

CFD SIMULATIONS OF HYDROGEN RELEASE AND DISPERSION INSIDE THE STORAGE ROOM OF A HYDROGEN REFUELING STATION USING THE ADREA-HF CODE

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ABSTRACT

The paper presents CFD simulations of high pressure hydrogen release and dispersion inside the storage room of realistic hydrogen refueling station and comparison to experimental data. The experiments were those reported by Tanaka et al. (2005), carried out inside an enclosure 5 m wide, 6 m long and 4 m high having 1 m high ventilation opening on all sidewalls (half or fully open) containing an array of 35 x 250 L cylinders. The scenarios investigated were 40 MPa storage pressure horizontal releases from the center of the room from one cylinder with orifices of diameters 0.8, 1.6 and 8 mm. The release calculations were performed using GAJET integral code. The CFD dispersion simulations were performed using the ADREA-HF CFD code. The structure of the flow and the mixing patterns were also investigated by presenting the predicted hydrogen concentration field. Finally, the effects of release parameters, natural ventilation and wind conditions were analyzed too.

1. INTRODUCTION

Growing energy security and environmental concerns have prompted the exploitation of hydrogen as an alternative to petroleum. Hydrogen delivery to its end use is an essential component of any hydrogen energy infrastructure. Hydrogen must be transported from the point of production to the point of use and handled within refueling stations so that it can be dispensed into the fuel cell vehicles.

Nowadays, new hydrogen refueling stations are built world wide for demonstration purposes. Apart from any possible technical problems in producing, storing and delivering H₂ there are also safety concerns since H₂ once mixed with air may explode. Thus, to demonstrate that H₂ refueling stations are designed with an acceptable level of safety is vital before introducing H₂ as a fuel for vehicles in a larger scale.

This paper presents CFD simulations of H₂ release and dispersion inside the storage room of a realistic refueling station and compares the results of the simulations with the experimental data reported by Tanaka et al. [1]. It aims to predict the dispersion of H₂ in realistic scenarios and therefore to contribute to the development of safe H₂ systems and facilities.

2. EXPERIMENTAL DESCRIPTION

Figure 1 shows the modeled site geometry of the layout of the hydrogen refueling station used for the dispersion and explosion experiments of Tanaka et al. [1]. This figure shows the case of the storage room with fully open vent openings. Figure 3 shows the modeled site geometry of the hydrogen refueling station with a storage room with half open vent openings. The design of the refueling station was selected by Tanaka et al. [1] to represent 300 Nm³/h H₂ production capacity, 500 Nm³/h H₂ compressor flow, 3500 Nm³ H₂ storage and two H₂ dispensers. The station consisted of a compressor room, a gas storage room located on the right of the compressor room used to store H₂ in 35 cylinders, a buffer tank, a natural gas reformer unit, a pure water unit, a pump and an extra compressor, a cooling tower, a ventilation stack, a service house and the previously mentioned two dispensers with a canopy construction for weather protection. Two of the four sides of the station were fenced by 2 m high and 150 mm thick walls. The other two sides were left partially open to represent a station located near a road junction. It should be noted that some dimensions of the layout were either missing or not clearly written thus they had to be assumed for the site geometry to be complete.

Figure 2 shows the modeled storage room with the cylinders of 250 L capacity placed inside the room. The room was 5 m wide, 6 m long and 4 m high. A gap of 1 m between the roof and the side walls was placed to provide natural ventilation. The gap was completely open, as shown in Figure 2, or meshed leaving a 50% open vent area. The authors of the experiments mentioned that the H₂ releases from one cylinder were taken to be representative worst-case scenarios. Finally, the initial pressure of the cylinder for the majority of the experiments was 40 MPa.

The dispersion experiments were carried out inside the storage room filled with 35 cylinders. The cylinders were placed in two arrays. The exact dimensions and the location of the cylinders were again assumed for the subsequent simulations. Three sizes of leak were employed (0.8 mm, 1.6 mm and 8 mm) while the ventilation openings were either fully or half open as mentioned above. Table 1 presents the experiments of the 250 L cylinder mentioned in the work of Tanaka et al. [1].

Table 1. Experiments' Matrix

Case 1	0.8 mm leak size, half open ventilation openings
Case 2	1.6 mm leak size, half open ventilation openings
Case 3	8 mm leak size, half open ventilation openings
Case 4	8 mm leak size, fully open ventilation openings

The location of the leak was at the centre of the storage room whilst its direction was horizontal. Again, there was no mention on the exact direction of the leak (either x directed or y directed leak). Consequently both of them were considered possible.

