SAFETY OF LABORATORIES FOR NEW HYDROGEN TECHNIQUES

Heitsch, M.[1], Baraldi, D.[2], Moretto, P.[3], Wilkening, H.[4]
[1]JRC, Institute for Energy, Postbus 2, NL-1755 ZG Petten, Netherland,
Matthias.Heitsch@ec.europa.eu
[2]JRC, Institute for Energy, Postbus 2, NL-1755 ZG Petten, Netherland, Daniele.Baraldi@jrc.nl
[3]JRC, Institute for Energy, Postbus 2, NL-1755 ZG Petten, Netherland, Pietro.Moretto@jrc.nl
[4]JRC, Institute for Energy, Postbus 2, NL-1755 ZG Petten, Netherland, Heinz.Wilkening@jrc.nl

ABSTRACT

In this paper, a case of hydrogen release in a typical research laboratory for the characterisation of hydrogen solid-state storage materials has been considered. The laboratory is equipped with various testing equipments for the assessment of hydrogen capacity in materials typically in the 1 to 200 bar pressure range and temperatures up to 500°C. Hydrogen is delivered at 200 bar by a 50 l gas bottle and a compressor located outside the laboratory. The safety measures directly related to hydrogen hazard consist in a distributed ventilation of the laboratory and air extraction fume hoods located on top of each instrument.

Goal of this work is the modelling of hydrogen accidental release in a real laboratory case, in order to provide a more fundamental basis for the laboratory safety design and assist the decision on the number and position of the safety sensors.

The computational fluid dynamics code (CFD) ANSYS-CFX has been selected in order to perform the numerical investigations.

Two basic accidental release scenarios have been assumed both at 200 bar: a major leak corresponding to a guillotine breaking of the hydrogen distribution line and a smaller leak typical for a not properly tight junction.

1.0 INTRODUCTION

Following initiatives at national and international level aiming at a quick progress towards the development and introduction of a hydrogen-based economy, many new R&D laboratories have been created or upgraded worldwide in the last years. They focus on hydrogen production methods, on fuel cells development and testing, or on hydrogen storage technologies.

Although guidelines, regulations and standards on the use of flammable gases are available at national and international levels, which assist and regulate the safety design of the laboratories, they are optimized for industrial applications and often disregard small-scale research laboratories. Specific aspects of hydrogen, such as its volatility and its wide flammability range, can cause doubts and uncertainties in the choice of the proper safety solutions. For example the selection of detector positions and ventilation strategies must be carefully optimized in order to detect and reduce the occurrence of flammable hydrogen-air mixtures due to accidental release of hydrogen.

To our best knowledge, there has been only one paper published recently tackling the case of the release of a considerable amount of hydrogen in the confined space of a laboratory [1]. However the authors disregard time-dependent release, and focus only on the consequences of ignition of the total amount of hydrogen released by means of simplified models such as the TNT-equivalency explosion model.

Investigations of release phenomena have been performed both with experiments and with Computational Fluid Dynamics (CFD) simulations. For example, several configurations of hydrogen release in a partially enclosed space have been presented by Swain et al. in [2].

In general, numerical studies require additional validation activities before a code can be applied to the safety design of a real laboratory equipped with forced ventilation and complex building geometry. Validation of the CFD code CFX related to hydrogen (or helium as a replacement of hydrogen because of safety concerns) gas release and mixing in complex geometries was performed by the authors [3], [4] and [5]. Another example of validation benchmark can be found in Gallego et al. [5]. The goal of this work is the simulation of two leakage scenarios in an existing laboratory for solid-state hydrogen storage by means of CFD. Further steps will be the identification of a most credible accident and the optimal positioning of hydrogen safety detectors.

2.0 METHODOLOGY

2.1 Description of the laboratory

The laboratory is located at the Institute for Energy of the Joint Research Centre (JRC) and it is equipped with various instruments for hydrogen sorption measurements in materials. The measurements are based on gravimetric, volumetric and spectrometric principles. They are performed typically in the 1 to 200 bar pressure range and with temperatures up to 500°C. The laboratory is approximately 18 m long, 8.5 m wide and 3.5 m high, with a volume of approximately 285 m^3. A picture of a part of the laboratory is given in Figure 1.

