CFD MODELING OF HYDROGEN DISPERSION EXPERIMENTS FOR SAE J2578 TEST METHODS DEVELOPMENT

Tchouvelev, A.V.[1†], DeVaal, J.[2], Cheng, Z.[1], Corfu, R.[2], Rozek, R., and Lee, C.

[1]A.V.Tchouvelev & Associates Inc., 6591 Spinnaker Circle, Mississauga, ON, L5W 1R2 Canada
[2]Ballard Power Systems, 9000 Glenlyon Parkway, Burnaby, BC, V5J 5J9 Canada

ABSTRACT

This paper discusses the results of validation of Computational Fluid Dynamics (CFD) modeling of hydrogen releases and dispersion inside a metal container imitating a single car garage based on experimental results. The said experiments and modeling were conducted as part of activities to predict fuel cell vehicles discharge flammability and potential build-up of hydrogen for the development of test procedures for the Recommended Practice for General Fuel Cell Vehicle Safety SAE J2578. The experimental setup included 9 hydrogen detectors located in each corner and in the middle of the roof of the container and a fan to ensure uniform mixing of the released hydrogen. The PHOENICS CFD software package was used to solve the continuity, momentum and concentration equations with the appropriate boundary conditions, buoyancy effect and turbulence models. Obtained modeling results matched experimental data of a high-rate injection of hydrogen with fan-forced dispersion used to create near-uniform mixtures with a high degree of accuracy. This supports the conclusion that CFD modeling will be able to predict potential accumulation of hydrogen beyond the experimental conditions. CFD modeling of hydrogen concentrations has proven to be reliable, effective and relatively inexpensive tool to evaluate the effects of hydrogen discharge from hydrogen-powered vehicles or other hydrogen containing equipment.

1.0 INTRODUCTION

The purpose of dispersion experiments conducted by Ballard Power Systems at Powertech Labs was to simulate potential accumulation of hydrogen in a single car garage due to fuel cell vehicle flammable discharges from the tailpipe. Since performance of such experiments leads to accumulation of flammable atmospheres inside enclosures and, thus, presents certain risks to the test personnel and equipment, it is desirable to minimize the number of experiments and replace them with validated numerical simulations. Hence, the purpose of this research is to validate the calibrated CFD modeling [1, 2, 3, 4, 5] of hydrogen release and dispersion against experimental results obtained by Ballard and to apply validated models for predicting hydrogen concentrations beyond experimental conditions and areas of concentrations where reliable experimental measurements were not possible.

2.0 SET UP AND RESULTS OF DISPERSION EXPERIMENTS

2.1. Experimental set up description

The set up of Ballard hydrogen dispersion experiments is presented below. The experiments were conducted in a rectangular metal container representing a single car garage. Figure 1-3 show the geometry and experimental settings inside the container. Nine hydrogen sensors are placed inside the container to capture the transient hydrogen concentrations. Figure 2 shows the H_2 sensor numbering scheme. The basic boundary conditions are as follows: the container is a metal box made of steel, roughly 2.44 m × 2.44 m × 5.79 m, where it is pretty-much airtight, except for a 3.81 cm hole about 10.2 cm up from the floor roughly half-way down the side of the container (i.e., mid-way between H_2 sensors 3 and 7). For the experiments, wiring and instrumentation lines were fed through this hole. The hydrogen injection point was installed in front of an electric fan (shown on Figure 3) to simulate a radiator fan of a vehicle. The container has corrugated sides, and its internal volume is estimated to be

† Corresponding author. E-mail address: atchouvelev@tchouvelev.org

about 31 m^3 as measured by the gas volume of N_2 which was injected into the container. The doors of the container were kept open and the door opening was sealed with a plastic sheet (See Figure 4). Due to constant movement of the sheet (that acted like a "pump") it is believed that some very small air leaks at a few spots along the perimeter might have existed during the experiments.

Figure 1. Experimental settings inside the container: hydrogen sensor located at the corner of the container.

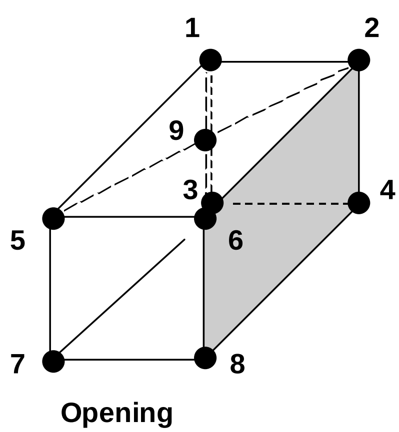

Figure 2. Locations of nine hydrogen sensors in the container.

