

# CFD SIMULATIONS ON SMALL HYDROGEN RELEASES INSIDE A VENTILATED FACILITY AND ASSESSMENT OF VENTILATION EFFICIENCY

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## ABSTRACT

The use of stationary hydrogen and fuel cell systems is expected to increase rapidly in the future. In order to facilitate the safe introduction of this new technology, the HyPer project, funded by the EC, developed a public harmonized installation permitting guidance (IPG) document for the installation of small stationary hydrogen and fuel cell systems for use in various environments. The work was strongly supported with experiments and related CFD simulations. The present contribution focuses on the safety assessment of a facility, inside which a small hydrogen fuel cell system (4.8kW<sub>e</sub>) is installed and operated. Dispersion experiments were designed and performed by partner UNIPI in collaboration to partner KI. Partner NCSR D assisted in the design by performing related pre-test calculations. The scenarios considered cover releases occurring inside the fuel cell, related to the low pressure hydrogen downstream of the pressure regulator, which controls the hydrogen flow to the fuel cell system. Hydrogen is expected to leak out of the fuel cell into the facility and from there outside in the open through the facility ventilation system. The initial leakage diameter was chosen based on the ATEX limits for classification of the facility as Zone 2. The release flow rate was calculated assuming 5 bars pressure. Two higher release flow rates (larger leak diameters) were also considered to address more dangerous cases. Several natural ventilation configurations were examined. The performed tests were simulated by NCSR D using the ADREA-HF code. The performed analysis took into account the full interior of the fuel cell, in order to investigate for any potential accumulation effects. The present contribution focuses on the performed CFD calculations. Comparisons between predicted and experimental hydrogen concentration at 4 sensor locations inside the facility are reported. Based on the performed calculations and experiments, an overall assessment of the ventilation efficiency of the facility is made.

## 1 INTRODUCTION

The HyPer project [1] was aimed at providing a comprehensive agreed installation permitting process for developers, design engineers, manufacturers, installers and authorities having jurisdiction across the European Union. The work within this scope is reported in the Installation Permitting Guidance document (IPG) [2] which provides recommendations for the safe installation of small stationary hydrogen and fuel cell systems and presents assessments of current knowledge on installation requirements and case studies of representative installations. A combining experimental and modelling work was carried out to address topics relevant to small stationary hydrogen and fuel cell installations covering scenarios of high pressure releases, small foreseeable releases, catastrophic releases and the

effects of walls and barriers. A summary of the modelling and experimental programme in the EC FP6 project HYPER is given in [3].

Specifically for scenarios on small foreseeable releases, the aim was to determine the ventilation requirements in enclosures containing fuel cells, such that in the event of a foreseeable leak, the concentration of hydrogen in air for zone 2 ATEX is not exceeded. A modeling and experimental work was carried out within this scope. Experiments with natural and forced ventilation were carried out by partner UNIPI in collaboration to partner KI. Partners UNIPI and KI also investigated experimentally the case of a fully closed facility. The modeling work was carried out by partners NCSR D, UU and KI. Pre-test calculations were carried out by partners NCSR D and UU whereas post-test calculations were done by partners NCSR D, UU and KI. This paper presents a part of the modeling work on small foreseeable H<sub>2</sub> releases performed by NCSR D within the EC FP6 HyPer project.

## 2 DESCRIPTION OF THE UNIPI EXPERIMENTS

The CVE facility was initially designed to test the effect of the vent area as a function of the pressure during deflagrations of explosive mixtures in uniform and non uniform conditions. The same facility was used to test the scenarios on small foreseeable releases. Its dimensions were 2753 mm, 3233 mm and 2814 mm providing an internal volume of 25 m<sup>3</sup> (Figure 1). The dimensions of the fuel cell Penta H<sub>2</sub> were 800mm x 688mm x 1024mm. The position inside the CVE is shown in Figure 2.

The leak of H<sub>2</sub> was assumed at the valve of the inlet gas pipeline just before of the pressure reducer. The internal pressure of the fuel cell was considered between 2 and 5 bars whereas after the pressure reducer the pressure value was 350 mbar. In order to take into account the worst probable loss, the highest pressure value was chosen, i.e. 5 bars. The calculations of the H<sub>2</sub> flow were performed with EFFECT-SGIS 7.3. The diameter of the leakage was chosen based on the ATEX limits in order to calculate Zone 2. The guide for pipelines with diameter up to 150 mm refers to a small accidental leakage from a valve which is exactly the case of the H<sub>2</sub> inlet pipeline. The ATEX loss value from a valve is analogous to a flux from a hole with diameter 0.25 mm<sup>2</sup>. Calculations of the H<sub>2</sub> flow were also done for diameters of 0.5 mm<sup>2</sup> and 1 mm<sup>2</sup> to study more dangerous cases than the one according to ATEX.

