CFD STUDY OF THE UNIGNITED AND IGNITED HYDROGEN RELEASES FROM TRPD UNDER A FUEL CELL CAR

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ABSTRACT

This paper describes a CFD study of a scenario involving the vertical downward release of hydrogen from a thermally-activated pressure relief device (TPRD) under a fuel cell car. The volumetric source model is applied to simulate hydrogen release dynamics during the tank blowdown process. Simulations are conducted for both unignited and ignited releases from onboard storage at 35 MPa and 70 MPa with TPRD orifice 4.2 mm. Results show that after TPRD opening the hazards associated with the release of hydrogen lasts less than two minutes, and the most hazardous timeframe occurs within ten seconds of the initiation of the release. The deterministic separation distances for unignited releases are longer than those for ignited releases, indicating that the separation distances are dominated by delayed ignition events rather than immediate ignition events. The deterministic separation distances for both unignited and ignited hydrogen downward releases under the car, are significantly shorter than those of free jets. To ensure the safety of people a deterministic separation distance of at least 10 m for 35 MPa releases is required. This distance should be increased to 12 m for the 70 MPa release case. To ensure that the concentration of hydrogen is always less than 4% at the location of the air intake of buildings, the deterministic separation distance should be at least 11 m for 35 MPa releases and 13 m for 70 MPa releases.

1.0 INTRODUCTION

The goal of a hydrogen economy has been pursued for decades. One of the most promising fields is the application of hydrogen fuel cells, especially fuel cell vehicles (FCVs). Lux Research Report forecasts that the FCVs market will reach a total of $2 billion by 2030, which is approximate 2/3 of the total fuel cell market, as shown in figure 1 [1]. In Europe, the number of FCVs is expected to reach 500,000 by 2020 [2]. This will inevitably introduce unfamiliar hazards that are different from those of conventional vehicles.

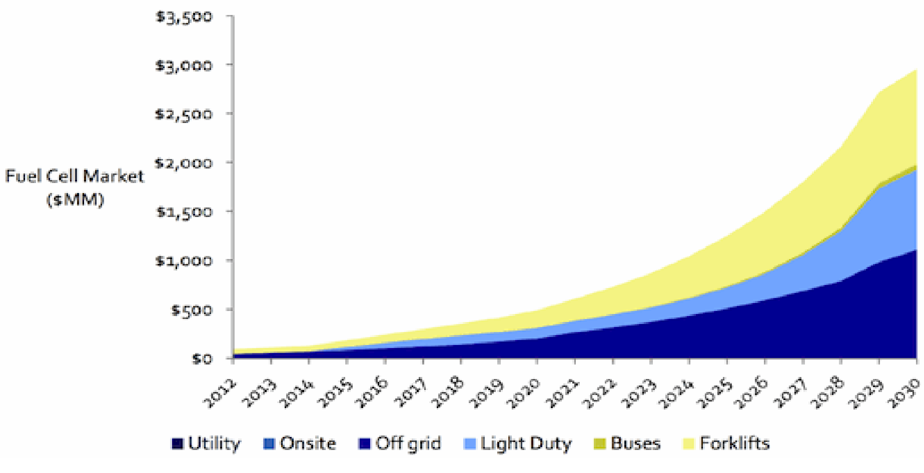

Figure1. Outlook of hydrogen fuel cell market [1]

Compared to conventional petrol vehicles hydrogen fuel cell vehicles usually require high storage pressures. In hydrogen fuel cell vehicles hydrogen is usually stored onboard at high pressures of up to 35 MPa or 70 MPa. Therefore such hydrogen storage tanks are commonly equipped with pressure relief devices to prevent tank explosion. Pressure relief devices significantly reduce the risk of tank catastrophic rupture by venting the high pressure hydrogen outside. However the released hydrogen could raise additional safety concerns. Compared with hydrocarbon fuel, hydrogen has a wider flammability range, lower ignition energy and higher burning rate. These unique properties of hydrogen bring new challenges to both the general public and first responders.