The air exchange of the container can be expressed by the number of times the container's air is replaced from outside in an hour, or "air changes per hour". Because of the flapping of this plastic sheet it was difficult to establish experimentally the actual air exchange inside the container. It was first believed to be around 0.3 air changes per hour (ACH). Later during modelling it was possible to determine that the air exchange was at 0.1 ACH.

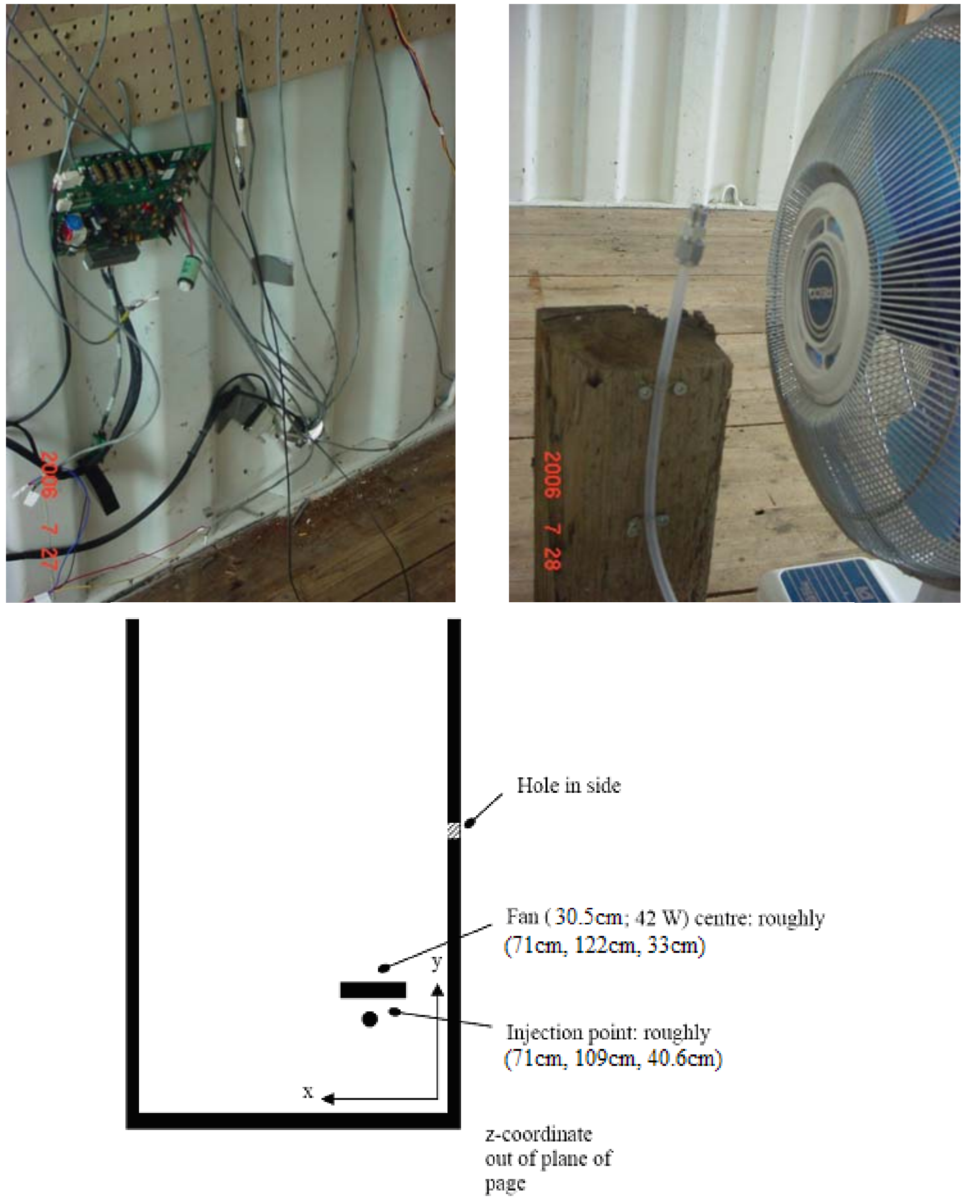

Figure 3. Pictures and schematic of the wiring hole, hydrogen injection point and electrical fan locations inside the container.

