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Development of a numerical capability for simulating non-ideal explosives and reactive materials

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Abstract

There is continuing motivation to develop and attain numerical modelling capabilities to better assess, understand and evaluate blast effects from explosive threats for UK Defence and Security. In line with this, significant efforts have been made by the Terminal Effects Simulation Team (TEST) at Defence Science and Technology Laboratory (Dstl) to introduce novel functionalities, such as a capability to model porous explosives, which has led to promising results, but ongoing work is required to validate outputs before advancing development. On the other hand, non-ideal explosives, including Home Made Explosives (HMEs) are an especially complex entity to understand due to various effects including metal particle combustion, non-ideal detonation and manufacturing variability. Long-term research investigations are ongoing into the methods by which the phenomena can be better understood and simulated, meanwhile, current available modelling capabilities are being explored in commercial codes such as APOLLO Blastsimulator to progress Dstl's ability to model non-ideal detonation and air blast events. This paper will detail the ever-evolving efforts to develop the numerical functionality described above, the role each capability plays in our competencies as an organisation and the future work required to further advance.

Introduction

There are currently some gaps in explosives modelling that need to be rectified in order to comprehensively simulate all aspects of energetic behaviour. To address this there are ongoing efforts to improve the understanding and modelling of explosives, which includes both longer-term research goals and short-term objectives, through innovative methods and the exploitation of available modelling capabilities. One specific area of interest is modelling non-ideal explosive detonation and blast. An explosive's detonation behaviour and subsequent blast effects can be described as acting either ideally or non-ideally:

- Ideal – Refers to a reacting explosive with a very small reaction zone, critical diameter[1] and run-to-detonation distance[2] with a near constant detonation velocity. Due to the small reaction zone, a simple programme burn model can be used to approximate the detonation behavior [1], where the reactant instantly transitions to its detonation products following a reaction front based on a constant detonation velocity
    - Ideal explosives will also behave non-ideally if the charge geometry is on a small enough scale (typically a size smaller than used in reality) [2]

- Non ideal – Having a larger reaction zone, critical diameter and a longer run-to-detonation distance with an accelerating detonation velocity. The explosive output is also dependent on the mass [3]. The larger reaction zone means that the energy release and build up to a detonation wave is slower and therefore the instantaneous transition that is assumed by a programme burn model would over predict the detonation behavior
    - Non ideal explosives can show approximate ideal behaviour if the charge is large enough, for example ANFO detonates ideally when it approximately has a mass of >100-200kg [2]

The non-ideal detonation behaviour is typically found in non-ideal explosives, including many HMEs. Non-ideal explosives are more challenging to model in comparison to ideal explosives for three main reasons:

- Explosive variability – Manufactured explosives, even with stringent regulations, will vary in their explosive make-up from sample to sample. This variability is far more exaggerated for HMEs as they are not manufactured with a consistent approach or regulation. The constituent ingredients will vary considerably and will often include commercially available products such as fertiliser to replace laboratory-grade materials. The difference in material quality, particle sizes and the quality of manufacturing technique will naturally result in significant variation
- Manner of energy release – Non-ideal explosives can contain other ingredients such as metal powders that change energy release of the explosive. These added materials can be inert during the detonation process but will react at a later stage and combust, releasing energy over a longer timescale [5]
- Initiation and detonation – As stated before, non-ideal explosives have larger reaction zones where the transition from reactants to detonation products occurs over a longer period than ideal explosives [6]. Due to this large reaction zone, they often have a large critical diameter and their detonation performance can heavily depend on their level of confinement and geometry as seen in internal tests, see *Figure 1*. Their detonation velocity is also typically slower, with a longer run-to-detonation distance and the detonation wave is more curved

[1] Critical diameter - The required diameter for an explosive for detonation to occur. [4]

[2] Run to detonation distance – The distance for a shock wave to travel until it transitions into a full steady-state detonation wave for a given input pressure. [4]

This paper will discuss the expansion of Dstl's high-fidelity physics functionalities for simulating aspects of the non-ideal behaviour of explosives to address these capability gaps.

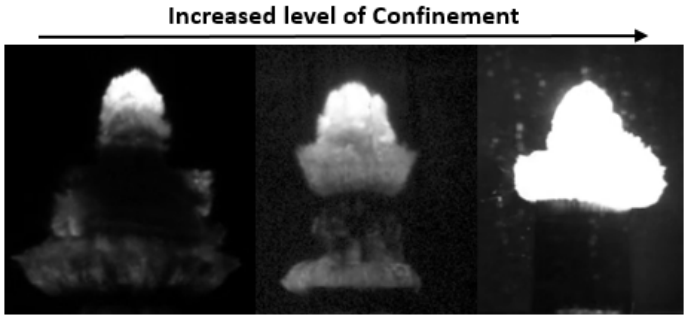

Figure 1. Confinement study using an underwater explosive

Software

Different software contains their own set of tools and functionalities to simulate explosives and their effects, which possess the ability to model the common relevant phenomena, however, there is no single code that can accurately model everything. Therefore, it is necessary to utilise multiple numerical codes, individually and/or (when possible) coupled[3] to other codes, to enable the combination of functionalities to tackle a single problem and aid in understanding certain behaviours of a given energetic material.