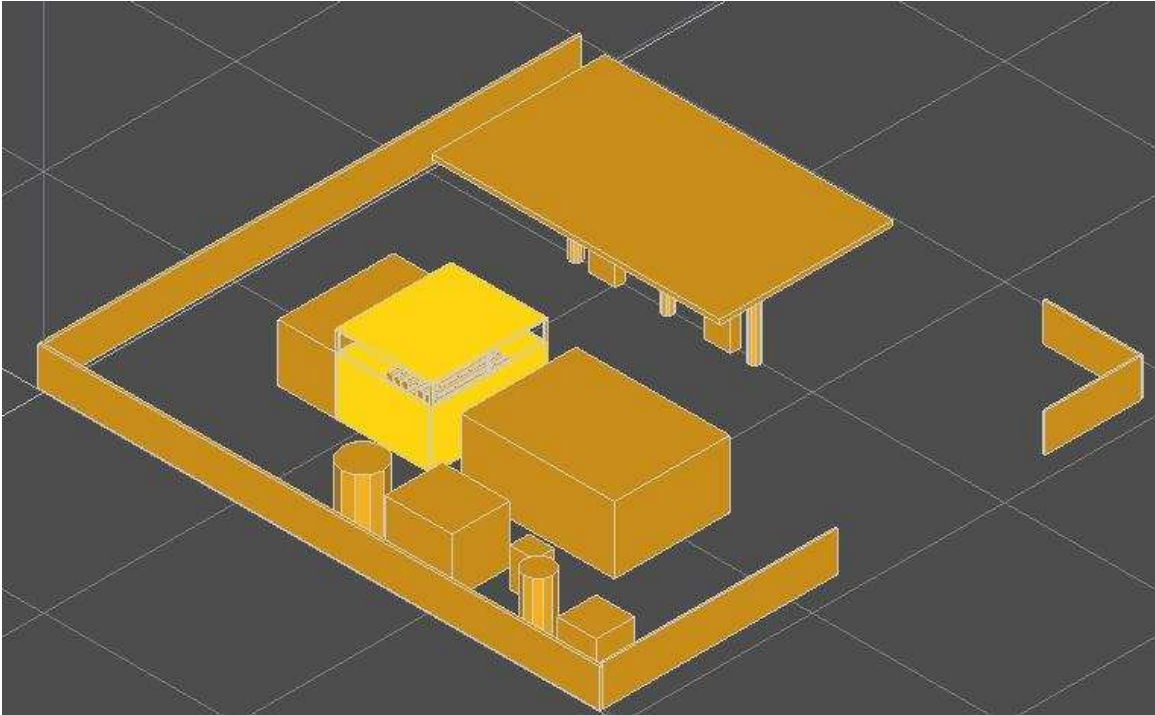


Figure 1. Modelled Site Geometry of the H₂ Refuelling Station (storage room -coloured in yellow- with fully open ventilation openings)

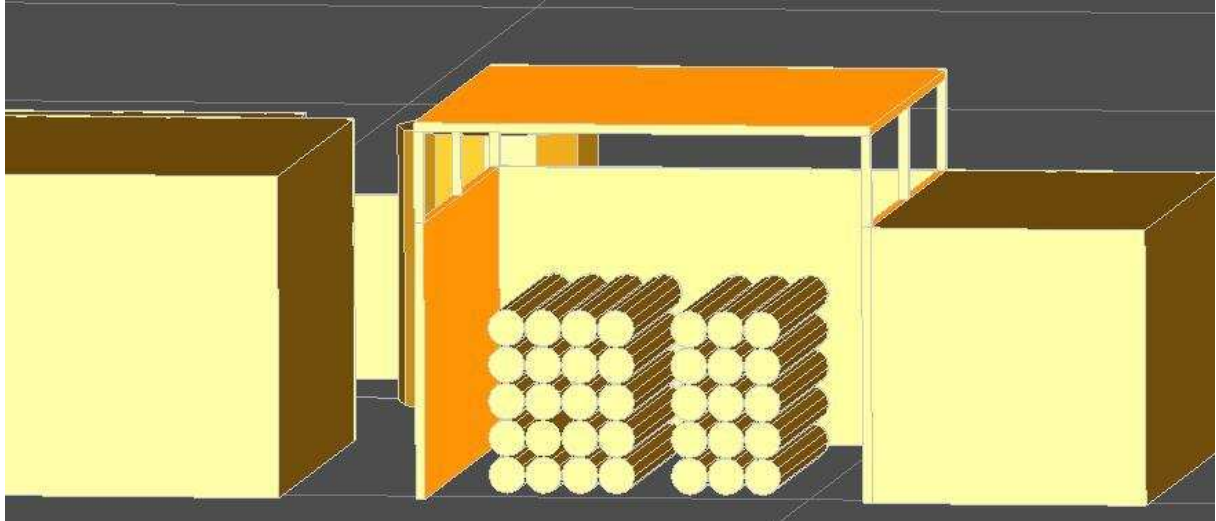


Figure 2. Interior of the Modelled Storage Room with the 35 Cylinders (room with fully open ventilation openings)

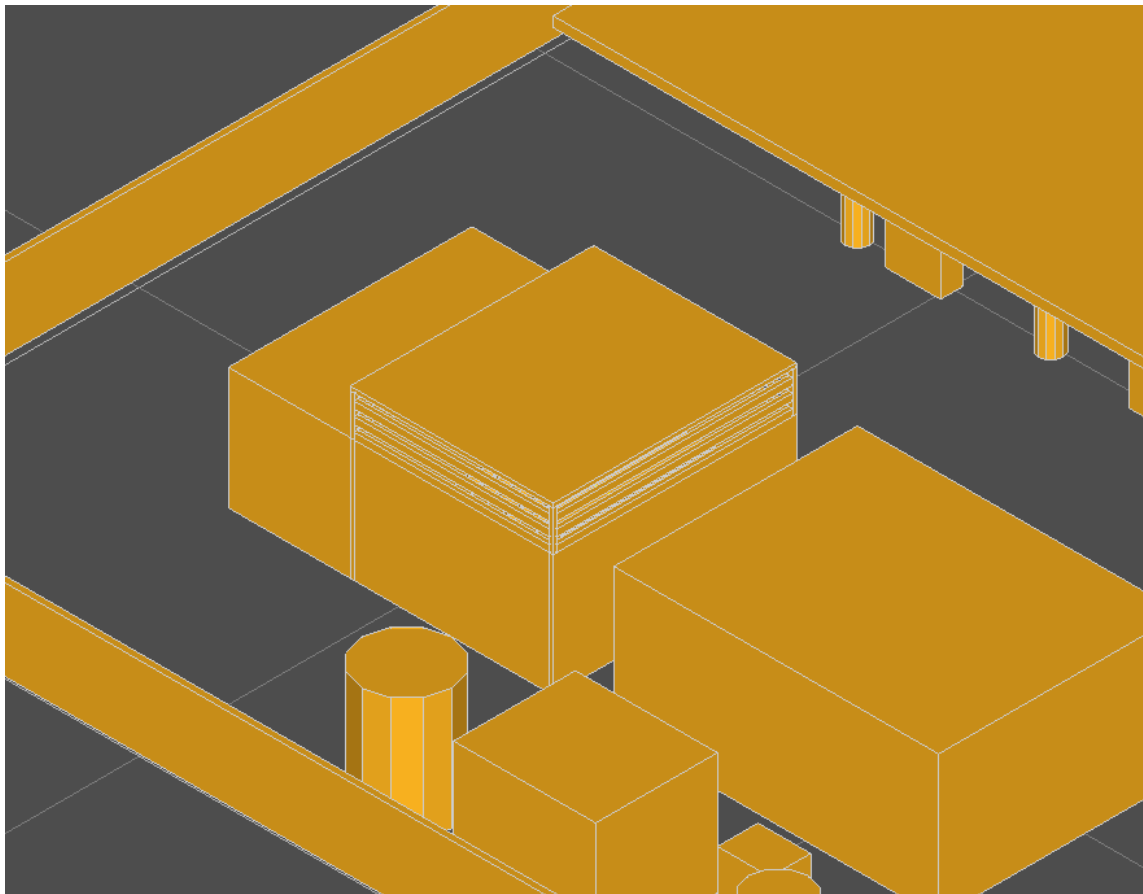


Figure 3. Modelled Site Geometry of the H₂ Refuelling Station (storage room with half open ventilation openings)

3. MODELING STRATEGY

The strategy adopted consisted of two stages. The first was the release source calculations and the second was the dispersion calculations. The release source calculations provided the necessary release conditions for the subsequent dispersion calculations.

