INVESTIGATION OF THE SUITABILITY OF VIPER::BLAST CFD SOFTWARE FOR HYDROGEN AND VAPOR CLOUD EXPLOSIONS

Wholey, W.A.[1], Aggromito, D.E.[2], Stirling, C.G.[3], and Abboud, J.M.[4]
[1] Arup, 77 Water Street, New York NY, 10005, USA will.wholey@arup.com
[2] Arup, 560 Mission Street, San Francisco CA, 94105, USA daniel.aggromito@arup.com
[3] Viper Applied Science, SSSL, 272 Bath Street, Glasgow, G2 4JR, UK chris@viper.as
[4] Arup, 10370 Richmond Ave, Houston TX, 77042, USA julia.abboud@arup.com

ABSTRACT

Many simplified methods for estimating blast loads from a hydrogen or vapor cloud explosion are unable to take into account the accurate geometry of confining spaces, obstacles, or landscape that may significantly interact with the blast wave and influence the strength of blast loads. Computation fluid dynamics (CFD) software Viper::Blast, which was originally developed for the simulation of the detonation of high explosives, is able to quickly and easily model geometry for blast analyses, however its use for vapor cloud explosions and deflagrations is not well established. This paper describes the results of an investigation into the suitability of Viper::Blast for use in modeling hydrogen deflagration and detonation events from various experiments in literature. Detonation events have been captured with a high degree of detail and relatively little uncertainty in inputs, while deflagration events are significantly more complex. An approach is proposed that may allow for a reasonable bounding of uncertainty, potentially leading to an approach to CFD-based Monte Carlo analyses that are able to address a problem's true geometry while remaining reasonably pragmatic in terms of run-time and computational investment. This will allow further exploration of practical CFD application to inform hydrogen safety in the engineering design, assessment and management of energy mobility and transport systems, infrastructure, and operations.

INTRODUCTION

Vapor cloud explosions (VCE) and other accidental blast risks are of increasing concern as renewable energy technologies continue to advance and are implemented more widely in both private and public industry. There is a strong desire from these industries, regulators, and those who insure them to quantify the impacts from associated blast risks. While many simplified methods for this assessment exist, such as the multi-energy method, these are unable to assess the impact of confinement and geometry in a detailed manner. Many computational fluid dynamics (CFD) codes also exist, though most of these focus on extremely detailed models of flame front characteristics and are not optimized to run on the latest high-performance computing (HPC) hardware parallelized for a graphics processing unit (GPU). There is a gap in the suite of available tools for a CFD code that features less detailed 'engineering' models of deflagration processes but is still able to incorporate complexities of geometry and run a suite of models efficiently and quickly, thus enabling Monte Carlo simulation and associated Quantitative Risk Assessment methodologies.

According to the American Institute of Chemical Engineers (AIChE), a VCE is the explosion resulting from the ignition of a cloud of flammable vapor, gas or mist in which flame speeds accelerate to sufficiently high velocities to produce significant overpressure. VCEs are generally seen as the result of an accident scenario of energy storage. Typically, energy storage is located in areas where complex geometry exists, whether it be the storage mechanism or the wider space that houses it. With this understanding how VCE acts in confining spaces can affect the gas cloud size, if turbulence develops and how it effects the combustion rate during the explosion [1].

Several experiments have been conducted to understand the deflagration of hydrogen air mixtures in large, vented enclosures. Bauwens et al [2], conducted several experiments to examine the similarities and differences between three mixtures of similar laminar flame speed, 18% hydrogen air, 9.5% methane

air and 4.0% propane air. Using a chamber with the dimensions of 4.6m x 4.6m x 3.0m and a vent on one side, they determined the despite having similar laminar flame speeds, the hydrogen mixtures experimentally measured flame speeds were much higher than methane and propane mixtures due to flame instabilities. Additionally, higher pressures were generated compared to the methane and propane mixtures due to the higher propagation speeds of the hydrogen flames. The authors of that study, generated pressure-time histories and plots of flame velocity as a function of distance for 18.1% Hydrogen, 18.2% Hydrogen and 18.6% Hydrogen. Wakabayashi et al. [3], conducted field explosion tests of several hydrogen air mixtures. In this study, the experiments were conducted in a $31m^3$ tent, with different concentrations of hydrogen-air mixtures of 21%, 28.7% and 52.9%. It was determined that the amplitude of the overpressure depends on the concentration of hydrogen. Overpressure increased in accordance with increased concentration of hydrogen and the shape of the pressure time histories were found to be dependent on the difference in ignition method, electric spark or explosives.

Predicting VCE without completing experiments is challenging, however there are three simplified methods, which are considered an alternative to computational fluid dynamics (CFD). These are the TNT equivalence method, the TNO multi-energy method and the Baker-Strehlow-Tang (BST) model. The TNO-multi-energy method [4] is based on experimental research which indicated that only the combustion energy generated in obstructed and/or confined regions result in lethal overpressures (DNV software). It assumes that an obstructed region is where obstacles generate turbulence accelerating the flame if a cloud is ignited within it. This method isolates each region as a separate explosion source, if the distance between regions is large enough, otherwise, the regions are combined to form larger confined sources. The Multi Energy method blast curves were derived from idealised ground level explosions, however due to the complex geometry used in energy plants, the division of the plant into different regions vary between analysts based on the assumptions made leading to widely different results depending on who is undertaking the analysis. The BST method [5] is one of the most common methods used to estimate overpressures and is particularly useful in the early stages of design where geometric details of the building are unknown. This methodology is effectively a look up table that includes flame speeds that are derived according to the confinement, congestion and cloud reactivity of the obstructed regions and a family of blast curves for the overpressure and impulse.