APOLLO Blastsimulator (referred to hereafter as APOLLO) [7] is a high-fidelity computational fluid dynamics (CFD) code that is developed by Fraunhofer Ernst Mach Institut (EMI) in Germany. The code uses an Eulerian framework with an explicit finite volume method and currently has 1D and 3D solvers, with a 2D solver currently under development. It is also computationally efficient due to its dynamic mesh adaptation[4] (DMA) and zoom[5] functionalities.

APOLLO is an Eulerian code, which is commonly used for modelling energetic events, and it does not have the option to use a spatial Lagrangian integration scheme, which can better represent structural deformation and small amounts of distortion. Additionally, since the code does not contain strength models that are required to simulate dynamic structural response or fragmentation it is therefore necessary to couple with a structural solver (e.g. LS-DYNA[6]) should this nature of output be the aim.

Dstl's current ecosystem includes LS-DYNA and IMPETUS AFEA with an aim of SOPHIA soon to be included, all of which possess two-way coupling capability to APOLLO. APOLLO has a library of equations of states (EoS) for a multitude of explosives, which can be used for modelling detonation and blast. Should additional EoS not present in the library be required, thermochemical codes, such as Cheetah and EXPLO5, can be utilised to develop entries for use within APOLLO. This method has

[3] Coupling is a functionality that allows the capabilities of Euler and Lagrangian codes to be utilised in the same simulation. This can be one-way wherein the Euler code outputs the full pressure-time history as input load for the Lagrangian code, or two-way wherein the codes run simultaneously, but alternating such that the output of one feeds into the input of the other and vice versa [7]

[4] Dynamic Mesh Adaptation (DMA) is a numerical capability within APOLLO which improves computational efficiency. The DMA algorithm selects at least one region, with the strongest gradient for the parameter of interest (e.g. pressure), resolves the region to the highest resolution specified, and applies a coarser resolution to areas with weaker gradients [7]

[5] The Zoom option is used to handle increasing length scales. It allows for a time and region dependent DMA method, where a fine resolution can be initially selected and lowers over time or distance as the blast wave expands [7]

[6] LS-DYNA – is a multi-physics explicit dynamics solver (based on finite element analysis) that is typically used to simulate extreme deformation of structures [9]

been employed for ideal explosives, such as PE4, PE8 and PE10 and extensively validated against experimental data.

A key strength of APOLLO is its ability to explicitly model afterburn (or secondary combustion), an additional combustion reaction that occurs in fuel-rich, oxygen-deficient explosives, characterised by insufficient oxygen required to fully oxidise. In such scenarios, this then leads to partially reacted and unreacted explosive material further reacting with external oxygen sources such as the surrounding ambient air, provided sufficient energy is present to initiate the reaction. [8]

APOLLO's base functionalities allow the code to be proficient at modelling air blast scenarios. This, in addition to its ability to couple to other structural solvers to simulate material response, highlighted it as software with significant potential eventually leading to the extensive contribution to the overall development of the code. It has grown to become the main high-fidelity blast code used within Dstl due to its efficiency and accuracy, having been extensively used and validated by the TEST team at Dstl over several years for ideal explosive air-blast simulations.

Porous functionality

Conventional physics codes are typically designed to represent explosives as homogenous materials (see Figure 2, left), when in reality they can be composed of multiple materials (see *Figure 2*, middle and right), and/or air in the form of pores, known as porosity. Developing a porous functionality therefore became an endeavour aimed at enabling the analysis of a more representative material to investigate this.

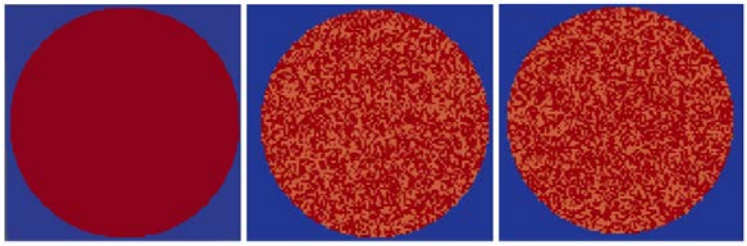

Figure 2. Standard smeared homogenous representation of CompB (left) and stochastically-filled CompB geometries (middle and right)

The porous functionality works by running an executable in conjunction with a text file containing: the desired charge geometry, including shape and size; resolution; ambient conditions, for temperatures and densities; pore and volume fraction, to stochastically generate the porosity within the charge; and a seed number. A seed number is assigned to allow the charge composition to be identically recreated at a later date or changed to produce a different geometry. This information is read to generate the charge in the form of a map file, which can be read in APOLLO, and introduced to the full global model.

