Numerical simulations of large scale hemispherical and pancake cloud detonation

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Abstract

The present study is motivated by the need to validate modeling approaches for detonation propagation pattern, pressure, velocity and drag impulse for consequence analysis of real scale accidental scenarios. Using the same modeling approach described in Heidari et al. [1, 2], numerical simulations were carried out for large scale hydrogen-air and propane-air detonations in a hemispherical geometry with 300 m^3 volume and a propane-air pancake cloud. The hemispherical hydrogen-air detonation was set up with the same configuration as the full scale tests of Groethe et al. [3]. The predictions were found to be in reasonably good agreement with the measurements for overpressure and impulse. Comparison of the predictions for the propane-air hemispherical and pancake cloud detonation has illustrated some differences that may have implications for accident investigation.

Introduction

Vapour cloud explosion is one of the most serious hazards in the process industries [4]. While in practice, vapour cloud can take different shapes, the most typical example include hemispherical and pancake type clouds. The latter was found to be the case in the recent Buncefield depot explosion on 11 December 2005 resulted in the largest fire in Europe since World War II [5]. While transition from deflagration to detonation is believed to be unlikely in an unconfined vapour cloud, the recent major incidents at Buncefield (Dec. 2005) [5], a fuel depots of the Caribbean Petroleum Corporation near San Juan, Puerto Rico (Oct. 2009) [17] and the Indian Oil Corporation (IOC) in Jaipur, India (Oct. 2009) [18] appeared to bear similar features that indicate the possibility of such transition. This has sparked renewed interests in consequence analysis for vapour cloud detonations.

Most experimental studies for hemispherical cloud detonations were conducted in the 1970s [e.g 6-7], mostly focused on the direct initiation of hemispherical detonation. The widely used multi-energy method [8] is actually based on numerical simulation of a blast wave from a centrally ignited hemispherical cloud with constant velocity flames. Detailed measurements are, however, rare, for the blast wave propagation and impulse values from large cloud detonations. Groethe et al. [3] carried out large-scale deflagration and detonation experiments of hydrogen and air mixtures with the aim to provide fundamental data needed to address accident scenarios and to help in the evaluation of predictive tools.

Sichel and Foster [9] carried out an analysis of planar detonation and found that the pressure behind the detonation front decreases quite rapidly and the positive phase duration near the centre of the cloud is extremely long even though the pressure is relatively low. Fishburn et al. [10] conducted theoretical and experimental studies of the blast effect from a pancake shaped fuel drop-air cloud detonation. The HEMO hydrocode, which is based on the CJ-volume burn method which assumes that the flow is one dimensional and the front of the detonation is a jump discontinuity with infinite reaction rate [11], was used to simulate centrally initiated detonation in a cloud. Heidari et al. [1-2, 12] developed a modelling approach for large scale detonations and applied it to study the pancake cloud configuration in the Fishburn et al. [7] tests.

Previous detonation simulations have been carried in both in 2-D [13] and 3-D [14-15] examining the detailed structures of the detonation front and cells size and pattern. Numerical simulations of detonation using single step reaction by Thomas and Williams [14] and Williams et al. [15] showed that the structure of transverse shocks in 3-D is much more complex than 2-D simulations. Tsuboi et al. [16] used detailed reaction kinetics for 3-D simulations. They found out that there are 2 modes of propagation based on the peak pressure history. In one of the modes the detonation cell size is the same as 2-D simulations and in the other, the cell size is about three quarter of 2-D mode. Due to the relatively large size of the domain and the need for the simulations to be carried out in 3-D, relatively large grid size was used to render the computation affordable. However, the adaptive mesh refinement technique is used to facilitate dynamically tracking the leading wave and refine the grid at the shock front. Even so, the resolution is not sufficient to capture the detailed cell patterns. Part of this study is to establish the reliability of such predictive techniques in capturing detonation propagation pattern, pressure, velocity and drag impulse for consequence analysis in real scale accident scenarios. Although the computationally less demanding hydrocode methods can predict the pressure decay with reasonable accuracy, such approach which assumes one dimensional flow will miss out important characteristics of the fully three –dimensional detonation, and hence will not capture the deviation of detonation pressure and velocity in complex geometries and in the presence of obstacles where the reflected shocks need to be taken into consideration.