Figure 4. Plastic sheet covering perimeter of the door opening of the container.

The experimental geometry setting was directly plotted in the PHOENICS VR [6] user interface for the domain geometry and for the numerical simulations.

2.2. Injection flow rate

Figure 5 shows the hydrogen release rate with time.

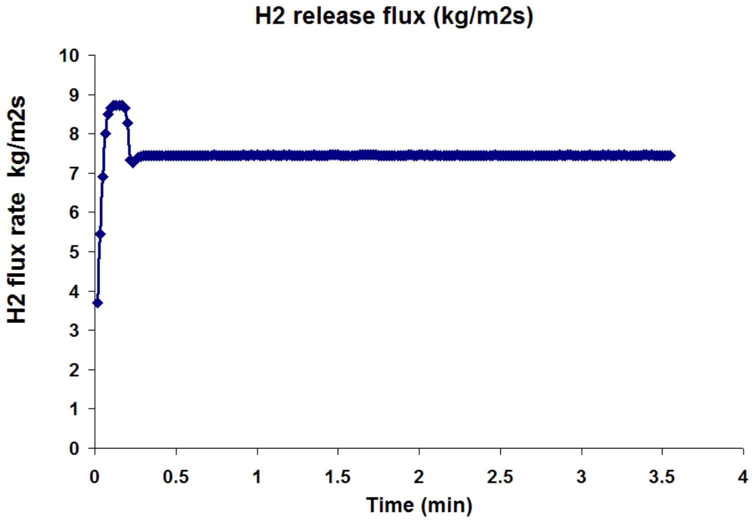

Figure 5. H_2 release rate with time (mass flux rate in kg/m^2s).

This H_2 flow rate is approximated to a formulation of polynomials for the time so that it can be easily implemented into our user-defined hydrogen release patch designed for the PHEONICS software package. The polynomial trend charts were obtained by the Microsoft Excel table.

Figure 6 top and bottom charts show the release flow rate from the onset of leak to 17 seconds and from 17 seconds to the end of the leak, respectively. The total duration of the release is about 214 seconds (3.6 minutes) and the average release rate is 5×10^{-3} m^3/s. The injection of 5×10^{-3} m^3/s H_2 occurred in front of an electric fan (Figure 3), where this stirred the room and (after a while) resulted in nearly uniform H_2 concentrations. The temperature was measured about waist-height roughly above the instrumentation hole on the side, but may be assumed to generally hold for the whole container. In the modeling scenario, it was assumed that the leak and dispersion are isothermal so temperature change was not considered because the hydrogen concentration distributions are nearly unaffected by the temperature.

