NUMERICAL MODELLING OF HAZARDS OF HYDROGEN STORAGE

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ABSTRACT

For the general public to use hydrogen as a vehicle fuel, they must be able to handle hydrogen with the same degree of confidence as conventional liquid and gaseous fuels. The hazards associated with jet releases from accidental leaks in a vehicle-refuelling environment must be considered if hydrogen is stored and used as a high-pressure gas since a jet release can result in a fire or explosion. This paper describes the work done by us in modelling some of the consequences of accidental releases of hydrogen, implemented in our Fire Explosion Release Dispersion (FRED) software. The new dispersion model is validated against experimental data available in the open literature. The model predictions of hydrogen gas concentration as a function of distance are in good agreement with experiments. In addition, FRED has been used to model the consequence of the bursting of a vessel containing compressed hydrogen. The results obtained from FRED, i.e. overpressure as a function of distance, match well in comparison to experiments. Overall, it is concluded that FRED can model the consequences of an accidental release of hydrogen and the blast waves generated from bursting of vessel containing compressed hydrogen.

1.0 INTRODUCTION

There is currently widespread interest in hydrogen and the role it may play as the fuel of choice for the clean fuel-cell vehicles of the future. Hydrogen is light gas and higher diffusion coefficient which means that hydrogen has higher tendency to go upwards and mix quickly with air (because of higher diffusion coefficient) in comparison to other hydrocarbons. However, it has wider limits of flammability (4 to 75% by volume), low ignition energy, very high burning velocity and susceptibility to detonation. These properties suggest that hydrogen presents different safety challenges than other hydrocarbon fuels [3]. These unique features of hydrogen have been safely managed on an industrial scale for many years but, in a retail environment for refuelling hydrogen powered vehicles, industrial safety measures would be inappropriate and the proximity of the public unavoidable.

In the last few years there has been an upsurge of interest in safety issues (see ISO/TR 15916 [1]) related to the use of hydrogen. In Europe, this has spawned the EU funded Safety of Hydrogen as an Energy Carrier (HySafe) Network of Excellence, and an increasing number of European Union funded research projects containing some aspects of hydrogen safety. In the US, there was hydrogen safety research funded by the Department of Energy, and in Japan research funded by the New Energy and Industrial Technology Development Organization. Recent international conferences on Hydrogen Safety [2,3], organised by HySafe, provide a good overview of the current status of hydrogen safety research worldwide and an overview of experimental databases relevant to hydrogen safety standards development is given by Houf et al. [4]. For the safe design of retail facilities, through the development of appropriate codes, it is essential to understand all the hazards that could arise following an accidental release of hydrogen and to have data to allow the appropriate standards to be developed. These data can be also used to develop and validate models used in quantitative risk assessment tools [5-13] and tools based on computational fluid dynamics (CFD) [14-17] or tool based on integral models e.g. Fire Release Explosion Dispersion (FRED) [18] or PHAST [19].

Present paper reports validation of FRED (Shell's in-house consequence assessment tool) against literature data for hydrogen dispersion and vessel burst.

The paper is structured as follows: Section 2 describes the modelling used in this paper. Section 3 describes the experiments which is used to validate FRED models described in this paper. Section 4 presents results of validation. Finally, overall summary and conclusions are presented in Section 5.

2.0 MODELLING

The modelling was performed using the Shell FRED[1] model. The code version used was 6.2. It is a system which models the consequence of a release of hydrocarbon, both accidental and intentional. Its aim is to assist designers to produce safe and cost effective modifications to existing or new site layouts and design. Alternatively, it may assist in the development of site operational procedures or provide a screening tool for "effect calculations" in Quantitative Risk Assessment studies.

The FRED code uses HGSYSTEM [20,21] suit of models to predict dispersion from a jet release. FRED is a GUI based software which requires user to provide the temperature, pressure, release location and size of the leak. In addition, user should provide information of the wind (i.e. speed and stability class). FRED then calculates exit temperature, pressure and expanded exit velocity. This information is then passed to dispersion module in FRED which is based on HGYSTEM.