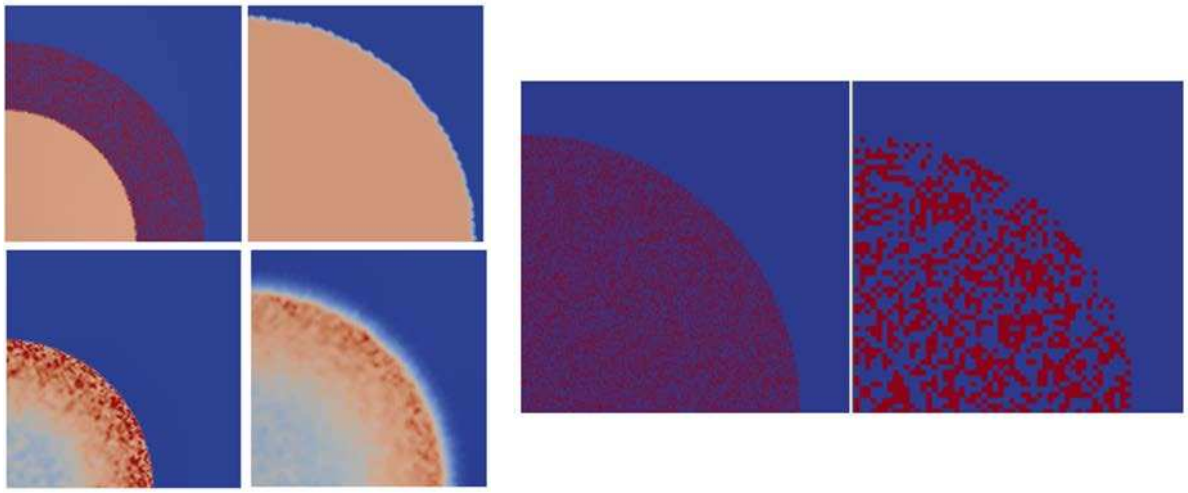

Figure 3. Conversion from reactants to detonation products following a spherical reaction front (top left) and pressure distribution of the reacting explosive (bottom left), resolution study geometry (right)

This functionality works robustly with APOLLO's Burn on Time (BoT) detonation model (also known as programme burn) wherein cells containing explosive material instantaneously convert from reactants to detonation products at a time calculated with the distance between the initiation point and the cell in question, whilst assuming a constant user-defined detonation velocity (see Figure 3) [7].

Furthermore, an initial study was conducted to understand the resolution dependence of the capability; five models ranging from 100 microns to 1mm in resolution were used to generate the charge geometry, and their blast effects were evaluated in both the near-field and the far-field. It was concluded that although there is a difference in how the explosive is physically represented (see *Figure 3*), there is minimal difference in the blast effects. This indicated that this capability was not resolution sensitive in this case, however, further investigations are required for a wider range of materials and scenarios to fully understand the resolution dependence of the functionality.

Powdered explosives are often represented as a smeared continuum with a single EoS for a specific bulk density within a numerical code, whereas in reality there are voids (air gaps) between the particles, which are randomly distributed. In addition to this, depending on the manufacturing quality and consistency, sometimes the bulk densities can vary from the expected bulk density between charges.

The porous functionality allocates random pores within the powdered charge and allows for the creation of random voids within the powdered charge, resulting in multiple charge geometries with different distributions of pores. This helps in understanding the differences and variations in blast effects based on the composition of the charge. Unlike the standard approach, which relies on a smeared continuum method and a single JWL[7] EoS with a fixed initial bulk density, the porous functionality enables users to adjust the bulk density by manipulating the pore fraction within the charge. As a result, a range of charges with different bulk densities can be simulated with a single EOS and a density-dependent detonation velocity that can be derived using a thermochemical code. This eliminates the requirement for derivation of multiple EOSs for a single explosive at different densities and associated validation processes.

This capability was originally derived to model free-field tests using powdered ideal energetic materials (HMX, RDX, Octoviton and PETN). Initially, the standard JWL at bulk density was used to model the experiments, however as the measured test bulk density was lower than the JWL bulk density of the explosives, the modelling results across the explosives were dissimilar and inconsistent to the

[7] An equation of state is an equation that relates the pressure, temperature and volume of a substance; the Jones-Wilkins-Lee (JWL) variety is used universally to describe the expansion of detonation products, particularly in a numerical modelling context.

experimental data. Therefore, the porous functionality was used and pores were introduced into the charge to achieve the test density without having to derive a new JWL.

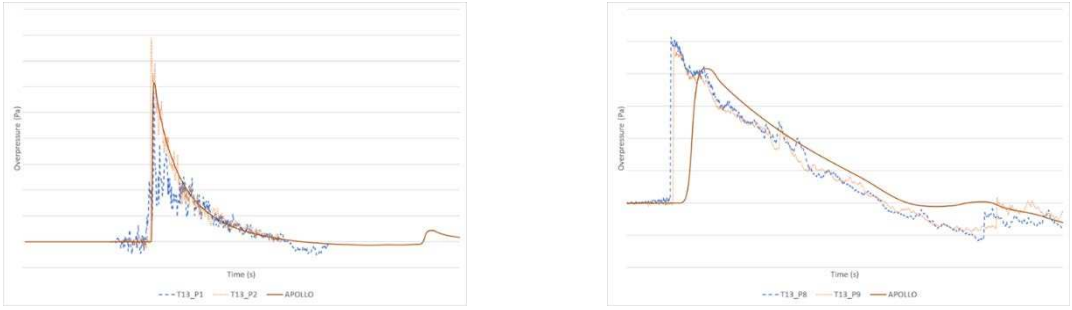

Figure 4. Overpressure comparison in the near field (Z ≈1.25 m/kg$^{1/3}$) (left) and the far field (Z ≈6.3 m/kg$^{1/3}$) (right) for a powdered charge

Using this method provided success with matching the test data very well in both the near field (Z ≈1.25 m/kg$^{1/3}$) and the far field (Z ≈6.3 m/kg$^{1/3}$) consistently for all of materials. As shown in Figure 4**.** for one of the powdered charge materials, the APOLLO results trend very well with the experimental data and simulate similar blast effects.

