EXPERIMENTAL RESULTS AND COMPARISON WITH SIMULATED DATA OF A LOW PRESSURE HYDROGEN JET

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ABSTRACT

Experiments with a hydrogen jet were performed at two different pressures, 96 psig (6.6 bars) and 237 psig (16.3 bars). The hydrogen leak was generated at two different hole sizes, 1/16 inch (1.6 mm) and 1/32 inch (0.79 mm). The flammable shape of the plume was characterised by numerous measurements of the hydrogen concentration inside of the jet. The effect of the nearby horizontal surface on the shape of the plume was measured and compared with results of CFD numerical simulations. The paper will present results and an interpretation on the nature of the plume shape.

1.0 INTRODUCTION

The scope of the work was concentrated on comparison of selected free and horizontal jets experiments with results from CFD simulations. This work directly contributes to the work plan of the Hydrogen Implementing Agreement/International Energy Agency Task 19 Hydrogen Safety [1]. This paper compares CFD simulation results and experimental data of hydrogen release and dispersion from free hydrogen jets using real gas law with identical jet releases but in a presence of a horizontal surface with variable proximity. The considered 21 scenarios are summarized in Table 1 below. They provide good guidance to planned experiments. All simulations were conducted using transient models. Measurements of the Hydrogen jet profile and concentration were performed in laboratory targeting the low flammability limit value (LFL) of 4% inside of the cloud produced.

Table 1. Simulation scenarios

Pressure at the nozzle	Hole diameter	Free jet	Distance to horizontal surface (ground)						
			1 cm	2 cm	5 cm	8 cm	10 cm	20 cm	30 cm
96 psig	1/32” 0.79 mm	0.71 m	?	?	?	?	?	?	?
236 psig	1/32” 0.79 mm	1.07 m	?	?	?	?	?	?	?
193 psig	1/16” 1.6 mm	1.96 m	?	?	?	?	?	?	?

2.0 EXPERIMENTAL SETUP AND RESULTS

2.1 Speed and accuracy of the hydrogen concentration measurement

Measurements of the hydrogen concentration profiles during leaks is of first importance for the experimental part of this study. It will be found later in the text that the nature of the hydrogen jet measured by the detector is having a wavy shape. So it is of first importance to get precise and accurate concentration results to get an exact size of the hydrogen cloud and to confirm the shape of the jet. To determine the shape of the jet, it was decided that the low flammability limit (LFL) of hydrogen was the targeted concentration we wanted to measure. The objective was to get a picture of the LFL cloud size and to compare the results with CFD simulations. The hydrogen detectors must have the following important specifications:

- **fast response time**
- **range of concentration between 1-10% (around the LFL)**
- **stability and reliability to perform measurements from hydrogen leaking out at a high flow rate**
- **accuracy of the detector**
- **low calibration frequency**

The hydrogen sensor used was the *Neodym Panterra* model and was based on thermal conductivity measurements. Some tests were made inside of a plexiglass chamber with different hydrogen/oxygen gas flows with concentrations ranging from 5 to 50%. The preliminary results confirmed the precision of the measurement. Additional experiments were performed by applying drastic changes in the hydrogen/oxygen ratio by changing the flow rate of the hydrogen meter. For example, by starting the detection at a hydrogen concentration of 70%, followed by a drastic changes of the concentration in few seconds, down to 10%. Overall, it confirmed that the time to detect changes of the hydrogen/oxygen concentration was less than 3 seconds inside of the chamber and possibly as low as 1 second. This fast response time was found to be acceptable for the needs of the project. In principle a hydrogen/air mixture containing nitrogen should give similar response time.

Experiments with hydrogen mixed with air (oxygen/nitrogen) were performed. Evaluations of the response time was made by filling a hydrogen bag with a known concentration of hydrogen/air mixtures below 10 %. The hydrogen detector was rapidly introduced inside of the bag containing hydrogen to perform concentration measurements. The detector gave a stable signal after less than 2 seconds.

Calibration procedures of the sensors were developed to evaluate the accuracy of the measurements. Hydrogen mixtures were prepared by filling a syringe with pure hydrogen and by adding known amount of air. The hydrogen/air mixtures were left for few seconds inside of the syringe to get a homogeneous mixture. The syringe was sealed during the mixing time to avoid leaks. Different ratios of hydrogen/air mixtures between 1 to 100% were prepared by using this procedure. The front end of the hydrogen sensors was then sealed by using a tape. The homogeneous hydrogen/air mixture was then introduced with the syringe, through the sealed tape, right at the front end of the sensor. A calibration curve for concentration ranging from 1 to 100.0% was made is shown on Figure 2a. There was a slight difference between the hydrogen concentration injected into the front end of the sensor and the value given by the detector. For example, the hydrogen sensor gave a value of 12% for hydrogen concentration of 10% (see Figure 2a). It demonstrates that the hydrogen sensor needs to be calibrated, all along the range of concentration. It was done by measuring the signal at various concentrations and by using a calculated polynomial curve. Numerous measurements confirmed that the accuracy and the reliability of the measurements were better than ± 5% using a calibration curve.