The purpose of the experiments was to determine the ventilation requirements, either natural or forced, in order to verify the size of Zone 2 ATEX in case of a small accidental leakage of the fuel cell. In this case the limit of H<sub>2</sub> in air is 2% H<sub>2</sub> by volume. Five sensors to measure H<sub>2</sub> concentration were available in order to define the volume around the fuel cell where the limit is not overtaken. The first sensor (sensor 1) was located in the middle of the back fan of the fuel cell to measure the H<sub>2</sub> coming out from the fuel cell. The last sensor (sensor 5) was placed close to Vent 1 (in the middle of the vent's height) to measure the H<sub>2</sub> leaving the facility from that vent. The rest of the sensors were placed at the same Y-Z plane as sensors 1 and 5. Figure 2 shows the location of the sensors inside the facility.

As mentioned above, the work consisted of natural ventilation and forced ventilation experiments. Concerning the natural ventilation experiments the ventilation was provided by openings on the two opposite walls of the facility. The area of Vent 1 could be fixed from a minimum value of 0.35 m<sup>2</sup> (Vent 1) to a maximum of 0.70 (0.35+0.35) m<sup>2</sup> (Vent 1 + Vent 1\_2) and the area of Vent 3 was 0.35m<sup>2</sup>. The areas of Vent 2 and Vent 4 were 0.14 m<sup>2</sup> each (Figure 3). Concerning the forced ventilation experiments, either a small air flow (0.14 m<sup>3</sup>/s) or a large air flow (0.28 m<sup>3</sup>/s) from the fan was investigated. The forced ventilation experiments were performed for the cases that the natural ventilation failed to provide adequate dilution of H<sub>2</sub> as defined by ATEX. All tests were performed in homogenous condition of temperature during winter. This condition is conservative because a gradient of

temperature between the internal and external part of the CVE can enhance the mixing of hydrogen [4].

UNUPI performed 31 experiments with natural ventilation, 1 experiment with the facility fully closed and 10 experiments with forced ventilation. Four of the natural ventilation experiments were done in collaboration with KI partner. Several natural ventilation configurations were examined whereas four different H<sub>2</sub> release locations were chosen. Two of them were inside the fuel cell, one horizontal and one vertical. The horizontal release was close to the back fan of the fuel cell directed to the outside environment and the vertical was close to the upper part of the fuel cell. The other two release locations (tests of UNUPI with collaboration with KI) were outside the fuel cell with directions either horizontal or vertical. The H<sub>2</sub> flow rate was approximately 40 lt/min (based on ATEX). As mentioned before, two higher release flow rates were examined (90 lt/min and 180 lt/min) to study more dangerous cases than the one specified by ATEX. Finally, wind conditions were measured for some tests. The wind velocity did not exceed the value of 6.7 m/s. Details of the experimental work of UNUPI can be found in [5] and [6].



Figure 1: CVE Experimental facility at UNUPI

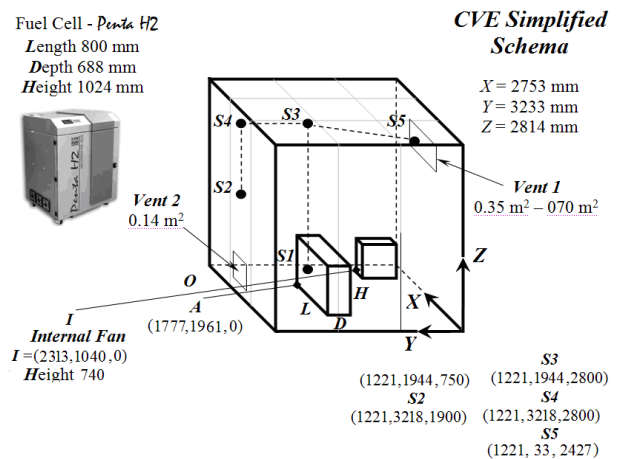


Figure 2: Simplified drawing of CVE facility and position of the Fuel Cell and sensors

### 3 CFD SIMULATIONS OF THE UNUPI EXPERIMENTS

Pre-test calculations were done assuming a release from the valve of the inlet gas pipeline before the pressure reducer with four different release directions (two horizontal, directed inside the fuel cell or outside to the environment and two vertical downwards or upwards). The purpose of the pre-test calculations was to identify the worst case related to the direction of the release. The suggestions were incorporated by UNUPI to finalize the set up of the experiments.

NCSR D simulated 10 of the UNUPI natural ventilation experiments. These covered scenarios with different ventilation configurations, two release directions (horizontal or vertical) and two release flow rates (40 lt/min or 90 lt/min). The horizontal release was close to the back fan of the fuel cell directed to the outside environment (y<sub>out</sub> release) and the vertical upwards was close to the upper part of the fuel cell (z<sub>up</sub> release). Details of the simulated cases and the ventilation configuration of each experimental case are given in Table 1 and Table 2. The interior of the fuel cell was included in the simulations to study possible accumulation of H<sub>2</sub> (Figure 4). The geometrical data used to reproduce the Penta fuel cell was provided by Arcotronics in cooperation with UNUPI. Details on the geometry of the fuel cell are given in [7] whereas the geometrical data to reproduce the CVE facility is given in [8].