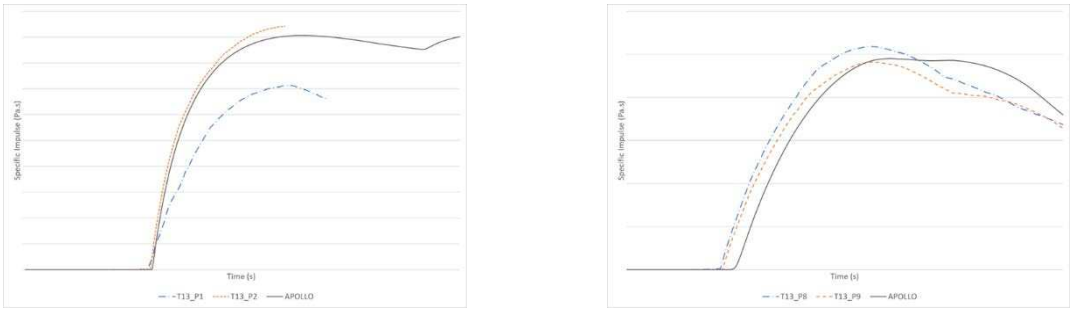

Figure 5. Specific Impulse comparison in the near field (Z ≈1.25 m/kg$^{1/3}$) (top) and the far field (Z ≈6.3 m/kg$^{1/3}$) (bottom) for a powdered charge

The porous functionality has now been expanded to model composite explosives, explosives with multiple energetic components. However so far only studies on explosives without additional binders have been conducted (e.g. CompB and Octol). In the standard approach to explosives modelling, mixed porous explosives such as CompB (≈60% RDX/40% TNT) [4] have typically been represented as a smeared continuum with a combined bulk JWL. However, with the porous functionality a CompB geometry can now be stochastically generated as a mixture of TNT and RDX. Similar to the porous charge development, the volume fraction of both TNT and RDX has to be specified to achieve the correct mass percentage of each explosive within the mixture.

To evaluate how well it can model mixed energetic explosives, five mixed TNT/RDX spheres representing CompB were stochastically generated and their blast effects were compared in the free field to a standard CompB JWL, where the CompB charge is modelled as a smeared continuum with a single CompB EoS.

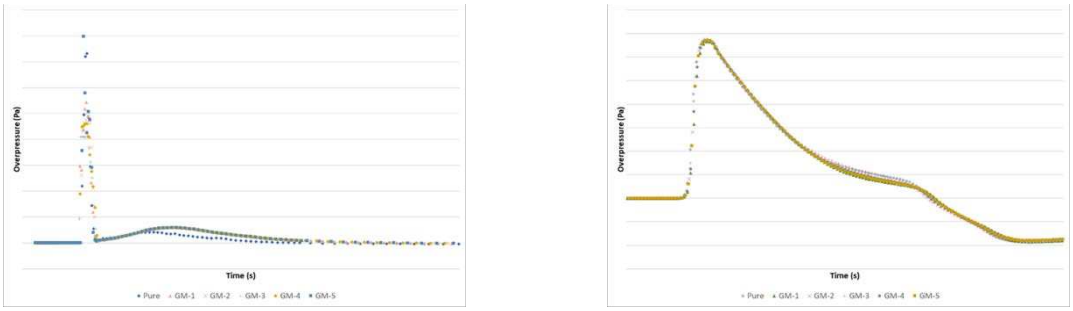

Figure 6. CompB porous functionality comparison against a standard JWL approach taken at a scaled distance of approximately 0.7 (left) and 11 m/kg$^{1/3}$ (right)

As shown in Figure 6, all five models show a variable output with a very fine spread in the far-field, with a larger spread in the near-field in terms of overpressure. This disparity could be due to potential localised extreme differences in the mixing. This difference is however minimal for specific impulse in both the near-field and far-field.

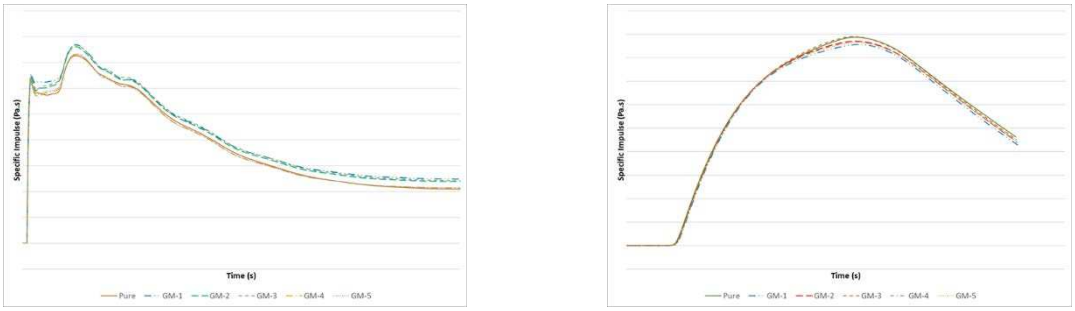

Figure 7. CompB porous functionality comparison against a standard JWL approach taken at a scaled distance of approximately 0.7 (left) and 11 m/kg$^{1/3}$ (right)