CFD software allows the designer to consider the influence of cloud and obstruction geometry on the propagation of the combustion front. When developing a method to simulate VCE in CFD, the ability to alter different parameters to appropriately model the chemical composition is paramount. These parameters include density, energy, ratio of specific heats, upper and lower flame speeds, and parameters related to combustion processes. This study develops a convergence method to vary these parameters based on literature and run multiple CFD analyses in Viper::Blast. The results are compared with two experimental studies including Bauwens et al and Wakabayashi et al.

VIPER::BLAST DETONATION AND DEFLAGRATION MODELING BACKGROUND

The Viper::Blast(Viper) CFD software was originally designed for simulating the air blast environment resulting from detonation of High Explosives (HE). Fundamentally, Viper solves the Euler equations which govern adiabatic and inviscid flow of fluids, but with particular attention being paid to accurately modelling the formation, propagation, and interaction of strong shock waves. Viper was also designed to be an optimal solution for use in a commercial consultancy environment where reliability, accuracy, robustness, and efficiency are all vital. Combined with additional features for handling very complex geometries, Viper offers a best-in-class tool for simulating complex air blast events.

Attempts have been made recently to enable Viper to simulate VCEs in a similarly efficient, robust, reliable, and accurate manner. Initial investigations revealed that Viper was already very capable of simulating *detonations* of vapours. The numerical methodologies and schemes in Viper are almost equally applicable to detonations of condensed phase explosives as well as detonation of vapours. This is primarily due to the fact that for detonation of a material, the wave speed is nearly constant and supersonic (for practical purposes within the scope of Viper), which means that interactions between the

flame front (or detonation front) and obstacles, turbulence, and mixing of the vapour and the surrounding gases, have very little influence on the detonation itself.

However, as soon as the velocity of the flame front (or shock front) drops below the speed of sound in that material, other physical processes become relevant, for example, turbulent mixing of the fuel vapour and surrounding gases. Various other CFD codes attempt to model the highly complex turbulent combustion processes that occur in a vapour cloud deflagration [2]. Due to the complexity of those physical and chemical processes, it is often the case that simulations outputs are associated with very high uncertainty levels, which can be problematic in many circumstances. The approach taken initially in Viper for simulating VCEs differs in that it attempts to simulate the principal features of a VCE without explicitly modelling the root physical and chemical processes. The idea being that producing relatively accurate simulations with relatively low uncertainty, in a rapid manner, is of potentially greater value than much more complex simulations that are exceedingly expensive to conduct but still have very high uncertainty associated with their outputs.

Viper considers only ambient air, unburned fuel-oxidizer mixture, and burned fuel-oxidizer mixture, as three separate fluids. Unburned fuel-oxidizer mixture contains energy available for combustion, calculated externally to be used as an input in the software. Unburned mixture is converted into burned mixture following some very simple functions of time, space, and properties relating to the fuel mixture. A VCE is initiated by igniting the unburned mixture in one or more computational cells. The unburned mixture is converted to burned mixture, and the energy available for combustion in the unburned mixture is added to the internal energy of the burned mixture in that cell. As a consequence, the temperature and pressure in that cell rise. A flame then propagates from each cell with burned mixture to each cell with unburned mixture, according to a flame speed and with some other constraints such as minimum temperature for combustion to propagate and an autoignition temperature.

The flame speed in Viper is variable and calculated independently in each computational cell. When a user is defining a fuel-oxidizer mixture, five parameters are provided to control flame propagation. First, an upper bound flame speed, often a theoretical detonation wave speed for that mixture but it may also be an estimated upper bound for a flame speed in a material that is known not to be detonable. Second, a lower bound flame speed. This would ideally be a laminar flame speed but VCE at laminar velocities is usually of little interest for most real-world applications of Viper, so a lower bound flame speed of interest is normally provided here, often related to the flame speed that might be expected for an unconfined deflagration of that mixture in a free-field environment. The flame speed in Viper varies dynamically between those two bounding values. The flame speed currently only varies as a function of pressure, which merits some explanation here.

In a VCE within a complex geometry, a flame accelerates when a flame front geometry is perturbed by interaction with obstacles. It also accelerates when pressure and temperature rise due to confinement and interaction of blast pressure/shock waves with obstacles. So, a flame might initiate in a free-field environment, propagate at a very low velocity, and then encounter an obstacle which results in acceleration due to turbulence/pressure/temperature evolution around that obstacle. Conversely, a flame exiting a region with obstacles may then slow down again. The schemes in Viper are well able to model the interaction of shockwaves with obstacles, including the evolution of pressure/temperature/density around those obstacles. So even excluding any combustion processes, a shock wave entering a confined environment will already result in increased pressure, temperature, and shock wave speeds. For simplicity in the initial implementation of VCE in Viper, it was thought that a simple link between the pressure in that environment and the flame speed would be able to replicate most of the important behaviours of a VCE in a complex geometry.

Two additional parameters are required: the upper and lower bound values for what is termed “burn duration” in Viper. These values relate to the time it takes all unburned material in a computational cell to be converted to burned mixture once that cell has been ignited. These values relate to both the cell size and scale of the model, but also physically to the fuel-oxidizer mixture and the pressure/temperature/density conditions in that cell. For simplicity, the burn duration in each cell is

calculated as a function of the upper and lower bounds using the same linear relationship as used for the flame speed. Thus, there are linkages between the thermochemical state of the fluid in a cell, the flame speed in the cell, and the duration of combustion in a cell, all of which are controlled by some very simple inputs from the user.

