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PHYSICS-INFORMED MODELING OF AFTERBURN IN EXPLOSIVE SIMULATIONS WITH GPU-ACCELERATED CFD

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ABSTRACT

Quasi-static pressure (QSP) in confined detonations is dominated by the internal-energy rise of the enclosed gases and, for oxygen-deficient charges, by post-detonation "afterburn" of detonation products and binder with atmospheric oxygen.

We present a new explicit afterburn model in Viper Blast and compare this to confined detonation experiments for PE10. The newly developed explicit afterburn model in Viper Blast is outlined, and it is shown how the model tracks both the detonation and combustion products through separate species, with the afterburn combustion process both limited by stoichiometry and temperature. This method is compared to the classic Miller-type afterburn process currently available in Viper Blast – and it is shown that it removes user input for both the amount of afterburn energy and time scales for combustion.

Initial results using the new Viper Blast implementation reproduce the experimental PE10 trends in air and nitrogen. We outline the variable gamma methodology used inside the explicit solver without sacrificing GPU performance.

INTRODUCTION

Confined detonations develop a long-duration QSP after multiple reflections and mixing. For fuel-rich explosive compositions, afterburn can dominate the final pressure. Afterburn is the process through which later time energy is released through the combustion of detonation products. This is primarily the case for oxygen deficient (fuel rich) explosives. These detonation products require sufficient oxygen (or in an air atmosphere) and temperature to combust. This process is therefore sensitive to the specific explosive (and related binder) composition, stoichiometry, problem geometry, timescales, and venting – among other factors.

Fast-running predictions are valuable for design and assessment but should honour the energy pathways and heat-capacity changes of realistic gas mixtures. Recent thermochemical work has demonstrated that an ideal-gas, composition-aware treatment can match chamber data for plasticised explosives across atmospheres with ≈1–3% error, providing a strong basis for embedded models [1].

Implementing such a scheme into an explicit solver has several challenges, and advantages, which we outline in this paper. Namely these are – the potential for a simplified user experience, increased accuracy of QSP, reduction in conservatism.

Initially we outline the current results from the afterburn implementation in Viper Blast as compared to a series of chamber experiments against the PE10 explosive, conducted by Sheffield University in Ref [2]. After this we discuss our improvements to the afterburn algorithm which we call 'Explicit' afterburn, and how this compares to the existing implementation. Finally, we discuss methods to improve agreement with experiment by implementation of a variable gamma formalism with Viper Blast.

BACKGROUND

Viper Blast is a finite volume computational fluid dynamics code for the simulation of blast effects, solving the Euler equations based with the AUSMDV scheme. Fundamentally, the numerical methodology is similar to that provided in Rose et al. [3]. The MUSCL-Hancock time integration is used, yielding a scheme that is second order in both space and time. GPU scalability yields significantly reduced computational time and massive scalability – with 100's of millions of computational cells tractable on a consumer laptop.

A standard methodology for treating afterburn in numerical simulations is a Miller-type approach. In the case of Viper Blast this involves only two inputs. Firstly, for a given explosive type the potential afterburn energy to be produced A_e (J/kg) and the time frame over which this energy is deposited, A_t. In Viper Blast this A_t defines the time frame from detonation which energy is deposited as a S-curve, where A_t defines the time when 99.99% of A_e has been deposited into the system. A_e is defined as the difference between the defined detonation energy and the total potential combustion energy of the explosive in ideal conditions. Detailed validation cases of this method are available in the Viper Blast User Manual [4].

This methodology is simple to use and can be made to be generally conservative and so is a popular and robust choice. However, in more complex scenarios – either novel explosives or complex geometry – deriving A_e and A_t may be non-trivial. Additionally, in the Miller-esque approach, the afterburn energy is deposited uniformly across the detonation products, which can lead to a degree of inaccuracy in more complex geometries.

To overcome some of these limitations in more complex problem types we have implemented a more robust, physics based explicit afterburn algorithm that remains GPU compatible with no performance penalty.