3.1 Release Source Calculations

The release source calculations were performed using the integral code GAJET [2]. An isentropic change was assumed and the flow was considered sonic. The temporal variation of temperature, pressure, density and velocity were calculated as exit conditions for the three different sizes of the leak (0.8 mm, 1.6 mm and 8 mm). The relevant model equations are given in detail in [2]. Figure 4 shows the variation of the pressure inside the storage cylinder with time, which is compared with the experimental data and with some predictions reported by Tanaka et al. [1]. The authors mentioned that their predictions were based on perfect gas behavior. As can be seen there is a very good agreement between the experimental data and the calculations for all leak sizes. Furthermore, the H₂ content of the cylinder from the 8 mm leak size was rapidly released into the environment (the first 20 seconds) whilst for the rest of the cases the contents were partially released at the end of 100 seconds. This fact makes the release from the 8 mm nozzle the worst case of all three as such a rapid release is difficult to be detected on time. Consequently, any further measures (shut of any valves) to prevent the H₂ supply before most of it is released is very difficult.

The results from GAJET [2] were then taken as inputs for the calculation of the fictitious area using the Birch approach [3]. Figure 5 shows the calculated fictitious diameter for the three initial leak sizes as function of time. The H₂ jet was modeled as a circular source area whose diameter changed with time according to Figure 5. Other conditions at the source were sonic velocity and atmospheric pressure and temperature. The size of the cell in which the jet was located was set approximately equal to the average (in time) fictitious diameter for each case.

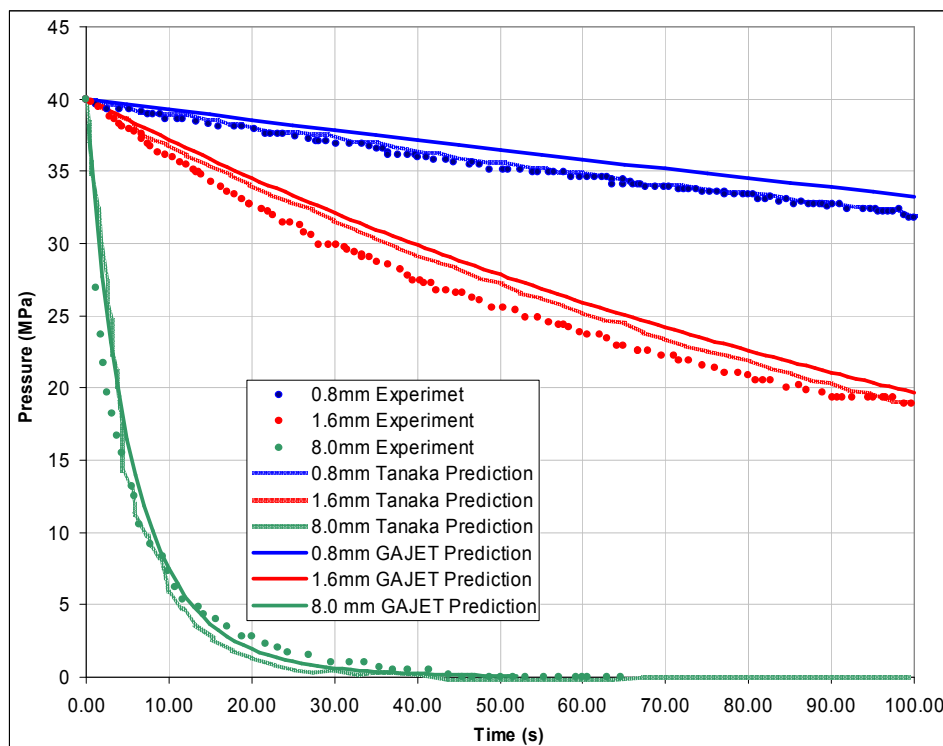


Figure 4. Comparison of Pressure Time History Plots Inside the Storage Cylinder

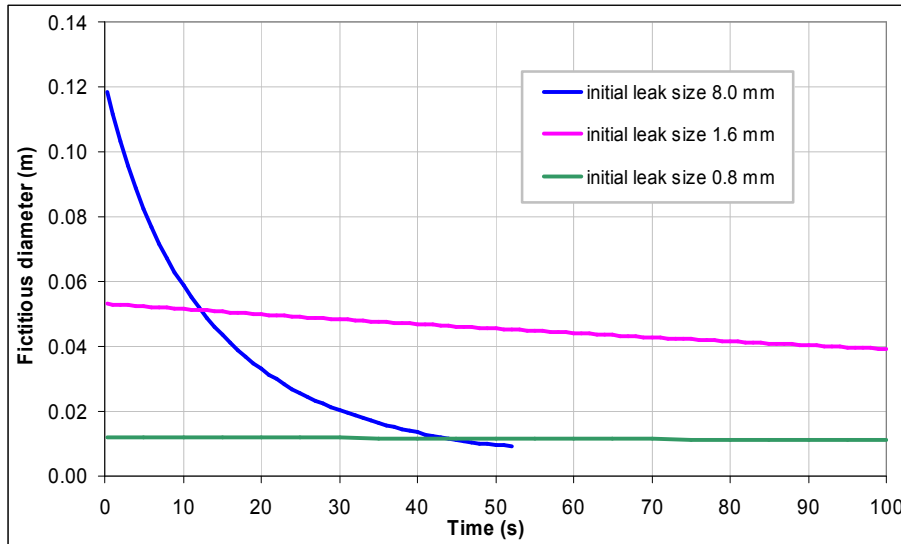


Figure 5. Calculated Fictitious Diameter Using the Birch Approach

3.2 Dispersion Calculations

The dispersion calculations were performed using the ADREA-HF CFD code [4]. Validation studies of the ADREA-HF code for gaseous H₂ release and dispersion can be found in Venetsanos et al. [2], Gallego et al. [5] and Papanikolaou et al. [9].