It has been found during the development process that this simple methodology for describing the very complex processes involved in a VCE has produced some very promising outputs for a wide range of VCE configurations, from very low velocity deflagration in open spaces, to detonations in confined spaces, as well as for configurations where flames accelerate or decelerate due to obstacle interactions. However, it was also found that the choice of the parameters to define the properties of the vapor was critical. It is not clear yet how to deterministically identify appropriate values for the vapor cloud property definitions used in Viper. These values are obviously closely linked to the physical and thermochemical properties of the fuel-oxidizer mixture, but the process by which a user may derive those simplified parameters for a specific vapor composition has not been adequately defined. Purposes of the work presented here include to examine that process but also to consider whether improvements to the VCE representation within Viper may be possible.

STUDY METHOD

Since Viper::Blast and its user manual do not identify recommended parameters for the combustion characteristics of specific vapors for a deflagration model, it is the task of the user to establish reliable input parameters. Where available, this study uses preexisting, well-established calculation methods to estimate input values. Established tools, such as NASA Chemical Equilibrium with Applications (CEARUN) [6] have been used to obtain the ratio of specific heats and the Chapman-Jouget velocity, which is used as the upper flame speed based upon a detonation event. Lower flame speeds were roughly estimated based upon multiple sources for laminar flame velocities of representative fuel-air mixtures.

Parameter Derivation

The parameters of the Pressure Threshold (Pt), Upper Burn Duration (Bd), and Lower Burn Duration (Bd_min) are proprietary features of the Viper::Blast combustion model that each require estimation based upon the specific characteristics of the vapor that is being modeled. The Upper and Lower Burn Duration relate to the rate at which energy is released into the model by combustion processes and the Pressure Threshold influences the burn duration and flame speed used by the combustion model in a given timestep. There are therefore two characteristics, flame speed and burn duration, which are defined by five interrelated input parameters. Three of these parameters require estimation dependent upon the specific fuel-air mixture under examination. In order to establish robust estimates for the three parameters in question, a convergence study was conducted that used a goal-seeking algorithm and the automation of Viper::Blast CFD modeling. The workflow is described in Figure 1.

Convergence Metrics

Three features of the pressure-time history were considered in order to estimate the quality of the model output: peak overpressure, impulse, and the time of the peak pressure. In addition to these three metrics, which can be objectively calculated, a subjective judgement was made of the model quality based upon the overall shape of the pressure-time history compared to the experimental results. These metrics were examined for the following reasons:

- Peak overpressure is used widely as an indicator of primary blast injury to humans exposed to a blast event. It is also a robust metric that is easily calculated and highly objective in nature.

- Peak impulse is very influential, along with peak overpressure, in estimating the effects of the blast loading on structures. It is another robust metric that is easily calculated and highly objective in nature.

- The timing of the occurrence of the peak overpressure is a broad indicator of the overall model behavior. While not as important for estimation of the impacts of a blast, it is a helpful, objective metric alongside the more subjective judgements made on model quality.

In this study, the parameters were optimized only with respect to peak overpressure and peak impulse, however, optimization with respect to all three parameters simultaneously is currently in progress. The models were considered to have converged when the peak overpressure and peak impulse match the experimental value to within a 5% error margin.

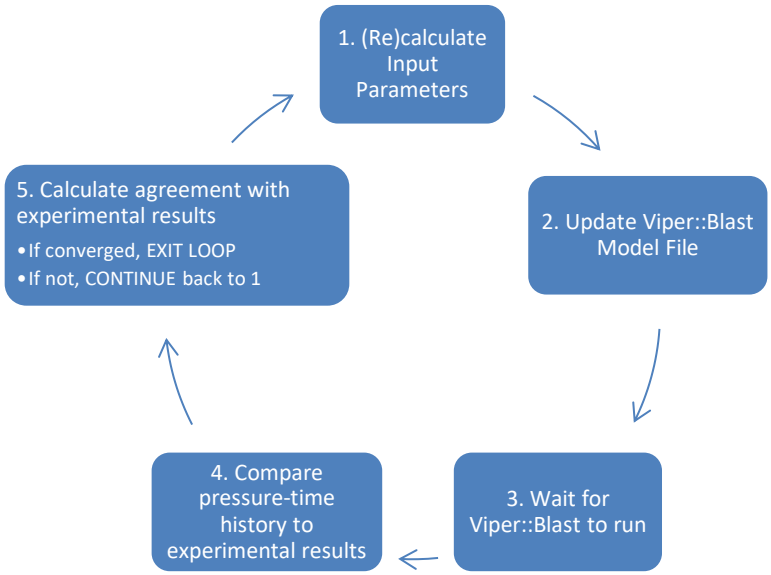

Figure 1 Schematic diagram of automated workflow for establishing model parameters

Preparation of Inputs

Table 1 summarizes the key inputs for running a vapor cloud deflagration model in Viper::Blast. The density, energy, ratio of specific heats, and upper and lower flame speeds have been calculated using established methods such as NASA CEARUN. The Pressure Threshold and burn duration parameters are tailored to each vapor and are the primary subject of examination in this modeling exercise.