CHAMBER EXPERIEMENT

The experiments conducted by Sheffield University have focused on Quasi Static Pressure (QSP) studies inside sealed chambers. In particular the data used for our comparison is set out in Ref [2]. We focus our comparison on the PE10 (30 g) experiment, which is detonated inside a 275 L chamber, the experimental setup is shown in Figure 1.

QSP was recorded in experiments in Air, N2 and Ar atmospheres. Full experimental data is available as part of the supplementary data in Ref [2].

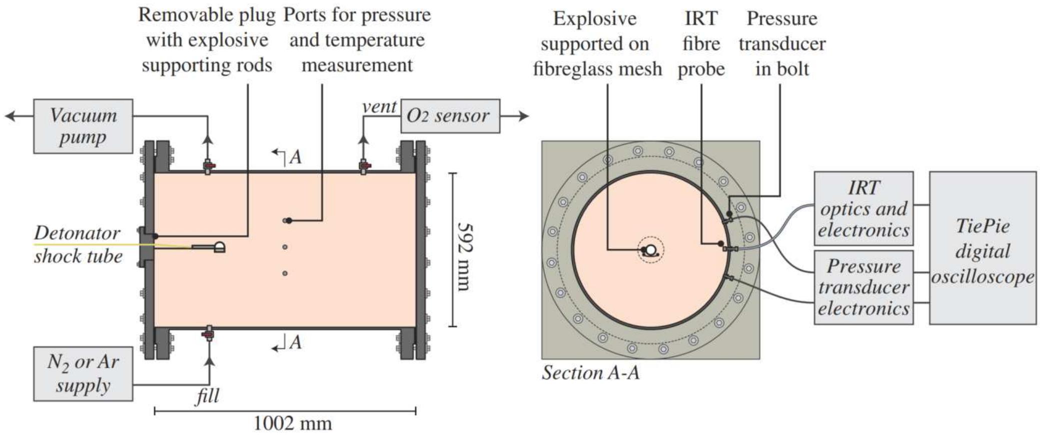

Figure 1: Experimental setup as outlined in Reference [2]

VIPER BLAST SETUP

JWL properties for PE10 are taken from Ref [5] and are shown in Table 1. The initial model setup is shown in Figure 2, and quarter symmetry is used. The location of the pressure gauge used for comparison is shown also in Figure 2. The simulation is run in 3D with a cell size of 2 mm and approximately 11 million cells.