The following table, Table 2, presents the simulated cases. From the description of the experiments there was no indication on the exact direction of the release apart from being horizontal. Thus, it was decided to simulate initially the two possible directions (x and y) of the 0.8 mm leak size and from the comparison of the results with the experimental ones to conclude on the direction that the experiments were done. Furthermore, even though it was mentioned at the experimental work [1] that wind conditions did exist, there was no other information on the meteorological conditions. Again, the conditions had to be assumed. It was decided to simulate dispersion with stagnant and D2 meteorological conditions, which refer to a wind speed of 2 m/s at 10 m height and neutral atmospheric stability. For the D2 meteorological conditions two different wind directions were examined, expressed below as west and north, based on where the wind is blowing from. The cases termed as West D2 Wind, refer to wind blowing from the negative X direction whilst the cases termed as North D2 Wind, refer to wind blowing from the positive Y direction. It should be noted that the selection of the two wind directions was random. The experiments of 8 mm leak size (with fully open and half open ventilation openings) were then simulated as they represent the worst case of the three release leak sizes as mentioned above. The case of 1.6 mm leak size was omitted as the authors thought that it will not contribute to any substantial additional information.

Table 2. Dispersion Calculation Matrix

	0.8 mm leak diameter with half open vents	8 mm leak diameter with fully open vents	8 mm leak diameter with half open vents
X directed leak	Stagnant Conditions	Stagnant Conditions	Stagnant Conditions
	West D2 Wind	West D2 Wind	West D2 Wind
	North D2 Wind	North D2 Wind	North D2 Wind
Y directed leak	Stagnant Conditions	Not simulated	Not simulated
	West D2 Wind	Not simulated	Not simulated
	North D2 Wind	Not simulated	Not simulated

The computational domain extended the domain of the experimental facility by 20 m in the x and y direction. This was decided following common methodology of computational domain design that suggests that in geometries that contain obstacles the domain should be extended at least 10 times the size of the obstacles. In this case, the walls and fences surrounding most of the refueling station had 2 m height. The computational domain dimensions were 69 m by 68 m by 20 m in the x, y and z direction respectively. Figure 6 shows the grid used of the 8 mm with x direction leak case (top view) whilst Figure 7 shows the grid inside the storage room of the same case. As mentioned above, the calculated fictitious diameter determined the minimum cells size of each case. Furthermore, when the leak was x directed, the minimum cell size was in the y and z direction whereas when the leak was y directed the minimum cell size was in the x and z direction. This was decided as experience has proved that it is acceptable to double or sometimes even triple the cell size in the same direction as the one of the leak without any loss of the calculations' reliability. Volume porosity and area permeability approach was used to model the complex geometrical layout with Cartesian grids. The geometrical pre-processing was performed with the DELTA-B Code [6]. Table 3 presents the main characteristics of the computational grid used in all cases.

Table 3. Computational Grid Main Characteristics

	0.8 mm leak diameter with half open vents	8 mm leak diameter with fully open vents	8 mm leak diameter with half open vents
X directed leak	Grid dimension: 75x92x56 Active cells: 361.698 Minimum cell size: 0.04 m	Grid dimension: 66x86x54 Active cells: 287.656 Minimum cell size: 0.05 m	Grid dimension: 66x86x54 Active cells: 287.624 Minimum cell size: 0.05 m
Y directed leak	Grid dimension: 87x71x56 Active cells: 325.846 Minimum cell size: 0.04 m	Not simulated	Not simulated

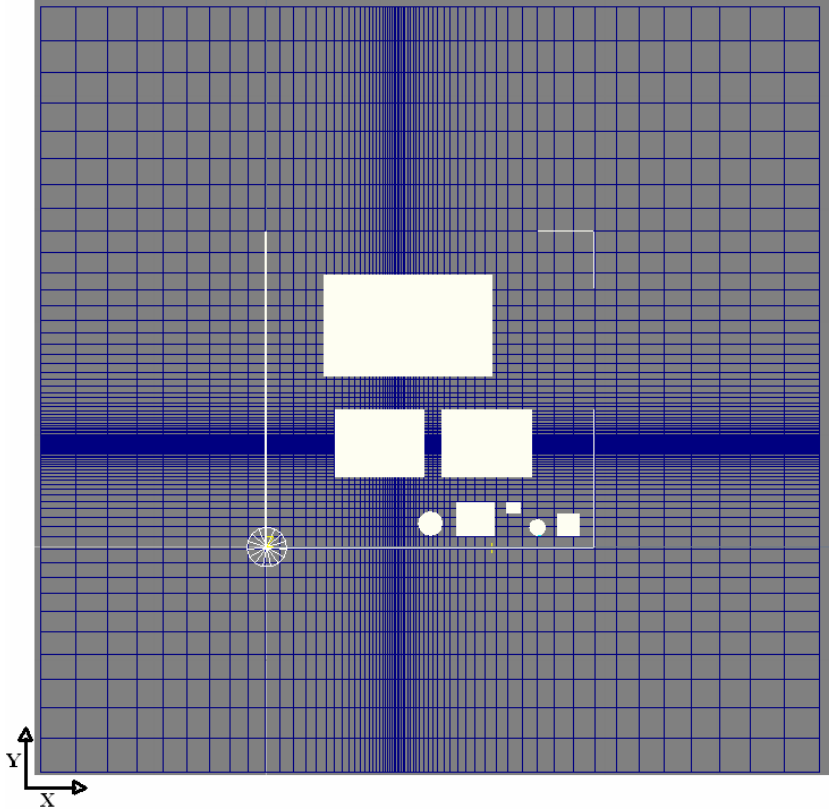


Figure 6. Grid Used (top view of 8 mm, x directed leak case)

Turbulence was modeled using the two equation standard k-epsilon model of Launder and Spalding [7], modified for buoyancy effects.

The mixing of H₂ with air was calculated by solving the three dimensional transient, fully compressible conservation equations for mixture mass (continuity equation), mixture momentum (for the three velocity components) and the H₂ vapor mass fraction transport equation.