Hydrogen is delivered at 200 bar by a 50 l gas bottle and a compressor located outside the laboratory. The maximum amount of hydrogen which would be released in the laboratory in case of failure of all the automatic and manual shut-down procedures can be calculated by considering a full gas bottle, a full compressor buffer tank, all the pipes at 200 bar and all the experimental equipments at full capacity. That amount is approximately 1.2 kg.

A distributed ventilation system guarantees constant exchange of the air for the whole laboratory. As shown in Figure 2, in the ventilation system there are 8 inlet openings located on the ceiling, and 10 extraction openings, 6 of which are placed on the ceiling and 4 on a wall, at the floor level (in Figure 2 the inlets are shown in blue while the exhaust openings are illustrated in red). In addition, air extraction fume hoods are located on top of each testing equipment in order to collect the hydrogen released during experiments and discharge it to the roof of the building.

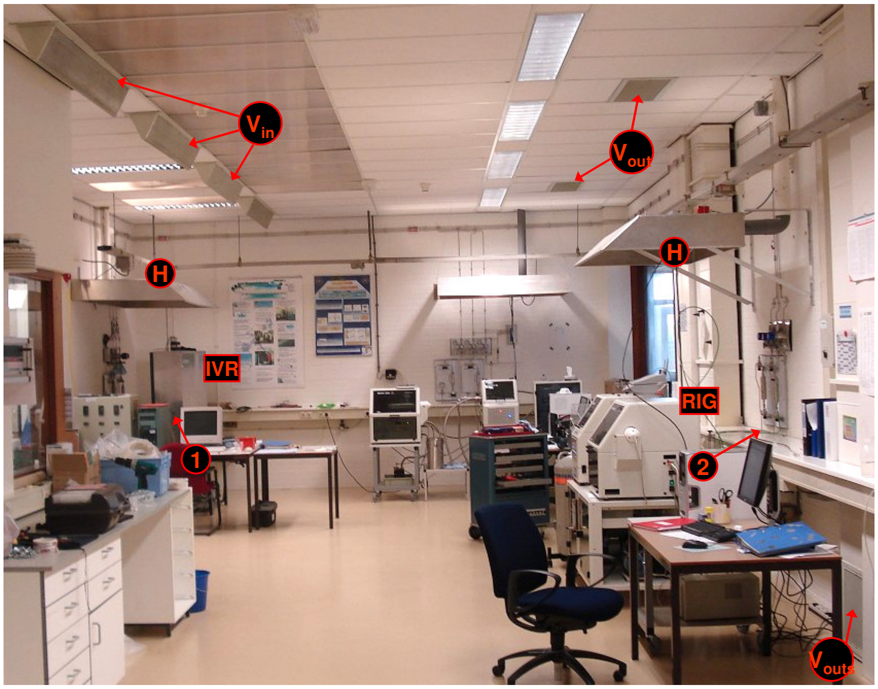

Figure 1. Picture of a part of the laboratory: V_{in} indicates the positions of the ventilation inlets, V_{out} the positions (on the ceiling and near the ground) of the ventilation outlets, H two of the fume hoods positioned on top of the test rigs. Numbers 1 and 2 indicate the positions of the two hydrogen releases that have been assumed in the simulations.

Local air velocities have been measured by means of a calibrated anemometer at all openings of the ventilation system and then averaged in order to obtain a single averaged value per opening. The velocities range is between 1 and 2 m/s, and the total airflow entering into the laboratory sums up to approximately 15000 m^3/h. The same procedure has been applied to the air extraction pipes under the fume hoods, where the air velocity range is between 1.5 and 5.5 m/s. These data have been fed into the CFD calculations as boundary conditions.

Two independent leak detection systems are available: an overflow valve in the main hydrogen supply line, and safety hydrogen detectors under each fume hood. If the flow rate in the hydrogen supply system or local hydrogen concentrations in the lab exceed certain threshold values, an automatic shut down procedure will start. In that case the hydrogen supply is interrupted and the distribution system is depressurized. The hydrogen concentration at which a detector will trigger the shut down procedure is 0.4% in air, corresponding to 10% of the low flammability limit (LFL).

