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Towards CFD Modelling of Multi-Peak Structure of Liquid Hydrogen Storage Tank “BLEVE”

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Liquid hydrogen (LH2) storage tanks are equipped with pressure relief devices (PRD) to vent hydrogen and avoid the pressure build-up in a tank due to heat transfer from the ambient, including in case of fire. In the event of a PRD failure, the tank structural integrity may be compromised leading to catastrophic rupture of the storage tank releasing the stored energy and producing destructive blast wave, fireball and projectiles. The present paper presents a CFD model to investigate the underlying physical processes of what is called “BLEVE” and assess the blast wave generated by an LH2 storage tank rupture in a fire. The proposed CFD approach advances the previous model (Cirrone et al., 2023) to include the effect of flash evaporation of LH2 during pressure drop after tank rupture and reproduce the multi-peak overpressure structure observed in experiments performed by BMW. Simulation results show that the observed maximum pressure peak is associated with the gaseous phase “explosion”, whereas the series of secondary pressure peaks, smaller in amplitude and of longer duration, are associated with the flash evaporation of the LH2 fraction stored in the tank. Simulations can reproduce the minimum and maximum overpressures measured at 3 m from the storage tank in BMW experiments. The simulated maximum blast wave pressure is seen to increase with the storage pressure and volumetric fraction of the gaseous hydrogen phase in the tank prior to rupture.

* 1. Introduction

Transport, storage and use of liquid hydrogen (LH2) is one of options for scaling up the hydrogen supply infrastructure and applications. LH2 storage requires temperatures as low as 20.3 K at ambient pressure, thus necessitating vacuum insulated vessels. Exchange of heat with the external ambient, e.g. due to a compromised insulation or a fire surrounding the tank, can cause a pressure build-up in the storage tank due to intensive evaporation. For this reason, LH2 storage systems are equipped with pressure relief devices (PRD) aimed at hydrogen venting to avoid the pressure build-up in the tank. In case of structural integrity or PRD failure before the hydrogen is released, a storage tank may burst with consequent blast wave, fireball and projectiles, as occurred in 1975 for a 76 m3 LH2 storage tank (Shen et al., 2024). The tank rupture results in what is called a boiling liquid expanding vapour explosion (BLEVE). This incident worst-case scenario needs to be fully understood and thoroughly investigated to properly assess hazards and associated risks. Expansive experimental research has been performed on hydrocarbons BLEVE (Birk, 1995; Birk et al., 2018), whereas only a few experimental tests have investigated LH2 storage system BLEVE. Experiments performed by BMW (Pehr, 1996) on the “controlled” rupture of LH2 storage systems at pressure in the range 0.20-1.13 MPa(a) revealed a multi-peak structure of the blast wave, as shown in Figure 1. Pehr (1996) associated pressure peaks with the following phenomena: peak 1 - explosive charge initiating the tank bursting; peak 2 - liquid hydrogen evaporation and expansion of gaseous hydrogen; peak 3 - additional pressure event followed by the acceleration of flames and expansion of burnt gas behind the progressing flame front. This interpretation of the pressure dynamics contradicts the experimental observations on the small-scale propane BLEVEs in (Birk et al., 2018) that the primary shock is mainly produced by the vapour space and not by the slower flashing liquid boiling process. To the best of authors’ knowledge, the only other experimental study available in literature on catastrophic rupture of LH2 storage systems was performed by Van Wingerden et al. (2022) on a tank with volume of 1 m3, which failed after 68 min of fire exposure.



Figure 1. Typical pressure transients at 3 m from the tank centre with one (a), two (b) and three (c) distinctive peaks in BMW experiments (Pehr, 1996)