Determination of the accuracy of the sensor for concentration around the LFL value was made by using a different experimental setup. Measurements of hydrogen/air concentrations were performed by using a 2.0 L glass container. Precise volumes of hydrogen were injected in one second, inside of the 2.0 L container. Mixing time to get a homogeneous mixture was observed to be around 20 seconds. A calibration curve for concentration between 1.0-10.0% was made. By using this procedure, it was found that the accuracy and the reliability of the measurements were better than ± 5%. It was also found that the procedure using injection at the front end of the sensor with concentration from 10-100% was enough to calibrate the sensors over the broader range of concentration (1.0-100%). In conclusion, we may say that each detector need to be calibrated with the best fit polynomial calibration curve and by using appropriate experimental setup.

2.2 Comparison of free jets for selected pressures (CFD simulations)

We first predicted the LFL hydrogen cloud extents for free jets for selected pressures and orifices and compared them with Birch model prediction [2]. In Birch's paper, the leak temperature was assumed to be the same as atmosphere, eg. $T_a \approx T_e$, so the pseudo orifice could be calculated by $d_{ps} = \sqrt{C_D (\frac{P}{P_a})(\frac{2}{\gamma+1})^{\gamma+1/2(\gamma-1)}}$. This simplification, however, causes larger extent values than they should be. The leak temperature should reflect real gas law and, thus, be around 243K. Birch's paper did not provide coefficients for hydrogen to adjust these values. Sandia has noticed it and adjusted the formulations in their paper by introducing the real temperature at the leak orifice [3]. Their formulation is a direct derivation including the real orifice temperature. By using this formulation, Birch's coefficients for hydrogen should be selected as: Cd=0.95 and K=5.4. We used these coefficients and the real orifice temperature (similar to Sandia's formulations) for calculating Birch's model predictions.

2.3 Flammable shape of the plume (Experimental and CFD simulations)

Hydrogen jet experiments were conducted inside of a closed room designed to sustain undesired blast events. The size of the room was big enough to remove any effect of the walls on the shape of the hydrogen plume leading to the free jet. The jet was produced at the height of 2 meters to remove any effect of the ground on the shape of the plume.

The flammable shape of the plume produced by the hydrogen leaking out from the nozzle (orifice diameter: 1/16" and 1/32") was characterized by performing numerous measurements of the concentration. Many trials were performed by displacing the hydrogen detector at different positions inside and outside of the plume. As soon as the hydrogen was released from the nozzle, the measurement of the concentration was taken until it had reached a steady state inside of the jet (stable concentration inside of the hydrogen cloud produced by the jet). About 10 seconds was necessary to reach the steady state and the hydrogen concentration was then taken. The pressure gauge was present at few centimetres from the nozzle releasing the hydrogen. Identification of the 4% vol. concentration was

performed inside of the plume to determine the shape, dimensions and length of the LFL cloud (namely LFL extent in Tables and Figures). To get a picture of the 4% vol. hydrogen cloud it was necessary to perform numerous trials, as reported in Table 2. Around 44 experimental data points were necessary to describe the 4% vol. hydrogen cloud produced by the jet, as shown in Figure 1.

Figure 1 shows a typical example of the shape of the plume from CFD simulations (generated by FLACS Hydrogen) compared to the experimental results. The number of data points collected was found to be enough to find that the plume was having a wavy shape. The wavy shape of the plume determined by experimental trials is consistent with observations found in literature and is slightly different from the CFD simulation that generated a time-averaged (smoothed) image of concentration distribution. This, in turn, is consistent with time-averaged images that can be found in literature. The results reported in Table 3 for three pressures (93psig, 236psig and 193 psig) confirmed that both the CFD simulations and Birch model produced very similar results to experimental data for the length of the LFL plume (namely LFL extent in Tables and Figures). Also, it was found that experimental data and CFD simulation results (not shown in Table 3) were giving very similar results in terms of the width and the size of the plume

Table 2 – Experiments performed to determine the shape of the LFL plume

	Pressure at the nozzle	**Orifice diameter**	**Number of trials**
Condition 1	**96 psig**	**1/32" 0.79 mm**	**361**
Condition 2	**236 psig**	**1/32" 0.79 mm**	**100**
Condition 3	**193 psig**	**1/16" 1.6 mm**	**185**
Condition 4	**96 psig**	**1/16" 1.6 mm**	**50**