Numerical Modelling

The reactive Euler equations are solved using finite volume method. The Van Leer flux limited method which is a total variation diminishing scheme is used for shock capturing. The chemical energy release is taken into account using a single step Arrhenius reaction. The numerical domain around the hemispherical vapour-cloud is extended in all directions to record the resulting blast pressure and impulse following the detonation phase. Euler equations are solved to model gas dynamics. The Euler equations should be solved along with a proper set of chemical reaction equations. These reactions model the consumption and production of each chemical element which is present during the detonation process. By using the production rate of each element and the resulting change in the enthalpy it is possible to calculate the energy source term and the progress rate of the phenomenon. However, a complete set of chemical reactions for a certain fuel contains tens and sometimes hundreds of reactions which are mostly stiff and very difficult to solve and their usage is limited to scales of a few millimeter or centimeter while a properly tuned single step reaction is enough for reproduction of overpressure, velocity and most other properties of detonation waves. A single step Arrhenius reaction is hence used here to model the chemical energy release. The pre-exponential factor and activation energy of the reaction are carefully tuned by running several 1, 2 and

3-D simulations to ensure it delivers accurate results for Chapman-Jouguet (CJ) detonation pressure (15.5 and 18 atm for hydrogen and propane, respectively) and propagation velocity (1980 and 1800 m/s for hydrogen and propane).

Numerical Domain and Mesh refinement

The schematic of the domain and mesh is presented in Figure 1. The diameter of the hemispherical cloud is 10.5 m, giving a volume of 300 m^3. The domain is extended to longer distance specifically at one side to cover a distance of about 20 m away from the ignition centre. The results are recorded at a monitoring point placed 15.61m away from the ignition centre to compare the predictions with the measurements of Groethe et al. [3].

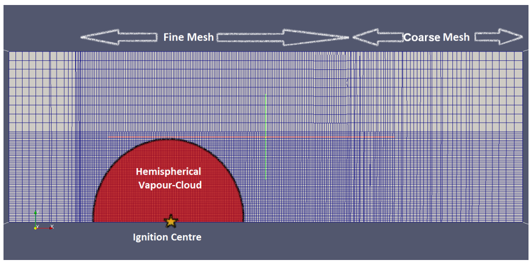

Figure1. The Numerical domain and the Mesh

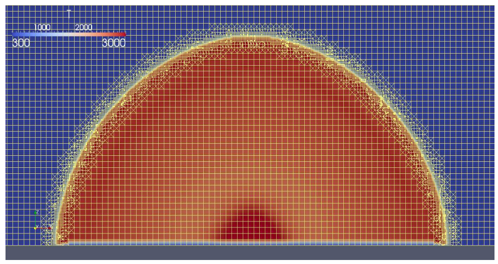

Figure 2. The mesh refinement at the shock front.

The red circle shows the location of the hemispherical cloud and the ignition point is shown by a star. The mesh is also shown in Figure 1. At the vicinity of the cloud, the grid size is around 6 cm and it is coarser further away from the cloud. The total number of cells is about 5.5 million. The adaptive mesh refinement (AMR) technique is adopted. It uses the gradient of pressure as the target variable and tracks the regions with high pressure gradient. The mesh at these areas is refined up to two levels therefore the minimum grid size is about 1.5 cm. Figure 2 shows that the mesh is finer at the wave front and coarser at the other areas which are not subjected to high pressure variations.