Three dispersion plume modules a) AEROPLUME, b) HEavy GAs Dispersion from Area Sources (HEGADAS) and c) PGPLUME (Pasquill/Gillford Plume) are invoked when performing dispersion.

AEROPLUME can be used to simulate the jet (plume) development of a release, from a pressurised vessel or from a stack, of a mixture of several non-reacting compounds, which can form one or more single or multi-compound aerosols. In the AEROPLUME calculation, the jet profile is assumed to be of top-hat type in both horizontal and vertical planes. The plume "average" properties calculated directly by AEROPLUME are identified as being concentration-weighted averages. In addition, it is assumed that the highest concentration in the profiled jet is always twice the average concentration calculated by AEROPLUME. It outputs parameters e.g., the horizontal distance travelled, the centroid height position, jet velocity, angle and jet temperature. These variables are then used in FRED to post process and provide contours of gas concentration.

HEGADAS is used for dense gas dispersion modelling i.e. modelling of heavier vapours generated from a pool. The model for far field passive dispersion is called PGPLUME. This is based on simple Pasquill/Gillford similarity model specifically designed to simulate passive gas dispersion downwind of a transition (momentum to buoyancy dominated regime) point with AEROPLUME.

The output from these module is then postprocessed to provide dispersion contours of various concentration.

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[1] As of FRED is Shell in-house software, but we are in the process of releasing FRED to outside world for their use.

In addition to the models for jet release, models have been built for vessel burst. The vessel burst model assumes physical explosion occurs due to the sudden release of mechanical energy. The explosion energy is calculated by work of Brode. It assumes explosion energy is same as what is required in raising the pressure of the gas from atmospheric pressure to the bursting pressure at a constant volume. The decay of overpressure generated from this explosion is calculated using Baker et al [22] overpressure decay curves.

3.0 EXPERIMENTAL FACILITY

This section summarizes the experiments used by us in validation of FRED for dispersion and vessel burst. Firstly, dispersion experiments are presented. Secondly, experiments used for validation of vessel burst/rupture model in FRED are presented.

DISPERSION EXPERIMENTS

A) SHIRVILL ET AL.

Several hydrogen release experiments were performed by Shell using the test facilities at HSL. These experiments are described in Shirvill et al. [23] and Roberts et al. [24]. These facilities were designed to have a maximum working pressure of 150 barg. The release direction was horizontal, at a height of 1.5 m above the test pad. The wind speed and direction were measured during the experiments using a Vector Instruments weather station fixed to the release pipe. Using this instrument (for this specific experiment) the average wind speed was measured to be 1.1 m/s, in the direction of release. The overall layout of the experimental setup is shown in Fig. 1.

(a) (b)

Figure 1: Experimental facility with oxygen depletion sensor for high pressure release a) behind release nozzle and b) towards release nozzle.

The hydrogen concentration in the experiments was derived from measurements of the oxygen concentration within the cloud. In the experiments, it was assumed that any decrease in the concentration of oxygen was due to displacement by hydrogen. 20 CiTicel AO2 Oxygen sensors were used during the experiments. The measurements accuracy of the sensors, including experimental variability, was of the order of ± 0.3% hydrogen. Video cameras (including thermal imaging) were used to monitor and record the experiments.

B) LI ET AL.

Li et al [25] conducted two different types of experiments to study the subsonic and sonic release of hydrogen. In the first experiments, the gas concentrations during subsonic releases of hydrogen and helium were measured for subsonic jets. The gas for the subsonic tests was released through a vertical tube having an inside diameter of 1.91 mm. In second experiments, a custom designed high-pressure stagnation chamber with an internal volume of 1.24 L was used to create under-expanded hydrogen jets with static pressures up to 60 bar. The downstream gas concentrations in these experiments were obtained using a Planar Laser Rayleigh Scattering (PLRS) system.