Table 1. Summary of Inputs for Vapor Composition in Viper::Blast

Input	Definition
Density	Density for fuel-air mixture
E0	Energy available for combustion
Omega	Ratio of specific heats for unburnt fuel-air mixture
Dcj & Fv_min	Upper and lower flame speeds, respectively
Pt	Pressure Threshold. The flame speed and burn duration will vary continuously between the upper and lower limits based upon a gradual function of pressure, with a maximum value when the model pressure is equal to or above the Pressure threshold, and a minimum value when the model approaches zero.
BD & BD_min	Upper and Lower Burn Duration, respectively

SIMULATION 1 STUDY RESULTS

Wakabayashi et al [3] conducted explosion tests on hydrogen-air mixtures under varying concentrations, geometries, and ignition conditions. This provides data for deflagration across a broad range of flame speeds and overpressures, which is helpful for assessing the capabilities of Viper::Blast.

Initial tests conducted by Wakabayashi et al [3] comprised cylindrical tents of hydrogen air mixtures at lean, rich, and approximately stoichiometric concentrations ranging from 21% to 52.9% of hydrogen by volume. These volumes were detonated by a spherical 0.1kg charge of C4 located at the center of the cylindrical tent as shown in Figure 2. These scenarios were modeled in Viper::Blast with a quarter-symmetry model with the C4 and hydrogen/air explosion sources modeled simultaneously as multiple charges. The detonation model for the C4 charge in Viper::Blast used the Jones-Wilkins-Lee equations of state [7] to model the detonation process. The propagation of this detonation wave out through the hydrogen air mixture ensured that the pressures and flame front speed were approaching the Chapman-Jouget velocity for the mixture, which is consistent with the modeling results.

Modeling of these tests was conducted in Viper::Blast using a relatively coarse mesh density of 50mm and exploiting the quarter-symmetry of the experimental setup in order to reduce model size further. Rather than undertake a convergence study to estimate the value of pressure threshold and burn durations for these experiments, initial modeling was conducted under the assumption that the C4 detonation at the center of the cylinder would result in detonation of the hydrogen cloud, resulting in flame front speeds approaching the Chapman-Jouget velocity for the mixture. Therefore, the Chapman-Jouget velocity was used as a constant burn velocity for the models, and the burn duration was reduced to a correspondingly short duration.

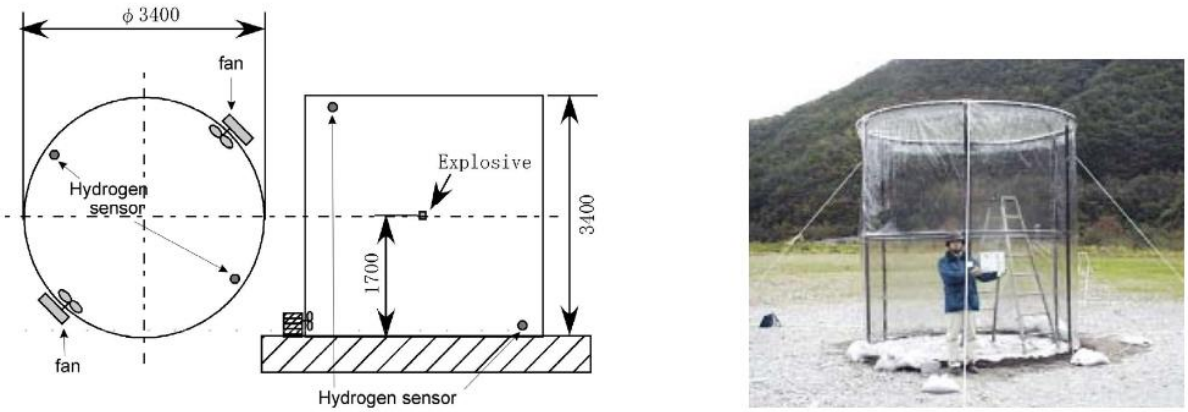

Figure 2. Experimental setup for explosion test with 31m^3 tent from [3]

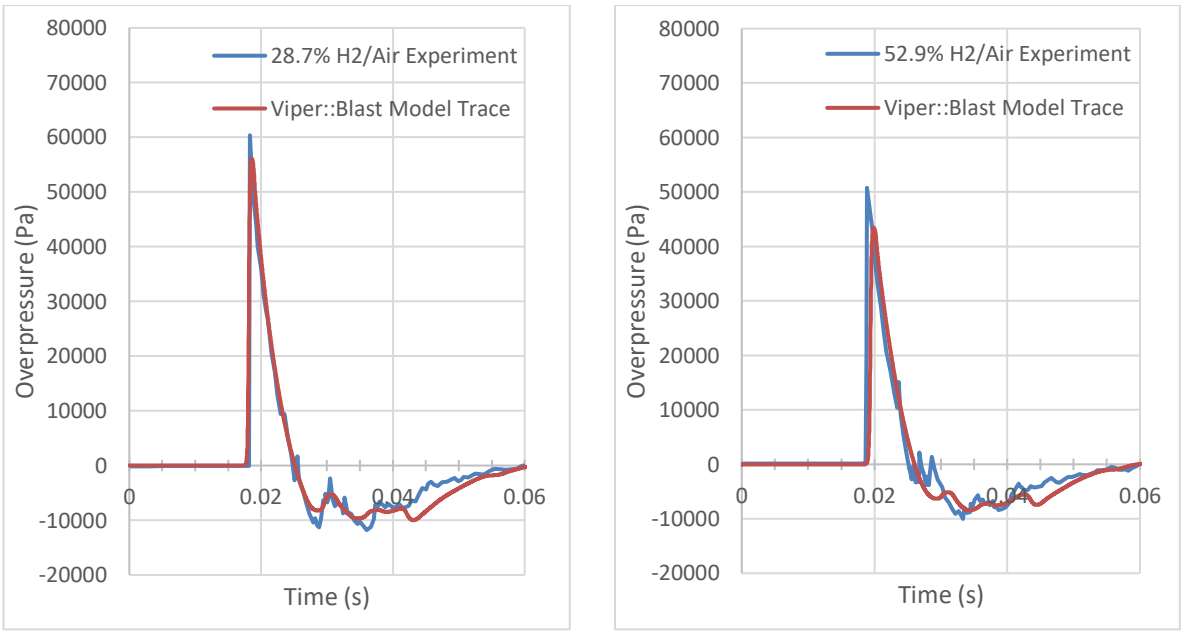

Figure 3. Vapor cloud detonation modelling and experimental results after [3]