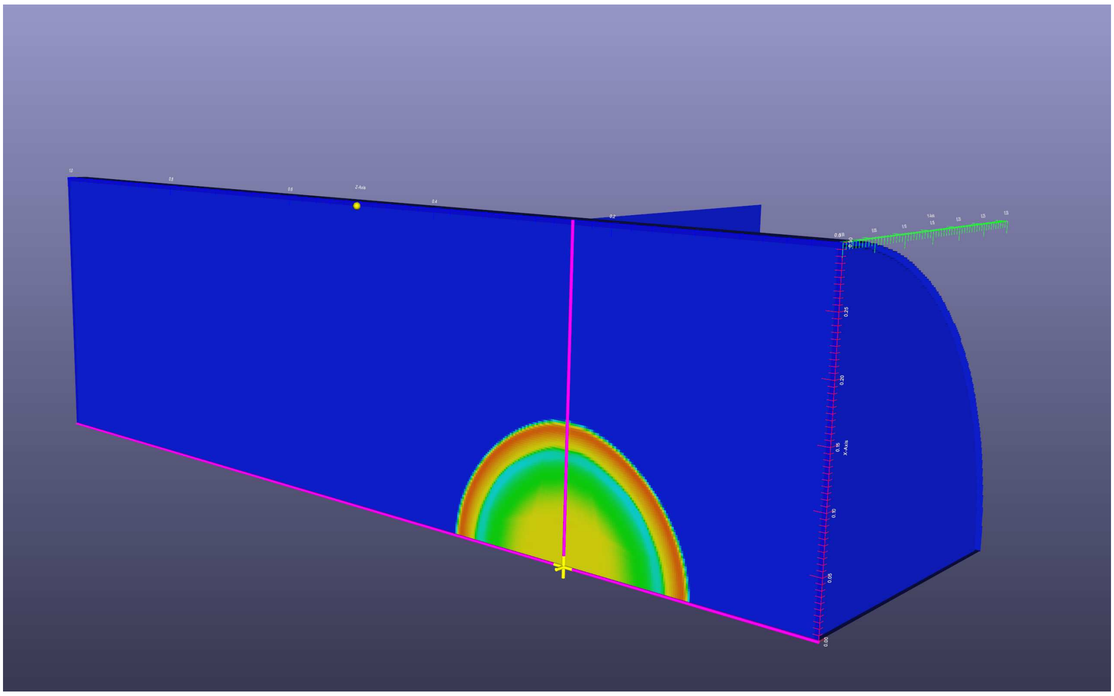

Figure 2: Viper model setup at early time.

Density (kg/m^3)	1550
A (Pa)	3.21E11
B (Pa)	9.40E9
R1	4.4
R2	1.228
Omega	0.271
Detonation Velocity (m/s)	7735
E0 (J/kg)	5.18E6

Table 1: Viper JWL Parameters for JWL PE10 [5].

CURRENT AFTERBURN ALGORITHM RESULTS

Figure 3 shows the results of the initial 40 ms of analysis time, comparing the experimental results from a detonation in an N2 atmosphere to Viper Blast simulation with No Afterburn and Standard Afterburn respectively. Note following on from the work in Ref [1] at this stage we do not take into account pyrolysis.

Generally good agreement can be seen between the experimental results and no afterburn case, the final QSP for the no afterburn case is obviously sensitive to the detonation energy and the EOS properties used.

Notable is the significantly higher QSP that is established with the user of afterburn, with a steady state QSP being reached shortly after the 10 ms – which is the defined AB_t value in Viper Blast for this example case. AB_e is selected as the difference between the combustion energy for PE10 as set out in Ref [1] and the JWL detonation energy in Table 1

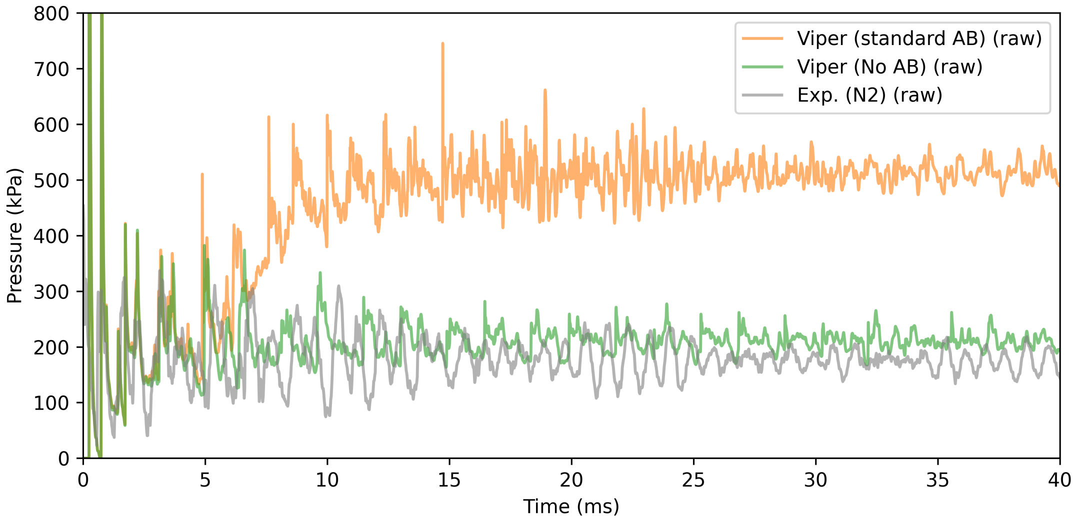

Figure 3: Comparison of Viper Blast results without afterburn, and with standard afterburn to experimental data for 30 g PE10 detonation in N2 atmosphere.

