SIMULATION OF AQUARIUM TESTS FOR PBXW-115(*AUST*)

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Aquarium tests have been performed on PBXW-115(*Aust*), the Australian analogue of the US Navy underwater explosive PBXN-111, and the results compared with hydrocode simulations. Due in part to differences between US and Australian grades of RDX, PBXW-115(*Aust*) has significantly different explosive properties to its US counterpart, including a lower shock sensitivity as measured by the Large Scale Gap Test, and a critical diameter nearly twice that of PBXN-111. This extremely non-ideal explosive is a challenging system to model, and to this end, simulations with 2D axisymmetric cylindrical geometry were performed using an explicit finite element hydrocode, LS-DYNA, with both an Ignition and Growth Model and a CPeX Reactive Model. The Ignition and Growth model accurately simulates small-scale aquarium tests, reproducing successive positions of the bubble and shock front. To test whether the models using parameters derived from small-scale tests can be applied to large-scale devices, both the Ignition and Growth Model in LS-DYNA and the CPeX Model in DYNA2D are applied to the simulation of mid-scale underwater tests of PBXW-115(*Aust*).

INTRODUCTION

The Australian version of the US Navy IM underwater explosive PBXN-111, based on indigenous ingredients and composed of 43% ammonium perchlorate, 25 % aluminium, 20% RDX and 12% HTPB binder, was developed and designated PBXW-115(*Aust*)[1]. Research by Bocksteiner and Whelan first addressed binder and formulation studies, compatibility and sensitiveness, then detonation properties including velocity of detonation, critical diameter, shock sensitivity and finally underwater explosive performance[1-3]. They found that PBXW-115(*Aust*) had significantly different explosive properties, particularly critical diameter and shock sensitivity from its US counterpart, believed due to the particle size distribution, grade and type of RDX used in the two formulations. These investigations resulted in PBXW-115(*Aust*) being qualified by Australian Ordnance Council for use as an insensitive main charge fill in large underwater blast weapons, and the proposal that the material could be qualified as an Extremely Insensitive Detonating Substance[4].

Turning attention to the modelling of Australian version of PBXW-115, i.e. PBXW-115(*Aust*), limited work reported so far[5] is confined only to modelling detonation velocity of unconfined PBXW-115(*Aust*) where the model was based on the results of experiments on relatively small charges. In order to validate extrapolation based on the experimental results on smaller charges to the larger explosive charges used in underwater devices, the Weapons Systems Division at DSTO- Edinburgh has been undertaking investigations into both modelling of realistic charge geometries and small scale to mid-scale underwater tests to record the "early-time" behaviour and performance of PBXW-115(*Aust*). The results of the small-scale aquarium tests[6,7] and the mid-scale underwater tests[8] are two of the experimental investigations carried out, which can be used for calibrating computer models.

This paper presents a comparison of the experimental and simulation results of small-scale aquarium tests for non-ideal explosive PBXW-115(*Aust*) using an explicit finite element hydrocode LS-DYNA[9] with an Ignition and Growth Model. By tracking the initial high-pressure shock front as it propagates along the explosive charge in the modelling results, the detonation velocities were determined and compared with the experimental results. Successive positions of bubble and shock front resulting from a detonation wave propagating down the explosive cylinder immersed in the water are successfully simulated, and show good agreement with the aquarium test results. Both the Ignition and Growth Model in LS-DYNA and the CPeX Model in DYNA2D[11] are also applied to the simulation of mid-scale underwater tests of PBXW-115(*Aust*).

EXPERIMENTS

Aquarium tests provide a photographic record of the early-time shock and bubble formation of an underwater detonation, and yield information on detonation velocity and pressure as well as boostering and confinement effects. Aquarium tests were performed on cylindrical charges of PBXW-115(*Aust*) 100mm in diameter and 200mm long.

Full details of the experimental arrangements and the measurement technique have been published previously[6,7]. Figure 1 shows a typical charge assembly showing piezoelectric pins and attached connectors used for measuring detonation velocity.