C) HAN ET AL. [26]

KIST (Korea Institute of Science and Technology) measured the concentration of a released hydrogen jet from a highly pressurized chamber which represents a high-pressure vessel. The hydrogen concentration was measured along the jet centreline for three cases of three different leak diameters of 0.5 mm, 0.7 mm and 1 mm. Different jet pressures (100 bar, 200 bar, 300 bar and 400 bar) were studied for this work.

VESSEL BURST EXPERIMENTS

Recently, two destructive tests were conducted by Weyandt [27, 28] which investigated the effects of bursting of high pressure hydrogen tanks, a stand-alone tank and an under-vehicle tank. These tests were modelled by [29]. The tank volume is 72.4 L capacity which is filled with hydrogen under initial pressure of 34.3 MPa and temperature 300.15 K. Table 1 provides parameters and test condition used for experiments. In his experiment, the blast wave overpressure was measured by pressure transducers located at different distances and directions (see Figure 2 which sensor locations). The blast wave overpressure measured at a distance of 4.2 m to the North is about 35% higher than at the same distance to the West. This essentially means that there is an asymmetry of the experimental pressure in different directions, possibly associated with the asymmetry of the tank. Molkov and Kashkarov [29] processed the pressure transients available from Weyandt's reports [27,28] to obtain the experimental values of impulse. These values were then used to compare FRED predictions.

Table 1: Parameters and test condition for experiments.

Test	Volume [L]	Gauge Pressure, [MPa]	Temperature [K]
Stand-alone Test [27]	72.4	34.3	300.15
Under-vehicle Tank Test [28]	88	31.8	306.15

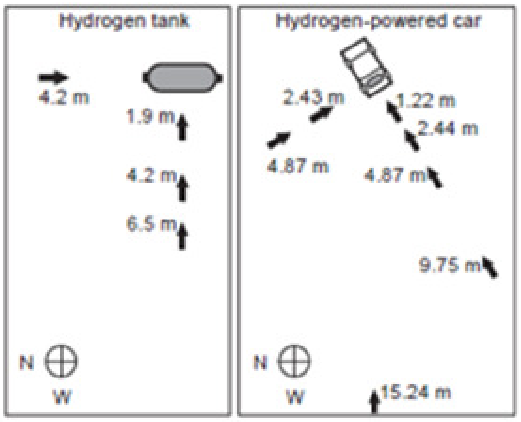


Figure 2: Location of pressure sensors in the stand alone tank test (left) and in the under vehicle tank test (right). This figure is taken from Weyandt [27,28].

4.0 RESULTS

DISPERSION VALIDATION

A) SHIRVILL ET AL.

Shell’s [23,24] dispersion experiments were used to validate FRED. FRED simulations were performed against 23 cases reported in [24]. Table 2 summarizes pressure, temperature and leak size of 14 experiments. Figure 3 shows the comparison of flow rate obtained from experiments and FRED. FRED can predict the mass flow rate within accuracy of 3 %. Next, concentration decay curves obtained from FRED are compared against experiments.

Table 2: Processed release data and calculated flow rate.

Case	Pressure (bar absolute)	Temperature (°C)	Leak Diameter (mm)
1	120	20	4
2	130	18	4
3	126	17	4
4	137	17	3
5	123	15	3
6	119	15	3
7	100	14	3
8	99	14	3
9	93	13.5	4
10	94	13	4
11	77	13	4
12	74	14	3
13	74	13.5	3

