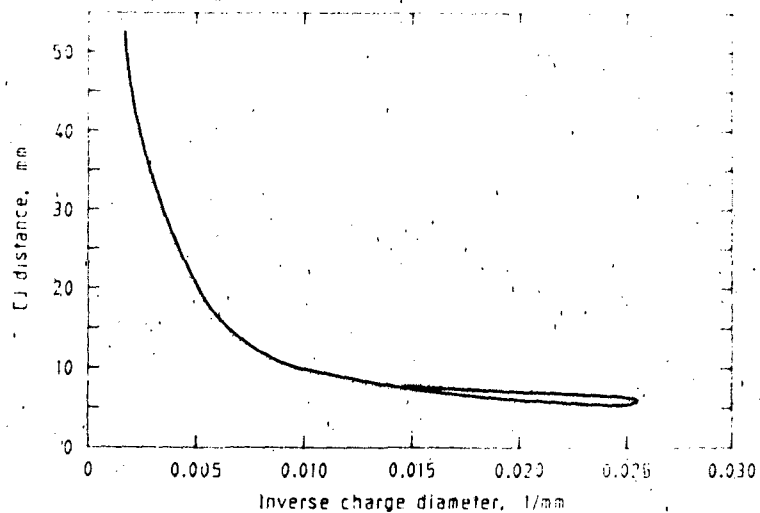


Figure 6: Distance between shock front and CJ point versus inverse charge diameter for unconfined PBXW-115 calculated by CPEX using the input data in Table 4.

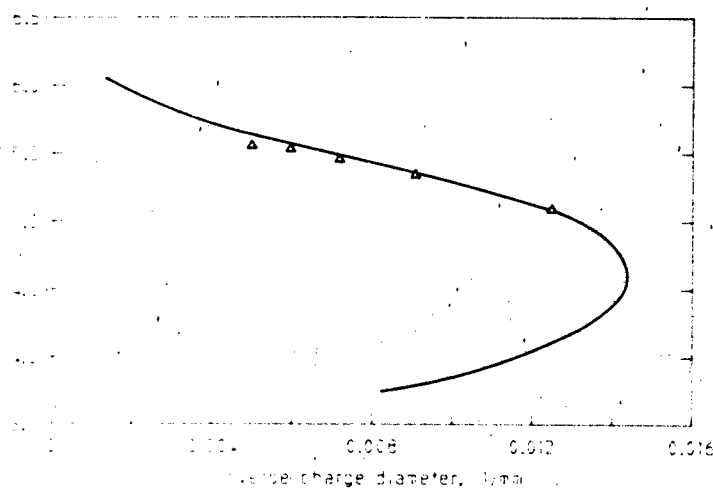


Figure 7: Detonation velocity versus inverse charge diameter for unconfined PBXW-115. The triangles are the experimental data from Bocksteiner et al. [9], the solid line is the CPEX fit using the data in Table 4, and the changes described in the text.

While the Australian and American formulations are nominally the same, there are differences in the nature of the RDX used in the two compositions because of differences in the method of manufacture. The American RDX contains approximately 8% HMX, while the Australian RDX is completely HMX free. The HMX content would make the US PBXW-115 slightly more shock sensitive, and hence may explain the smaller critical diameter. The different sensitivities of the RDXs used in the two compositions will also change the time constants in the reaction rate law for those processes connected with the RDX decomposition. To obtain the CPEX fit to the data shown in Figure 7 we increased the hot spot reaction time from 34 μ s to 110 μ s and the intermediate reaction time from 380 μ s to 800 μ s. The values of all other constants were the same as used in obtaining the CPEX fit to the NSWC data shown in Figure 5. The excellent fit to the data shown in Figure 7 is encouraging evidence that we are correctly modelling the basic reaction mechanisms occurring in PBXW-115.