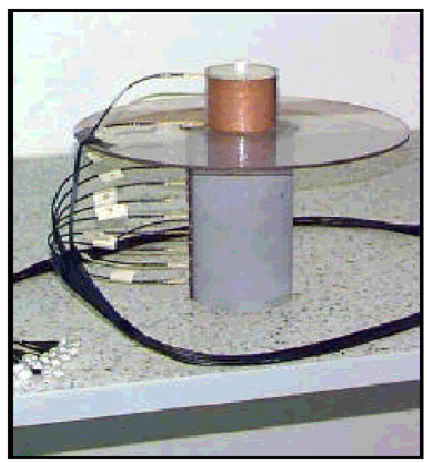

FIGURE 1. PHOTOGRAPH OF THE PBXW-115 CHARGE ASSEMBLY SHOWING PIEZOELECTRIC PINS.

For each firing, four frame images and a streak record were taken with an Imacon 468 CCD camera to measure the initial shock and bubble formation of bare PBXW-115(*Aust*). Images of one aquarium test are shown in Figure 2. The detonation front of PBXW-115(*Aust*) is difficult to distinguish in these frame images due to low self-illumination. This effect was also reported[16] for PBXN-111. However, illumination from later-time reactions is readily discernable, and attributed to combustion of aluminium.

These effects are also apparent in the accompanying streak image shown in Figure 3. The low levels of illumination necessitated a large slit width (100μm), resulting in a temporal resolution (± 0.5 μs) too low for precise detonation velocity measurements. However, there is a clear record of illumination due to aluminum combustion, which produces high levels of light approximately 25 μs after the initial front.

Estimates of detonation pressure can be derived from the streak and frame photographs by using the detonation detonation velocity of the explosive and the shock properties of water. From the velocity of the shock exiting the end of the charge in the streak record, the detonation pressure was estimated to be 9.8GPa[7]. Based upon the angle of the shock exiting radially from the charge in frames (B) and (C) of Figure 2, the detonation pressure is approximately 9.6 GPa.

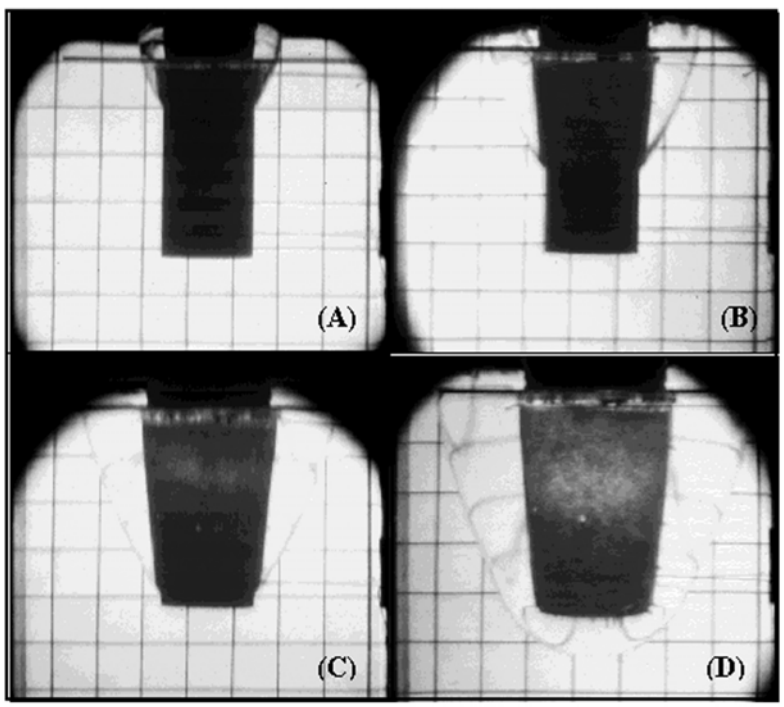

FIGURE 2. IMAGES OF AQUARIUM TEST SHOWING EARLY-TIME SHOCK AND BUBBLE FORMATION OF PBXW-115(*AUST*) DETONATION TAKEN APPROXIMATELY (A) 22μS, (B) 32μS, (C) 41μS AND (D) 56μS AFTER INITIATION OF BOOSTER.