2.0 SCENARIO DESCRIPTIONS

2.1 Typical Scenarios and Potential Hazards

A typical accident scenario can be considered as a representative example of an accident with high credibility, i.e. a scenario that is known to occur in real world conditions. The release of hydrogen from a thermally activated pressure release device (TPRD) can be considered as a typical accident scenario as the release of hydrogen from the TPRD is an inherent safety feature of onboard storage systems. If the temperature reaches more than 110 ^{o}C, the TPRD will be activated and hydrogen will be released. TPRDs are commonly located under the hydrogen fuel cell vehicle, orientated vertically downwards and therefore the release hydrogen will impinge on the ground. This typical scenario is studied in this paper.

The hazards associated with this scenario depend on the time of ignition. If the scenario of immediate ignition is considered, the impinging hydrogen jet flame (under the car) will spread outwards and create a high temperature fire environment which is hazardous to people and property. Without immediate ignition, the released hydrogen will form a flammable cloud that has the potential to result in flash fire. For such a delayed ignition event, occasionally the flammable cloud could result in an explosion if it is located in a confined space. This explosion event will not be studied in this paper. This present study will focus on the deterministic separation distances for releases in the open atmosphere.

An ignited release from a TPRD is mostly likely to occur in an event of a car fire, independent of whether the car is parked or driven on a road. A car fire can be caused by a variety of reasons such as a fire following a road collision accident, a battery fire or autoignition due to strong sunlight exposure, etc. An unignited hydrogen release from a TPRD may occur in extreme cases such as a faulty TPRD following a severe car crash or if the hydrogen tank is affected by a fire located at the opposite side of the tank to the TPRD location, etc.

2.2 Car Parameters and Environmental Conditions

The car is a typical saloon with dimensions of 5.16 m long, 1.83 m width and 1.47 m height, as shown in Figure 2. The car is assumed to be parked in the open and the onboard hydrogen tank is assumed to be at full capacity, in order to investigate the worst case credible scenario. Hydrogen storage parameters are adopted from the specification of the Honda FCX [3]. The onboard hydrogen tank is at pressure of 35 MPa with a volume of 171 litres. The TPRD is assumed to be located near the rear wheel under the vehicle as shown in Figure 2, and its orifice diameter is 4.2 mm, according to Tamura [4]. The ambient pressure and temperature are assumed to be at 1 atm and 20 °C. There is no wind in the environment.

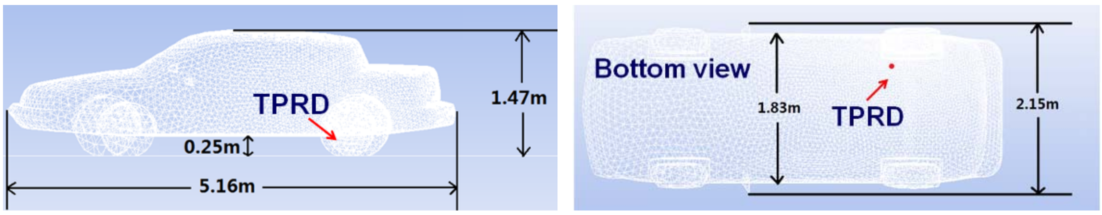

Figure 2. Geometry of the sedan and location of TPRD

2.3 Harm Criteria

The harm criteria for the determination of separation distances are listed in Table 1. For unignited releases, the 4% hydrogen mole concentration level is commonly acknowledged as the lower flammability limit in the literature and has been widely used as the harm criteria for the determination of separation distances to people. This is a relatively conservative harm criterion in our case (TPRD downward releases) as 4% hydrogen concentration can be ignited only for upward releases but not for downward releases in which the lower flammability limit is approximately 8.5% [5]. Therefore in this paper, 4% hydrogen concentration is applied as the harm criterion to the general public for the reason of conservatism, while 8% is applied as the harm criterion to first responders without thermal protective clothing, such as policemen and emergency medical technicians. For the firefighters with bunker gear, the hydrogen flammable cloud in the open will not harm them as their bunker gear will protect them from being injured by the potential hydrogen flash fire. In addition to the harm criteria to people, 4% hydrogen concentration can also be taken as the harm criterion to the air intake of buildings. If the flammable envelope of 4% hydrogen concentration reaches the location of an air intake into high-rise buildings, then the consequences for both occupants and the structure of the building could be catastrophic [5].