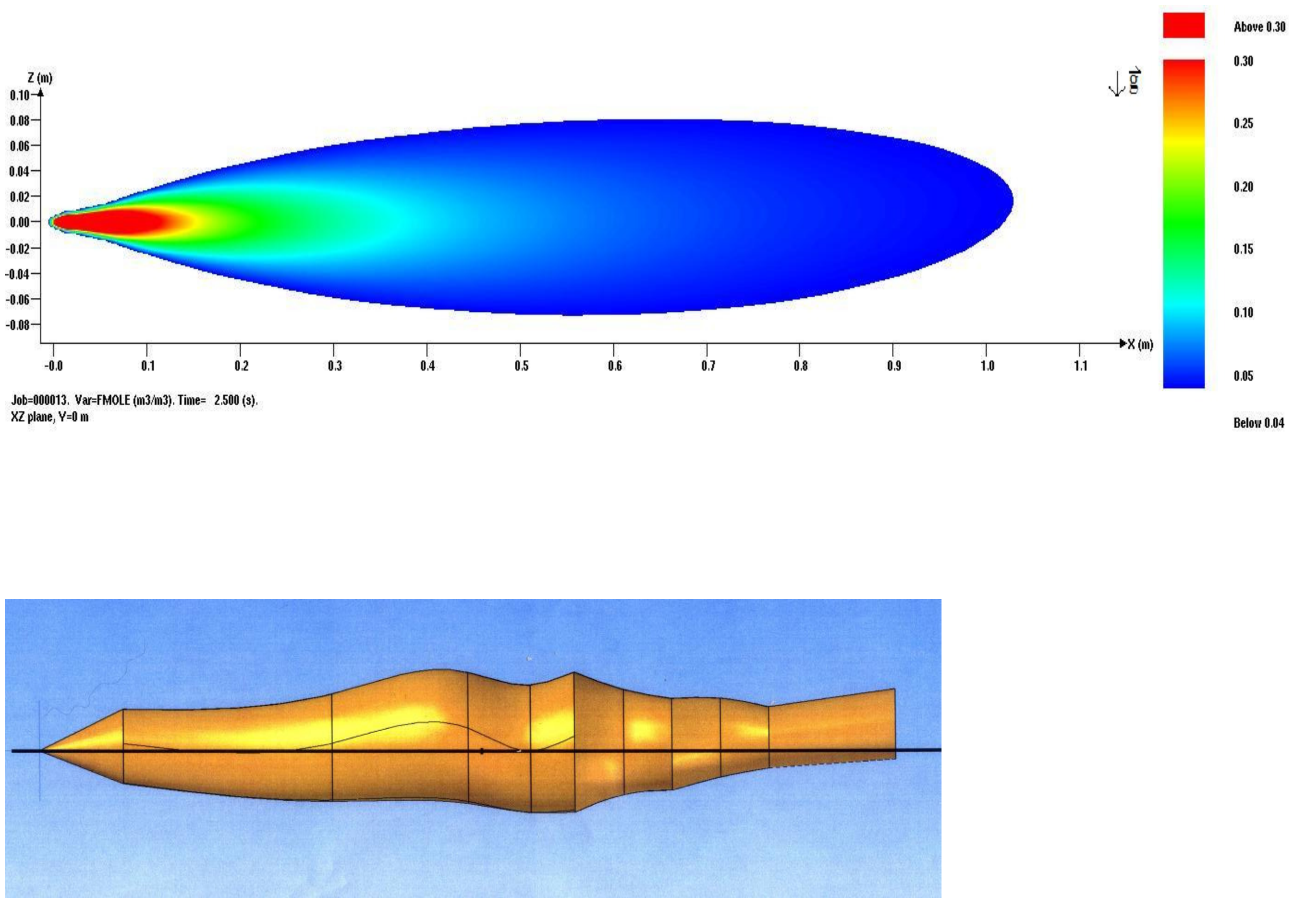
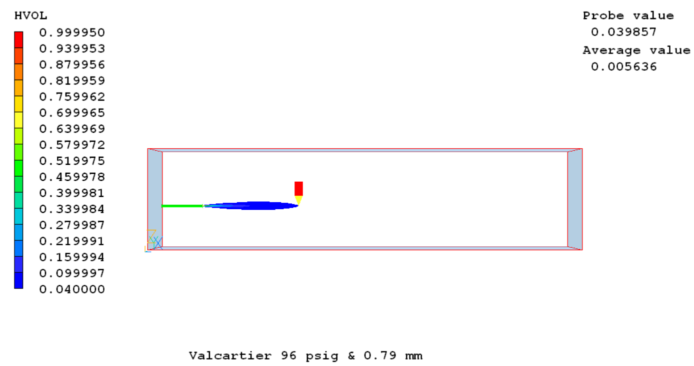
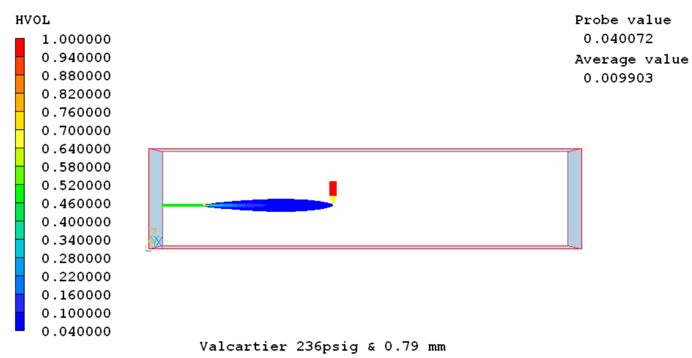
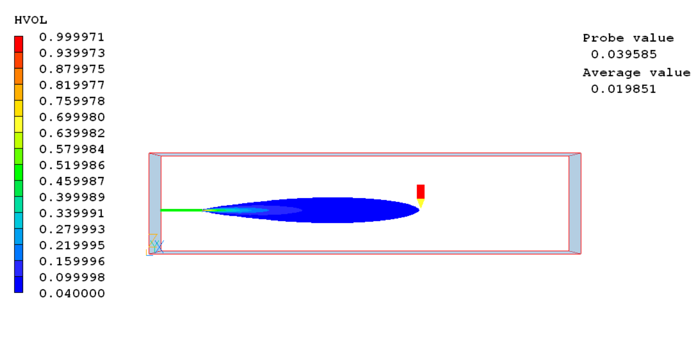