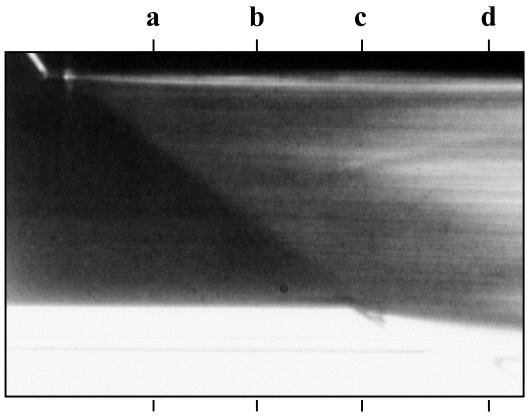

FIGURE 3. STREAK RECORD OF PBXW-115(*AUST*) AQUARIUM TEST. LABELS MARK APPROXIMATE TIMES OF FRAME IMAGES.

IGNITION AND GROWTH REACTIVE MODEL IN LS-DYNA

The Ignition and Growth Reactive Model in LSTC-DYNA is derived from the original work of Lee and Tarver[12], which permits the resolved reaction zone simulation of initiation (or failure to initiate) and detonation wave propagation of solid high explosives. According to Tarver et al.[13], shock initiation of heterogeneous solid explosives should be modelled as at least a three-step process. The first step is the formation of hot spots created by various mechanisms (void closure, viscous heating, shear banding, etc.) during shock compression and the subsequent ignition (or failure to ignite due to heat conduction losses) of these heated regions. The second step in the process is assumed to be a relatively slow growth of reaction in inward and/or outward "burning" of the isolated hot spots. The third step in the shock initiation process is a rapid completion of the reaction as the reacting hot spots begin to coalesce. This model requires[14]:

- An unreacted explosive equation of state;
- A reaction product equation of state;
- A reaction rate law that governs the chemical conversion of explosive molecules to reaction product molecules, and a set of mixture equations to describe the states attained as the reactions proceed.

Both unreacted and product equations of state are of Jones-Wilkins-Lee (JWL) forms

$$p = Ae^{-R_1 V} + Be^{-R_2 V} + \frac{\omega C_v T}{V} \tag{1}$$

where p is pressure, V is relative volume, T is temperature, and A, B, R_1, R_2, ω (the Gruneisen coefficient) and C_v (the average heat capacity) are constants. The chemical reaction rate equation in the three-term ignition and growth model is of the form[15]:

$$\frac{\partial F}{\partial t} = I\left(1-F\right)^b \left(\frac{\rho}{\rho_0} - 1 - a\right)^x + G_1\left(1-F\right)^c F^d p^y + G_2\left(1-F\right)^e F^f p^z \tag{2}$$

where F is the fraction reacted, t is time, ρ_0 is initial density, ρ is current density, p is pressure, and I, G_1, G_2, b, x, a, b, c, d, y, e, f, and z are constants. Three more constants are added to the model: F_{mxig}, F_{mxGr} and F_{mnGr} which limit the contributions of the three terms to respectively a maximum reacted fraction F_{mixg} for the first term, a maximum fraction F_{mxGr} for the second term and a minimum fraction F_{mnGr} for the last term.

Table 1 lists the parameters in the Ignition and Growth Reactive Model fitted to the detonation velocity versus diameter effect experimental data for unconfined PBXN-111[16,17] and PBXW-115(*Aust*)[2].

TABLE 1. PARAMETERS FOR THE IGNITION AND GROWTH OF REACTION MODEL[18].