For ignited releases, three temperature limits are adopted as harm criteria for different vulnerable targets. For the general public, a temperature of 70 °C is taken as an acceptance criterion for no harm. For the first responders without thermal protective clothing, a temperature of 115 °C is assumed as the pain limit acceptance criteria for individuals who are able to promptly evacuate from such temperatures. For first responders with thermal protective clothing, it is conservatively assumed that they should not work in an environment where the temperature is higher than 260 °C, as the bunker gear is designed not to ignite, melt, drip, or separate when exposed to such temperatures for five minutes[6].

It should be noted that the harm effects near the ground are defined as adverse effects under a height of two metres above the ground.

Table 1. Harm criteria for hydrogen releases from TPRD under a car.

<table>
<tr><th colspan="2">Vulnerable targets</th><th>Unignited releases</th><th>Ignited releases</th></tr>
<tr><td colspan="2">General public</td><td>4% v/v</td><td>70 °C</td></tr>
<tr><td colspan="2">Air intake of buildings</td><td>4% v/v</td><td>-</td></tr>
<tr><td rowspan="2">First responders (firefighters, police, emergency medical technicians, etc.)</td><td>Without bunker gear</td><td>8% v/v</td><td>115 °C</td></tr>
<tr><td>With bunker gear</td><td>-</td><td>260 °C</td></tr>
</table>

3.0 MODELLING

3.1 Notional Nozzle Model and Blown Down Process

Hydrogen releases from high pressures of either 35 MPa or 70 MPa are under-expanded jets, where the pressure at the exit of the nozzle is above atmospheric pressure. Calculation of this expansion with complex shock structure from the nozzle exit to the Mach disk requires intensive computation. In many practical situations, it is not necessary to fully resolve these shock structures if the main concern is not focused on the near field around the nozzle. For the determination of separation distance for hydrogen releases, the far field parameters are the major concern. Therefore, it is convenient for our case to substitute the under-expanded jet with an expanded jet by applying the nozzle model that was introduced by Molkov et al. [7].

In real world conditions, a hydrogen release from a high pressure tank is not a steady release but a blowdown process with pressure decay in the reservoir until the tank is empty. The notional nozzle model mentioned above can be applied to simulate pressure dynamics in the hydrogen storage tank during an underexpanded jet release. The experimental validation proves that the adiabatic calculation gives a better prediction than that from the isothermal calculation undertaken in [7]. Therefore for the particular cases investigated in this present study, the adiabatic blowdown process is applied in our modelling procedure to describe the blowdown of the tank. The obtained results are shown in Figure 3 below. For the release from the 4.2 mm orifice, 171 L tank at 35 MPa, the total blowdown time is less than 110 seconds, and the transition from an underexpanded jet to an expanded jet occurs at 85 s. For the release from the 4.2 mm orifice, at 70 MPa with identical mass, the total blowdown time is less than 75 seconds, with the transition from an underexpanded jet to an expanded jet occurring at about 58s.

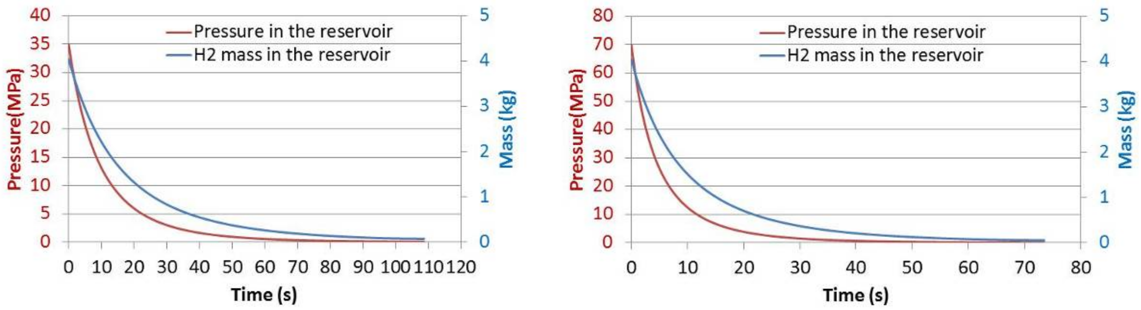

Figure 3. Adiabatic blowdown of 4.2mm releases from 35 MPa (left) and 70 MPa (right) tanks