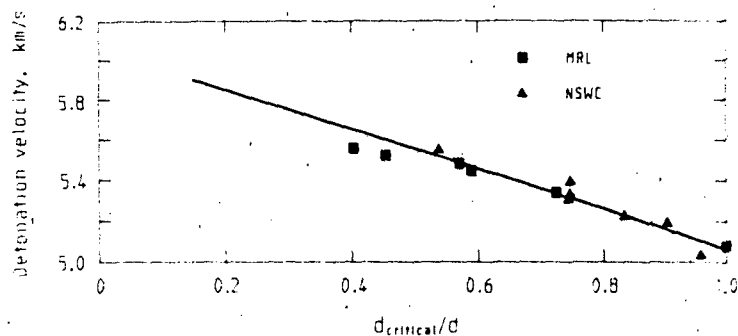


Figure 8: Detonation velocity as a function of scaled inverse diameter for the data of Forbes *et al.* [1] (triangles) and Bocksteiner *et al.* [9] (squares).

We intend to further validate this model by comparing its predictions against a variety of experimental data. The effect of both brass and steel confinement on failure diameter will be calculated and compared with the results of experiments currently in progress at MRL (Bocksteiner [22]), and we also intend to use a version of the DYNA2D code containing the CPEX reaction rate scheme and equation of state to model aquarium test data obtained using the US formulation. A reactive Flux-Corrected Transport code will then be used to simulate the corner turning experiments of Forbes *et al.* [1].

5. Discussion and Conclusion

The application of CPEX to PBXW-115 enables us to calculate many explosive properties as a function of the charge radius. It also allows us to obtain information on the reaction time scales of the various components and the degree of reaction at the CJ point. CPEX provides a complete model for a slightly divergent non-ideal detonation for explosives of commercial interest. Other methods have been published which estimate the performance of commercial or non-ideal explosives and it is pertinent to mention some of these here.

Johnson *et al.* [3] have used data from the aquarium test and combined this with BKW and two-dimensional code calculations to infer information about the degree of chemical reaction at the detonation front for several commercial explosives. A BKW calculation was made using the initial density and chemical composition of the explosive assuming thermodynamic equilibrium

and complete chemical reaction at the detonation front. The BKW calculations were then compared with the measured detonation velocity. Generally, the measured detonation velocity was well below the theoretical prediction, indicating that reaction was incomplete at (or very near to) the detonation front.

Additional BKW calculations were then performed with varying amounts of the constituents withheld from chemical reaction at the detonation front until agreement was achieved between measured and calculated detonation speed. If the explosive contains several non-energetic components then some chemical knowledge is required at this stage to decide which components should be reacted. An equation of state of the detonation products can then be constructed and used in a two-dimensional hydrocode calculation to simulate the aquarium test data and predict the position of measured shock wave and confinement/water interface positions.

Additional assumptions regarding post CJ reaction are then necessary to match measured and predicted positions. Johnson and co-workers [3] have applied this approach to ANFO, aluminized ANFO and several other commercial products. For 11% aluminized ANFO the results could be described by assuming that 60% of the AN and all of the aluminium react by the CJ plane, with the remaining AN reacting within a few microseconds. Similarly, their calculations for ANFO indicated that 55% of the AN remained inert at the CJ plane, and then complete reaction occurred within a few microseconds.

However, these studies employed an artificial burn model to advance the detonation front in the hydrocode simulations. This imposed an artificially large radius of curvature on the detonation front, distorting the hydrodynamic flow in the vicinity of the explosive/confinement interface. Furthermore, this procedure imposed an artificially short reaction zone length, and hence ignored the energy delivered to the surroundings by expansion within the reaction zone. By performing a proper two-dimensional resolved reactive flow simulation using the hydrocode DYNA2D modified to include the CPEX equation of state and reaction kinetics, Kennedy [23] was able to reproduce the ANFO aquarium data of Johnson *et al.* [3] with no a priori assumptions. The predicted CJ zone length was 16 mm, with the extent of reaction at the CJ surface being 95% (cf. 55% from Johnson *et al.*) on the charge axis, dropping to 83% at the ANFO/confinement boundary.

Wanniger *et al.* [24] have investigated the detonation properties of a variety of ammonium perchlorate explosives using an approach similar to Johnson *et al.* They have varied the fraction of AP reacting in the detonation front in a BKW calculation until agreement is obtained with experimental detonation velocity measurements. They have then combined these reaction schemes with an underwater hydrocode to calculate relative shock and bubble energies.