14	50	12.5	3

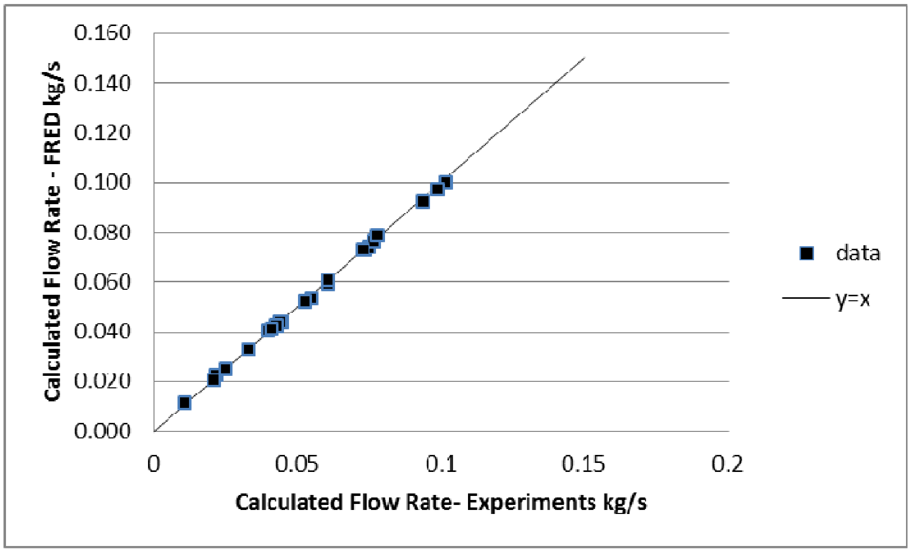
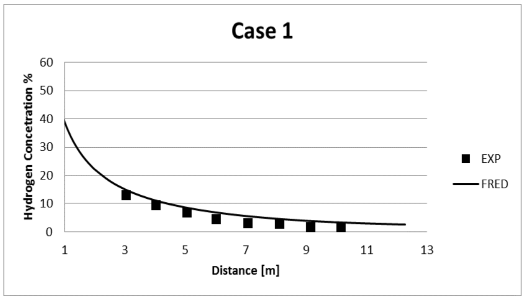
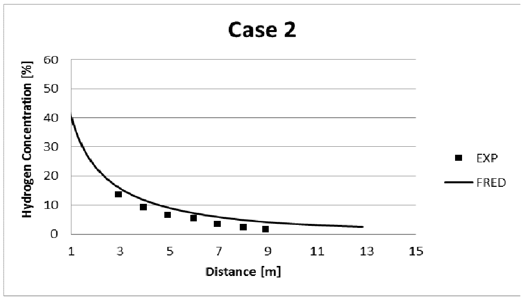


Figure 3: Shows the comparison of flow rate calculated from experiments and FRED.





(a)

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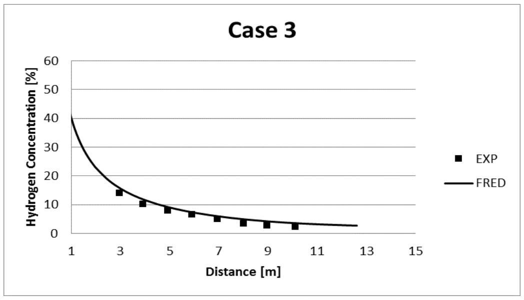
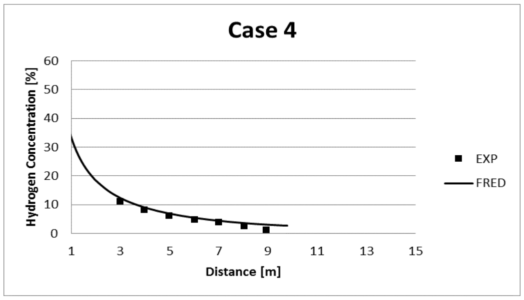
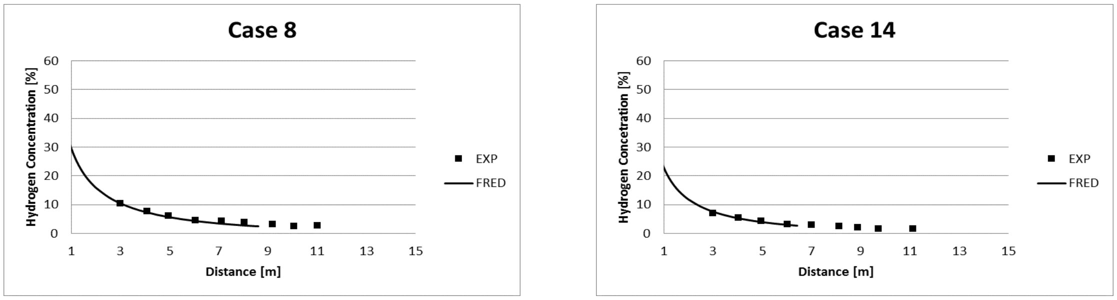