Furthermore, a cylinder expansion (CYLEX) test was simulated to validate the functionality. Five stochastically generated CompB mixtures were generated and placed as the explosive fill with a copper cylinder wall encapsulating the energetic material. The explosive is initiated from the bottom and the wall velocity of the cylinder is tracked. This model was also set up and run in Autodyn[8] using Autodyn CompB JWL values. As seen in Figure 8, when the CompB charge initiates and detonates, the detonation products are formed which expands the cylinder, driving it outwards.

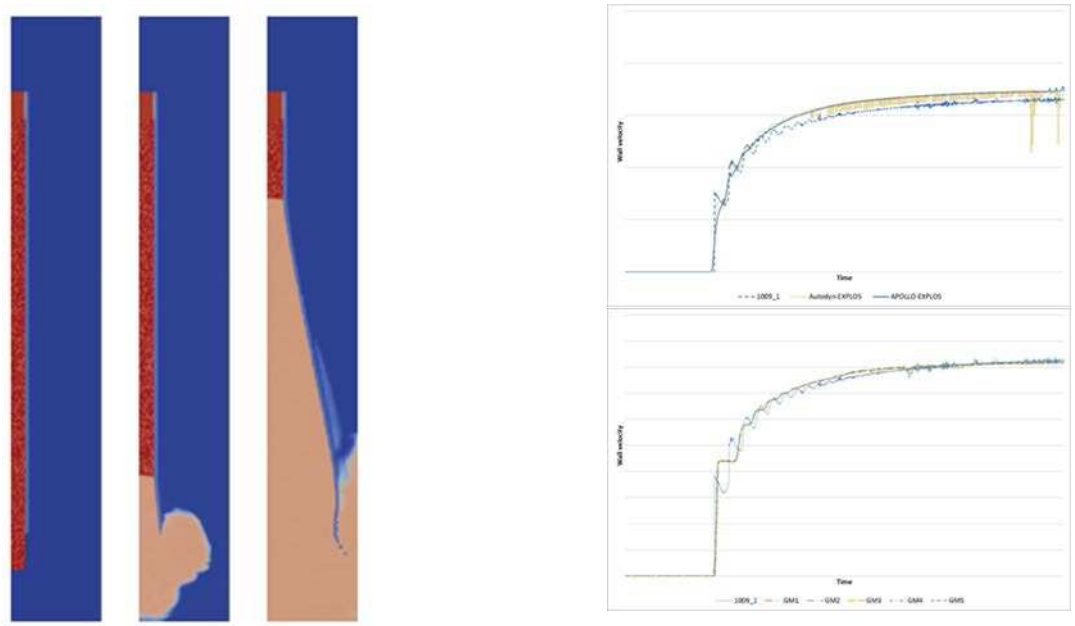

Figure 8. CYLEX simulation using the porous functionality (left), comparison of CompB EoS to test data (upper right) and Porous EoS to test data (bottom right)

With this study, the results of the porous functionality are compared to the standard JWL approach, experimental data as well as Autodyn results using an EoS generated in EXPLO5 [10]. In *Figure 8*, both Autodyn and APOLLO outputs slightly over predict the wall velocity in comparison to the experimental data. However, when using the porous functionality the results trend very well with the Autodyn results and experimental data throughout the simulation. Both simulation results and comparisons show a successful application of the porous functionality to develop mixed explosives.

[8] Autodyn is a commercial code developed by ANSYS US. It is a Finite Volume code and has a wide range of functionalities including simulating blast.

There is also great interest in investigating packed prilled explosives (such as ANFO) for a given geometry. This can be achieved by pairing the porous functionality, to generate the individual prills, with an algorithm, to pack the prills together, which constructs the prilled explosive.

Two algorithms (obtained from open sources [11] [12]) were incorporated into a Python script: one to perform uniform packing of equal spheres (see Figure 9, left) and one to perform non-uniform packing of both equal (see Figure 9, middle) and unequal (see Figure 9, right) spheres. In both cases the script calls for a bounding radius to be prescribed as a constraint for placing spheres in three-dimensional space, the logic being that any given sphere centre, plus its radius, cannot exceed the bounding radius. It is at this point that the similarities end between the two algorithms.