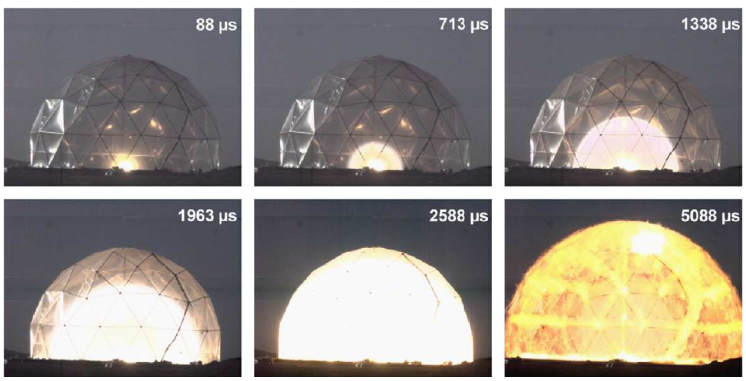

Figure 3. The experimental images from Groethe et al. [3]

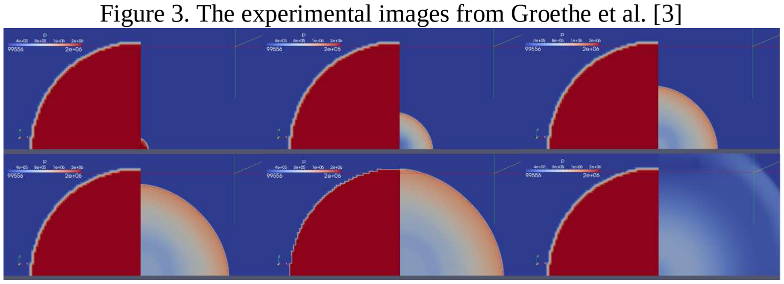

Figure 4. The pressure field and cloud position at the same time intervals as Figure 3.

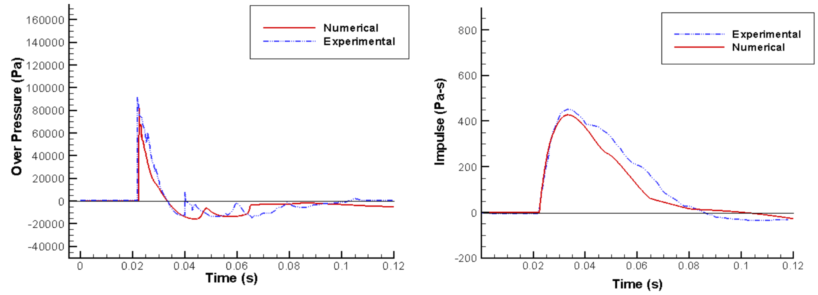

Figure 5. Comparison of the predicted and measured overpressure and impulse for hydrogen-air cloud

Numerical simulations and results

The mixtures are stoichiometric propane-air and hydrogen-air at atmospheric condition. The detonation wave is initiated by using a small region of high pressure and temperature at the ignition point. The initial pressure and temperature of the ignition point are selected to be roughly equal to CJ values for each reactive mixture. The simulation is run for 0.12 second.

Figure 3 shows the images recorded by Groethe et al. [3] illustrating the detonation propagation in experiments. Figure 4 shows the pressure fields at the same time intervals as in Figure 3. The cloud location is shown on the left half of each frame while the right half is the pressure wave.

Figure 5. shows the recorded pressure and impulse at a monitoring point located 15.61 m away from the ignition centre. The timing of wave arrival and the pressure history shows good agreement with the experimental results. However the numerical peak pressure is slightly lower than the measured value.

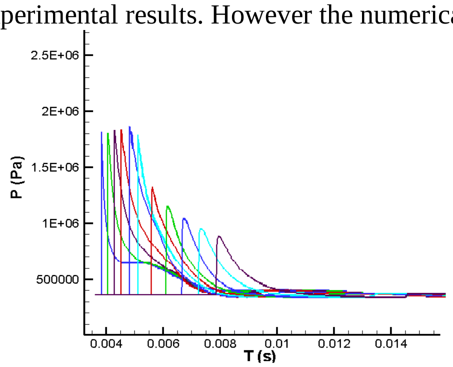

Figure 6. Pressure diagram for propane-air cloud, Pressure drop for hemispherical cloud