(b) (d)



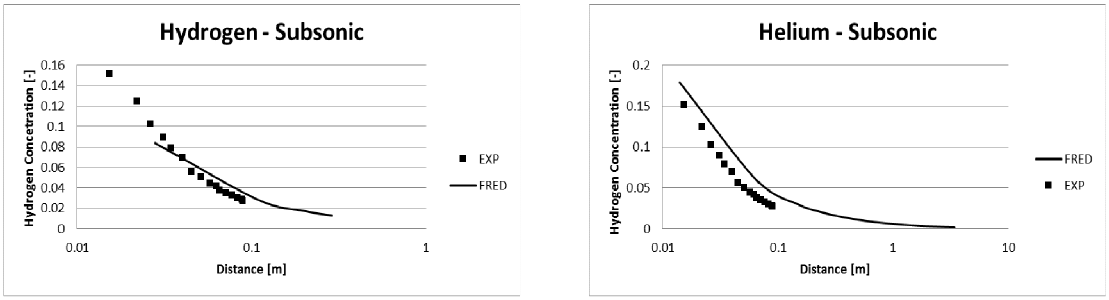
(e) (f)

Figure 4: Comparison of decay of centreline hydrogen concentration as a function of distance. Symbols represent Shirvill et al. [23] experiments, while lines represent modelling results using FRED. Results for different cases are presented in a) Case 1, b) Case 2 c) Case 3, d) Case 4, e) Case 8 and f) Case 14 (refer to Table 1 for the pressure, temperature and leak size of the cases).

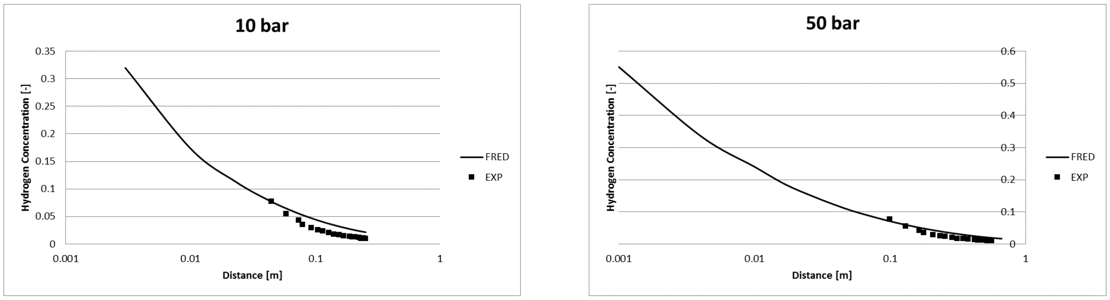
A detailed comparison of simulated versus reported concentration decay (see Fig. 4) from experiments indicates that there is a reasonable agreement between predictions and experiments for the cases considered here. It is worth noting that simulation results are plotted only up the concentration of 4 % (LFL of hydrogen).

B) LI ET AL.

To further validate the FRED dispersion modelling simulations were performed for different experiments performed by Li et al for subsonic (expanded) and sonic (under expanded) jets. Figure 5 shows the decay of hydrogen concentration in the centreline as a function of distance. The x-axis is plotted in logarithmic scale to highlight the predictions of decay behaviour. Symbols represent experiments while lines show FRED simulations results. Cases a) and b) correspond to subsonic jets of hydrogen and helium. There is a slight over prediction in near field for helium and slight over prediction for hydrogen case. However overall decay of hydrogen concentration with distance is correctly predicted. Case c) and d) correspond to hydrogen jets with initial pressures of 10 bar and 50 bar. In this case both the near field and far field is correctly predicted.