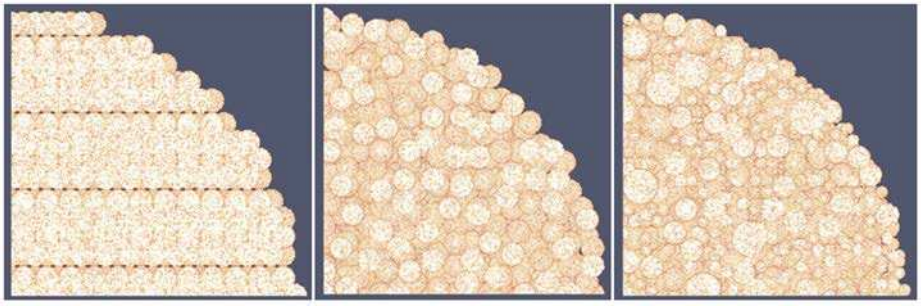

Figure 9. Packing methods: uniform spheres fixed packing (left), uniform spheres random packing (middle), random packing of different sphere sizes (right)

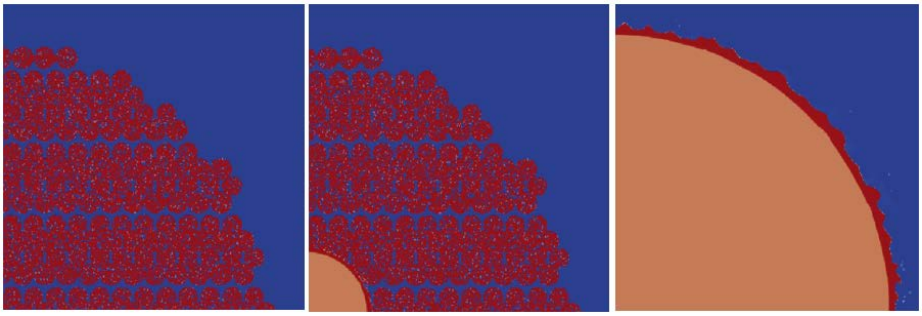

Figure 10. Conversion from reactants to detonation products following a spherical reaction front for a prilled explosive

A generic mix has been modelled in 1/8th symmetry and centrally detonated (see Figure 10). Although not obvious in the middle image of Figure 10 at this scale, the right-hand image displays evidence of imperfections in the shock front (at the extremities) as well as behaviour similar to spalling, potential evidence of this has been seen in ANFO tests and is being investigated as part of a study into the detonation of ANFO. Whilst the results look promising at first glance, this is by no means considered as a valid functionality and therefore requires further verification and validation. For instance, a known issue of incorrectly represented spheres at symmetry boundaries is currently under investigation.

Reactive burn model

The implementation of the HVRB (History Variable Reactive Burn) model in LS-DYNA is part of a collaborative effort between the University of Oxford and Dstl. The HVRB model is a reactive burn model that controls the transition from the unreacted EoS to a reacted EoS. It is a pressure-based model used to treat shock-induced initiation that grows to detonation for a heterogeneous explosive material [13].

The HVRB model was selected to be incorporated into LS-DYNA via user subroutine as both organisations had access to the code and it did not require source code access to implement the model, however it has been produced in a format that can be integrated into any commercial code.

To ensure that the HVRB model was correctly implemented into LS-DYNA, a verification study based on Gustavsen's flyer plate tests was conducted. This experiment was used to derive the explosive's initiation threshold and run-to-detonation distance and time, by impacting a PBX9501 explosive with flyers at varying velocities [14].

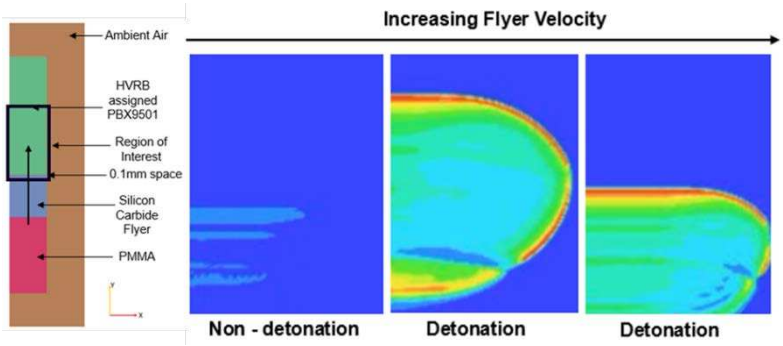

Figure 11. 2D HVRB Eulerian impact initiated PBX9501 model with a uniform fixed mesh (left), simulating an input pressure run to detonation distance

The model was set up as a 2D axisymmetric Eulerian impact initiated explosive to match the experiment (see Figure 11), where a silicon carbide flyer impacted a HVRB assigned PBX9501 at various velocities. It was modelled in LS-DYNA using amended HVRB values and reactant and detonation product PBX9501 EoS parameters found in online literature.

As seen in Figure 11, within the region of interest, when the flyer impacts the explosive and provides sufficient input pressure, the explosive initiates and detonates. However, when the flyer travels at a lower velocity it does not provide the required input pressure to detonate the energetic material. Furthermore, the implemented HVRB model can capture a pressure-dependent run-to-detonation distance, where the distance is decreased with increased flyer velocity. This verification study provided confidence that the HVRB model was correctly implemented into a commercial code as it was able to capture both non-detonation and a pressure-dependent run-to-detonation distance.

An optimisation tool has been developed by the University of Oxford to derive HVRB parameters from experimental data, such as pop plot and particle velocity data. It uses a metamodel-based optimisation procedure, where an approximate surrogate model is optimised against experimental data using LS-DYNA simulation results. Starting HVRB parameters are set at the beginning with a minimum and maximum range and the three Lagrangian shock to detonation (SDT) models are run simultaneously, with each model assigned a different flyer velocity, providing a different input pressure. Pressure-time histories are then extracted along the elements across the centre axis of the explosive. The HVRB values which provides the lowest mean squared error difference value (how far the average model value is away from the target experimental data) for both the pop plot and flyer optimisation is then selected.