Figure 1 – Comparison of the CFD simulated data (upper diagram) generated by FLACS Hydrogen and the experimental result (lower diagram) for a jet produced at 96psig from a orifice with a diameter of 1/32" (0.79mm)

Table 3. Comparative LFL extents obtained by CFD modeling (generated by PHOENICS), Birch model and experimental results

Pressure at the nozzle	Hole diameter	Experimental extent of 4% vol.	Birch	CFD
96 psi	1/32 0.79 mm	88 cm	72 cm	71 cm 
236 psi	1/32 0.79 mm	118 cm	109 cm	107 cm 
193 psi	1/16 1.6 mm	225 cm	201 cm	196 cm 

2.4 Effect of the nearby horizontal surface

The length of the low flammability limit cloud (4% vol.) was measured by displacing the detector at different positions from the nozzle. The finding of the exact position of the 4% vol. hydrogen cloud boundary inside of the plume was determined by doing more than 5 experiments for each point in Figure 2. The graph on this figure shows the effect of the nearby horizontal surface on the LFL extent. The ground was composed of a steel plate. The graph in Figure 2 shows that the ground started to have an effect on the length of the plume at a distance of 8 cm for a 96 psig jet with an orifice size of 1/32" (0.79 mm). Results from the CFD simulation (PHOENICS) were very similar as shown on Figure 2. It demonstrates that the CFD model predicts very well the effect of the nearby horizontal surface on the LFL extent.

Further experiments were performed with the following parameters:

- hole size of 1/32" (0.79mm) at 236 psig
- hole size of 1/16" (1.6mm) at 96 psig
- hole size of 1/16" (1.6mm) at 193 psig (not done yet)

The results are shown on Figure 3 and 4. CFD simulations (PHOENICS) were done for the case of the 1/32" (0.79 mm) orifice at 236 psig. Though the experimental results shown in Figure 3 are in general agreement with the CFD modeling, the experimental data for distances closer than 5 cm to the surface clearly deviate from the trend. This is thought to be attributed to the interference of the sensor (appr. 5 cm in diameter) with the hydrogen flow close to the surface. There are still additional CFD simulations and experiments to be done over the next few months for the bigger orifice size (1.6mm); those will be added to Figures 4 and 5. The results for the bigger orifice, shown on Figures 4 and 5, demonstrate that the ground started to have an effect on the LFL extent of the plume at a much higher distance (20 and 30 cm from the ground).

A LFL plume for the 96 psig with orifice size of 0.79 mm is described in Table 4. Substantial increase in LFL extent was noticed when a horizontal jet was released at close proximity to surface.