Explosive	PBXN-111	PBXW-115(Aust)
Unreacted Equation of State and Constitutive Values		
ρ_0 (g/cm^3)	1.792	
A (GPa)	4.066E+03	
B (GPa)	-133.9	
R_1	7.2	
R_2	3.6	
$R_3=\omega * C_v$ (GPa/K)	2.091E-03	
Yield Strength (GPa)	0.2	
Shear Modulus (GPa)	4.54	
Reacted Product Equation of State and CJ Values		
A (GPa)	372.9	
B (GPa)	5.412	
R_1	4.453	
R_2	1.102	
$R_4=\omega * C_v$ (GPa/K)	4.884E-04	
E_o (KJ/cc)	12.95	
D_{cj} (mm/µs)	6.476	
P_{cj} (GPa)	20.84	
Reaction Rate Parameters for 3 Term Model		
I (µsec^{-1})	30	15
b	0.6667	0.6667
a	0	0
x	4.0	4.0
G_1 (GPa^{-y}µsec^{-1})	0.045	0.0195
c	0.6667	0.6667
d	0.1111	0.1111
y	1.0	1.0
G_2 (GPa^{-z}µsec^{-1})	1.805E-03	8.00E-04
e	1.0	1.0
f	0.1111	0.1111
z	2.0	2.0
F_{mixg}	0.015	0.015
F_{mxGr}	0.25	0.25
F_{mnGr}	0	0

Note: E_o is the internal energy.

Figure 4 summarises the DYNA predictions of detonation velocity in axisymmetric geometry, together with experimental data. For comparison purpose, the results[18] using kinetic CHEETAH[19] are also included in the figure. Agreement is seen to be excellent between the DYNA predictions and the experimental results for both PBXW-115(*Aust*) and PBXN-111 (US). The curve predicted by DYNA and that predicted by CHEETAH follow similar trends. It is seen that even though CHEETAH overestimates the detonation velocities, it can still predict the trend of the detonation velocity versus diameter effect.

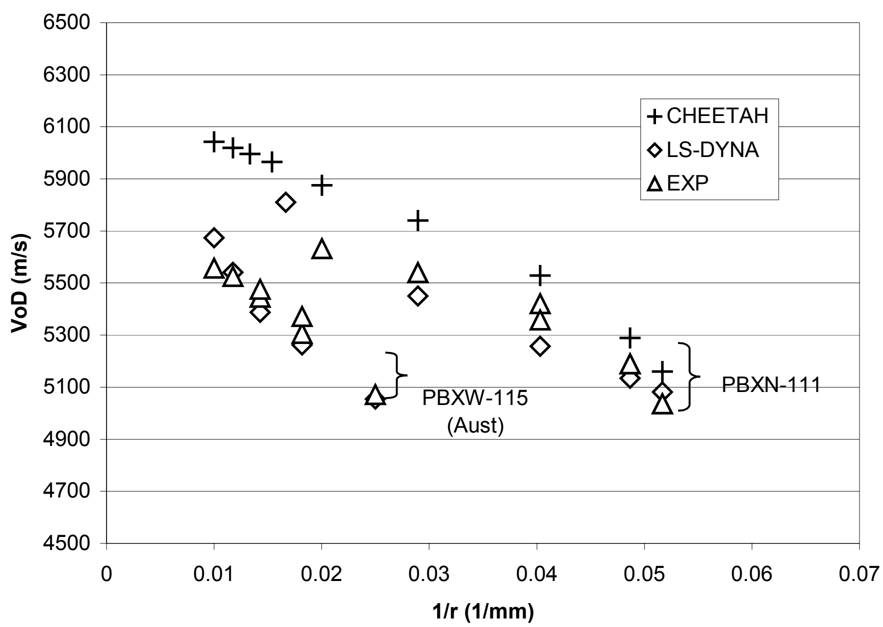

FIGURE 4. PBXW-115 DETONATION VELOCITY.

CPEX REACTION MODEL

The CPeX (Commerical Performance of explosives) reaction model is based upon the Wood-Kirkwood theory of slightly divergent detonation. Like the Ignition and Growth model, this model also involves a three-stage process to describe varying rates of combustion among the ingredients of a composite explosive. There are four adjustable parameters – three characteristic reaction times (hotspot, intermediate and final stages of the reaction) and the critical pressure that inhibits the onset of the hotspot reaction[11], which can be calibrated against the experimentally observed dependence of detonation velocity on charge diameter. For both PBXN-111 and PBXW-115(*Aust*), these parameters are based on the assumption of the initial ignition and consumption of the RDX, the intermediate decomposition of the AP plus binder, and the later reaction of the Al. The CPeX model has been incorporated into both the explicit finite difference two-dimensional in-house multi-material

Eulerian hydrocode "MULTI"[10] and the explicit finite element hydrocode DYNA2D[11] to permit the simulation of time-dependent reactive flow in non-ideal explosives.