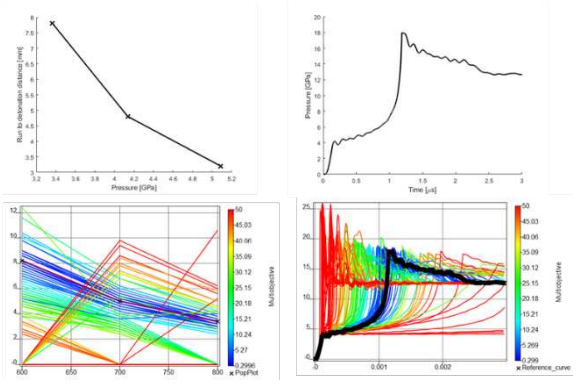

Figure 12. Target Pop plot and Particle velocity data (Top) and optimised surrogate models (below)

Aluminised Explosives

Within APOLLO, reactive particles are Lagrangian particles that are modelled as mass points and interact with fluids through drag forces, chemical reactions and the transfer of heat. They can also interact with rigid objects in APOLLO through momentum exchange. Reactive particles can be implemented in various sizes, materials and velocities. Reactions with oxidisers are explicitly calculated and can lead to the formation of new combustion products such as aluminium oxide, which are modelled as a continuum condensed droplet phase.

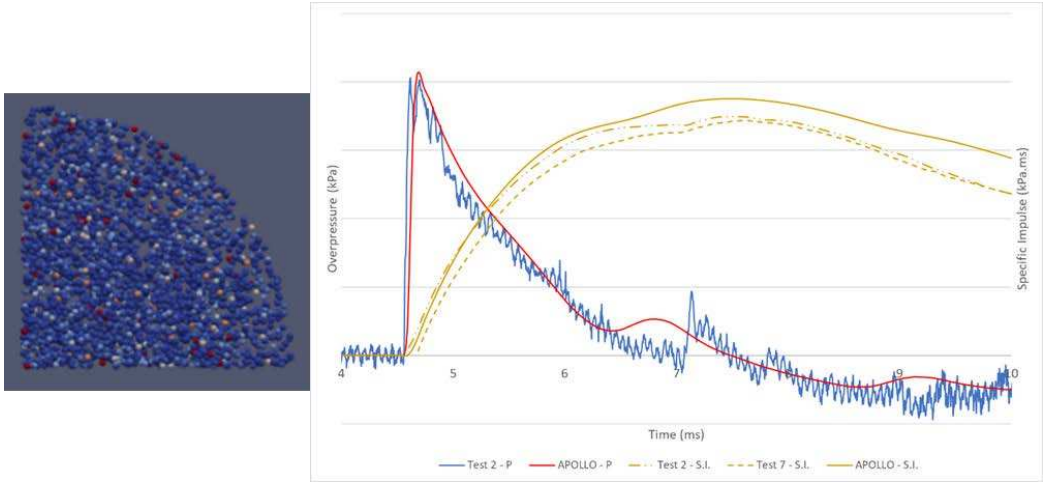

Figure 13. Hemispherical PBXN-109 geometry developed using reactive particles (left) and ground burst overpressure and specific impulse comparison (right)[9]

This option is used to simulate the details of dispersion and combustion of metallic particles in high explosives interacting with a gas flow. For aluminised explosives, the aluminium powder can release a large amount of energy after detonation has occurred. Metallised explosives are modelled within APOLLO by using a continuum JWL to model the explosive as a base layer with a lower density (without the metal powder) and then reactive particles are used to model in the aluminium powder (see Figure 13). This function has been used to model hemispherical ground burst (see *Figure 13*) and confined PBXN-109 experiments with success (the EoS and reaction parameters used in this study were developed in a blind study by EMI).

As seen in Figure 13, the APOLLO results trend very nicely with the hemispherical ground burst experimental data and for the confined PBXN-109 experiments.

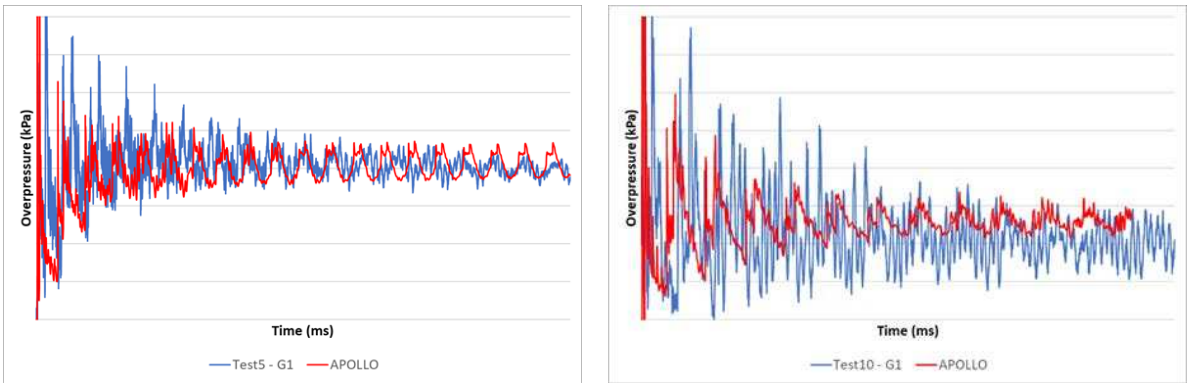

Figure 14. Spherical confined PBXN-109 overpressure and specific impulse comparison in air (left) and nitrogen (right)

[9] Early arrival time of the secondary shock is a known general issue (not specific to these models) in APOLLO when afterburn is included, which is under investigation

The APOLLO results lie between the peaks and troughs of spherical confined PBXN-109 overpressure and specific impulse comparisons for both in air and in nitrogen (see Figure 14).