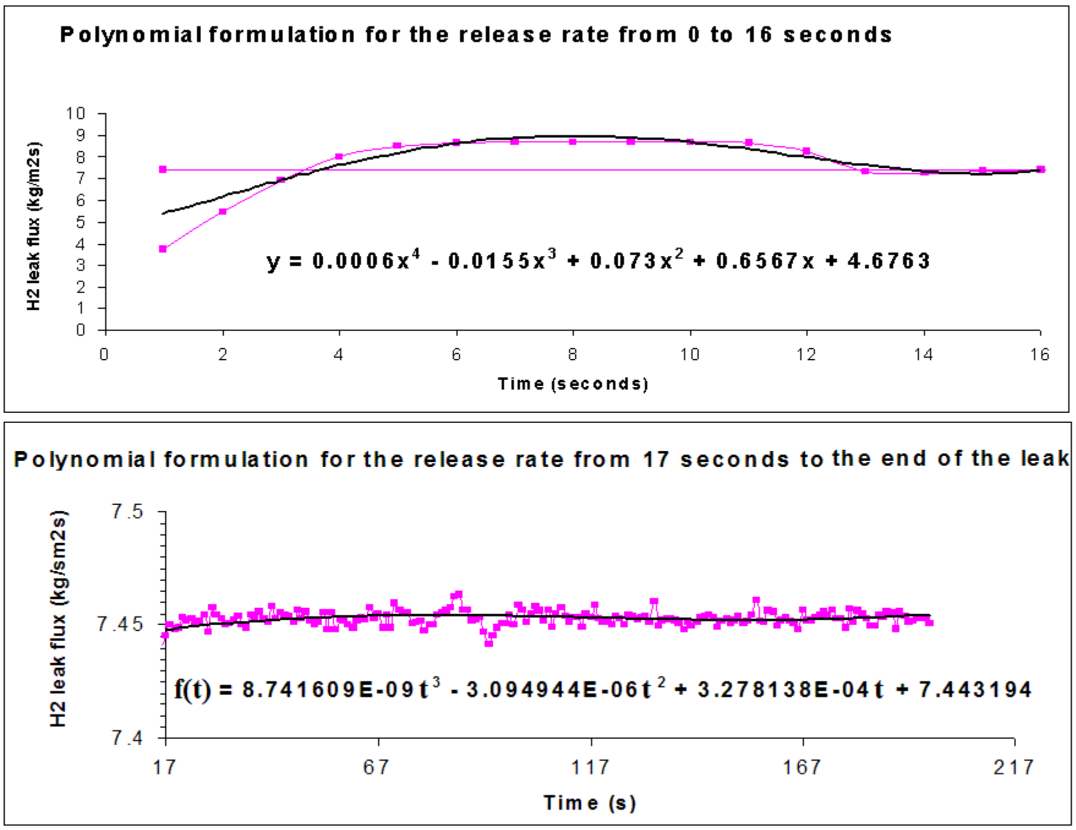

Figure 6. H_2 release flux rate (kg/m^2s) approximated by the polynomial formulations with time (seconds) (top: from the start of the leak to 16 seconds; bottom: from 17 seconds).

The hydrogen release flux (kg/m^2s) f(t) with time (seconds) can be approximated as follows:

$$f(t) = \begin{cases} 6.0\times10^{-4}t^4 - 0.0155t^3 + 0.073t^2 + 0.6567t + 4.6763 & 0 \le t \le 16 \\ 8.741609\times10^{-9}t^3 - 3.094944\times10^{-6}t^2 + 3.278138\times10^{-4}t + 7.443194 & 17 \le t \le 213 \end{cases}$$

The RKI H_2 sensors used in this test were generally brand new, and can likely be trusted to be accurate within about +/-0.01 (percent H_2) up to 4% vol.

2.3. Combined dispersion experimental results

The combined dispersion experimental results are presented in Figure 7.