Blast overpressures were measured for the referenced pressure-time history traces at 10.6m from the cylinder. Time zero corresponds to the initiation of the vapor cloud using the booster charge. When modeling the two scenarios, one of which is nearly stoichiometric and the other of which is rich, the energy available was assumed to be capped at the value for the stoichiometric mixture. This assumption was made to reflect the fact that the speed of the detonation wave precludes mixing that would allow substantial additional oxygen from outside the tent to burn the excess hydrogen fuel in a way that significantly contributes to the blast wave. Furthermore, the properties of the hydrogen/air mixture, namely the lower density, results in a lower overall mass of mixture present and available for detonation. Based upon the agreement of the modeling with the experimental results, these assumptions appear to be reasonable for this particular modeling method. The specific values for Viper inputs are tabulated below.

Table 2 Summary of inputs for vapor cloud detonation experimental modelling

Parameter	Value – 28.7% H2 / Air Mixture	Value – 52.9% H2 / Air Mixture
Mass (kg)	27.3243	18.9971
Density (kg/m^3)	0.88143	0.61281
E0 (J/kg)	2.95E+06	2.95E+06
Omega	1.34	1.34
Dcj (m/s)	2000	2000
FV_min (m/s)	2000	2000
PT (Pa)	Not applicable	Not applicable
GUB	1.4	1.4
BD (s)	0.001	0.001
BD_min (s)	0.001	0.001

SIMULATION 2 STUDY RESULTS

Wakabayashi et al [3] also conducted explosion tests in a 9.4m^2 rectangular tent with a hydrogen air mixture of 29.5% that were initiated with a spark plug. These deflagrations, with minimal obstruction or congestion, provide a helpful indication of Viper's capabilities at the other extreme of the deflagration

strength spectrum; from strong detonations modeled previously to extremely weak deflagrations of well-mixed vapor. The width of the tent in the experiments was 2.5m, and the height was 1.5m with the blast wave measured at a distance of 4.4m from the center of one side of the cuboid as shown in Figure 3 below. Table 3 summarizes the composition of the vapor cloud input parameters for Viper obtained by the convergence algorithm for the 29.5% hydrogen-air mixture when matching peak pressure. The algorithm had not reached full convergence for impulse, and the model overpredicted the impulse by approximately 20%.

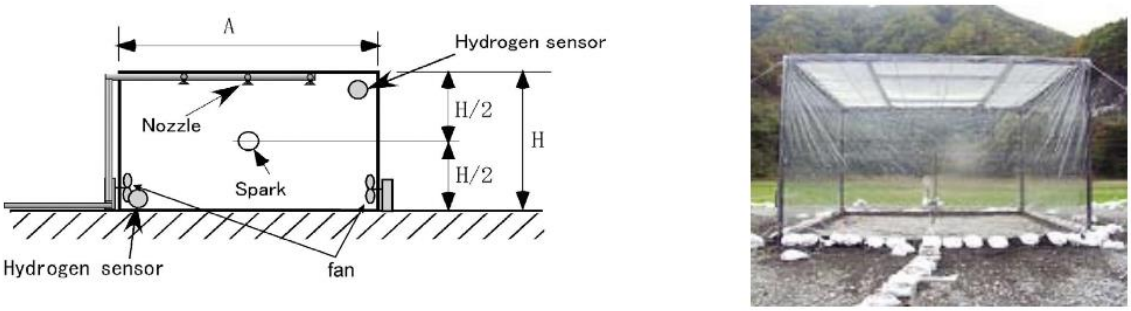

Figure 3. Experimental Set-up for cuboid tent from [3]

Table 3. Summary of inputs for vapor cloud deflagration experimental modelling

Parameter	Value – 29.5% H2 / Air Mixture
Mass (kg)	8.4
Density (kg/m^3)	0.888
E0 (J/kg)	3.11e+06
Omega	1.34
Dcj (m/s)	2021
FV_min (m/s)	6.47
PT (Pa)	1953119
GUB	1.4
BD (s)	0.019131876
BD_min (s)	0.001

The results of the modeling indicate that Viper is displaying broadly the correct behavior when compared to the experimental results albeit with a temporal offset. The peak pressure has converged in this modeling effort to within 5% of the measured peak pressure from experimental pressure-time histories. The impulse is approximately 20% higher than the measured value. While this is in error, it is in the same order-of-magnitude and conservative.

Initial convergence simulations demonstrated very large, sometimes order-of-magnitude variability in model outputs based upon small changes in model input. This was common throughout the analyses and is a reflection of the high sensitivity of VCE intensity to the conditions of the vapor cloud and its immediate environment. This effect is also captured by the analyst's ability to identify a degree of confinement when using the TNO multi-energy method, which has a similarly large impact on calculated impacts of a given VCE. In the convergence analyses within this study, a small example of this variability is given for Simulation 3.