Reactive Materials

Reactive materials (RM) are of increasing interest in the defence industry, to maximise blast effects while reducing inert materials. APOLLO, along with SOPHIA, have had initial functionality development to allow reactive materials to be simulated and allow full start to finish simulations to be conducted, including:

- Explosive detonation
- Casing fragmentation
- Fragment break-up on impact
- Fragment/particle burning
- Pressurisation and structural response

Work is ongoing to be able to simulate natural fragmentation effects as well as experimentally characterise reactive materials for validation of numerical models. SOPHIA is not yet available to Dstl but Fraunhofer EMI have provided initial proof of concept simulations, demonstrating the available functionality, as can be seen in Figure 15 and Figure 16.

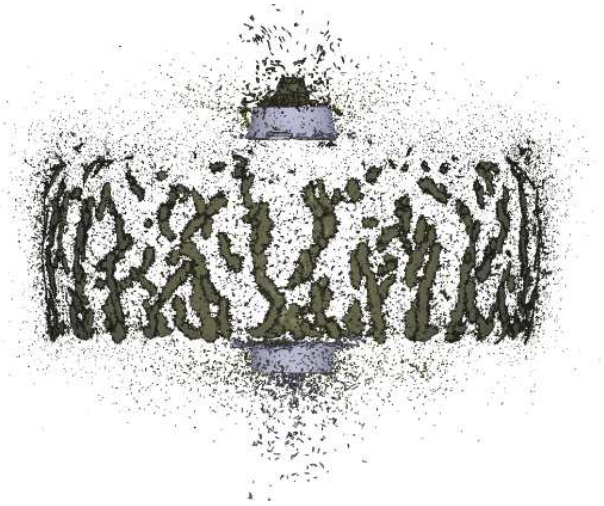

Figure 15. Natural fragmentation of a cased charge in IMPETUS

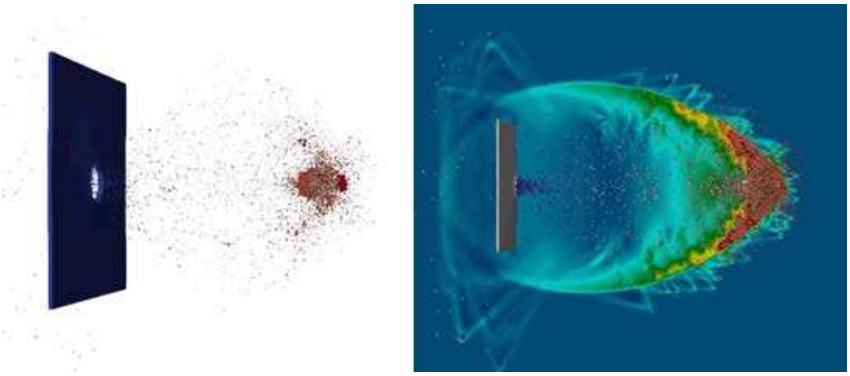

Figure 16. Impact and break-up of a RM fragment on a steel plate (left) and pressure release through combustion of developed particles (right)

Conclusions and Ongoing Work

The work discussed in this paper is ongoing capability development work, therefore although promising results have been seen, further validation and development is required.

- Porous functionality
  - Excellent initial results have been produced for a range of ideal powdered explosives. Additional data is required, including for confined and near-field tests to further validate this method
  - For mixed material explosives although very promising results have been seen, simulation of a wider range of materials is required to ensure this method is appropriate for a wide range of scenarios
  - An aim for future work is to develop a methodology to include binder materials withing the simulations. This would allow a wide range of explosive materials to be simulated with a relatively small number of EoS, which are not density dependent
  - A non-constant detonation velocity has also been included in APOLLO, this will be tested to see if any non-ideal behaviour can be captured by this
- Reactive burn models
  - The implementation of the HVRB model allows inclusion of a reactive burn model with additional functionality, as well as the use of the optmisiation software to develop HVRB parameters
  - Future work is aimed at investigating the use of HVRB for non-ideal explosives as well as investigating the development of a physics based predictive initiation model
- Reactive particles
  - The use of reactive particles within APOLLO has been very promising for aluminised explosives in both far-field and confined scenarios
  - Generating EOS for a wider range of aluminised explosives and simulation of a wider range of regimes for aluminised explosives (e.g. CYLEX and near-field) is required
  - Expansion of this capability to UNDEX explosives where there are both aluminium and ammonium perchlorate particles
  - Validation of reactive burn break-up and combustion

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