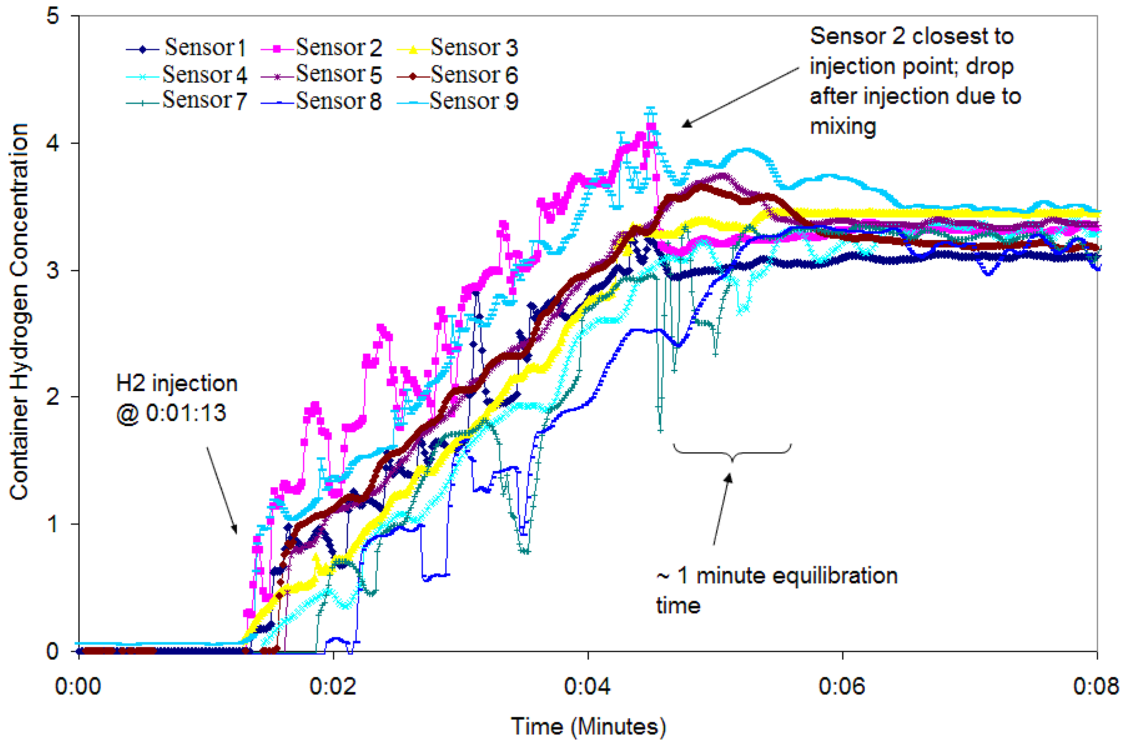

Figure 7. Combined dispersion experimental results

All nine sensors show similar behaviour during hydrogen injection and dispersion: first displaying continuous concentration increase during the injection phase, then collapsing around 3.3% vol. after the injection has stopped due to the strong convection force caused by the ventilation of the fan inside the container.

3.0 PHOENICS GEOMETRY AND NUMERICAL APPROACH

The electrical fan was running at speed 3, which produces 1.888 m^3/s (4,000 SCFM) swirl flow rate. A swirl number of 0.1 was used for the simulations. In the PHOENICS software package [6], the swirl number is defined as the ratio between the tangential and the axial velocity. The tangential velocity is constant across the fan diameter and the swirl number is also the tangent of the swirl angle. To set the boundary conditions (momentum attributes) at the fan, the PHOENICS interface was used for inputting the volumetric flow rate (1.888 m^3/s) and the specific swirl number (0.1) for the fan. The swirl direction is clockwise and the fan axis direction is positive in the current setting for the simulations.

3.1. The geometry for the PHOENICS software package

Table 1. Geometry of the objects in the current CFD modeling scenarios:

Objects	Dimensions			
	Location	X (m)	Y (m)	Z (m)

Domain	Location	0	0	0
	size	2.4384	5.7912	2.4384
Hole	Location	0	2.8956	0.1
	size	0.03378	0	0.03378
Electric fan	Location	0.6366	4.572	0
	size	0.362	0.24765	0.478
Leak orifice	Location	0.7112	4.7	0.4064
	size	0.00848	0.00848	0

3.2. Numerical approach

The RNG k-ε model (renormalization group k-ε turbulence model) was selected as the turbulence model for computational tasks in this project.

To account for the effect of hydrogen buoyancy, the gas mixture density was calculated from the mass concentration of hydrogen, C1, with coefficients based on the gas constants of air and hydrogen under the specified conditions. The buoyancy force, acting on the fluid particles, was proportional to the difference between the transient local gas mixture density and the constant reference density of air under the specified conditions. As a result, the significance of the buoyancy force in various container locations depended on the transient 3-D, C1 distribution. The latter was calculated from the standard mass conservation equation of hydrogen.

For dispersion experiment, the simulation was performed first by the non-leak transient state run for the 73 seconds so that the fan effect can be captured. This is the exact time period when the injection of hydrogen starts as shown in Figure 7. After that, a transient leak period for 213 seconds was simulated using the incompressible hydrogen mass transport equation. Finally, the hydrogen dispersion after the stop of the leak was simulated for 200 seconds. The time steps and sweeps for each time step used during the non-leak and leak period are shown as follows:

Table 2. Numerical steps and sweeps for the simulations

Period	Time (s)	Steps	Time per step	Sweeps	Leak type
Before leak	0 – 73	365	0.2	50	No leak
Leak	0 – 17	340	0.05	70	Leak
	17 – 214	3940	0.05	30	Leak
After leak	0 – 200	1000	0.2	30	No leak

A structured mesh of 39×37×34 with the local mesh refined near the leak injection was used for the simulations. The sensitivity study performed in the current research showed that this is the optimal mesh. Figure 8 shows the domain and the mesh used, with a red pencil, which marks the leak location, in front of the fan. The sensor locations are marked by green blocks.