EXPLICIT AFTERBURN ALGORITHM

The first stage in the explicit afterburn algorithm remains the standard JWL equation of state, this, by definition defines the detonation energy of the explosive. The second requirement is then the total combustion energy – the total maximum possible afterburn energy (before air-fuel stoichiometric considerations) is the difference between these two values.

A complex plasticized explosive, such as PE10, may not have the full chemical composition freely available for plasticizers and binders – however the percentage of binder, filler is generally available.

The combustion energy of the explosive itself can be calculated according to a set of simplified CHNO rules (Kistiakowsky–Wilson style). One can go directly from the chemical formulae of the explosive to the combustion energy in such an approach. A similar approach can be taken for binders. In fact – all that is required is the total amount of C, H, N & O.

This then generates the total amount of energy per kg that can be deposited by afterburn process in perfect conditions.

Detonation products from the JWL EOS are tracked, and when sufficient air is available detonation products are converted to combustion products, assuming a sufficient activation energy has been exceeded with in the cell, and the appropriate amount of energy is seeded into the cell. The combustion products are modelled with an ideal gas equation of state.

In this way, afterburn energy is released on a cell-by-cell basis, at locations where there are sufficient energy and temperature for the process to occur – on a per mass basis. This is a simple and effective method for a more robust and physically accurate afterburn process than is captured using the Miller-esque process.

In our testing thus far, there is no appreciable loss in performance for this methodology vs the standard JWL solver.

RESULTS: VIPER BLAST AFERBURN MODELS

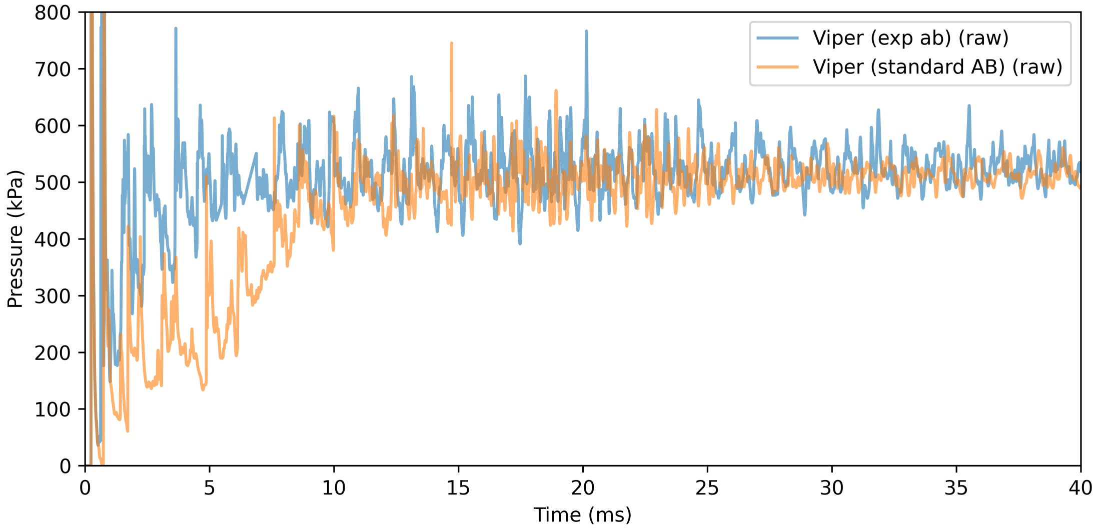

Figure 4: Comparison of Viper Blast with explicit afterburn and standard afterburn models.

Figure 4 shows a comparison of the explicit afterburn algorithm to the existing afterburn algorithm, previously shown in Figure 3.