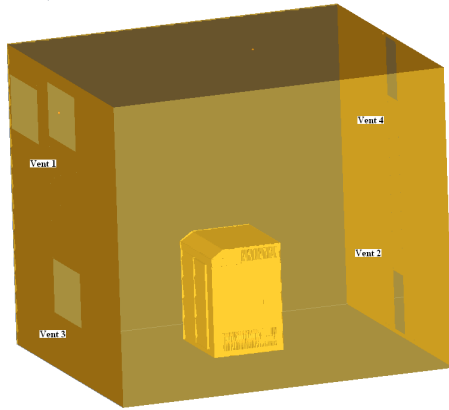


Figure 3: Vent locations on the CVE facility (geometrical processing with DELTA- code)

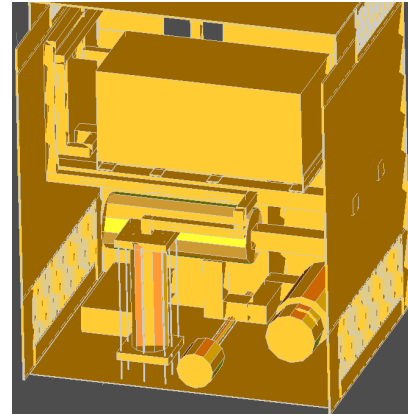
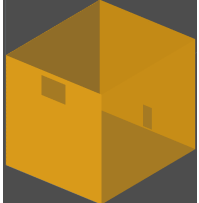
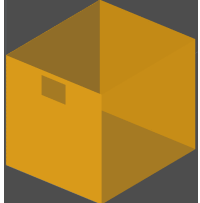
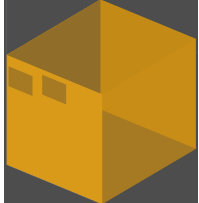
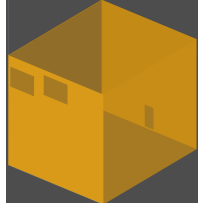
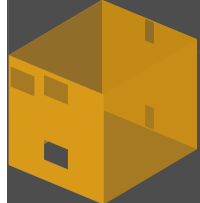


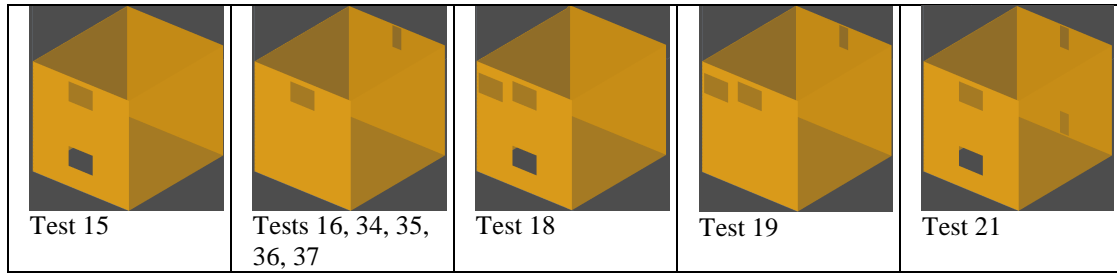
Figure 4: Interior of fuel cell

Table 1: Specifications of simulated experiments

Test	Temp (K)	H2 flow (l/min)	Vent area (m2)	Release time (s)	Leak direction	Hole diameter (m)	Pipe diameter (m)
3	288.65	40	0.35(up) 0.14(down)	1200	y_out	1.00E-03	1.00E-03
5	283.15	40	0.35(up)	900	y_out	1.00E-03	1.00E-03
6	283.15	40	0.35(up) 0.35(up)	1200	y_out	1.00E-03	1.00E-03
14	290.15	40	0.35(up) 0.14(down)	1200	z_up	1.00E-03	6.00E-03
15	293.15	40	0.35(up) 0.35(down)	770	z_up	1.00E-03	6.00E-03
16	295.15	40	0.35(up) 0.14(up)	900	z_up	1.00E-03	6.00E-03
11	290.85	90	0.35(up) 0.14(down)	420	y_out	6.00E-03	6.00E-03
12	292.35	90	0.35(up) 0.35(up) 0.14(down)	373	y_out	6.00E-03	6.00E-03
18	298.15	90	0.35(up) 0.35(down)	900	z_up	1.00E-03	6.00E-03
19	301.15	90	0.35 (up) 0.35(up) 0.14(up)	900	z_up	6.00E-03	6.00E-03

Table 2: Ventilation configuration of the experimental tests

				
Tests 3, 4, 9,10, 11, 13, 14, 17, 23, 28, 39, 40	Tests 1, 2, 5	Tests 6, 7, 8	Test 12	Tests 20, 22



### 3.1 Modeling Strategy

The dispersion calculations were performed using the ADREA-HF CFD Code [9]. Validation studies of the ADREA-HF code for gaseous H<sub>2</sub> release and dispersion can be found in [10], [11] and [12] whereas a general overview of the validation of the ADREA-HF code for hydrogen applications can be found in [13].

Turbulence was modelled using the two equation standard k-epsilon model of Launder and Spalding [14], [15] modified for buoyancy effects [16], [17]. The mixing of H<sub>2</sub> 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 H<sub>2</sub> vapour mass fraction transport equation.

Standard wall functions (no slip condition) were used for velocity, turbulent kinetic energy and dissipation rate on solid surfaces. A hydrodynamic roughness of 1 mm was assigned to all solid surfaces including the ground. Zero gradient condition for H<sub>2</sub> mass fraction was assigned to all solid surfaces. 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.