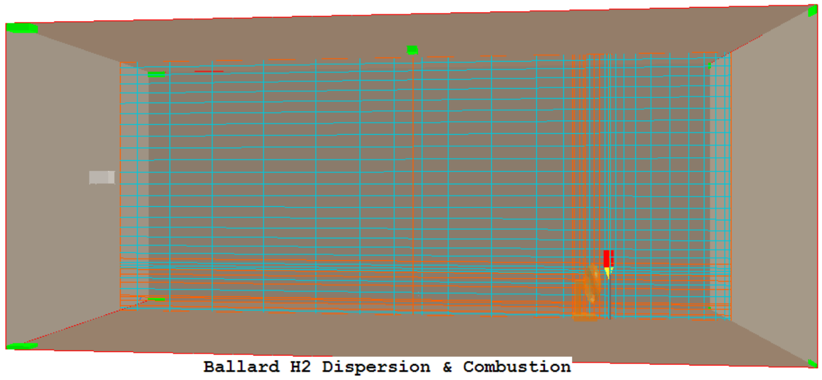

Figure 8. The domain and the structured mesh for the simulations.

4.0 NUMERICAL RESULTS

4.1. Before leak simulation results

Figure 9 shows the Y-Z plane velocity profile inside the domain (front view). Strong velocity vectors caused by the 42 W electrical fan across the leak orifice enhance the hydrogen dispersion inside the domain. Figure 10 shows the velocity profile in the X-Z plane, in which the swirl effects of the fan are clearly visible. The fan caused complicated vortices in the hydrogen leak direction.

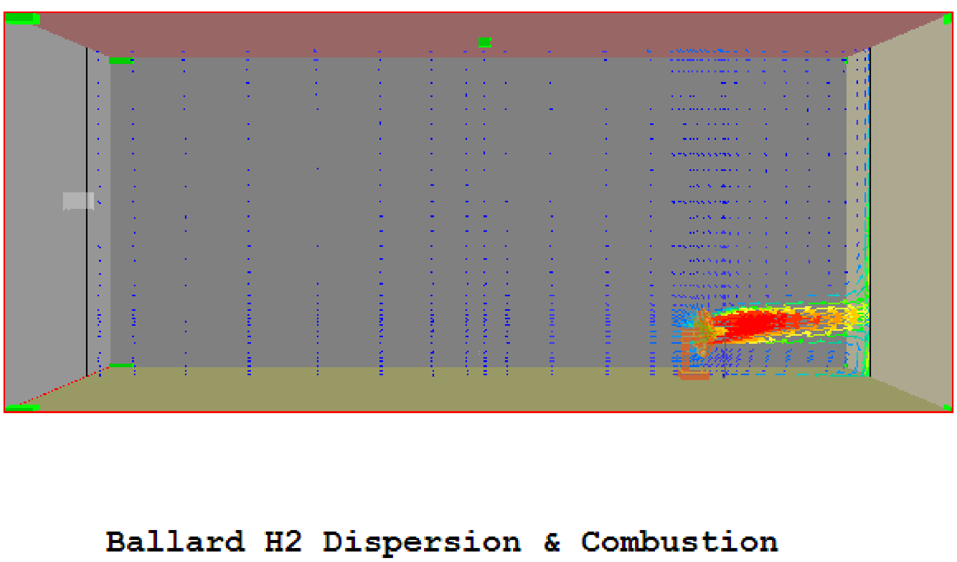

Figure 9. Velocity profile inside the domain before the hydrogen injection. (It shows the fan's potential effect on the H_2 leak)