3.2 Volumetric Source Model

During tank blowdown, the notional nozzle diameter will decrease with the decay of pressure in the reservoir. It would be difficult to change the effective diameter during a CFD transient calculation. Instead, hydrogen mass inflow was treated as volumetric sources of hydrogen mass, momentum, and energy in order to avoid having to constantly change the effective diameter with time during the simulation. Using this approach the release volume can be kept constant, but the volumetric sources change to reflect changing parameters at the notional nozzle. This approach was validated against HSL experimental data [8] of hydrogen releases through a 3 mm diameter orifice. The results reveal that if the volumetric source size is smaller than 4 times of the notional nozzle diameter then concentration decay in under-expanded jets is reproduced accurately, as shown in Figure 4 below.

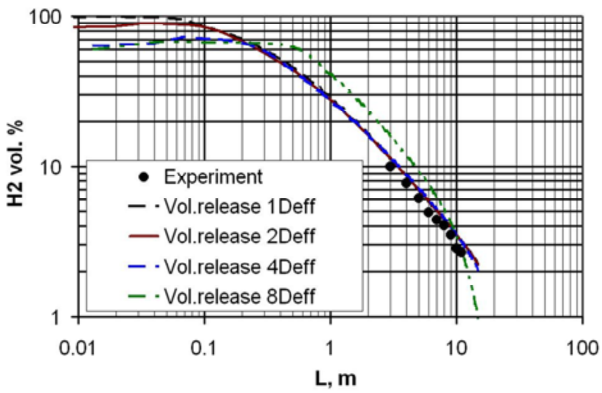

Figure 4. Validation of volumetric source model for free hydrogen jets [7]

3.3 Other CFD Models

Considering the viscous model implemented, the shear-stress transport (SST) k-ω model was applied in the turbulence calculations performed, as this model is known to allow for a more accurate near wall treatment than k-ε model. The SST k-ω model was developed by Menter [9] to effectively blend the robust and accurate formulation of the k-ω model in the near-wall region with the freestream independence of the k-ε model in the far field. For combustion modelling the eddy-dissipation model is applied. It is a turbulence-chemistry interaction model based on the work of Magnussen and Hjertager [10]. In this model, reaction rates are assumed to be controlled by the turbulence, so expensive Arrhenius chemical kinetic calculations can be avoided. The model is computationally cheap and effective for one or two step heat-release mechanisms.

3.4 Mesh, Calculation Domain and Boundary conditions

Although the tetrahedral grid is good for meshing an irregular geometry such as the complex shape of a car, from the perspective of the gradient calculations to be performed, a tetrahedral mesh would be not suitable for such a jet impingement scenario comprising large velocity gradients. A major disadvantage of tetrahedral meshes is that tetrahedral control volumes have only four neighbours, so computing gradients can be problematic because neighbouring nodes may all lie in nearly one plane, making it impossible to evaluate the gradient in the direction normal to that plane. As a result, the calculation will have “preferential” diffusion directions. To overcome this problem, a polyhedra grid is applied in the simulation. A polyhedra grid can overcome this disadvantage because they have many neighbours, so gradients can be much better approximated.

The calculation domain is a rectangular cuboid with dimensions of L x W x H = 50 x 40 x 30 m. As for boundary conditions, the ground and the car surface are set as wall boundaries and other boundaries are set as pressure outlets. Simulations are carried out using ANSYS Fluent 14.5.

4.0 RESULTS AND DISCUSSIONS

4.1 Deterministic Separation Distances for Unignited Releases

It can be seen from Figure 5 that for the first responder without thermal protective clothing, the longest separation distance is about 8.8 m and 10.5 m, for 35 MPa and 70 MPa releases respectively. The separation distance for the 70 MPa release increases nearly 20% compared with that of 35 MPa release. For both cases the largest 8% hydrogen envelopes near the ground occur at about 5.5 seconds after the opening of the TPRD. Afterwards, the envelopes will shrink and the separation distances will decrease.