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 [18]. An automatic time step increase/decrease mechanism was applied with 10<sup>-3</sup> seconds initial time step. The CFL number was set to 10.

The computational domain extended the experimental facility by 3 or 4 computational cells in the y direction when the wall in the x-z plane had ventilation openings. When the leak had a y axis direction, the minimum cell size was in the x and z direction whereas when the leak had a z axis direction the minimum cell size was in the x and y direction. The minimum cell size was 0.012 m for the majority of the simulated tests. An aspect ratio of 1.12 (maximum value) was used to increase the cell size far from the source. Volume porosity and area permeability approach was used to model the complex geometrical layout with Cartesian grid. The total number of active cells ranged from 130.000 to 240.000 depending on test by test. The geometrical pre-processing was performed with the DELTA-B Code [19].

The initial conditions for all tests were atmospheric pressure and temperature depending on each test as given by UNIPI. The initial conditions at the source depended on each test too. Velocity was assigned a value to give the indicated by the experiments mass flow-rate based on the corresponding release area.

### 3.2 Results and discussion

Due to size limitations, not all the results of the simulated tests are presented here. The work presented covers six of the ten simulated cases which are thought to be most indicative of the overall simulation work. Figure 5 to Figure 10 show the H<sub>2</sub> volumetric concentration of

sensors 2, 3, 4, and 5 of UNIPI experiments and NCSR simulations for Tests 3, 6, 11, 12, 14, 15 and 18. It can be seen that generally there is a good agreement between the experiments and the simulations. Comparison between the experimental and simulated results of sensor 1 is not included due to the technical characteristics of the sensors. The sensors cannot measure values higher than 20% of H<sub>2</sub> concentration (they get saturated). Therefore, sensor 1 (the sensor located close to the release) cannot measure correctly tests with H<sub>2</sub> flow-rate higher or equal to 90 lt/min.

For tests 3, 6 and 14 neither the experiments nor the simulations showed a H<sub>2</sub> concentration reaching 2% which is the ATEX limit for non-catastrophic H<sub>2</sub> accidents (classification of the facility by ATEX as zone 2). The release flow rate of these tests was the lowest, 40 lt/min. For test 18 only the experiment showed a H<sub>2</sub> concentration exceeding 2% (sensor 3). However, this value did not exceed 2.5%. For tests 11 and 12 both experiments and simulations showed a H<sub>2</sub> concentration exceeding 2%. However, for test 11, both the experimental and simulated value of sensor 3 did not exceed 2.5%. The simulation also showed sensor 5 to slightly exceed 2%. For test 12, both experimental and simulated value of sensor 3 slightly exceeded 2%. The last three tests, test 18, 11 and 12 had a release flow rate of 90 lt/min.

Concerning the differences between the experiments and simulations and specifically for test 3, the maximum difference was found in sensors 2 and 3 and did not exceed 0.6%. For test 6, the maximum difference between the experiment and the simulation was in sensor 4 and did not exceed 0.35%. For the rest of the sensors, the agreement is very good. For test 11, the experiment showed a slight excess of 2% of H<sub>2</sub> concentration for sensor 3 while sensor 5 almost reached that value. In simulations sensors 3 and 5 exceeded that value following the trend of the experiment. Both simulation and experiment show a decline in the H<sub>2</sub> concentration in all sensors after approximately 360 seconds. This is due to the rapid decline of the release flow rate starting at 360 seconds giving a zero flow-rate at 420 seconds. For test 12, the maximum difference between the experiment and the simulation was found in sensor 4 and did not exceed 0.7% whereas for test 14 it was in sensor 2 and did not exceed 0.96%. The experimental values of sensors 2 and 4 of test 14 were almost zero during the release time. For test 18 the maximum difference between the experimental and simulated value was in sensors 2, 3 and 4 and did not exceed 0.5%. The differences between the results can be attributed to the sensitivity of the experimental measurements as it was reported that the sensors had a precision of 0.2% H<sub>2</sub> concentration. Additionally, the presence of wind could have influenced the experimental results as the facility was located outdoors and measurements on the wind were either not reported for some experiments or for the tests that was reported the measurement of the wind velocity was not taken throughout the experiment whereas its direction was not reported. Furthermore, temperature could have also influenced the results as the roof and one side of the facility were entirely covered with panels of glass.

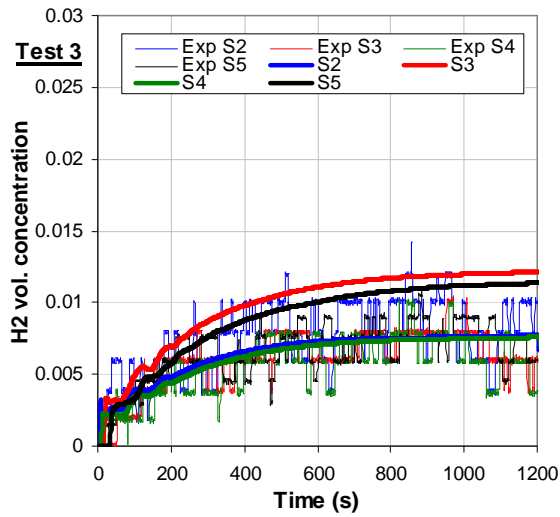


Figure 5: Experimental versus simulated results (Test 3)