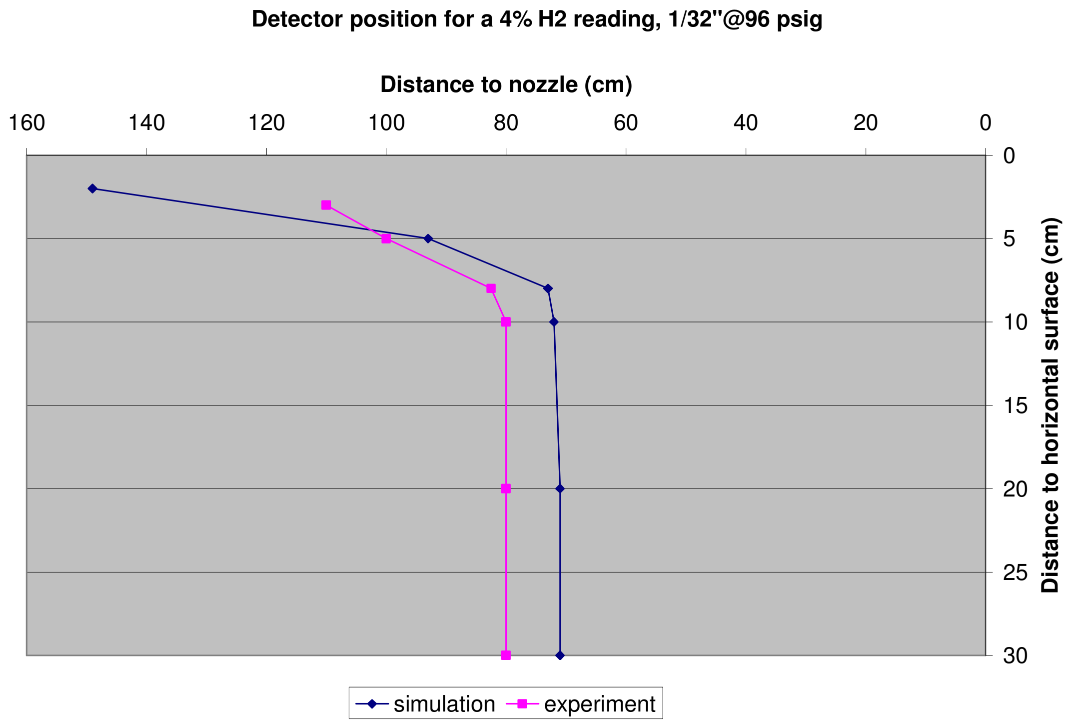


Figure 2 – Effect of the nearby ground (horizontal surface) on the length of the LFL cloud

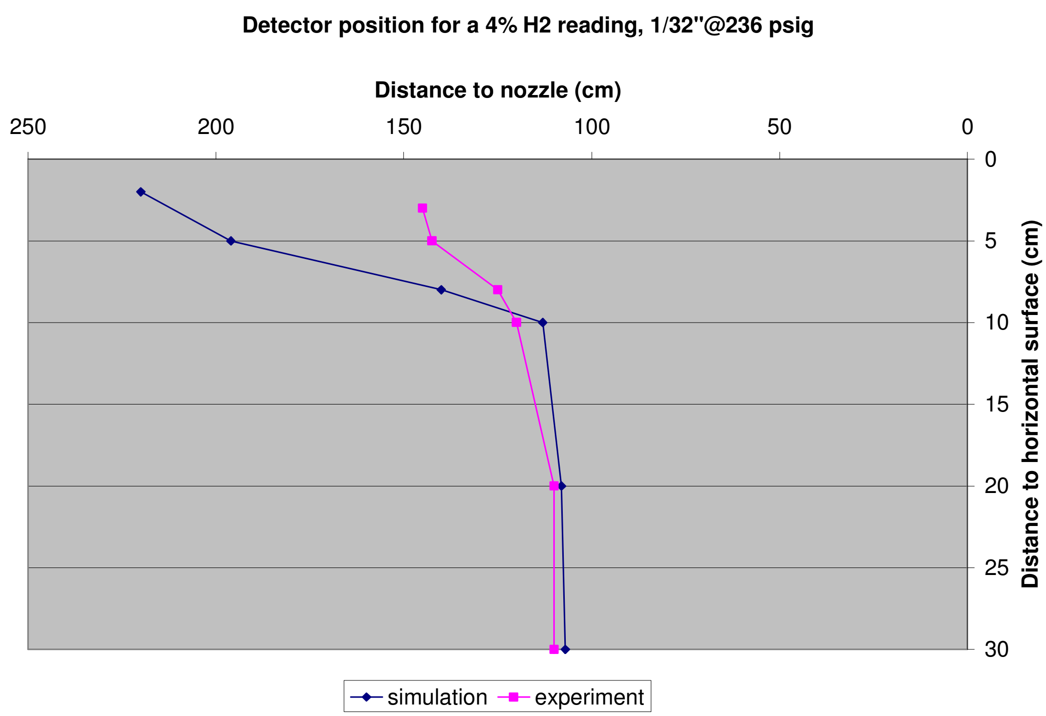


Figure 3 – Effect of the nearby ground (horizontal surface) on the length of the LFL cloud