(a) (b)

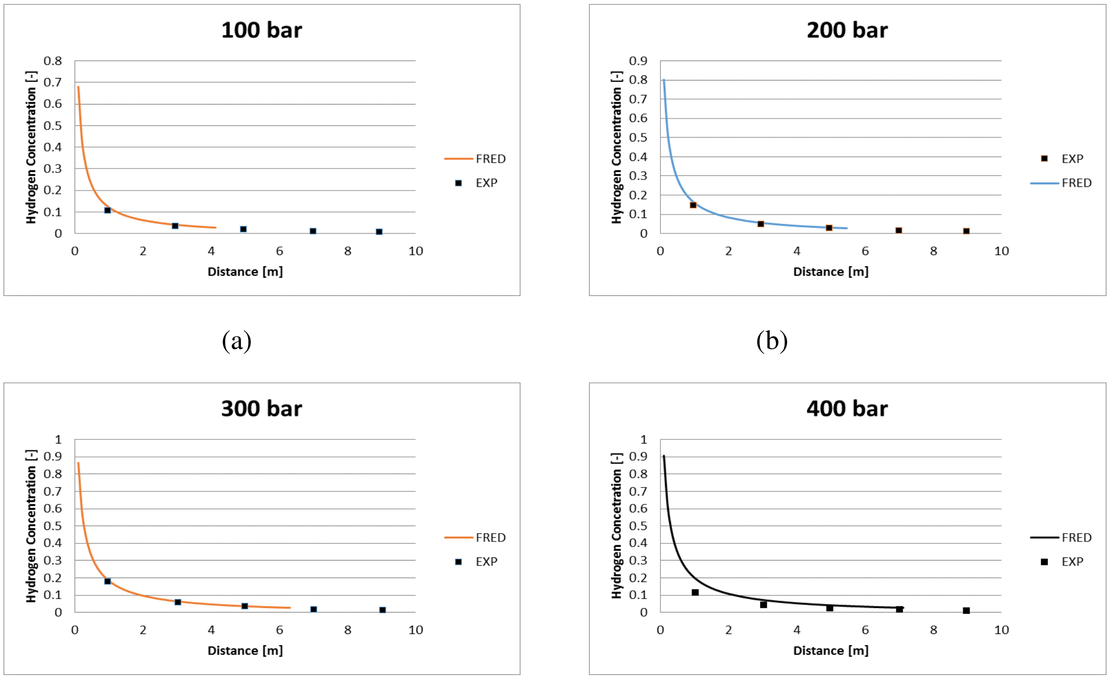


(c) (d)

Figure 5: Comparison of decay of centreline hydrogen concentration as a function of distance. Symbols represent Li et al. [25] experiments while lines represent modelling results using FRED. Results are shown here for a) hydrogen, b) helium subsonic releases. Sonic hydrogen releases are then shown with initial pressure of c) 10 bar and d) 50 bar.

C) HAN ET AL.

The typical operating pressure in hydrogen retail stations is around 450-750 bar, therefore comparison with the Han et al. experiments is particularly relevant. Figure 6 shows comparison of FRED prediction and experimental data for different initial pressure of a) 100 bar, b) 200 bar, c) 300 bar, and d) 400 bar. The release size is 1 mm. Symbols correspond to experiments while lines show FRED simulation results. There is a slight over prediction in the near field for 400 bar cases, but overall the concentration decay is predicted very well.