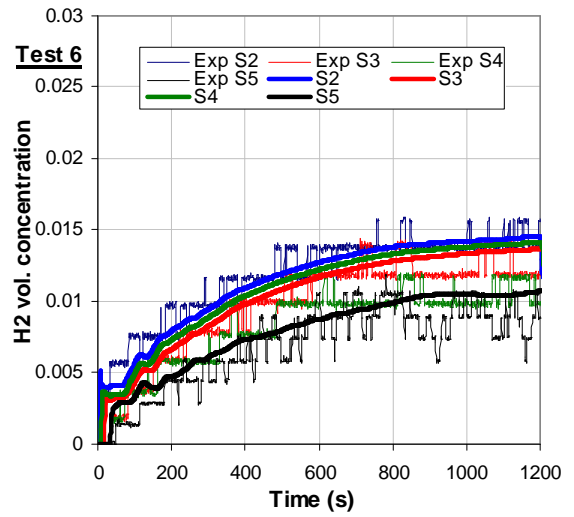


Figure 6: Experimental versus simulated results (Test 6)

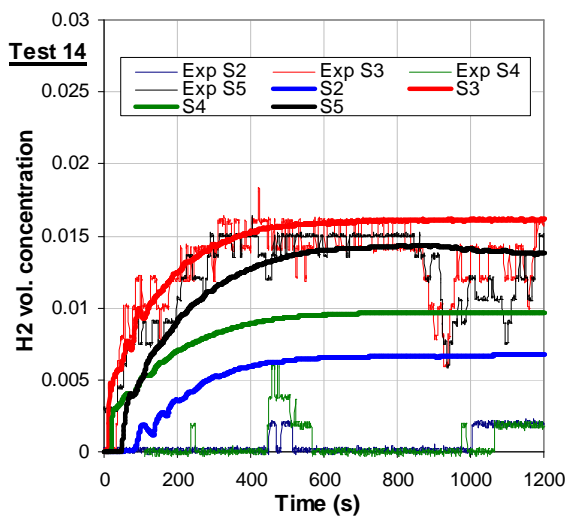


Figure 7: Experimental versus simulated results (Test 14)

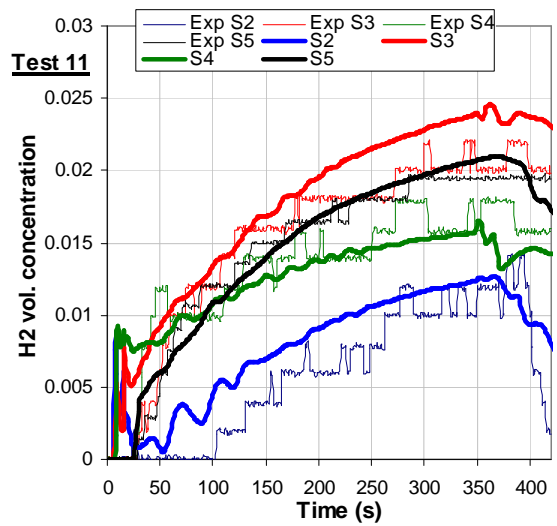


Figure 8: Experimental versus simulated results (Test 11)

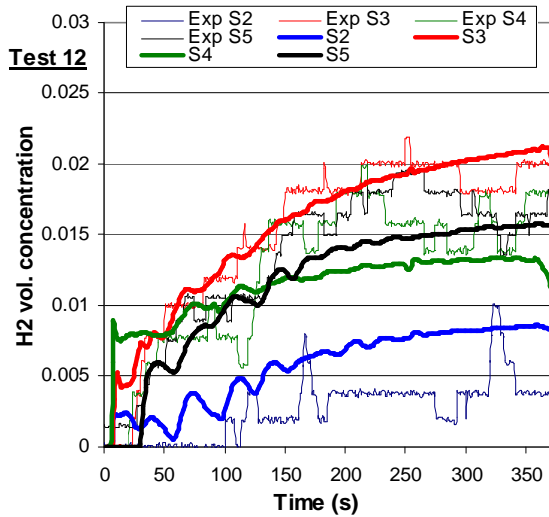


Figure 9: Experimental versus simulated results (Test 12)

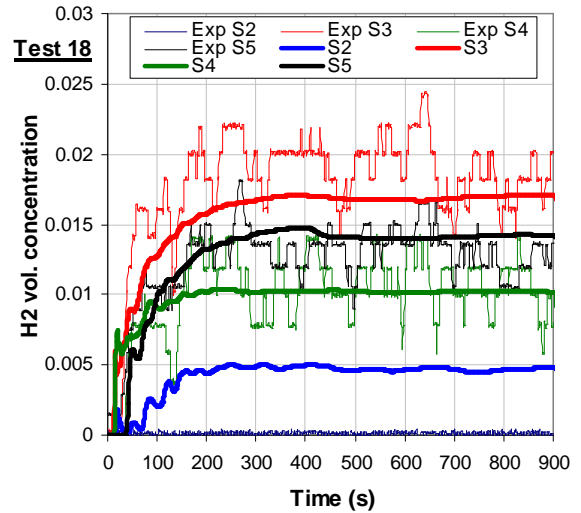


Figure 10: Experimental versus simulated results (Test 18)

## 4 OVERALL ASSESSMENT OF VENTILATION EFFICIENCY

### 4.1 UNIPI tests

Non-dimensional ventilation rates versus concentration at the top opening of a residential naturally ventilated garage were addressed by Barley (2007) [20]. Following this earlier work of Barley the ratio  $Q_{AV}/Q_{H2}$  versus  $H_2$  concentration (v/v) at the top vent (sensor 5), based on the UNIPI experimental results is plotted in Figure 11.