SIMULATION OF AQUARIUM TEST

The Ignition and Growth Reactive Model incorporated into the LS-DYNA described above has been used to simulate the small-scale aquarium tests reported previously[6,7]. The simulation used some 63000 elements in axisymmetric cylindrical geometry with a cell size of 1mm. The PE4 booster with a diameter of 64mm and a length of 65mm was detonated using the programmed burn option in LS-DYNA with the JWL parameters given in Table 2. The PBXW-115(*Aust*) charge with a diameter of 100mm and a length of 200mm was burnt by the Ignition and Growth Reactive Model. The surrounding water was modelled with Gruneisen equation of state with the parameters as given in Table 3.

TABLE 2. JWL PARAMETERS FOR PE4 BOOSTER[20] .

ρ_0 (g/cm^3)	1.59
A (GPa)	774.054
B (GPa)	8.677
R_1	4.837
R_2	1.074
ω	0.284
E_o (KJ/cc)	9.381
D_{cj} (mm/µs)	7.9
P_{cj} (GPa)	24.0

TABLE 3. GRUNEISEN PARAMETERS FOR WATER[21].

ρ_0 (g/cm^3)	1.00
γ_0	0.1
C(mm/µs)	1.65
S	1.92

Note: γ_0 is the Gruneisen gamma, C is the intercept of the shock velocity vs particle velocity curve and S is the coefficient of the slope of this curve .

By tracking the initial high-pressure shock front as it breaks out through the surface of the explosive charge in the modelling results, the apparent detonation velocities were determined and plotted in Figure 5, together with the experimental results[6,7]. It is seen that the hydrocode model can reproduce accurately the experimental results.

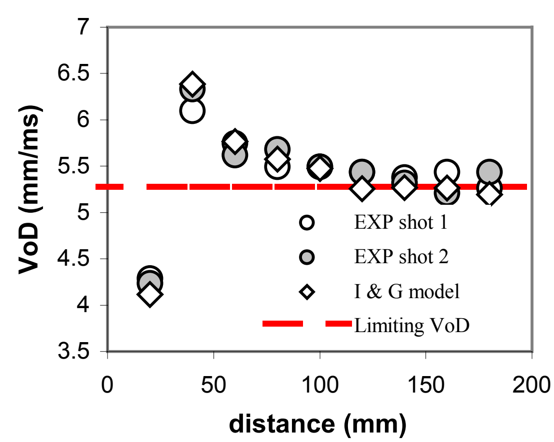

FIGURE 5. COMPARISON OF PREDICTED AND MEASURED APPARENT DETONATION VELOCITY ALONG THE CHARGE AXIS.

Figure 6 presents the results of the simulation after the resolved reaction zone detonation in the PBXW-115(*Aust*) has run approximately 32 μs. The calculated contours are of pressure in 1.4 GPa internals. The positions of the measured shock front and the bubble (explosive/water) interface (after correction for index-of-refraction effects[22]) are included as open circles[6,7]. The simulated water shock profiles off the end of the charge together with the experimental data after the detonation has run approximately 56 μs are shown in Figure 7. It is seen that the simulated shock and explosive/water interface are in excellent agreement with the experimental observation.

The good agreement between the hydrocode modelling and experimental observation showed that the Ignition and Growth Reactive Model, although determined from the detonation velocity versus diameter effect experimental data for unconfined explosives, could faithfully model the reaction rate characteristics for experiments carried out in other configurations. This gives us confidence in applying the mentioned models to simulation of the mid-scale underwater tests reported by Wilkinson[8] which are presented in the following section.