The manner in which we have measured the reactions of the various components of PBXW-115 to the reaction rate model in CPEX is similar to the schemes used by Murphy *et al.* [25] and Tarver and Green [26] to model composite explosives and propellants. Murphy *et al.* have studied a family of explosives containing HMX/AP/ZrH₂/binder using a three term ignition and growth model. The first term in the expression for the rate of reaction is the hot spot ignition term and their model assumes that the initial hot spot fraction is equal to the initial void fraction. The second term describes the growth of the ignited hot spots; previously published rates for HMX were used for this.

The third term describes the rate of reaction of the remaining components. Tarver and Green have studied a propellant composition containing HMX/AP/Al/binder using a similar scheme; the first term describes hot spot ignition, the second the growth rate of these hot spots using previously published HMX rates, and the third term describes the global reaction for the rest of the propellant (AP/Al/binder). The unknown constants in the reaction rate terms were estimated by fitting to experimental data from embedded multiple manganin pressure gauges in sustained pulse experiments using a four inch gas gun. Tarver and Green then used this calibrated reaction rate model with the DYNA2D hydrocode to estimate the failure diameter for this particular composition.

Leiper *et al.* [8] have also used the CPEX reaction rate model in the DYNA2D code to model an air sensitized water-in-oil emulsion explosive of composition 78.7% AN, 16% water and 5.3% oils and surfactants. They calculated density profiles and other flow field variables and found good agreement with experiment.

Interest at MRL is centred on the estimation of relative shock and bubble energy for PBXs of the PBXW-115 type. One possible approach to this problem is to use the reaction rate parameters obtained from CPEX, calibrating these to experimental data on the unconfined detonation velocity-diameter effect, and then using this reaction scheme in a one-dimensional hydrocode to simulate underwater blast. A one-dimensional hydrocode for detonation calculations has recently been developed at MRL [27] and is currently being modified for application to problems of this type [28]. Such an approach however requires the availability of a code such as CPEX, and experimental data for calibration purposes. It should be noted that CPEX took 10 man years to develop and, while a similar code could probably now be developed in less time, it is unlikely that MRL could devote the necessary resources to this.

Another approach would be to follow the method of analysis of Johnson *et al.* [3]. This has the advantage of the ready availability of all necessary codes, but would require the establishment of facilities to enable aquarium test data to be obtained for PBXW-115. It should be noted also that Bdzil and co-workers [29, 30] have developed a slightly different analysis of divergent flow theory based on the original Wood-Kirkwood paper and have developed a Detonation Shock Dynamics (DSD) code to model flows for which the local radius of curvature is very much greater than the local reaction zone width [31].

Whichever approach is adopted, it is evident that far more detailed experimental characterization of the particular explosive under study is required. Hydrocodes are unable to make reliable predictions of relative shock and bubble energies unless considerable experimental data is available to allow accurate parameterization of the appropriate reaction rate equations. Once this initial information has been obtained modelling techniques can then be used to investigate the effect of small changes in the formulation on the underwater performance of the explosive. These techniques will decrease the requirement for expensive field testing and provide efficient and relatively fast methods for estimating trends in underwater performance.

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Application of CPEX non-ideal explosive model to PBXW-115

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ABSTRACT

We present a detailed description of the use of the ICI non-ideal detonation code CPEX to model the performance of the composite underwater explosive PBXW-115 (20% RDX, 43% AP, 25% Al and 12% HTTB). We use both the ICI chemical equilibrium code IDEX and Mader's BKW code to first estimate the Chapman-Jouguet parameters for PBXW-115. Two different reaction rate models are assumed for the decomposition of the explosive components and the time constants for each are found by fitting to experimental US data on the variation of detonation velocity with charge diameter. The data is best fitted by a three term reaction rate model which equates hotspot content to some fraction of RDX content, the intermediate scale reaction primarily to the AP decomposition, and the slowest process to the Al reaction. After adjusting some of the reaction time constants because of differences between the US and Australian compositions the model then accurately reproduces the variation of detonation velocity with charge diameter found for Australian PBXW-115.

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