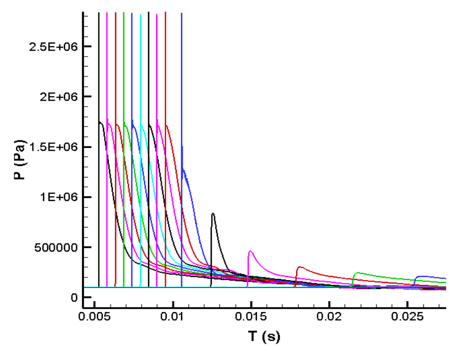

Figure 7. Pressure diagram for propane-air cloud, Pressure drop for pancake cloud [2]

For comparison, numerical simulations were also carried out for a pancake cloud with a diameter of 20 m (Figure 7). The minimum grid resolution is 10 mm. In Figures 6, the peak pressure of the hemispherical simulation is between 17 to 18 atm which is in agreement with CJ pressure, which is also well captured by the pancake cloud simulation. However, the Von-Neumann peak is not recorded in the hemispherical detonation. This is believed to be due to the use of relatively coarser grids in the spherical cloud simulations. However, the duration of Von-Neumann and other high pressure transients is so short that their effect on integral of pressure with time (impulse) is quite limited and “post C-J pressure history with its much larger integrated impulse is a greater threat” [4]. Therefore correct reproduction of the CJ parameters should be sufficient for safety analysis. Figures 6 and 7 show that the pressure drops sharply at the edge of both the spherical and pancake clouds. However, the drop is gentler in the spherical cloud in comparison to that of the pancake cloud. The left images shows roughly 8 atm pressure drop in about 3 ms right after the detonation phase is finished and the blast wave continues to propagate. The right image shows roughly 12 atm pressure drop in about 5 ms.

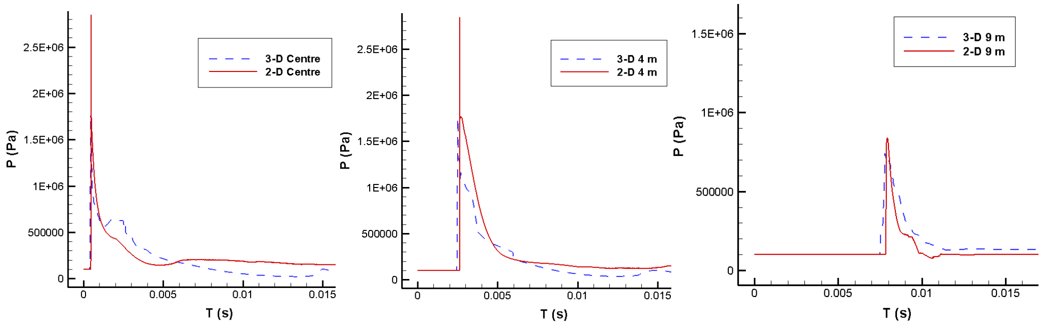

Figure 8. Comparison of pressure vs-time curve (propane-air mixture) at 3 monitoring points between the pancake (solid-red line) and the hemispherical clouds (blue-dashed line)

To provide a better comparison between pancake cloud and hemispherical results 3 monitoring points, one close to the cloud centre, one close to cloud edge and one at about 5 m away from the cloud edge are selected and the results for pressure, velocity and impulse are compared at these 3 points. Figure 8 shows the comparison for the predicted pressure-time curves. The time of shock arrival and the peak CJ pressure are found to be very close in both cases.

Horizontal velocities (U_x) at the monitoring points are compared in Figure 9. The previously predicted long period of high negative velocity shortly after the initial positive velocity phase is also seen here for both the spherical and pancake clouds. This is due to high pressure gradient behind the detonation wave which forces the detonation products to move in the opposite direction of detonation and compensates the pressure gradient behind the leading shock.