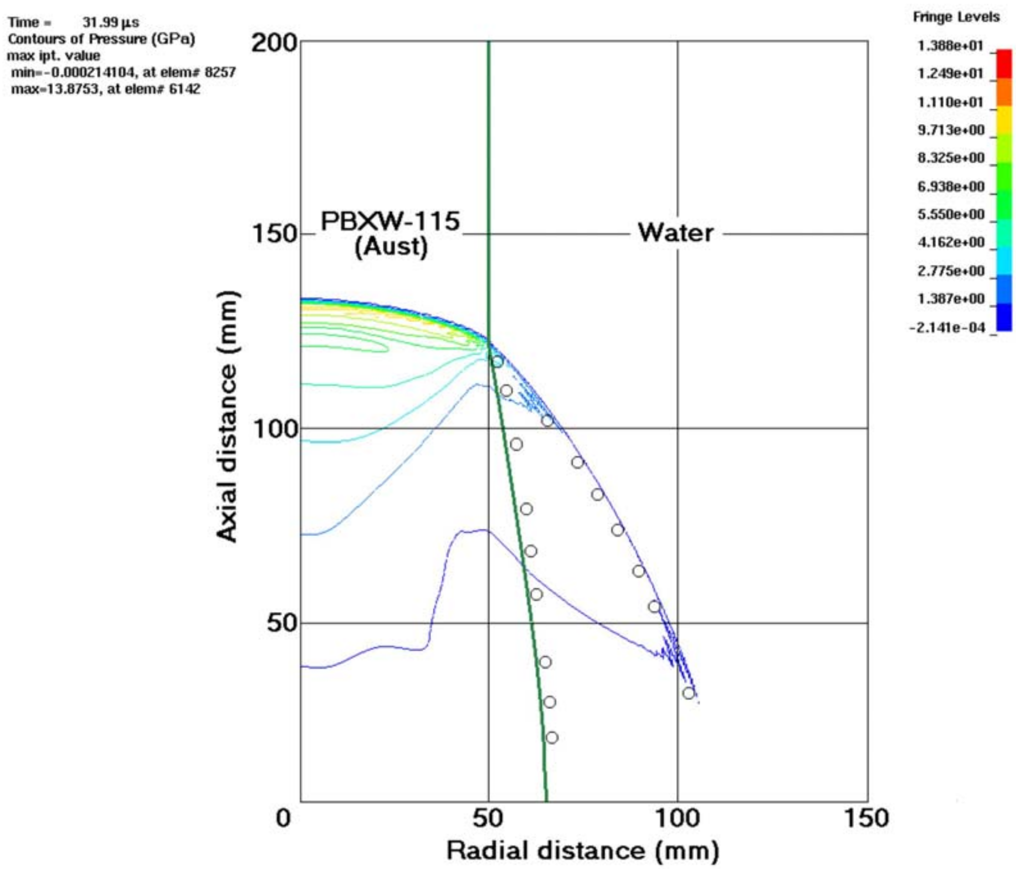

FIGURE 6. THE SIMULATION RESULTS BY LS-DYNA (SOLID LINES) OF THE PBXW-115(*AUST*) AQUARIUM TEST[6,7] (OPEN CIRCLES REPRESENT THE EXPERIMENTAL DATA) .