Standard wall functions were used for velocity (no slip), turbulent kinetic energy and its dissipation rate on solid surfaces. A hydrodynamic roughness of 1 mm was assigned to all solid surfaces including the ground. A zero gradient condition for H₂ mass fraction was assigned to all solid surfaces.

A constant pressure boundary condition was applied at the top of the domain. Consequently, the normal velocity of this surface was obtained from the continuity equation. For the rest of the variables a zero gradient was automatically assumed in case of outflow from the computational domain and a given value (equal to the one existing at time zero) in case of inflow.

Inflow boundary conditions (a given value and zero gradient) were applied at the inflow plane for the cases with wind. On non clearly defined inflow lateral planes, a zero gradient was applied for normal velocity and zero gradient or given value (equal to the one existing at time zero) was automatically applied for the remaining variables, depending on whether outflow or inflow was calculated through the surface.

The numerical options used were the first order implicit scheme for time integration and the first order upwind scheme for the discretization of the convective terms [8]. An automatic time step increase/decrease mechanism was applied with 10⁻³ seconds initial time step. The increase of the time step was bounded by a maximum allowed time step of 5·10⁻² seconds.

When wind was present the simulations consisted of three steps. In the first step, the steady state one dimensional vertical profile of the wind velocity and turbulence was calculated. In the second step, the three dimensional flow field over the refueling station was calculated using the previously obtained profiles spread over the three dimensional domain as initial conditions. Finally, in the third step, the H₂ dispersion was calculated using the previously obtained three dimensional steady state field as initial condition. In cases where wind was absent the first and second step was omitted.

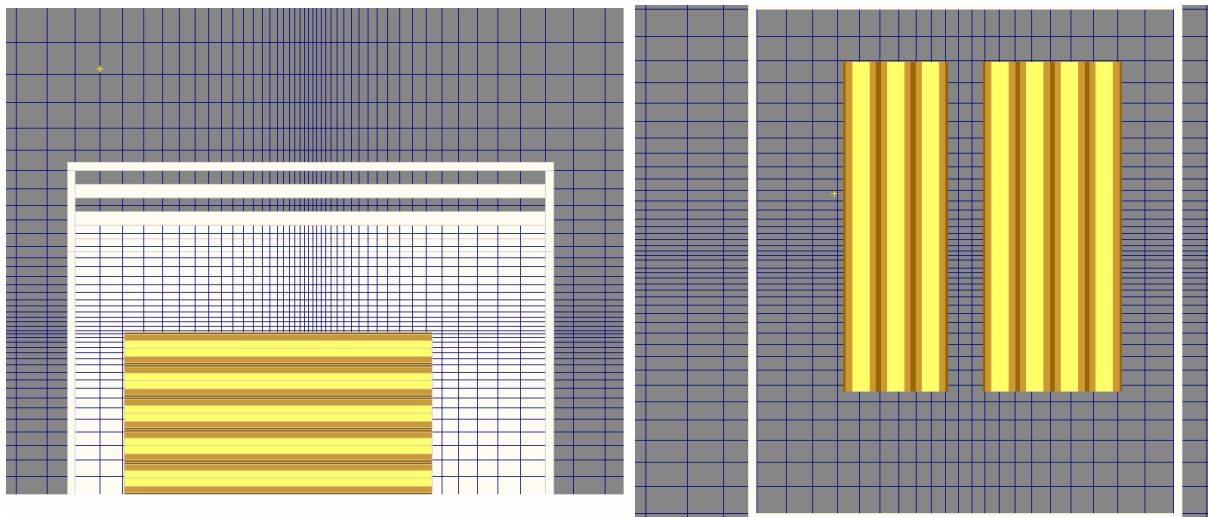


Figure 7. Grid Used Inside the Storage Room (8 mm, x directed leak) – Side View (left figure) and Top View (right figure)

4. RESULTS AND DISCUSSION

Figure 8 shows the predicted average H₂ concentrations (% by volume) versus the measured and the predicted given in Tanaka et al. [1] inside the storage room of the 0.8 mm leak release case. The average H₂ concentration (\bar{C}) was calculated using the following equation:

$$\bar{C} = \frac{\int_{M_{initial}}^{M_{last}} C \cdot dV}{\int_{M_{initial}}^{M_{last}} dV} \quad (1)$$

where C is the H₂ concentration (% by vol.) of each computational cell, V is its volume (m³) and $M_{initial}$ and M_{last} is the first and last cell located inside the storage room.

Comparing the red with the blue line one concludes that the direction of the leak affects the results significantly. Clearly, the blue line (case of x directed leak) is closer to the experimental. This can be attributed to the, relative to the leak direction, position of the obstacles which are the 35 cylinders. A closer look at the storage room reveals that when the leak is directed in the x axis, the H₂ hits the cylinders almost immediately after its release. Furthermore, the free path of the H₂ stream is by far less than the one that it will have to travel before meeting the first obstacle when it is directed in the y axis. It should be mentioned that when the leak is directed in the y axis the first obstacle that the H₂ meets is the wall after traveling 3 m whereas when the leak is directed in the x axis the H₂ meets the cylinders after traveling 0.4 m. Thus, the presence of obstacles enhances the diffusion of H₂.

Comparing the red with the purple and yellow line and the blue with the green and brown line one concludes that the presence of wind affects the results too. The wind irrespective of its direction sweeps the released H₂ and creates more turbulence compared to the stagnant cases.

From the results of the 0.8 mm leak size the authors believed that the x direction was more likely to be the direction of the leak used in the experiments. Furthermore, even the presence of weak wind affects the simulated results.

Figure 9 and Figure 10 shows the predicted LFL (Lower Flammability Limit) cloud of the 0.8 mm, x directed leak West D2 case at 10 and 50 seconds respectively whilst Figure 11 shows the predicted LFL cloud inside the storage room of the same case. As can be seen most of the LFL cloud is limited inside the storage room while it exits from the side of the ventilation openings opposite the wind direction. These figures reveal the wind aided ventilation of the storage room.