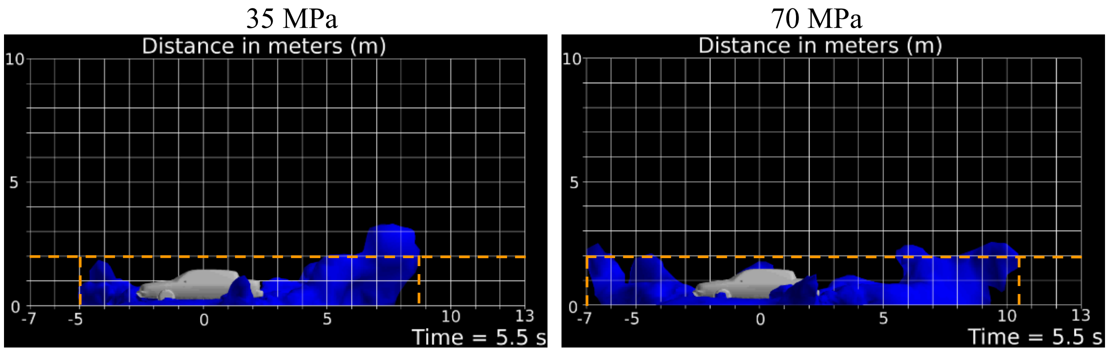

Figure 5. 8% v/v largest hydrogen envelope (extents cut off at 2 m height)

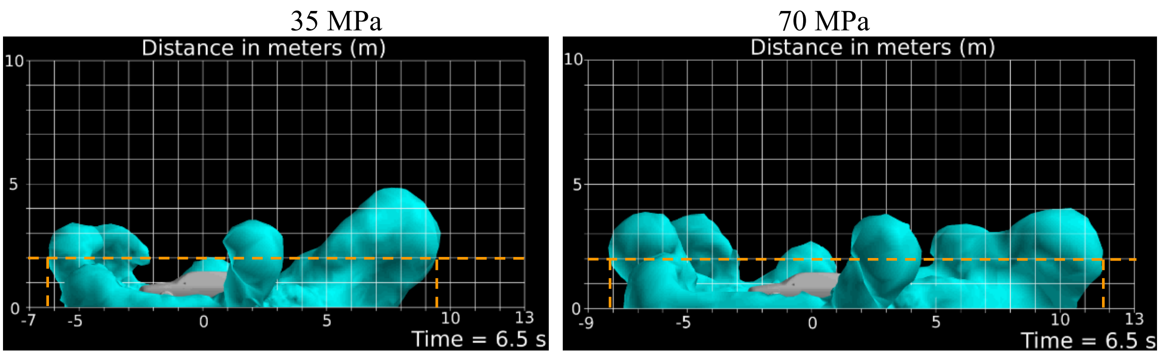

Figure 6. 4% v/v largest hydrogen envelope (extents cut off at 2m height)

It can be seen from Figure 6 that for the general public near the ground, the longest separation distance is about 9.4 m and 11.8 m, for 35 MPa and 70 MPa releases respectively. The separation distance for the 70 MPa release increases nearly 26% compared with that of the 35 MPa release case. For both cases the largest 8% hydrogen envelopes near the ground occurs at about 6.5 seconds after the opening of the TPRD. Afterwards, the envelopes will shrink and the separation distances will decrease.

Figure 6 only gives the largest envelope of 4% hydrogen below 2 m height. If we measure the largest flammable envelope for the total domain, as shown in Figure 7, the separation distances for the surroundings will be obtained.

It can be seen from Figure 7 that for the air intake of buildings, the longest separation distance is about 10.7 m and 12.3 m, for 35 MPa and 70 MPa releases respectively. The separation distance for the 70 MPa release increases nearly 15% compared with that of the 35 MPa release. For both cases the largest 4% hydrogen envelopes occurs at about 9.5 seconds after the opening of the TPRD. Afterwards, the envelopes will shrink and the separation distances will decrease. If the separation distances from these impinged jets are compared with the separation distances with those of free jets, the results show a significant reduction of more than 60% and 65%, for the 35 MPa and 70 MPa releases respectively, as shown in Figure 7.