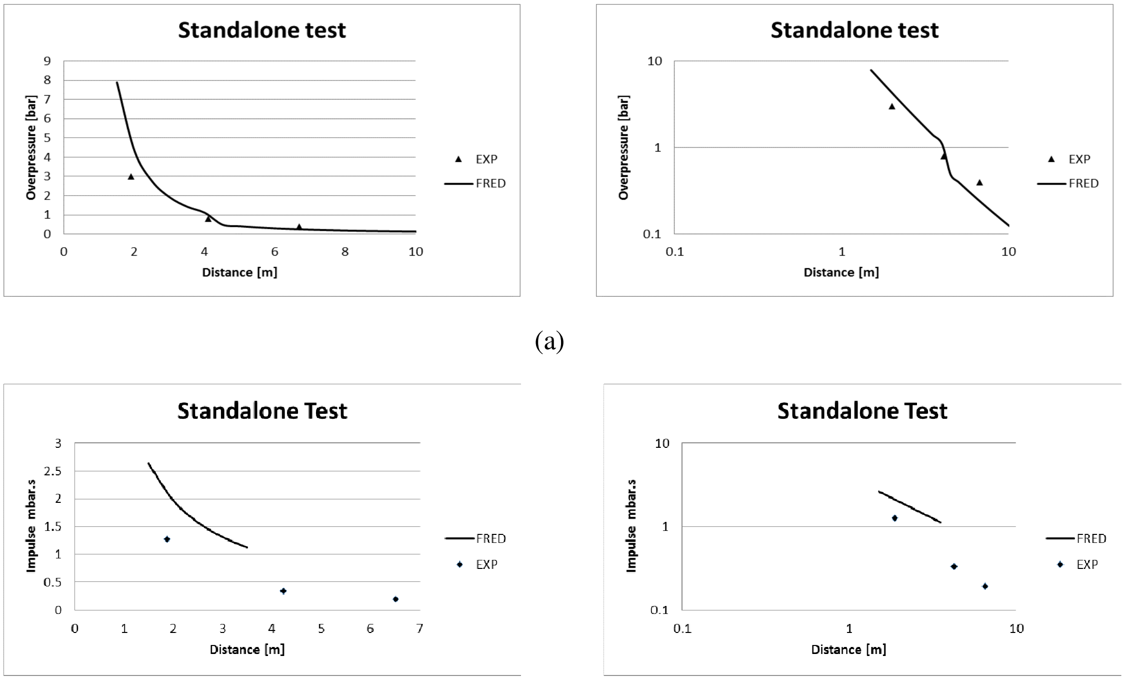
(a) (b)

(b) (d)

Figure 6: Comparison of decay of centreline hydrogen concentration as a function of distance. Symbols represent Han et al. [26] experiments, while lines represent modelling results using FRED.

Results are shown here for sonic release with an initial pressure of a) 100 bar, b) 200 bar, c) 300 bar and d) 400 bar sonic release. The leak size used in the calculation was 1 mm.

VESSEL BURST VALIDATION



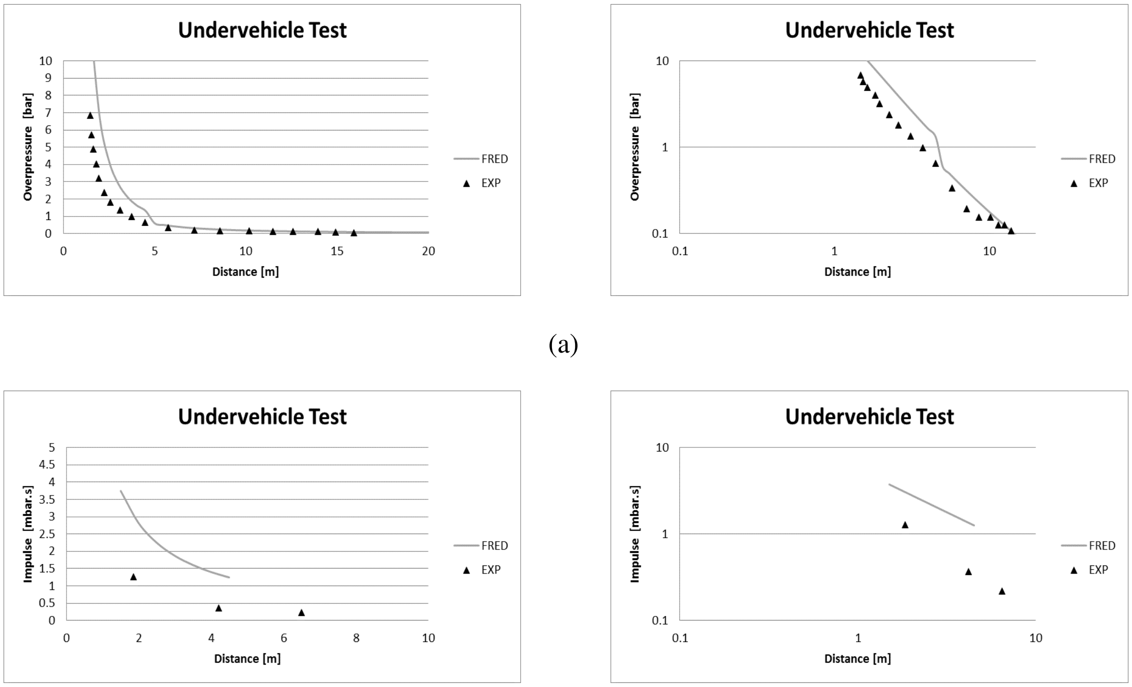
(a)