Further research is needed to close knowledge gaps on the underlying mechanisms and physical phenomena behind LH2 storage tank BLEVE. Computational Fluid Dynamics (CFD) can provide a powerful tool to address this knowledge gap and provide a better understanding of pressure dynamics and thermal hazards. Yakush (2016) carried out a 2D numerical study on liquefied propane BLEVEs. Simulation results shown a weaker blast wave in comparison to high explosive detonations and single-phase gas at the same burst pressure. The energy release rate for the BLEVE was concluded to be limited by the time of propagation of the “boiling wave” through the superheated liquid bulk. Hansen and Kjellander (2016) performed 3D RANS simulations on propane and butane BLEVEs, finding a good agreement with experimental measurements of overpressure when the vapour head was considered as the only energy source. Similar conclusions were reached in (Li and Hao, 2020). Ustolin et al. (2022) employed a RANS multiphase model to simulate the BMW test with storage pressure of 1.1 MPa(a), concluding that the maximum overpressure is generated by both vapour and liquid flashing energy sources. The CFD approach did not include combustion modelling and contribution to the blast wave strength. Recently, Cirrone et al. (2023) performed the numerical analysis of these BMW tests and proposed a different interpretation of the multi-peak structure observed in experiments. It was concluded that the maximum blast wave pressure (peak 2 in Figure 1c) is generated by the gaseous phase starting shock enhanced by combustion of hydrogen at the contact surface with air heated by the shock. It was assumed that the BLEVE pressure peak (peak 3) follows the maximum pressure of the blast generated by gaseous phase “explosion” and is of smaller amplitude but of longer duration. The numerical study demonstrated the significant combustion contribution to the blast wave pressure peak. The process of LH2 evaporation was not simulated in previous study (Cirrone et al., 2023), as it was assumed to not be fast enough to contribute to the first maximum overpressure peak generated by the vapour’s release starting shock and associated combustion at the contact surface.

This study presents a CFD model that advances the previous model (Cirrone et al., 2023) to include the effect of flash evaporation of liquid hydrogen and combustion contribution to the blast wave dynamics. The aim is to develop a model able to give insights and simulate the multi-peak structure of overpressure of what is called BLEVE and observed experimentally by (Pehr, 1996).

* 1. Validation experiments

The experiments used for comparison against simulations were carried out by BMW in 1996 (Pehr, 1996). The test campaign investigated the consequences of rupture of LH2 storage tanks of 0.12 m3 volume and burst pressure within the range 0.2-1.5 MPa(a). The mass content in the storage tank varied from 1.8 kg to 5.4 kg, but the exact mass content is not known. An explosive charge surrounding the tank circumference was used to induce a “controlled” burst of the tank. The blast wave overpressure was recorded by a pressure sensor located at 3 m from the storage tank. Table 1 shows the initial pressure in the tank before burst and the maximum blast wave overpressure recorded for each experimental test. The measured overpressure is seen to increase with the storage pressure, with the exceptions of Tests 1 and 7, which larger overpressures were associated by experimentalists to the contribution of the explosive charge and defective tank insulation, respectively.

Table 1: BMW tests - LH2 tank storage pressure and measured blast wave overpressure at 3 m (Pehr, 1996)

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **BMW test No.** | **1** | **2** | **3** | **4** | **5** | **6** | **7** | **8** | **9** |
| Tank storage pressure, MPa(a) | 0.20 | 0.21 | 0.37 | 0.40 | 0.40 | 1.10 | 1.10 | 1.13 | 1.50 |
| Blast overpressure at 3 m, kPa(g) | 16.7 | 3.3 | 6.0 | 7.7 | 11.0 | 13.3 | 47.0 | 15.0 | 16.0 |

* 1. Numerical approach and details

The CFD model for simulating the blast wave overpressure generated by the rupture of the LH2 storage tank employs a Large Eddy Simulations (LES) approach. The multiphase fluid is modelled via the VOF method, described in detail in (Kangwanpongpan et al., 2023). The Lee’s model is used for simulation of phase transition between hydrogen vapour and liquid (Lee, 1980) and employs evaporation and condensation coefficients equal to 10, as per the research in (Ma et al., 2022) on BLEVE of LPG storage tanks. A combined Finite Rate/Eddy Dissipation model is used to simulate hydrogen reaction at the contact surface, as this was seen to significantly contribute to the generated maximum blast wave overpressure in (Cirrone et al., 2023). The exact amount of hydrogen mass in the storage tank for each BMW test is not known. The only available information is that the mass for the entire set of experimental tests varied in the range 1.8-5.4 kg. Numerical experiments in this study were performed for the two extremes of the mass range for the six storage pressures within 0.2-1.13 MPa(a) in Table 1. For the cases with burst pressure 1.10 and 1.13 MPa(a) the minimum storable mass is 2.0 and 2.1 kg respectively. Simulations of each BMW test with the two mass limits would correspond, respectively, to the largest or smallest fraction of gaseous hydrogen in the storage tank and, apparently, to the maximum and minimum blast wave overpressure respectively. The multiphase fluid is composed by a primary phase for the hydrogen-air-water vapour gaseous mixture and a secondary phase for liquid hydrogen. The primary phase was modelled via the ideal gas equation of state (EoS) upon scaling the real tank ullage space before burst to conserve the internal energy of the real gas. The secondary phase is set as liquid hydrogen with properties defined according to the NIST database (2024). The computational domain is hemispherical with 60 m diameter and cylindrical storage tank located at its centre. The minimum control volume (CV) size is set as 2 cm in the storage tank zone and grows with increasing distance from the tank. The total number of CVs varies from 400k to 700k depending on the simulated test. The external boundaries are set as pressure outlets with gauge pressure equal to zero. The hydrogen storage tank region is initialised with pressure according to that in the simulated test and corresponding saturation temperature. Depending on the specific filling ratio, the storage tank is initialized with the top tank fully occupied by the compressed gaseous hydrogen (CGH2), and the bottom portion filled with LH2. The tank outer layer was initialized with higher temperature and presence of water vapour to imitate the explosive charge and trigger combustion. The domain is initialised with a temperature equal to atmospheric 288 K, pressure 101,325 Pa and normal air composition. Calculations employ a constant Courant-Friedrichs-Lewy (CFL) number equal to 0.1, as found to provide convergence by CFL (Cirrone et al., 2023).