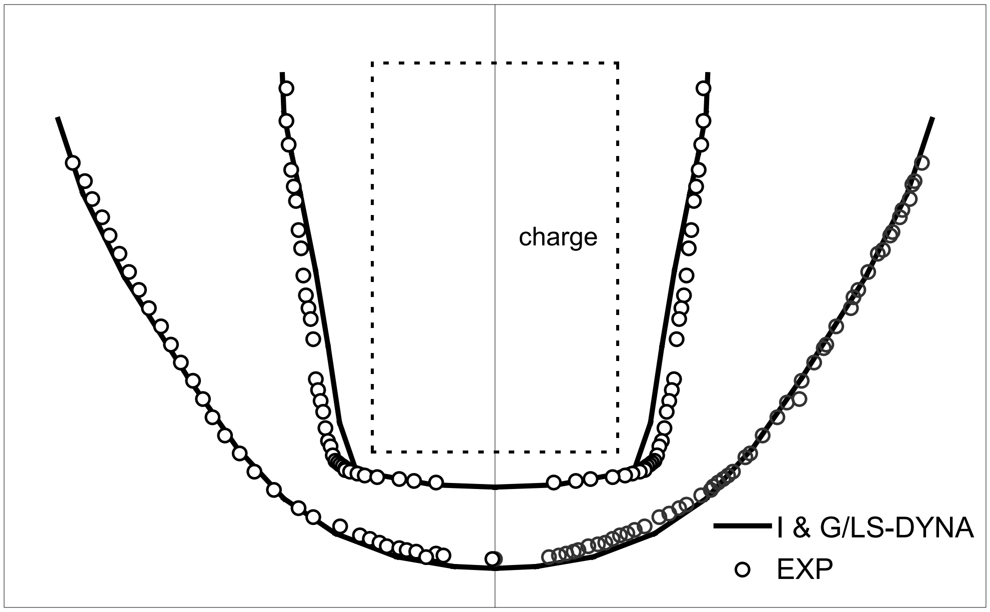

FIGURE 7. SIMULATED WATER SHOCK PROFILES OFF THE END OF THE CHARGE AT 56μS (OPEN CIRCLES REPRESENT THE EXPERIMENTAL DATA[6,7]).

SIMULATION OF MID-SCALE UNDERWATER TESTS

It is expected that the Ignition and Growth Reactive Model and CPeX Model described above using data from small-scale tests can be applied to large-scale devices. To test this extrapolation, both the Ignition and Growth Model in LS-DYNA and the CPeX Model in DYNA2D[11] have been used in the simulation of the mid-scale underwater tests reported by Wilkinson[8]. The size of the calculation configuration was set to Φ530mm x L1200mm in axisymmetric cylindrical geometry. The dimensions of PE4 booster, PBXW-115(*Aust*) charge and water are 34, 126 and 53mm in radius and 68, 400 and 1200mm in length, respectively. The thickness of the fibreglass confinement case is 9mm. The material properties and equations of state for PE4, PBXW-115(*Aust*) and water used in the calculation are the same as those used in the aquarium test simulation. The model parameters for the fibreglass case are given in Table 4.

TABLE 4. MATERIAL AND GRUNEISEN PARAMETERS FOR FIBREGLASS.

Yield stress	0.2GPa
Shear modulus	15GPa
ρ_0 (g/cm^3)	1.70
γ_0	1.01
C(mm/μs)	3.016
S	1.005

Figure 8 shows the initiation process and the intermediate expansion of the water shock and bubble. It should be noted that the images from 10 to 80 microseconds are plotted using the linear pressure scale and the images at 120 and 180 microseconds are plotted using a log scale. Good agreement is seen between the Ignition and Growth Model and the CPeX Model. The maximum pressure in the PBXW-115(*Aust*) occurs at the end of the booster, but since the curvature of the resulting detonation wave is too large for it to sustain, the shock attenuates down the center line until at about the center of the charge, the shock pressure begins to build up again as its curvature steadily decreases. The detonation propagates most strongly in a 45 degree cone out from the booster, again because of dependence on the curvature. Work on simulating the farther field for late-time effects with a calculation configuration of Φ530mm x L5000mm using the Ignition and Growth Model to compare the predicted peak overpressure with available experimental data is currently underway.