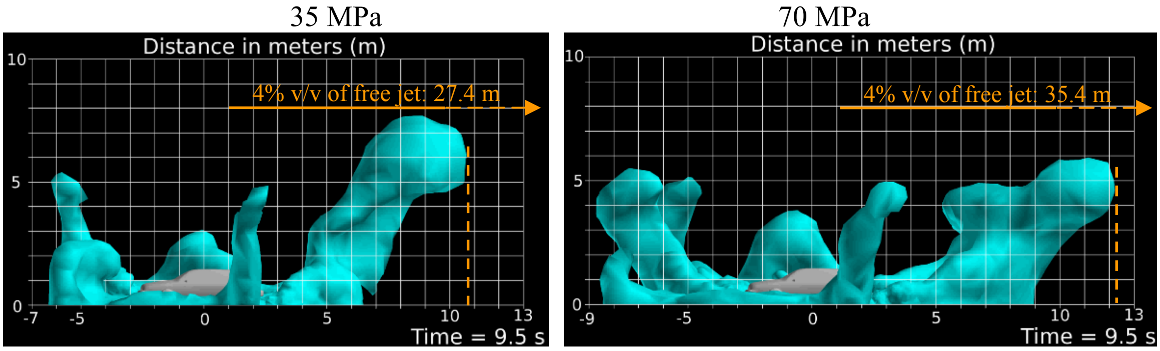

Figure 7. 4% v/v largest hydrogen envelope extents

4.2 Deterministic Separation Distances for Ignited Releases

It can be seen from Figure 8 that for the flame length, the longest separation distance is about 5.2 m and 8.4 m, for the 35 MPa and 70 MPa releases respectively. The flame length for the 70 MPa release increases more than 60% compared with that of the 35 MPa release. For both cases the largest flame envelopes near the ground occur at about 1.3 seconds after the opening of the TPRD. Afterwards, the flame will shrink and the separation distances will decrease. If the separation distances from these impinged jet fires are compared with the separation distances with those of free jet fires, the results show a significant reduction of more than 50% and nearly 40%, for the 35 MPa and 70 MPa releases respectively, as shown in Figure 7.

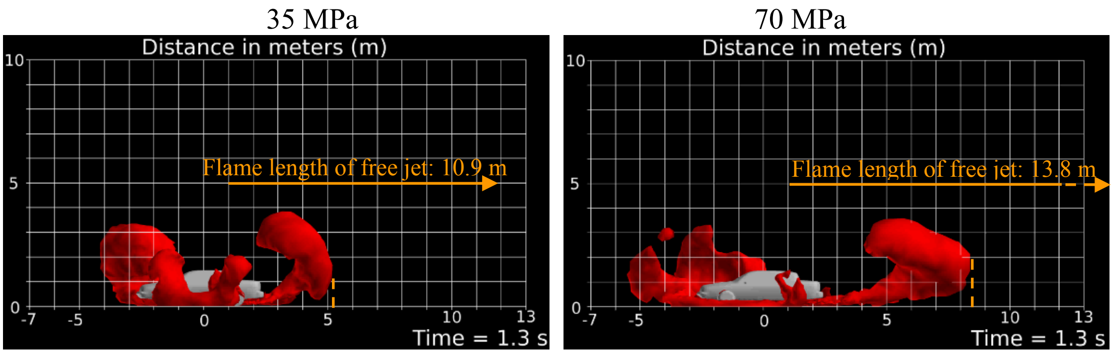

Figure 8. 1300 °C largest hydrogen flame envelopes

It can be seen from Figure 9 that for the first responder with thermal protective clothing, the longest separation distance is about 5.8 m and 9.2 m, for 35 MPa and 70 MPa releases respectively. The separation distance for the 70 MPa release increases more than 58% compared with that of 35 MPa release. For both cases the largest 260 °C temperature envelopes near the ground occur at about 1.5 seconds after the opening of the TPRD. Afterwards, the envelopes will shrink and the separation distances will decrease.