The final QSP for both are approximately the same, however the timescale over which the energy is deposited is significantly different. With the explicit algorithm depositing energy fast. While the standard algorithm is based purely on user input. The explicit algorithm requires neither user input for energy nor timescales.

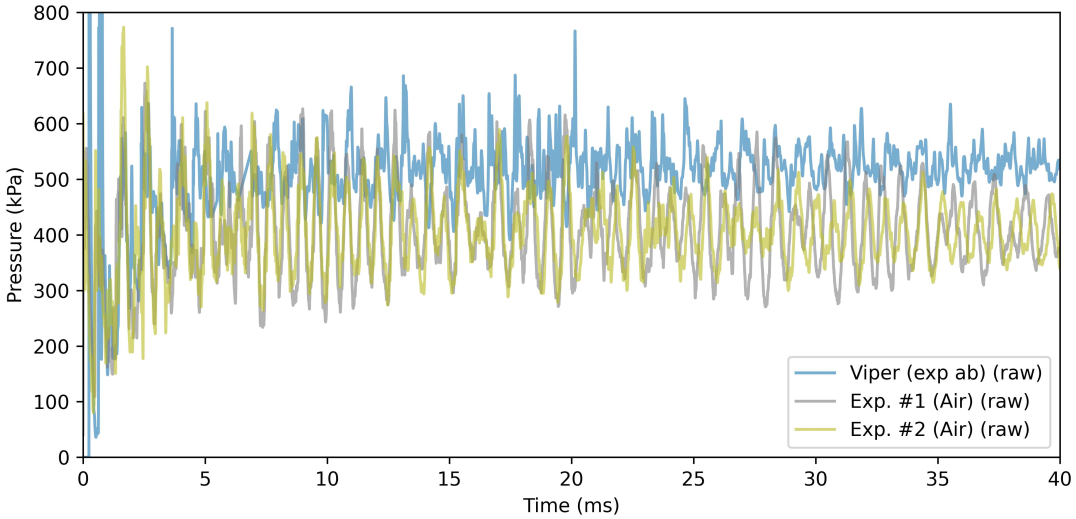

Figure 5: Comparison of Viper Blast with explicit afterburn to experimental results in air atmosphere.

Comparison to the experimental results in Figure 5 and 6 shows that the timescales calculated by the explicit afterburn method align closely with the those seen in experiment.

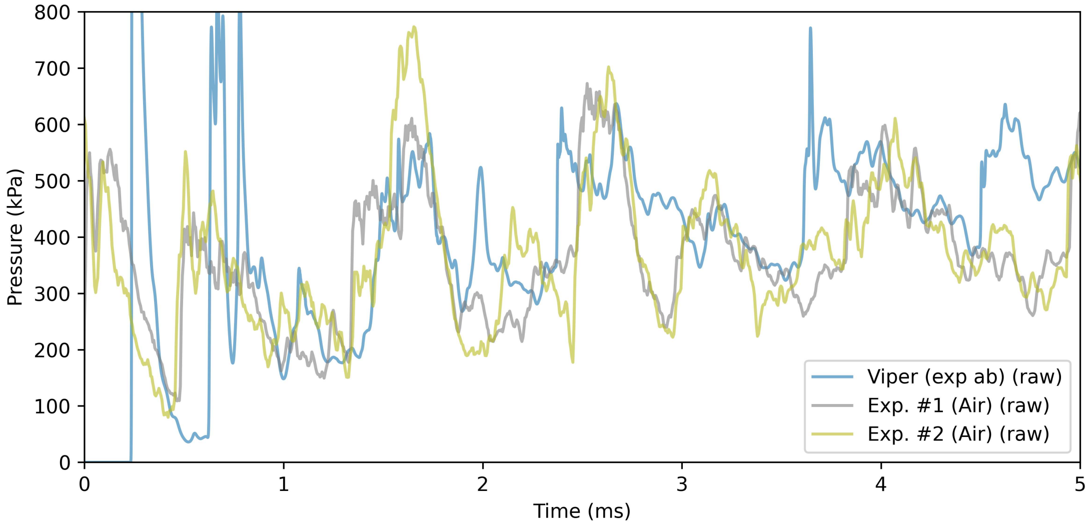

Figure 6: Comparison of Viper Blast with explicit afterburn to experimental results in air atmosphere – close-up view over first 5 ms.