* 1. Results and discussion

Simulation results are used to get insights into the physical processes responsible for the generated blast wave pressure dynamics after an LH2 storage tank rupture in a fire. Figure 2 shows the simulated overpressure dynamics at 3 m perpendicularly to the storage tank axis for the two limiting cases with minimum possible stored mass equal to 2.0 kg, corresponding to a full content of CGH2 phase in the tank, and maximum stored total mass of 5.4 kg for the numerical test burst pressure of 1.1 MPa(a). It can be observed that simulated overpressure dynamics for the limiting case with only gaseous content (mass=2.0 kg) shows only one peak followed by a negative pressure phase, closely resembling the experimental pattern observed in Figure 1a. On the other hand, the overpressure dynamics for the numerical test with maximum total mass of 5.4 kg presents a first pressure peak followed by a series of secondary pressure peaks smaller in the amplitude and with a comparable or larger impulse. The first peak is associated with the CGH2 shock with contribution of combustion and the secondary peaks are associated with LH2 evaporation during flash boiling in the tank due to fast pressure drop. Simulated overpressure dynamics resembles the experimental overpressure pattern presented in Figure 1b and 1c. It is estimated that the evaporated LH2 mass is about 7.4% at 8 ms and 23% at 30 ms. Hydrogen mass imbalance in simulations was within -1.5% up to 30 ms of simulated time and the required computational time on a 64-cores workstation was approximately 3.5 days. Figure 2 compares simulation results to the range of overpressures (from minimum to maximum) measured in the experiments with 1.1 MPa(a) burst pressure (with unknown exact hydrogen storage mass). The minimum experimental overpressure is well reproduced by the simulation with largest LH2 filling (mass=5.4 kg). The maximum experimental overpressure is about 36% lower than simulation results for a full CGH2 content (mass=2 kg), suggesting that the experimental test might have been performed for a higher LH2 filling, and thus larger mass of stored hydrogen.



Figure 2. Simulated overpressure dynamics at 3 m perpendicular to the tank axis for tests with maximum GH2 filling (m=2.0 kg) and LH2 filling (m=5.4 kg) at burst pressure of 1.1 MPa(a) against BMW experimental data

Figure3 provides insights into the blast wave propagation and combustion dynamics through the contours of pressure, temperature, GH2 mole fraction in the gaseous GH2-air mixture, LH2 phase volume fraction, and phase mass transfer rate in the time range 0-8 ms for the test with total mass of 5.4 kg and burst pressure of 1.1 MPa(a). The shock wave originated from the CGH2 phase is seen to move away from the tank zone at about 2 ms, reflect off the ground within 4 ms and catch up with the primary wave at about 6 ms. This primary blast wave front is responsible for the first pressure peak in Figure 2. The combustion development at the contact surface between hydrogen and heated by the shock wave is shown by the temperature contours in Figure 3. Combustion contributes to the blast wave and is estimated that 0.2% of the initial total mass has burnt by the time of 8 ms. The contours of the LH2 volume and GH2 mole fractions show that the volume occupied by the flashing mixture expands in time as well as the zone occupied by GH2. The flash boiling is triggered by the rapid decrease of pressure in the storage tank, as shown by the increase of phase mass transfer rate in the entire LH2 phase region with enhancement towards the tank sides due to the presence of the surrounding “fire”.