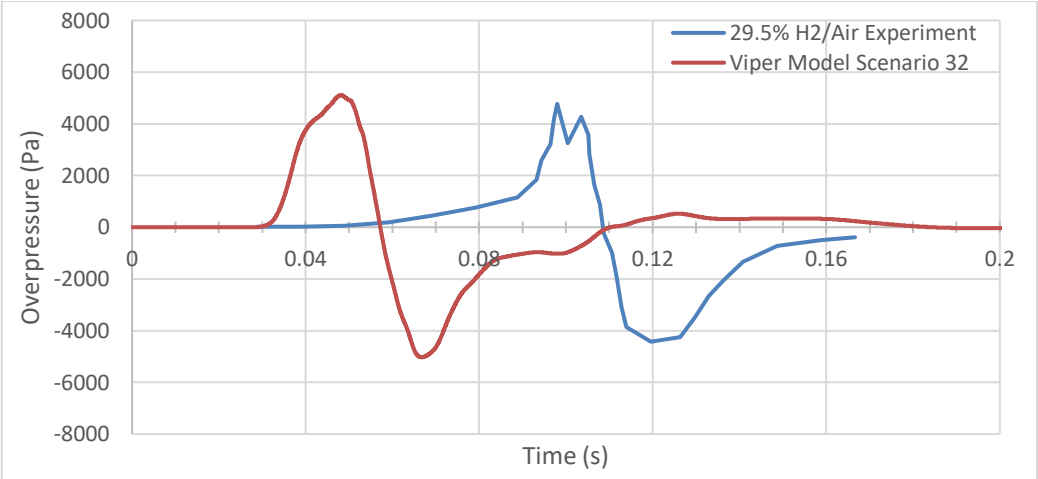

Figure 4. 29.5% Hydrogen/air mixture deflagration comparison of experimental and model results for cuboid experiments after [3]

SIMULATION 3 STUDY RESULTS

Bauwens et al [2] completed several explosion tests in a chamber with the dimensions of 4.6 m x 4.6 m x 3.0 m in two configurations featuring either a vent of 2.7 m^2 in area or 5.4 m^2. The deflagration was initiated either at the center of the volume or at the rear of the volume, on the side opposite the opening indicated with 'I' in Figure 5. In addition to these variations, the concentration of hydrogen also varied in the experiments. Three scenarios from the experimental results were modelled in Viper::Blast, all of which were at nearly 18% concentration of hydrogen in the volume. Two rear-ignition scenarios are presented, and one central ignition scenario is presented, as summarized in Table 3.

Table 3. Summary of models and distinguishing features

Model Setup Index (Simulation 3 Only)	Vent Area (m^2)	H2 / Air Concentration (%)	Ignition Location	Gauge Location
1	5.4	18.2	Rear	P1
2	5.4	18.2	Center	P1
3	2.7	18.6	Rear	P1

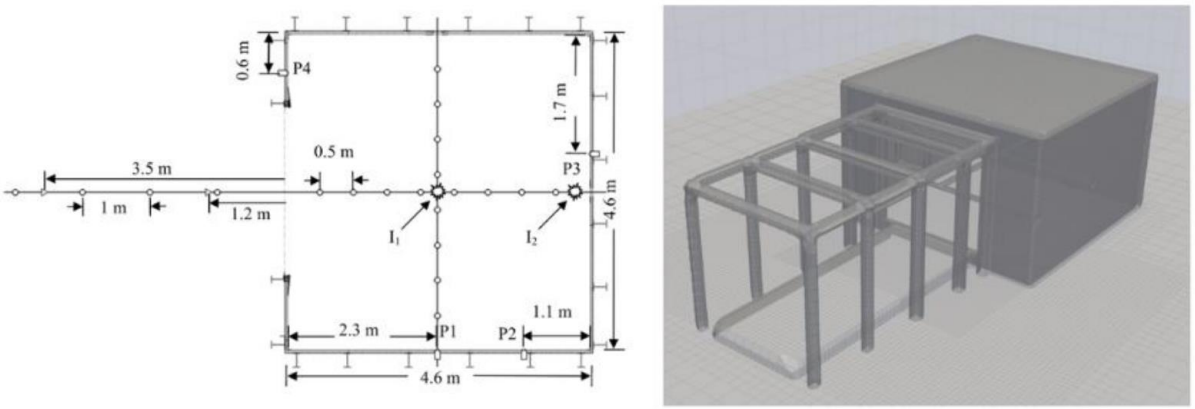

Figure 5. Left) Diagram of experimental set-up Right) CAD used in Viper::Blast from [2]

Table 2 summarizes the composition of inputs calculated for the different hydrogen-air mixtures. An example of the intermediate results in the convergence process is provided in Figure 6, while Figure 7 on the following page displays the results of the Viper modeling overlaid on the experimental pressure-time histories. It should be noted that these are all converged for peak pressure with an error of less than 5% between the model and experimental data, while only Setup 1 and Setup 3 converged for the impulse measurements. Setup 2 has an impulse error of approximately 20%, overestimating the impulse compared to the experimental data.