Figure 12 shows the predicted average H₂ concentrations (% by vol.) versus the measured and the predicted given in Tanaka et al. [1] inside the storage room of the 8 mm leak size release with half open ventilation openings. The results of the previous case lead to the decision to simulate only the leak with x axis direction. Again, stagnant and the two wind directions were simulated. The predicted average H₂ concentrations follow the trend of the experimental data while showing an overprediction of the maximum concentration at 10 seconds. Furthermore, a small effect of the presence of wind is still present.

Figure 13 shows the predicted average H₂ concentrations (% by vol.) versus the measured inside the storage room of the 8 mm leak release with fully open ventilation openings. Again, the predicted average H₂ concentrations follow the trend of the experimental data showing the first peak of the concentration at 10 seconds overpredicted. Stagnant and North D2 cases predicted the second smaller peak of the experimental data at 20 seconds.

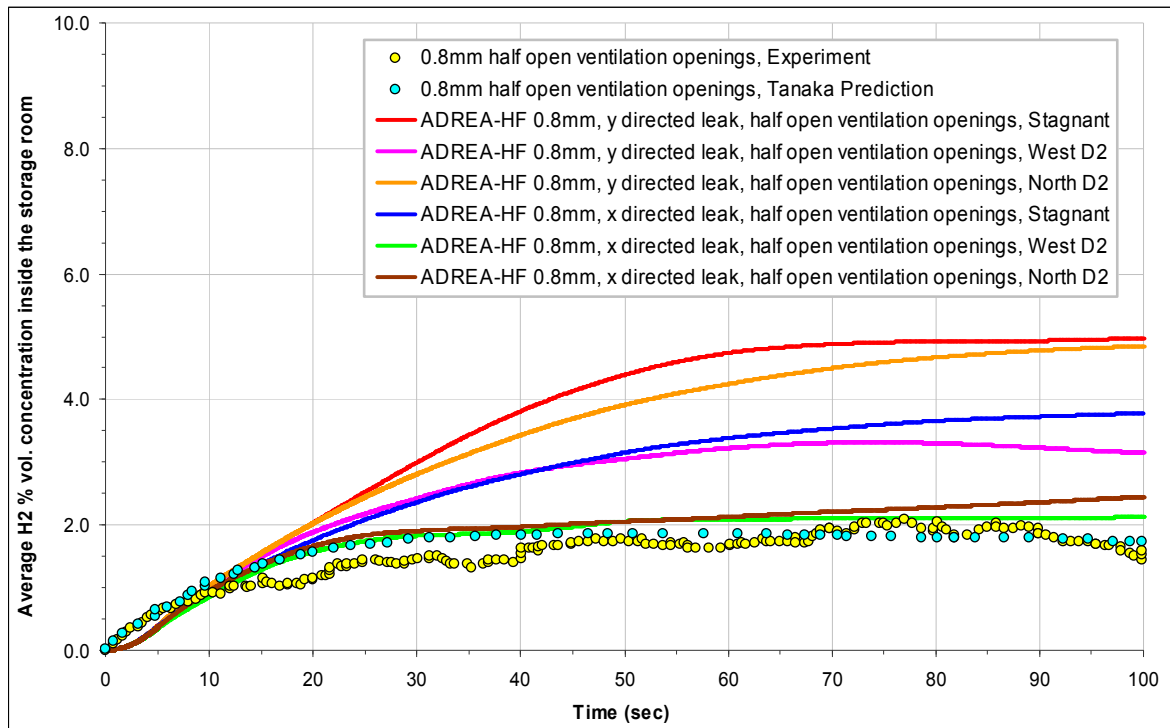


Figure 8. Average H2 % Concentration in the Storage Room (0.8 mm initial leak size, half open vents)

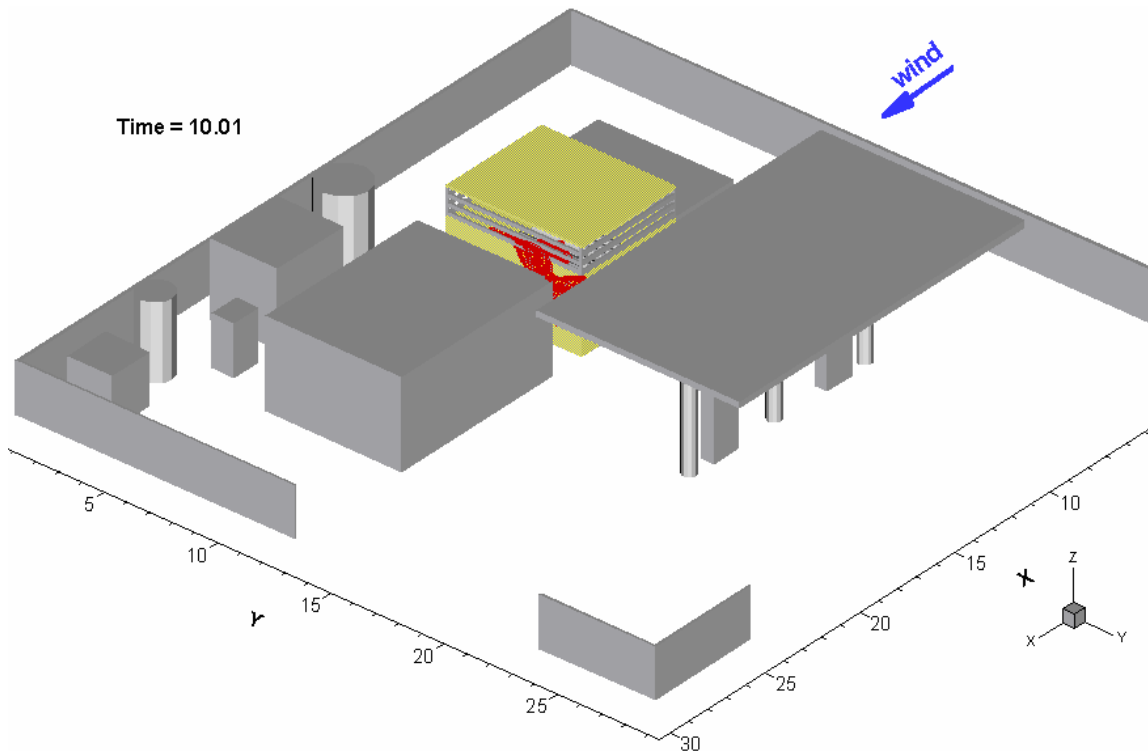


Figure 9. Predicted LFL Cloud of the 0.8 mm, x directed leak West D2 at 10 seconds