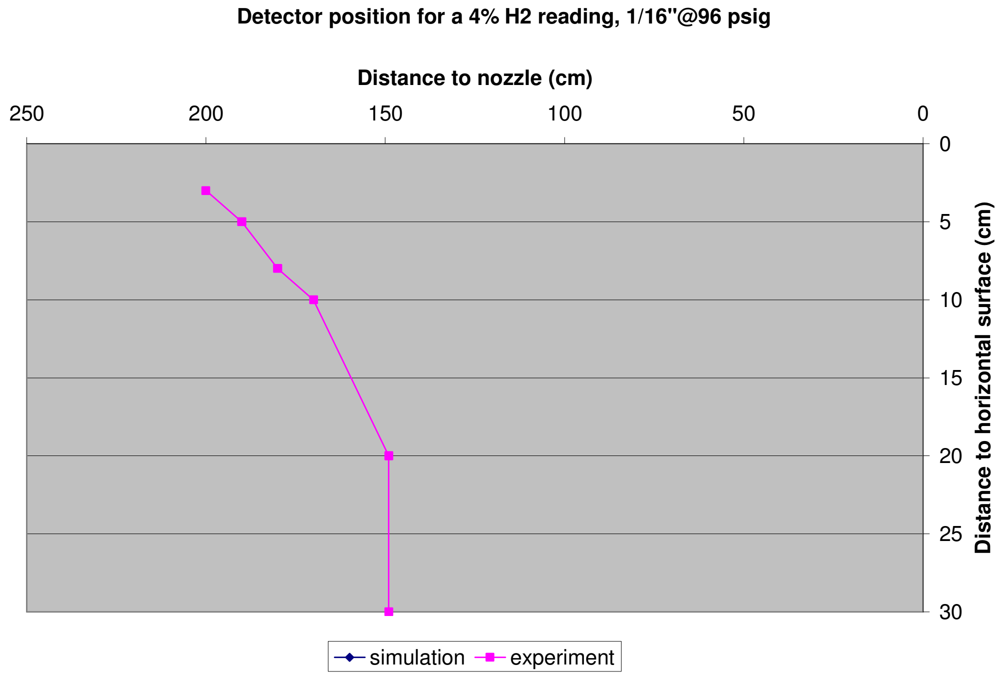


Figure 4 –Effect of the nearby ground (horizontal surface) on the length of the LFL cloud

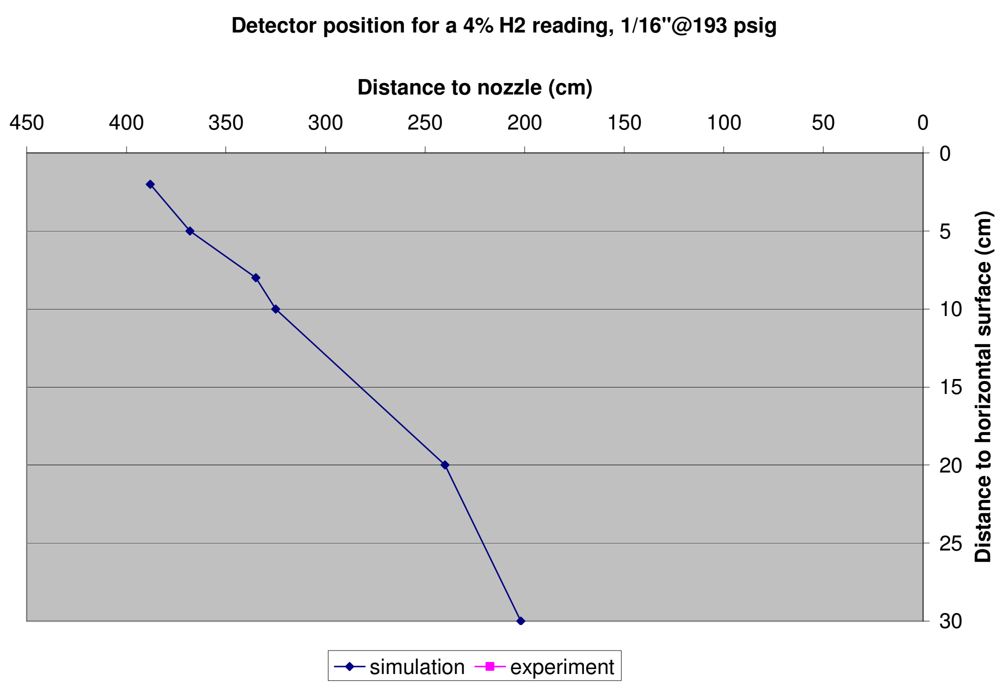
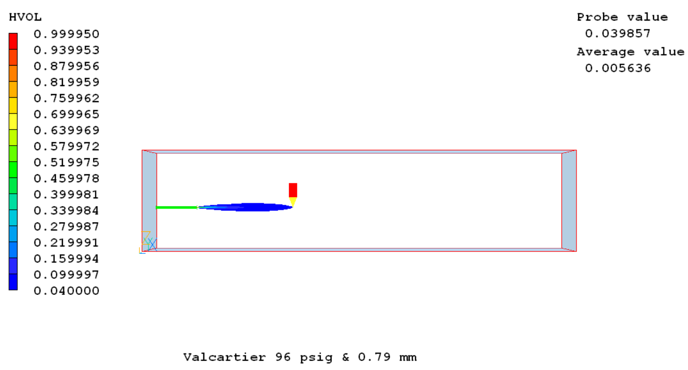
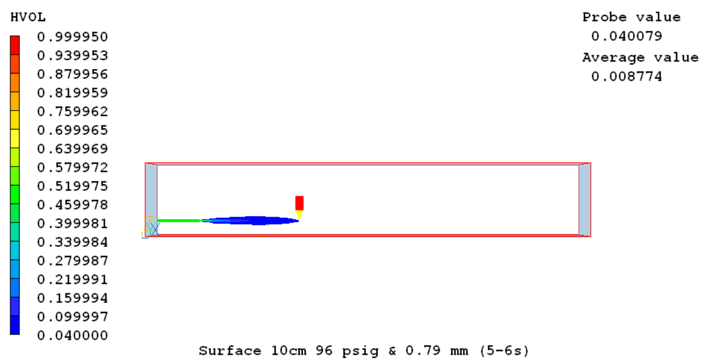
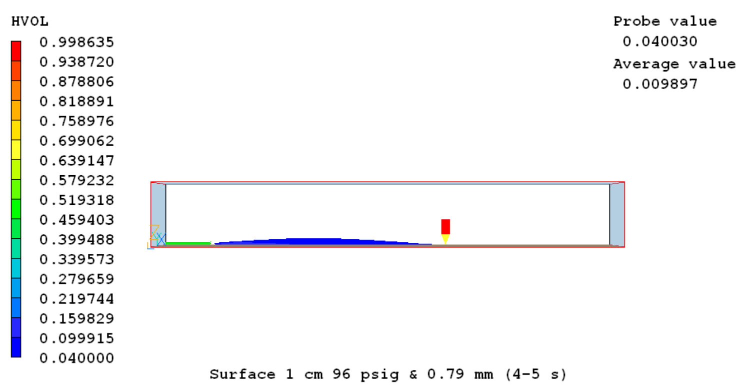