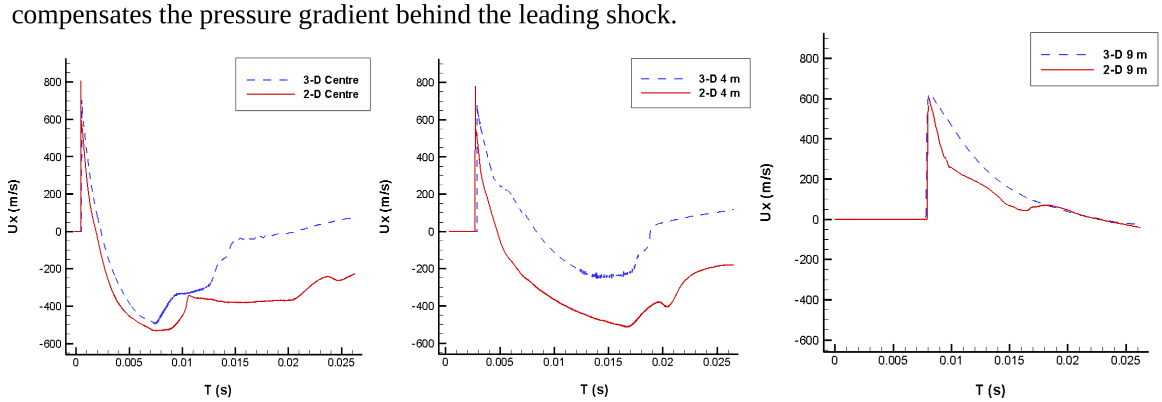

Figure 9. Comparison of the horizontal velocity (propane-air mixture) at 3 monitoring points between the pancake (solid-red line) and the hemispherical clouds (blue-dashed line).

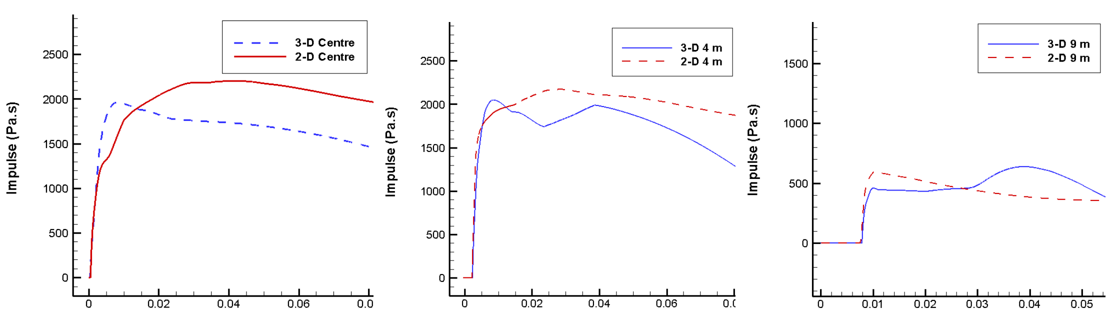

Figure 10. Comparison of pressure impulse (propane-air mixture) at 3 monitoring points between the pancake (solid-red line) and hemispherical clouds (blue-dashed line)

Although the predicted positive velocity phase for the pancake cloud is found to be very similar to that of the spherical cloud, the transition to the negative phase is found to be much sharper and the magnitude of negative velocity is higher in the pancake cloud. This is consistent with the shaper reduction in over pressure at the edge of the pancake could as shown in Figure 7. Figure 10 shows that the predicted pressure impulse of the pancake cloud is similar to that of the hemispherical clouds.

Conclusion

The numerical approach of this work which is based on solution of reactive Euler equations is proven to be reliable for detonation analysis in large scale geometries. The presented results in current work show good agreement with experimental measurements of Groethe et al. [3] for the blast wave resulting from a large scale hemispherical hydrogen detonation. The comparison of the hemispherical and pancake cloud results also shows, in spite of some discrepancies, the predictions are in good agreement. Although the peak Von-Neumann pressure might be missing in some simulations due to large computational grid size, the overall impulse wouldn't be much different because the Von-Neumann spike duration is extremely short. The presented numerical approach can be properly modified by feeding the code with proper thermo-physical properties and reaction mechanism to simulate detonation in different gas mixtures such as the propane-air simulations which are included in this work.

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