(b)

Figure 7: Standalone tests. Comparison of decay of a) blast wave overpressure and b) impulse as a function of distance. Symbols represent Weyandt [27] stand-alone experiments, while lines represent modelling results using FRED. Data are the same in the left and right graphs but those on the right are plotted on logarithmic axes.

Figure 7(a) presents the experimental data on a decay of blast wave overpressure as a function of distance from the standalone hydrogen tank after its rupture. Blast wave overpressures calculated by FRED are also compared. The overpressure in the near field (1.9 m) is over predicted by FRED. However, at far field locations of 4.1 m and 6.7 m FRED predicts overpressure very well.

Figure 7(b) compares the FRED prediction and experimental data on decay of blast wave impulse as a function of distance from the stand-alone hydrogen tank test. The prediction of impulse is slightly over predicted in near field and far field, however the decay behaviour is correctly predicted using FRED. It is worth noting that FRED does not output values of impulse lower than 1 mbar.sec.



(a)

(b)

Figure 8: Under-vehicle test. Comparison of decay of a) overpressure and b) impulse as a function of distance. Symbol represents Weyandt [28] under vehicle experiments, while lines represent modelling results using FRED. Data are the same in the left and right graphs but those on the right are plotted on logarithmic axes.

For the under-vehicle test, Figure 8 a) and b) show decay of blast wave overpressure and impulse as a function of distance. FRED over predicts the blast wave overpressure and impulse slightly in near field but decay behaviour of overpressure and impulse is correctly predicted.

5.0 SUMMARY AND CONCLUSION

Managing the hazards associated with hydrogen in a retail environment requires and understanding of the behaviour of potential accidental releases. In this paper, we report the validation of Shell's in-house software FRED against hydrogen dispersion and vessel burst experimental data available in the literature.

FRED codes use the HGSYSTEM suite of models to model the behaviour of jet. For the present purpose, we have used AEROPLUME to model jet release and concentration decay.

In the first step, FRED is validated against three different experiments a) Shirvill et al, b) Han et al. and c) Li et al. Experiments were performed for expanded (hydrogen and helium) and under-expanded (hydrogen) jets. The initial pressure in under-expanded experiments was varied from 50 bar to 400 bar, while the leak size was varied from 1 mm to 4 mm. In all the experiments, hydrogen concentration was measured in the centreline of the jet for different leak size and exit pressure of the jet. Although there is some slight over prediction in far field for certain cases, overall, FRED modelling very well predicts the concentration decay in these experiments.

In the second step, FRED is validated against vessel rupture experiments of Weyandt [28]. Two sets of experiments (using stand alone and under-vehicle tanks respectively) were performed. The decay of blast wave overpressure and impulse as function of distance was measured at different locations. FRED models slight over predict both impulse and blast wave overpressure, but overall decay behaviour is correctly predicted.

6.0 ACKNWOLEDGEMENT

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