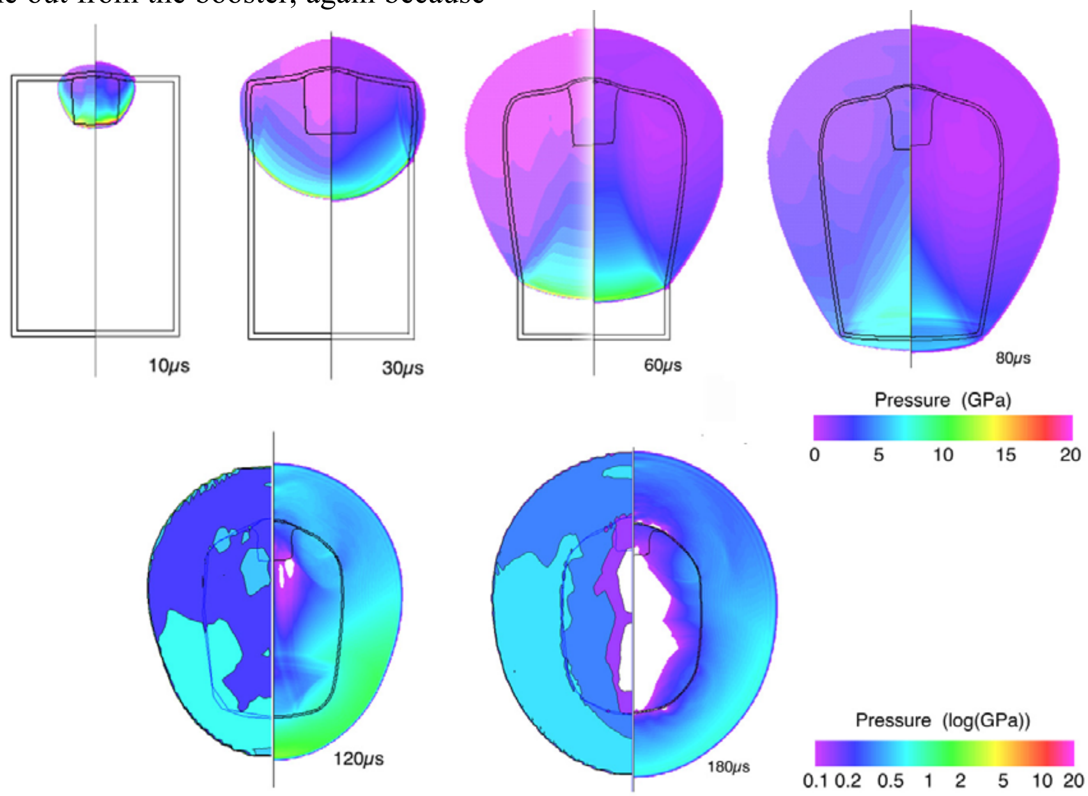

FIGURE 8. CALCULATED PRESSURE CONTOURS AT DIFFERENT TIMES WITH I & G MODEL PLOTTED ON THE LEFT SIDE OF EACH DIAGRAM WHILE THE CPEX MODEL IS PLOTTED ON THE RIGHT.

CONCLUSIONS AND FUTURE PLANS

From the simulation results of detonation velocity tests, aquarium tests and the mid-scale underwater tests with the parameters developed for both the Ignition and Growth Reactive Model and CPeX Model, the following conclusions have been reached.

- The Ignition and Growth Reactive Model can capture the physics of detonation inside the explosives accurately and successfully simulate successive positions of bubble and shock front resulting from a detonation wave propagating down the explosive cylinder observed in the aquarium tests.

- Both models, although determined from the detonation velocity versus diameter effect experimental data for unconfined explosives, could faithfully model the reaction rate characteristics for experiments carried out in other configurations.
- As part of the program of evaluating the ultrafine aluminium powder 'Alex' in explosive formulations, aquarium tests of Alex-based PBXW-115(*Aust*) will be carried out to measure Alex reaction rates in polymer-bonded explosives. These experimental results, together with the results[23] of VoD and plate dent depth tests and aquarium test of Tritonal (80:20 TNT/Al) explosive formulations containing 'Alex', will be used to calibrate the Ignition and Growth model in LS-DYNA for study the role of aluminium and particle size effects.
- The good agreement between the Ignition and Growth Model and the CPeX Model for the simulation of mid-scale underwater tests implies that these two models using parameters derived from small-scale tests could be applied to large-scale devices. Current work on simulating the farther field for late-time effects with a calculation configuration of Φ530mm x L5000mm using the Ignition and Growth Model and the available experimental peak overpressure data will provide the validation.

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