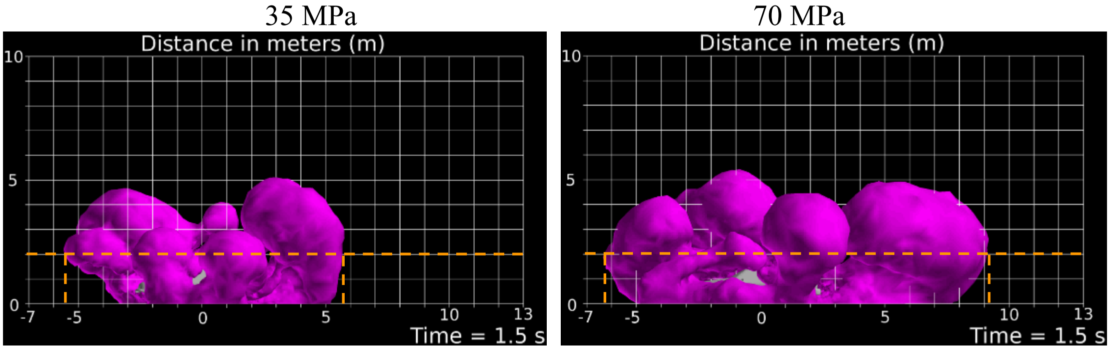

Figure 9. 260 °C largest extents cut off at 2m height

It can be seen from Figure 10 that for the first responder without thermal protective clothing, the longest separation distance is about 6 m and 9.4 m, for 35 MPa and 70 MPa releases respectively. The separation distance for the 70 MPa release increases nearly 57% compared with that of the 35 MPa release. For both cases the largest 115 °C temperature envelopes near the ground occur at about 1.5 seconds after the opening of the TPRD. Afterwards, the envelopes will shrink and the separation distances will decrease.

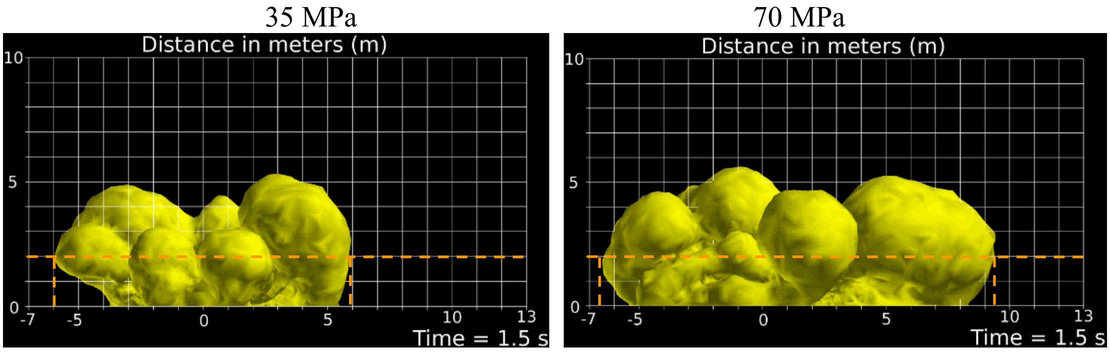

Figure 10. 115 °C largest extents cut off at 2m height

It can be seen from Figure 11 that for the general public, the longest separation distance is about 6 m and 9.5 m, for the 35 MPa and 70 MPa releases respectively. The separation distance for the 70 MPa release increases more than 58% compared with that of the 35 MPa release. For both cases the largest 70 °C temperature envelopes near the ground occur at about 1.5 seconds after the opening of the TPRD. Afterwards, the envelopes will shrink and the separation distances will decrease.