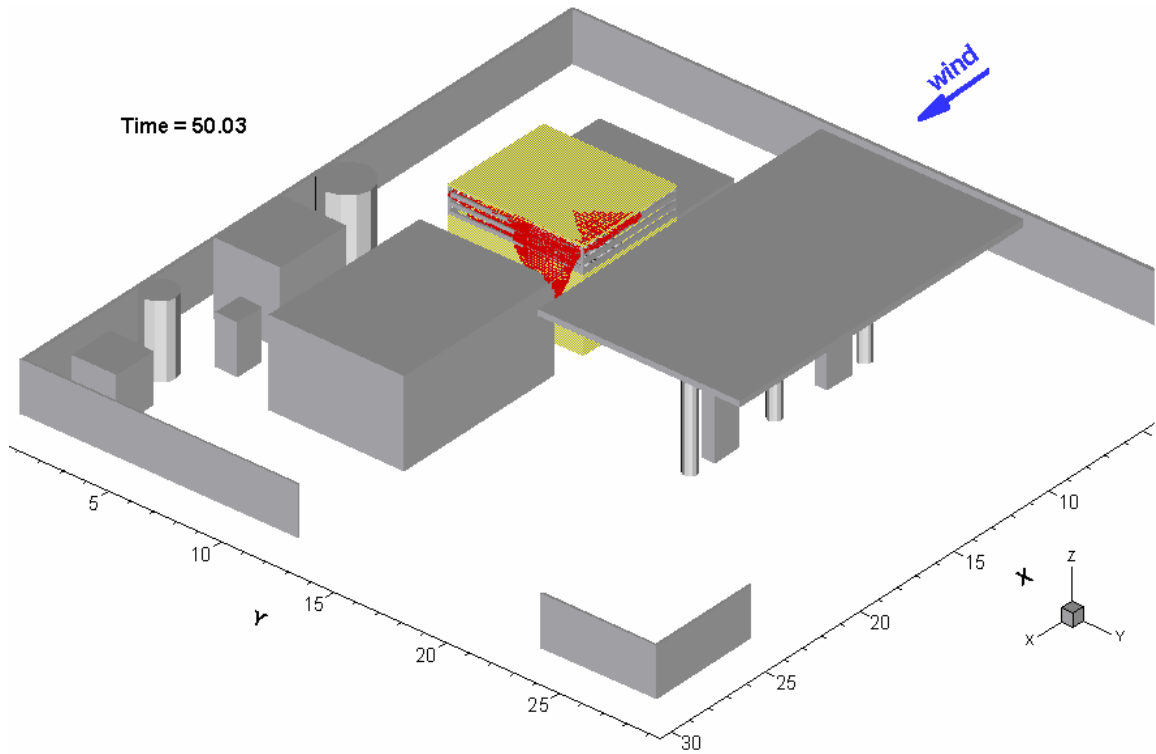


Figure 10. Predicted LFL Cloud of the 0.8 mm, x directed leak West D2 at 50 seconds

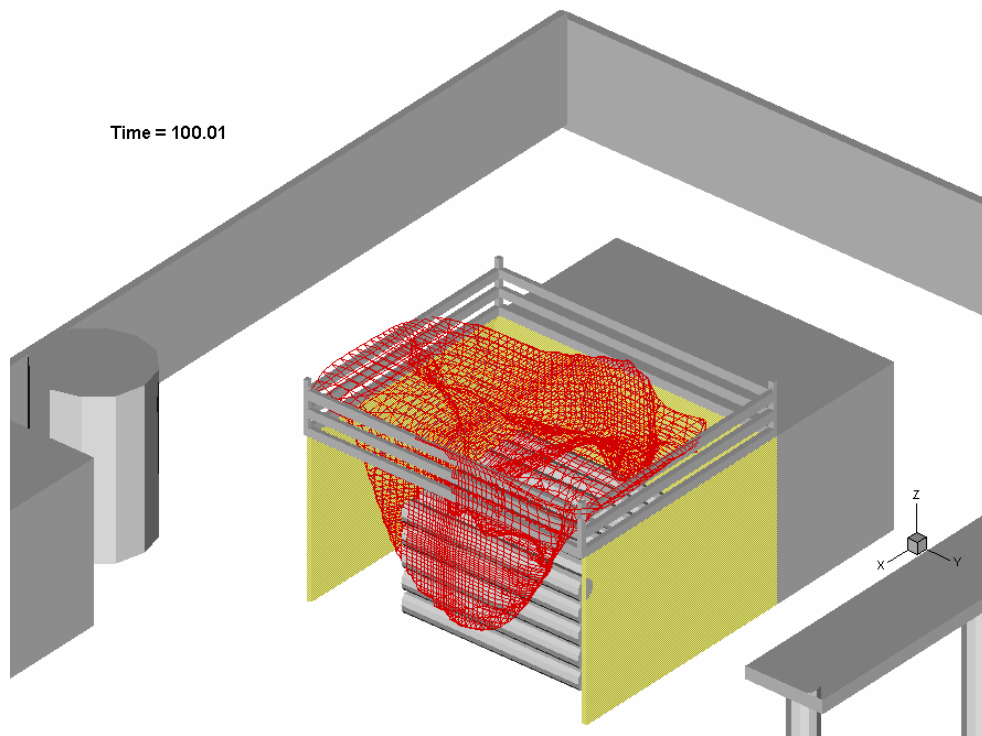


Figure 11. Predicted LFL Cloud Inside the Storage Room of the 0.8 mm, x directed leak West D2 at 100 seconds