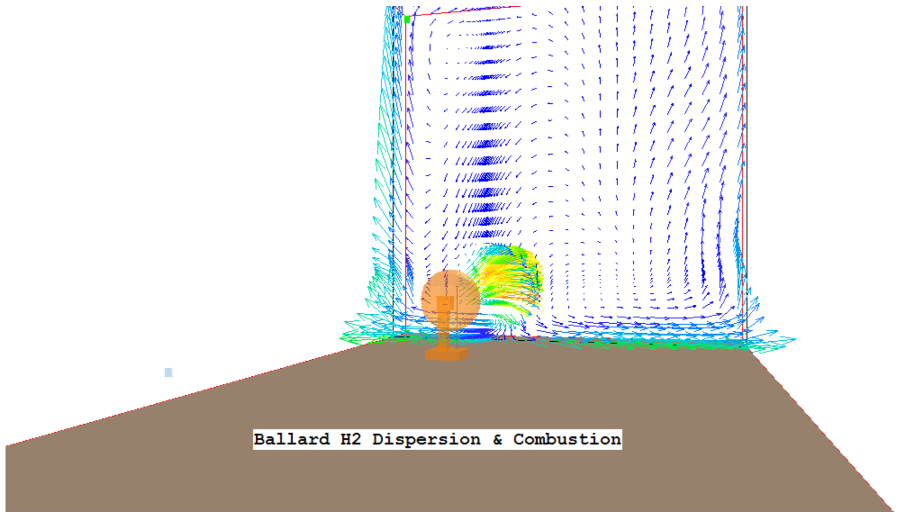

Figure 10. Swirl velocities caused by the electric fan in front of the leak.

4.2. Comparison of experimental and simulation results

Figures 11 to 14 show as examples the comparison of the experimental data with the simulation results for sensors 1 and 2 (top sensors), and 7 and 8 (bottom opposite sensors). The simulation results are within 10% to 15% for all nine sensors.