Table 2. Converged parameters derived for the different model Setups

	Setup 1 – 18.2% H_2	Setup 2 – 18.2% H_2	Setup 3 – 18.6% H_2
Mass (kg)	64.58	64.58	64.29
Density (kg/m^3)	1.02	1.02	1.02
E0 (J/kg)	2.19903e+06	2.19903e+06	2.23727e+06
Omega	1.39	1.39	1.39
Dcj (m/s)	2326	2326	2328
FV_min (m/s)	6.47	6.47	6.47
PT (Pa)	1.70e+07	2.00e+08	2.34375e+07
GUB	1.4	1.4	1.4
BD (s)	0.01329	0.0405	0.01569053
BD_min (s)	0.001	0.001	0.001

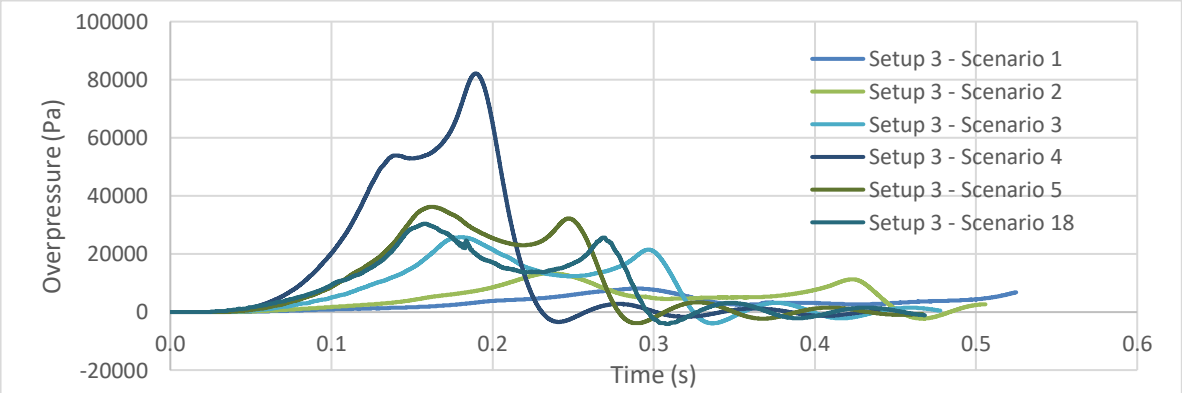

Figure 6. Example of large variability of model outputs based upon small input changes. These results are intermediate stages in the convergence process for Setup 3.

SUMMARY

This study has examined the quality of output from Viper::Blast modeling of hydrogen-air deflagrations under a variety of conditions from detonation through to weak, unconfined deflagration as well as varying degrees of venting. As demonstrated in the Simulation 1 results, for detonation conditions Viper::Blast produces very accurate results, predicting the peak pressure, peak impulse, and overall shape and timing of the blast wave based upon inputs defined by independent calculations. Simulation 2 demonstrated that Viper::Blast is capable of reproducing the broad shape of the blast wave including close estimation of the peak pressure and peak impulse for unconfined, weak deflagration events. The blast pressure-time history for the weak deflagration of Simulation 2, while converged for peak pressure and reasonable for impulse, is shifted to occur much earlier than the experimental observations. This trend is not uncommon in the deflagration events examined within this study.

Simulation 3 demonstrates the sensitivity of the model quality to the input parameters. In Setup 1, the blast wave appears to arrive earlier in the model than in the experimental data, while in Setup 2 the blast wave arrives later than the experimental data. Despite the difference in timing and overall shape of the