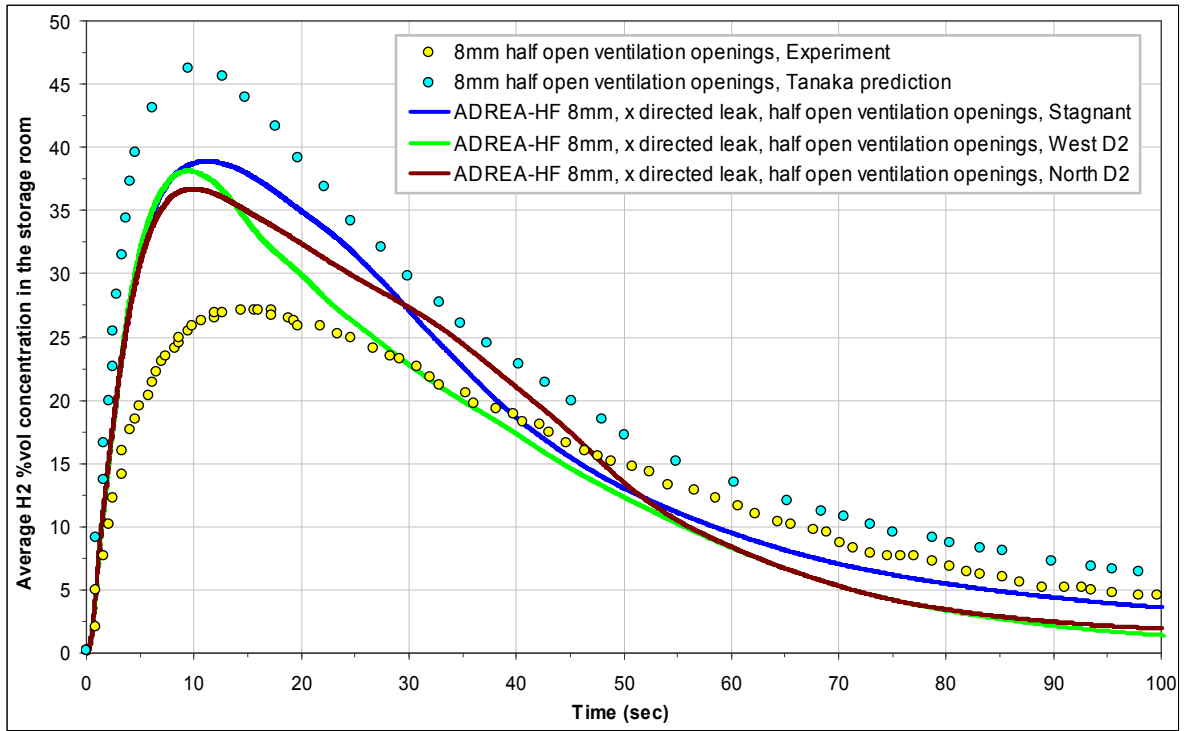


Figure 12. Average H2 % Concentration in the Storage Room (8 mm initial leak size, half open vents)

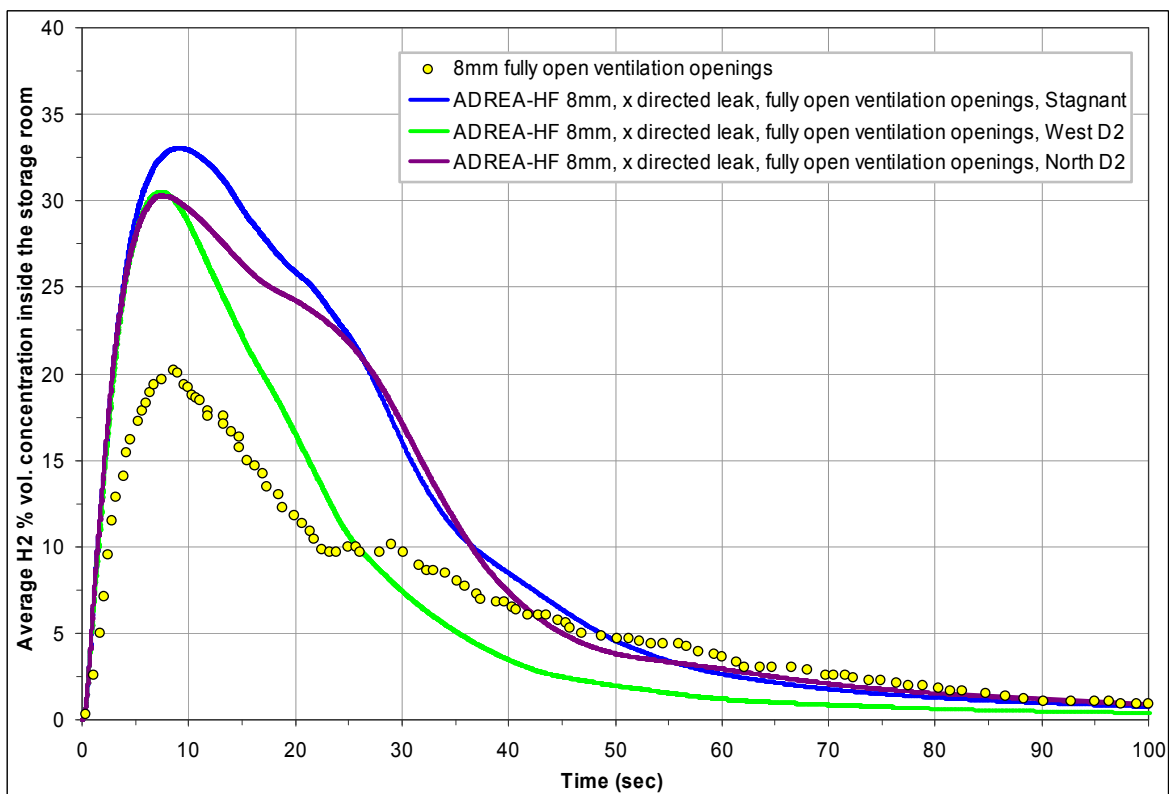


Figure 13. Average H2 % Concentration in the Storage Room (8 mm initial leak size, fully open vents)

5. CONCLUSIONS

The ADREA-HF CFD code was successfully applied to simulate three H₂ release experiments in a storage room of a full scale H₂ refueling station. The predicted average H₂ volumetric concentrations (%) inside the storage room were compared with the measured and some predictions given in the experimental work of Tanaka et al. [1]. The results followed the trend of the experimental data. It was found that the direction of the leak which is related to the presence of the obstacles and their relative position to the release and even the presence of weak wind affects the results significantly.

Finally, the calculations underline the importance of applying CFD methodology to evaluate possible hazards in complex geometries such as a storage room of a refueling station containing a large amount of cylinders.

6. ACKNOWLEDGEMENTS

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7. REFERENCES

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