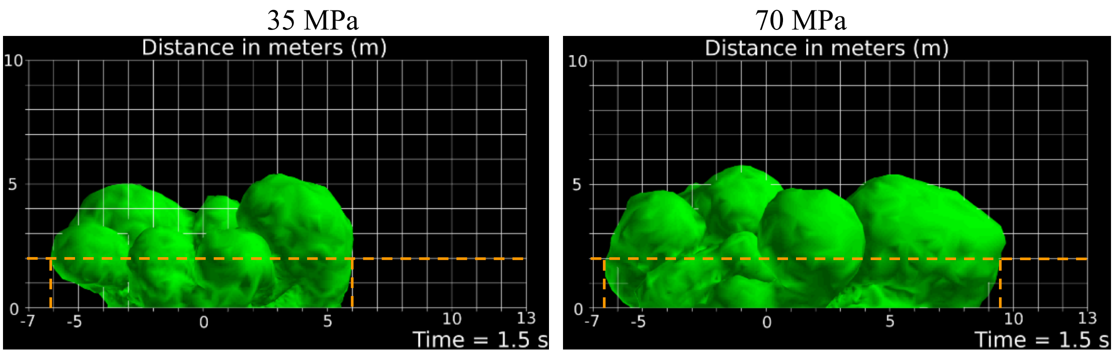

Figure 11. 70 °C largest extents cut off at 2m height

4.3 Summary of Deterministic Separation Distances

A summary of separation distances for different vulnerable targets is provided in Figure 12. In general, the unignited releases produce longer separation distances than the ignited releases. For all the 35 MPa release scenarios analysed in this study, the longest deterministic separation distances do not exceed, 10 m for the unignited case and 6 m for the ignited case respectively. For all the 70 MPa releases scenarios, the longest deterministic separation distances to people do not exceed, 12 m for the unignited case and 10 m for the ignited case respectively. For the air intake of buildings, the deterministic separation distances should be no less than 11 m and 13 m, for the 35 MPa and 70 MPa releases respectively. If a "safety factor" of 2 is applied, then about 26 meters would be a suitable "safety distance" for all scenarios.

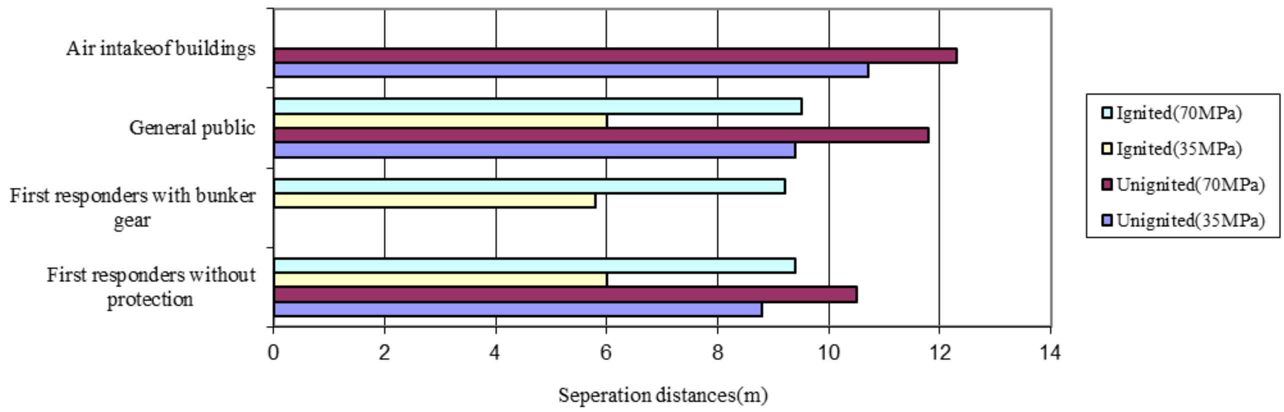

Figure 12. Summary of deterministic separation distances for different vulnerable targets

5.0 CONCLUSIONS

This paper investigates the deterministic separation distances required from vertically downward releases from a 4.2 mm TPRD located on an onboard hydrogen storage tank. Simulations are conducted for both 35 MPa and 70 MPa releases using real world car geometry. The results from this analysis are summarized below:

(1) For 35 MPa storage pressure, 171 L onboard storage, the blowdown time is less than 110 s. At storage pressure of 70 MPa with identical mass the blowdown time is less than 75s. For both 35 MPa and 70 MPa releases, the longest separation distances occur within 10 s after the opening of the TPRD. This indicates that the duration of the hazards associated with the release of hydrogen is less than two minutes, with the most hazardous timeframe occurring within ten seconds of the initiation of the release.

(2) For both 35 MPa and 70 MPa releases, the deterministic separation distances for unignited releases are longer than the comparative distances associated with ignited releases. This indicates that for such impinged jets, the deterministic separation distances are dominated by delayed ignition events rather than immediate ignition events.

(3) The deterministic separation distances for both unignited and ignited hydrogen releases, when the release is orientated vertically downwards from a TPRD under a car, are significantly shorter than those of free jets.

(4) In our case study, to ensure the safety of people a deterministic separation distance of at least 10 m for 35 MPa releases is required. This distance should be increased to 12 m for the 70 MPa release case. To ensure that the concentration of hydrogen is always less than 4% at the location of the air intake of buildings, the deterministic separation distance should be at least 11 m for 35 MPa releases and 13 m for 70 MPa releases.

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