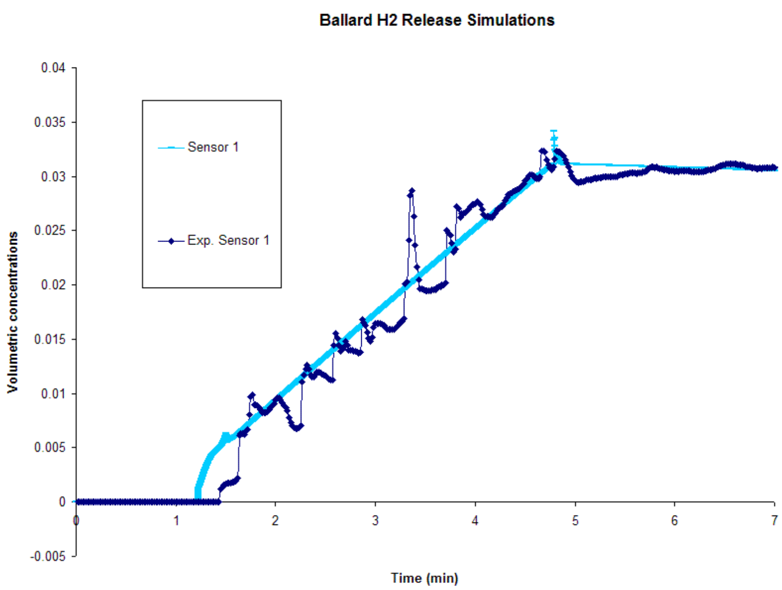

Figure 11. Simulation results vs. experimental data at sensor 1

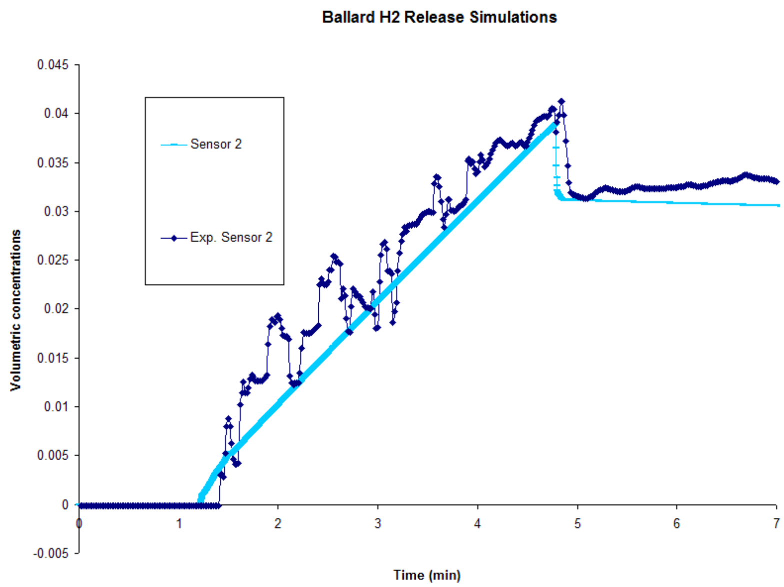

Figure 12. Simulation results vs. experimental data at sensor 2

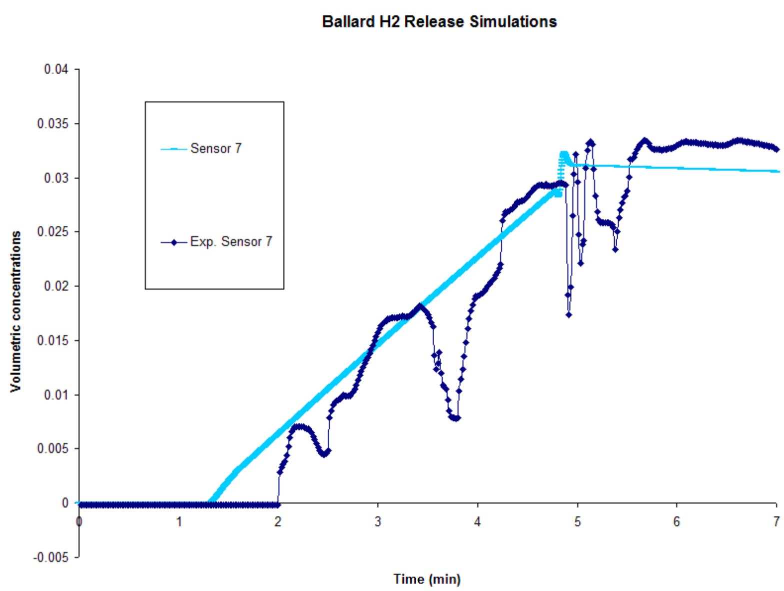

Figure 13. Simulation results vs. experimental data at sensor 7

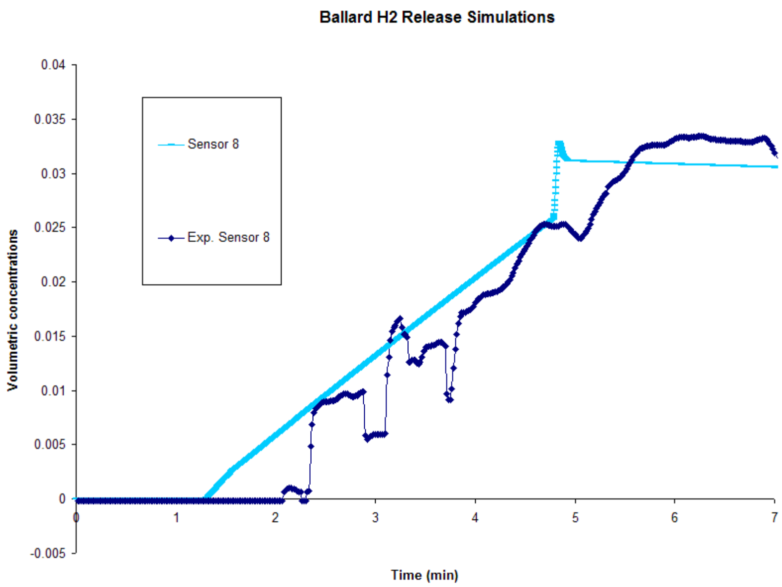

Figure 14. Simulation results vs. experimental data at sensor 8

5.0 CONCLUSIONS

This paper presented the results of validation of Computational Fluid Dynamics (CFD) modeling of hydrogen releases and dispersion inside a metal container imitating a single car garage based on experimental results. The said experiments and modeling were conducted as part of activities to predict fuel cell vehicles discharge flammability and potential build-up of hydrogen for the development of test procedures for the Recommended Practice for General Fuel Cell Vehicle Safety SAE J2578. The PHOENICS CFD software package was used to solve the continuity, momentum and concentration equations with the appropriate boundary conditions, buoyancy effect and turbulence models. Obtained modeling results matched experimental data of a high-rate injection of hydrogen with fan-forced dispersion used to create near-uniform mixtures with a high degree of accuracy (within 15%). This supports the conclusion that CFD modeling will be able to predict potential accumulation of hydrogen beyond the experimental conditions. CFD modeling of hydrogen concentrations has proven to be reliable, effective and relatively inexpensive tool to evaluate the effects of hydrogen discharge from hydrogen-powered vehicles or other hydrogen containing equipment.

6.0 REFERENCES

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