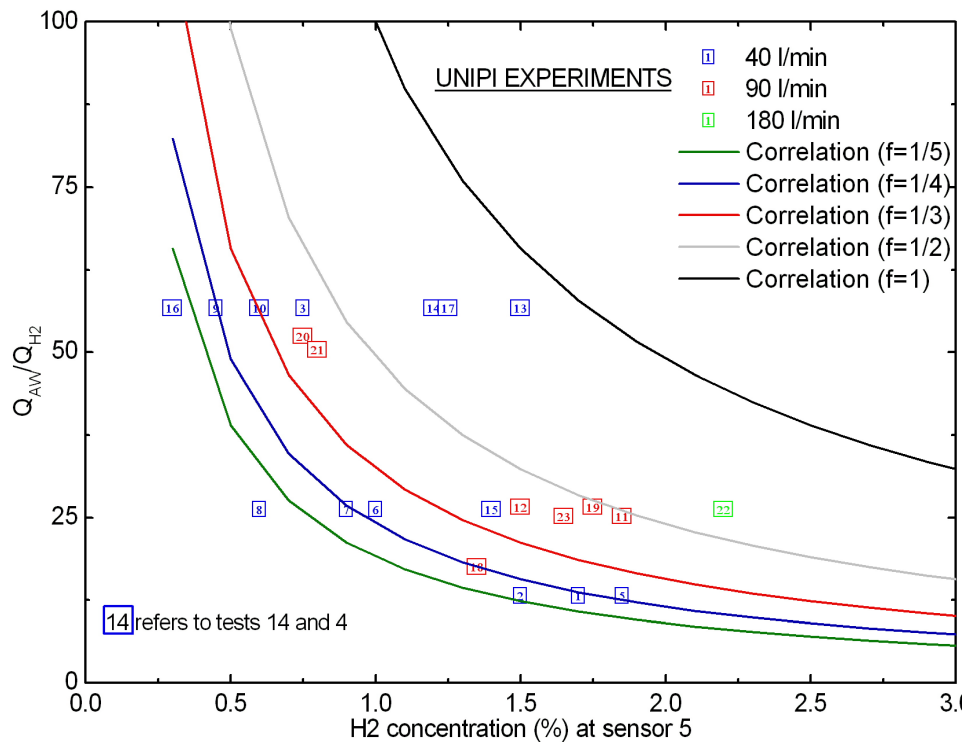


Figure 11:  $Q_{av}/Q_{H2}$  (UNIPI tests) versus  $H_2$  concentration at sensor 5



Here QH2 is the measured H2 volumetric release rate and Qaw is the volumetric air flow in, estimated based on the ATEX formulas provided by UNIPI (Table 3). In the calculation of Qaw, wind was assumed to have 1 m/s velocity for all cases. Figure 11 shows the experimental results as squares, where the number of each square is the number of the corresponding UNIPI experiment. The solid lines in Figure 11 represent the following correlation, which is described in paragraph 4.3:

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The factor f represents the fact hydrogen is not homogeneously distributed within the enclosure, but occupies a layer of certain size close to the ceiling. The stratification factor f is the ratio between the volume of the H2-air layer divided by the volume of the enclosure.

Table 3: Qaw values for UNIPI tests

Unipi Test	1,2,5	3, 4, 9, 10, 11, 13, 14, 17, 23	6, 7, 8	15	16	12	18	19	20, 22	21
Qaw	0.00875	0.03778	0.0175	0.0175	0.03778	0.0399	0.02625	0.0399	0.07864	0.07557

Based on Figure 11, the correlation  $f=1/3$  seems to be a good fit of the experimental data except for tests 4, 13, 14, 17 and 22. Furthermore, the graph shows that the values of Qaw are some how insensitive to the different ventilation configurations. More specifically, the value of  $Qaw/QH2$  is the same for tests 16, 9, 10, 3, 14, 4, 17, 13 which have the same release conditions (same QH2) but test 16 has different ventilation configuration (Table 2). The same holds for tests 8, 7, 6 and 15 which have the same QH2 but test 15 has different ventilation configuration. Additionally, close values of  $Qaw/QH2$  are shown in the graph for the group of tests 20, 21 and 12, 23, 19, 11. However tests 20, 21 and tests 12, 11 have different ventilation configurations.

**4.2 NCSR calculations**

Non-dimensional ventilation rates versus concentration at the top opening, based on the calculations performed with the ADREA-HF code is shown in Figure 12. In this case Qaw was calculated from the simulations as the sum of air flowing inside the facility from any ventilation opening present in each test.