However, the final QSP is significantly over predicted. Recent work by Barr et al [1] has shown the importance of considering the effects changes on the specific heat capacity with temperature. This has been shown to significantly reduce the QSP and bring results more in line with experimental records.

In the context of Viper Blast this would correspond to a gamma value (C_p/C_v) that is temperature (energy) dependent.

INITIAL VARIABLE GAMMA CALCULATIONS

In the same way that the combustion energy can be approximated using the K-W rules, combustion product specific heat capacities as a function of temperature (energy) are available.

In our initial approach, these are pre-tabulated for a variety of combustion products across a range of applicable temperatures. The gamma value is then allowed to vary on a cell-by-cell basis for both the air and combustion product species, both of which are modelled as ideal gases. This is used in combination with the explicit afterburn algorithm previously described.

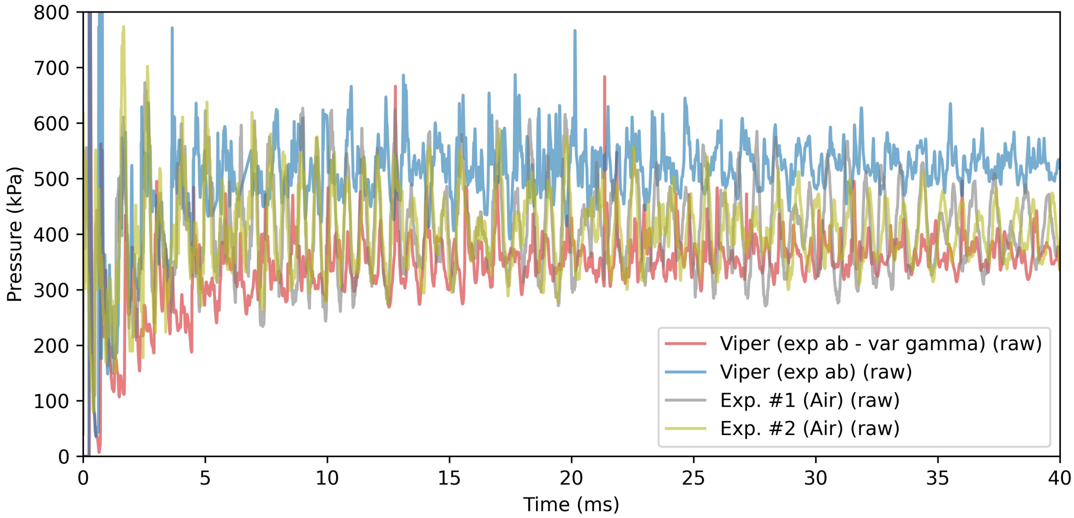

Figure 7: Comparison of Viper Blast with explicit afterburn and variable gamma to experimental results in air atmosphere.

This results in a significant reduction in QSP when compared to either the standard or explicit afterburn methodologies.

CONCLUSIONS & FUTURE WORK

The explicit afterburn implementation shown here shows good agreement with experimental results for both time scales in the case of the explicit afterburn algorithm and final QSP for the initial variable gamma implementation. The proposed methodology continues to be both user friendly and robust, allowing for implementation into commercially available CFD tools such as Viper Blast.

Performance has been shown to be generally unaffected by the inclusion of this additional explicit afterburn methodology, with Viper Blast retaining its GPU acceleration.

Future work will focus on more complex geometric validation cases, and other explosive compositions. Additional work will be undertaken on the variable gamma approach to ensure thermodynamic consistency across a wide range of temperatures.

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