Figure 5 – Effect of the nearby ground (horizontal surface) on the length of the LFL cloud

Table 4. Comparison of free jet with wall jets CFD simulations (generated by PHOENICS) at 10 and 1 cm respectively at 96 psig and 0.79 mm release orifice

1	**Free jet**	**0.71 m**	
2	**10 cm to surface**	**0.72 m**	
3	**1 cm to surface**	**1.59 m**	

2.5 Comparison of free and wall jets at 0.79 mm orifice and various pressures

To further investigate the effect of pressure on LFL extent at the presence of a horizontal surface, the comparison was made between to pressure release conditions, namely 96 and 236 psig, at the same orifice size 0.79 mm or 1/32". The CFD modeling results (generated by PHOENICS) showing comparison of free jets and wall jets at 1 cm proximity to horizontal surface are shown in the Table 5 below.

As it can be seen from the table, proximity to ground may have a greater effect on LFL extent than an increase in pressure. Increase on pressure by 2.4 times from 96 to 236 psig resulted in 50% extent increase from 0.71 to 1.07 m, while moving the surface to 1 cm increased the extent from 0.71 to 1.59 m, i.e. 2.24 times! The effect of surface proximity at 236 psig is similar

2.6 Comparison of orifice and pressure effects on LFL extent in the presence of a surface: additional CFD results

Similar comparisons were performed at a different orifice, 1.6 mm, and pressure, 193 psig. Combined results are presented in Table 6 and Figure 6. below.

Table 5. Comparison of free and wall jets CFD simulations (generated by PHOENICS) at 1 cm from the ground at 96 and 236 psig respectively

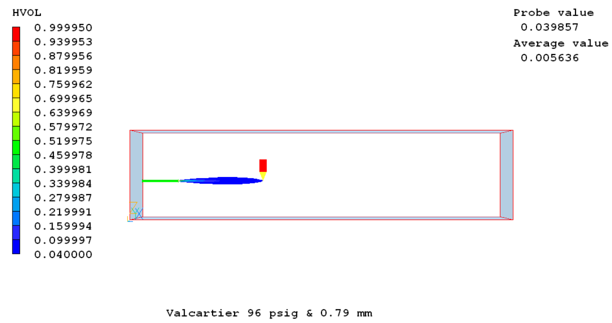
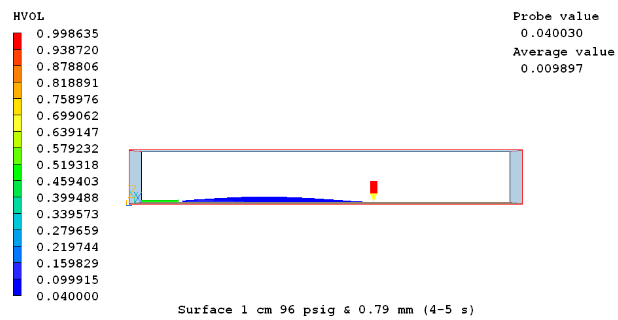
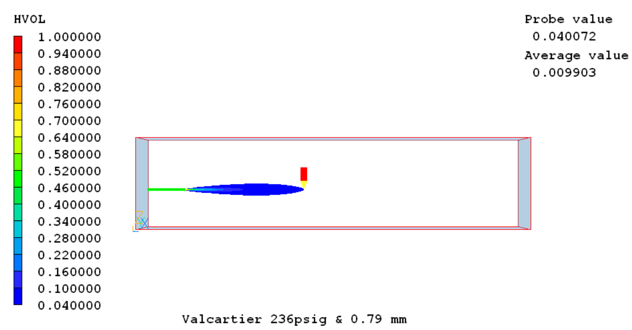
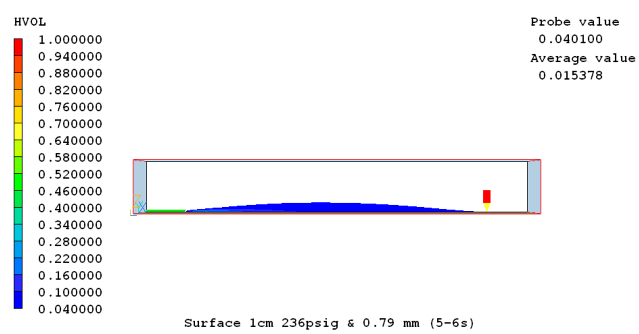
No	Designation	Extent	Results
1	Free jet at 96 psig	0.71 m	
2	1 cm from surface at 96 psig	1.59 m	
3	Free jet at 236 psig	1.07 m	
4	1 cm from surface at 236 psig	2.38 m	