Figure 3. Simulation results on parameters distributions in time on the plane perpendicular to storage tank axis for the numerical test with burst pressure of 1.1 MPa(a) and m=5.4 kg: (frame scale dimensions: 9.6x5.0 m)

* + 1. Advancements from the single-phase to multiphase CFD model

The proposed multiphase CFD model with phase transition advances the previous single-phase model (Cirrone et al., 2023) to include the effect of flash evaporation of LH2 during pressure drop after tank rupture on the blast wave pressure dynamics. The novelty of the present CFD approach in comparison to the multiphase model in (Ustolin et al., 2022) lies into the inclusion of combustion contribution to the blast wave dynamics. Simulation results on overpressure dynamics for the two models developed by the authors are compared in Figure 4 for the numerical tests with minimum and maximum burst pressures of 0.2 MPa(a) of 1.1 MPa(a). The maximum overpressure peak generated by the CGH2 phase is closely reproduced by both the “CFD, Single-phase Model” and “CFD, Multiphase Model”. For “CFD, Single-phase Model” this peak is followed by a significant negative pressure phase due to the absence of flashing evaporation of LH2. The maximum overpressure peak simulated by the “CFD, Multi-phase Model” is followed by either a less pronounced or absent negative pressure phase, and then by a series of secondary pressure peaks generated by the slower process of flash boiling of LH2, reproducing the experimentally observed multi-peak structure of LH2 BLEVEs.



(a) (b)

Figure 4. Simulated overpressure dynamics by single-phase and multiphase models at 3 m perpendicularly to the tank axis for the numerical tests with mass of 5.4 kg and burst pressures: a) 0.2 MPa(a), b) 1.1 MPa(a)

* + 1. Maximum overpressure for all BMW tests: simulations versus experiment

Simulations were carried out for all the BMW tests with storage pressure 0.2 to 1.1 MPa(a). The stored hydrogen mass in the tank is not known, therefore simulations were performed for the limiting cases corresponding to the possible minimum and maximum quantity of CGH2 phase in the tank, and corresponding maximum and minimum calculated overpressures are shown as lines with bars in Figure 5. It can be observed that simulations’ results considering the minimum mass of CGH2 are in excellent agreement with experimentally measured overpressure. Simulation results may be conservative as the mechanical energy lost with the tank fragmentation and ground catering is neglected. Maximum experimental measurement for the test with burst pressure of 1.1 MPa(a) is well within the simulated pressure range, indicating that it could be characterised by an amount of LH2 larger than the minimum employed in simulations. The numerical underestimation of maximum experimental overpressure for test with Ps=0.2 MPa(a) could be associated with contribution of explosion of the cutting charge, not considered in simulations. The simulated maximum blast wave pressure is observed to increase with the storage pressure and CGH2 phase volumetric fraction in the tank prior to rupture, potentially leading to greater hazard distances by overpressure thresholds. It should be remarked that the present research is limited to the analysis of the blast wave. The analysis of a fireball development and associated thermal hazards, which instead are expected to increase with larger LH2 phase fraction and H2 stored mass, is beyond the scope of this study. Future research should assess and compare both thermal and pressure hazards to conclude on accurate scientifically-based assessment of hazard distances from LH2 storage infrastructure.



Figure 5. Simulated minimum and maximum overpressure at 3 m perpendicularly to the tank axis versus experimentally measured in Tests No. 1-8 (Pehr, 1996)

* 1. Conclusions

This paper proposes a comprehensive three-dimensional multiphase CFD model capable of simulating the multi-peak structure of the blast wave observed in the LH2 BLEVE experiments. The numerical experiments allow to conclude that the maximum blast wave pressure is generated by the gaseous hydrogen shock enhanced by combustion reaction of hydrogen at the contact surface with air heated by this primary shock. The slower process of LH2 flash boiling produces a series of secondary pressure peaks with smaller amplitude but comparative or larger impulse. The model accurately simulated the pressure dynamics beyond the shock overpressure peak generated by the vapour phase, resembling the experimental observations (Pehr, 1996). Future research is planned to assess thermal hazards from the fireball to compare them with pressure hazards for an accurate scientifically-based assessment of hazard distances from LH2 storage infrastructure.

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