The assumption that inside the facility exists a H2-air layer in its upper part, was verified by inserting 75 monitor points (at the same y-z plane with the release) measuring H2 concentration in all tests. These simulations showed that the part of the facility from the ground up to the height of the release contains minimum or zero H2. This part is almost 1/3 of the total volume of the facility.

Unlike Figure 11, Figure 12 shows that the simulated tests lie between the lines with correlation  $f=1/2$  and  $f=1$ . Furthermore, the values of  $Qaw/QH2$  for the tests with the same release flow rate are now different for different ventilation configurations. Additionally, the values of Qaw of tests with the same ventilation configuration but with different release flow rates were different. The CFD predictions of the values of Qaw take into account not only the ventilation configuration but also the presence of H2 release. Figure 13 shows a comparison between calculated Qaw from simulations and Qaw based on ATEX. In most of the tests, Qaw based on ATEX is under-predicted as compared with the calculated. The under-prediction is higher in cases where all openings are in the same wall (tests 5, 6, 15 and 18). In test 14, which has one opening close to the ceiling and the other close to ground at opposite walls, the calculated Qaw is very close to the one from ATEX.

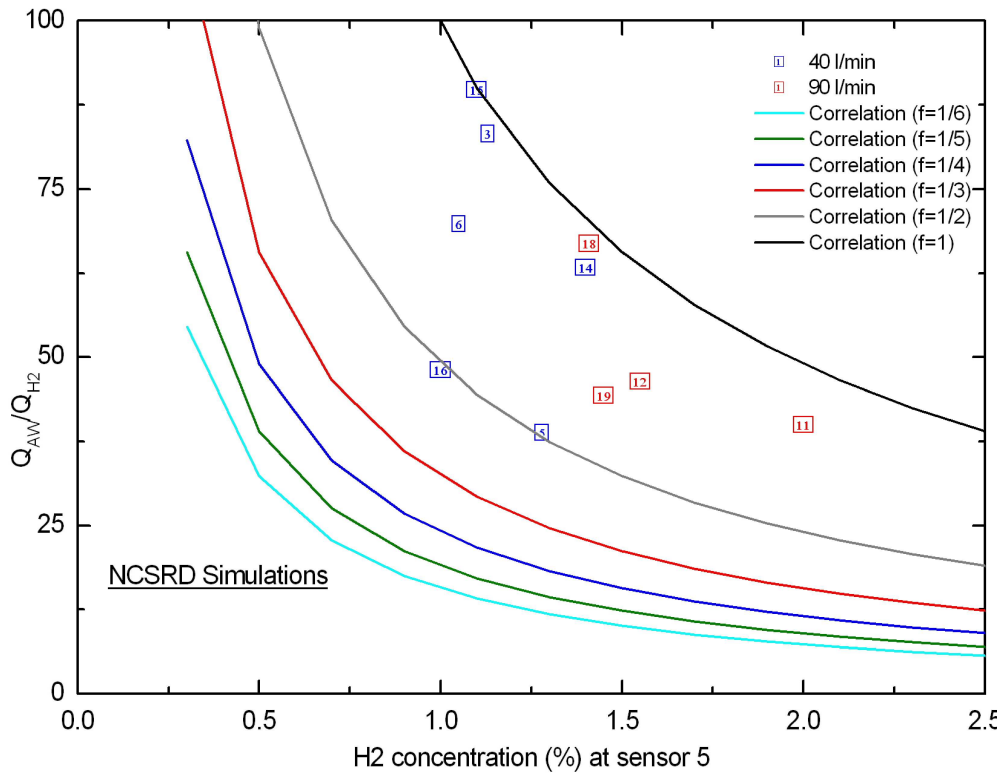


Figure 12:  $Q_{aw}/Q_{H2}$  (NCSR tests) versus H2 concentration at sensor 5

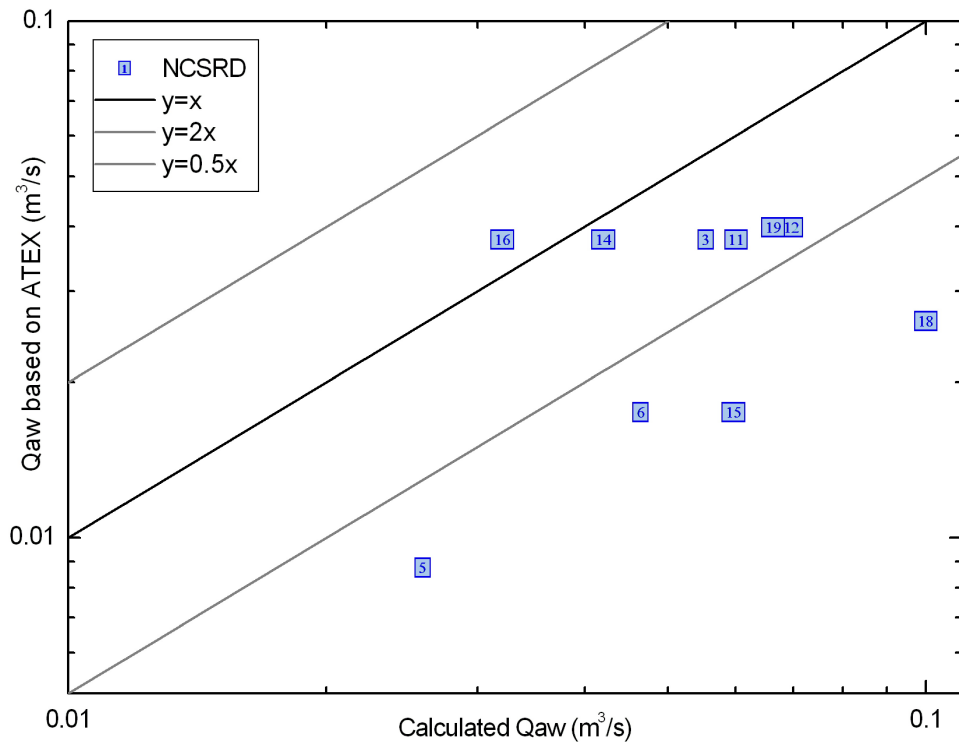


Figure 13: Comparison between calculated  $Q_{aw}$  from simulations and  $Q_{aw}$  based on ATEX

### 4.3 Normalized ventilation correlation

The simplified model considers a H<sub>2</sub> leak within an enclosure with two vents, one near the top and the other close to the bottom of opposite wall. Steady-state and isothermal conditions were assumed.

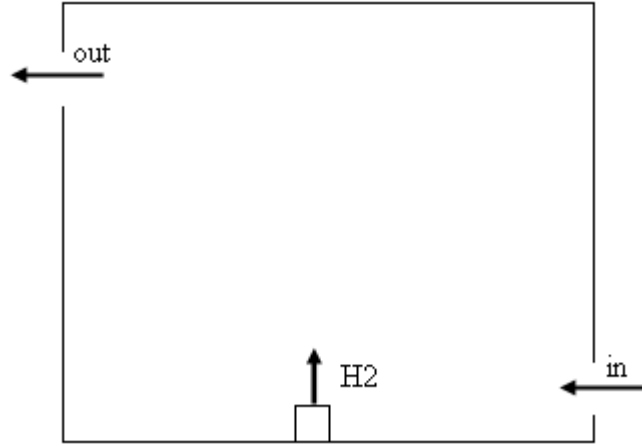


Figure 14: Simplified model

The following relationships were used: H<sub>2</sub> mass conservation:  $\rho_{H_2} Q_{H_2} = q_{out} \rho_{out} Q_{out}$ , total mass conservation:  $\rho_{air} Q_{in} + \rho_{H_2} Q_{H_2} = \rho_{out} Q_{out}$  and mixture density:  $\frac{1}{\rho_{out}} = \frac{q_{out}}{\rho_{H_2}} + \frac{1-q_{out}}{\rho_a}$  to derive

the relationship:  $c_{out} = \frac{Q_{H_2}}{Q_{in} + Q_{H_2}}$ . If to consider stratification inside the enclosure, the assumption of