Table 6. Comparison of free jets with horizontal wall jets CFD simulations (generated by PHOENICS) at various pressures and orifices vs proximity to horizontal surface

Pressure at the nozzle	Hole diameter	Free jet	Distance to horizontal surface (ground)						
			1 cm	2 cm	5 cm	8 cm	10 cm	20 cm	30 cm
96 psig	1/32 0.79 mm	0.71 m	1.59m	1.49 m	0.93 m	0.73m	0.72m	0.71m	0.71m
236 psig	1/32 0.79 mm	1.07 m	2.38m	2.20m	1.96 m	1.4 m	1.13 m	1.08m	1.07 m
193 psig	1/16 1.6 mm	1.96 m	4.04m	3.88m	3.68m	3.35m	3.25m	2.4m	2.02m

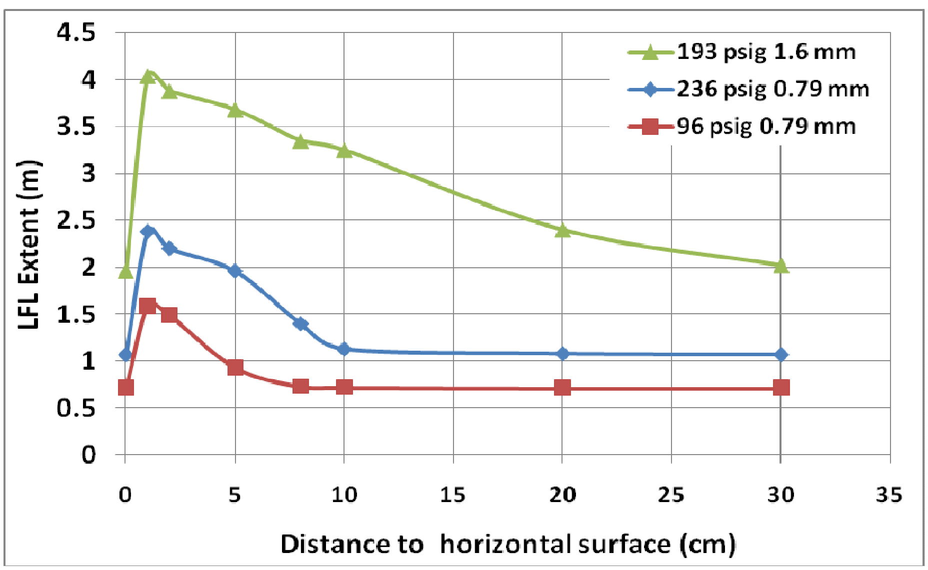


Fig. 6. LFL extent vs proximity to horizontal surface.

3.0 CONCLUSIONS

Experimental trials conducted with horizontal surfaces seem to qualitatively agree with CFD modeling predictions.

- **It appears that 1 cm proximity to horizontal surface results in approximately. doubling the LFL extent vs free jet at the same conditions of release**
- **Most of the effect occurs relatively close to the surface – within 10 cm for considered low pressures**
- **LFL extent appears to be more sensitive to release orifice size than to the release pressure.**

4.0 ACKNOWLEDGEMENTS

We thank the Natural Resources Canada for providing appropriate funding for this research project

5.0 REFERENCES

1-IEA HIA Task 19 Hydrogen Safety Work Plan, November 2007.

2-A. D. Birch, D. R. Brown, M. G. Dodson and F. Swaffield, "The structure and concentration decay of high pressure jets of natural gas", Combustion Science and Technology, 1984, Vol. 36, pp. 249-261.

3-W. Houf and R. Schefer, Predicting Radiative Heat Fluxes and Flammability Envelopes from Unintended Releases of Hydrogen, International Journal for Hydrogen Energy, 2006.