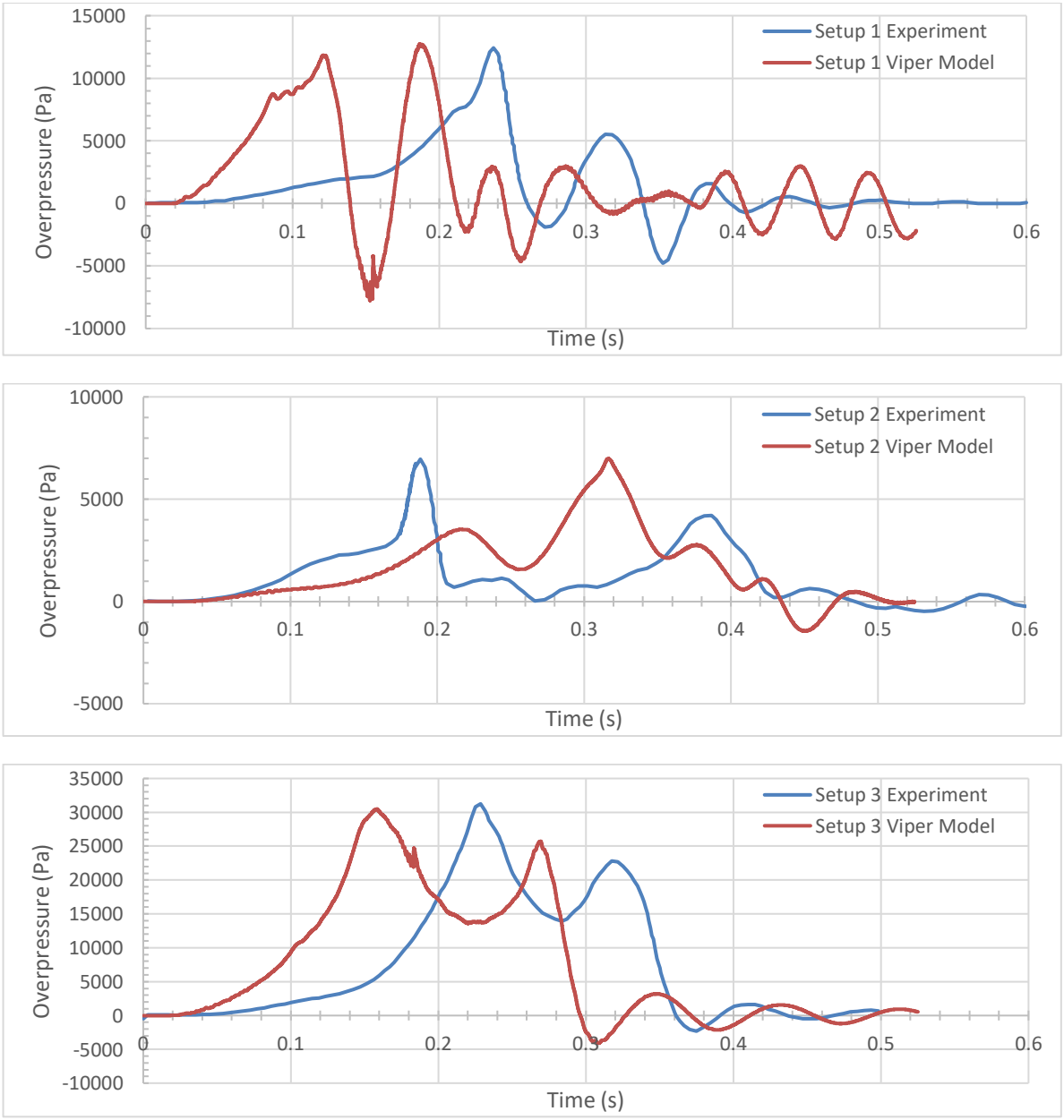

Figure 7. Pressure-time history traces for three setups of the Bauwens et al deflagration experiments overlaid with Viper::Blast converged model results. Each Setup was analyzed for convergence independently of the others.

blast wave, the impulse and peak pressure of Setup 1 and Setup 3 have both converged, reaching a value within 5% of the experimental data. It is interesting to note that Setup 1 and Setup 3, which are both more accurately reproduced in model data, are both rear ignition rather than central ignition. Setup 2 features central ignition, which is potentially reflected in the strongly bifurcated peaks of similar magnitude in the experimental data.

Consistent with the convergence methodology, model parameters were developed for all Simulations that achieve a prediction of peak overpressure within 5% of experimental data. Multiple models have also demonstrated the capability of the convergence algorithm to arrive at input parameters that match the peak impulse within the same 5% margin of error.

CONCLUSIONS AND RECOMMENDATIONS

This study has demonstrated that Viper::Blast is capable of modeling the detonation of hydrogen-air mixtures to a high degree of accuracy and with a high confidence based on externally derived inputs. The study demonstrates that Viper::Blast is capable of modeling deflagration events, however, it also demonstrates the sensitivity of the software to the selection of appropriate inputs, which are not currently standardized or summarized within the software user manual or in other literature. It is likely true that this sensitivity is common within most CFD codes that are used for modeling these types of deflagration events, however the onus is placed more heavily by Viper upon the analyst to make defensible, robust technical selections of input values than for other software.

While this is a challenge for the reproduction of specific experimental data, it is worth noting the high variability of results within a very similar experimental configuration. For example, Simulation 3 features a peak overpressure value that varies by a factor of approximately five, even though it is measured at the same point with almost the same hydrogen concentration across all three Setups. Given this high variability within similar experimental conditions, it is reasonable to consider the benefit that Viper::Blast offers by including features that allow sensitivity analysis and Monte Carlo analysis inherently built-in. By bounding certain parameters, such as flame speed, within prescriptive values or distributions that are subject to scrutiny at the input level, it may be possible to bound the outputs of modeling efforts more confidently than with more deterministic approaches to the same problem.

Further convergence studies, incorporating the time of peak pressure and potentially additional error metrics, are recommended in order to establish robust parameters for a given hydrogen-air mixture model in Viper. Additionally, it is recommended that the values derived in each of the simulations within this study are examined through the simulation of additional scenarios that are independently derived from separate experiments. This use of the converged input parameters in new situations will help to identify the robustness of input parameters or reveal shortcomings that should be addressed.

The speed of Viper::Blast, evidenced in the fact that many of these individual scenarios took approximately 20mins to run, combined with the software's features focused on Monte Carlo analysis make it attractive for further development as a potential tool for quantitative risk assessments of hydrogen deflagration impacts. It is recommended that future work continues to establish robust, generalized modeling parameters that can be deployed confidently not only for detonation simulation, but for a broad range of potential blast events.

REFERENCES

1. Qiao, A and Zhang, S., Advanced CFD modelling on vapor dispersion and vapor cloud explosion, *Journal of Loss Prevention in the Process Industries*, **23,** No.6, 2010, pp.843-848
2. Bauwens, C.R., Chaffee, J. and Dorofeev, S.B., Vented explosion overpressures from combustion of hydrogen and hydrocarbon mixtures, **36**, No. 3, 2011, pp.2329-2336.
3. Wakabayashi, K., Mogi, T., Kim, D., Abe, T., Ishikawa, K., Kuroda, E., Matsumura, T., Nakayama, Y., Horiguchi, S., Oya, M. and Fujiwara, S, A field explosion test of hydrogen-air mixtures, Research Center for Explosion Safety, National Institute of Advanced Industrial Science and Technology (AIST).
4. Bosch, C. and Weterings, R., Methods for the calculation of physical effects – 'Yellow Book', CPR14E, 1997, The Hague: The committee for the Prevention of Disasters
5. Melton, T.A., and Marx, J.D., Estimating flame speeds for use with the BST Blast Curves, *Process Safety Progress*, **28**, No. 1, 2009, pp. 5-10
6. Gordon, S., and McBride, B.J., Computer program for calculation of complex chemical equilibrium compositions and application, Nasa Reference 1311, 2009
7. Urtriew, P. A., and Hayes, B., Parametric Study of the Dynamic JWL-EOS for Detonation Products. Third International Lavrentiev's Readings Conference, Novosibirsk, USSR. Published by Lawrence Livermore Laboratory. March 1990. https://www.osti.gov/servlets/purl/6750269