a homogeneous mixture only in a part (upper) of the enclosure is made, were  $f = \frac{V_{upperpart}}{V_{total}}$  thus

$$c^* = \frac{V_{H_2}}{V_{upperpart}} \stackrel{(9)}{=} \frac{V_{H_2}}{f \cdot V_{total}} = \frac{1}{f} c \text{ and finally } c_{out}^* = \frac{1}{f} \frac{Q_{H_2}}{Q_{in} + Q_{H_2}}.$$

## 5 CONCLUSIONS

This paper presents a part of the modeling work performed by NCSR D on small foreseeable H<sub>2</sub> release experiments within the EC FP6 HyPer project. The aim of this work was to determine the ventilation requirements in enclosures containing fuel cells, such that in the event of a foreseeable leak, the concentration of hydrogen in air for zone 2 ATEX is not exceeded. The experiments with natural and forced ventilation were carried out by partner UNIPI in collaboration to partner KI.

In general good agreement was found between predicted and experimentally measured concentration time histories for all simulated cases. The differences between the results can be attributed to the sensitivity of the experimental measurements and the outdoor location of the facility. For the cases with 40 lt/min flow rate neither the experiments nor the simulations showed a H<sub>2</sub> concentration reaching 2% which is the ATEX limit for non-catastrophic H<sub>2</sub> accidents (classification of the facility by ATEX as zone 2). For the cases with 90 lt/min release flow rate both experiments and simulations showed a H<sub>2</sub> concentration exceeding 2% in some sensors. However the values did not exceeded 2.5% H<sub>2</sub> concentration.

Assessment of the ventilation efficiency was done for both UNIPI experiments and NCSR D simulations. It was found that the air flow in based on ATEX is some how insensitive to the different

ventilation configurations. CFD predictions of the air flow in were sensitive to both ventilation configurations and the presence and strength of the H<sub>2</sub> release. In some of the tests, Q<sub>av</sub> based on ATEX is under-predicted as compared with the calculated with higher under-prediction in cases where all openings were in the same wall. It is believed that the under-predictions would lead into too conservative ventilation requirements in enclosures containing fuel cells.

## 6 ACKNOWLEDGMENTS

The authors would like to thank the European Commission for co-funding of this work in the framework of the FP6 STREP HYPER project [1].

## 7 REFERENCES

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