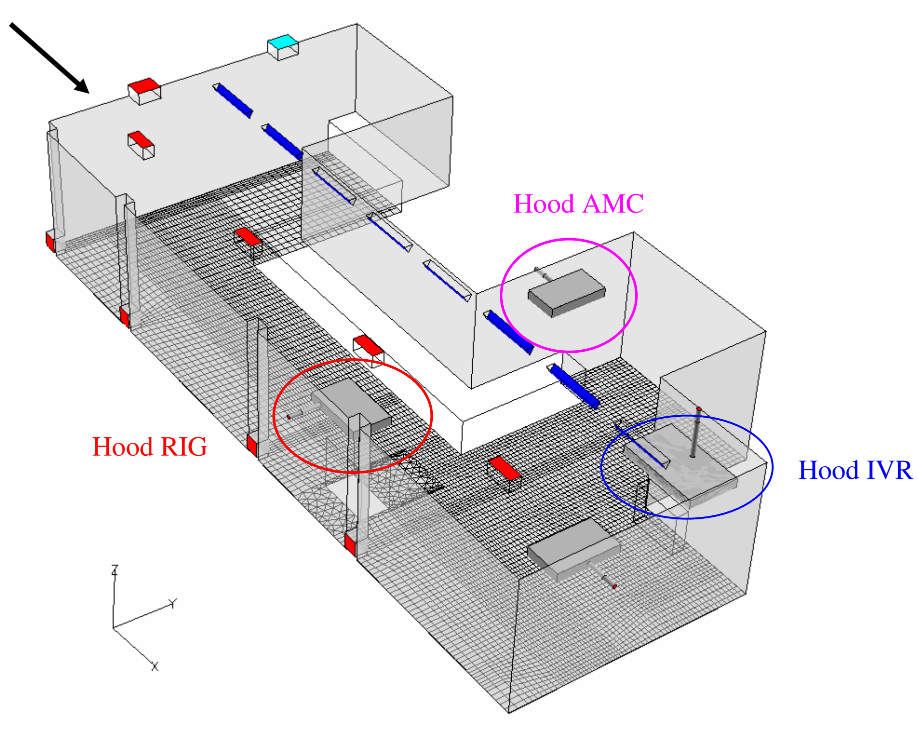

Figure 2. Model of the laboratory including the ventilation system. The black arrow identifies the viewing direction of the observer in the photo in Figure 1

2.2 Release Scenarios

Two release scenarios have been selected for this work, corresponding typically to accidents that were considered as possible in the laboratory safety assessment, although with different likelihood. They differ basically in terms of flow rates and position in the laboratory. As non-mitigated scenarios it has been assumed that the mitigation measures such as depressurization and interruption of hydrogen supply are not working.

The first release scenario (scenario A) is similar to a real event that occurred in the laboratory. The accidental release was caused by the non-complete tightening of a pipe fitting during maintenance work. For un-explained reasons, hydrogen started to leak approximately 24 hours after the end of the maintenance. The leak was detected according to the safety design by a hydrogen sensor, with successful completion of the automatic shut down procedure.
The release for the simulation has been assumed to occur at the hydrogen inlet of the testing equipment indicated with the acronym IVR in Figure 1 and Figure 2. With respect to the fume hood, the most external pipe position has been chosen for the release, so that only a fraction of the hydrogen cloud remains under the hood, while another fraction diffuses up to the ceiling.

The second scenario (scenario B) corresponds to the highly improbable, but still possible, case of the full opening or breaking of a high-pressure piping which occurs instantaneously. The pipe has an internal diameter of 4 mm. The rupture has been assumed at the wall behind the test rig indicated with the acronym RIG in Figure 1 and in Figure 2.

In both scenarios it has been assumed that the hydrogen release jet is directed horizontally towards the centre of the laboratory.

3.0 NUMERICAL SIMULATION OF RELEASE SCENARIOS

The two hydrogen release scenarios described in the previous paragraph have been investigated in order to evaluate the risk of formation of flammable clouds. The case of scenario A is characterised by a low speed release. The assumption of a not fully tight junction leads to a flow with high-pressure losses through the leak. It appears realistic to use a more distributed release area modelled as a ring with 1 mm width. This case involves a subsonic outflow. The second and more severe release scenario (scenario B) consists of a rupture with outflow through the full pipe cross section from one of the connecting pipes of the hydrogen delivery system. In this second case the exit flow speed is sonic.

The code used for all the simulations is CFX (version 10) [7]. The physical description of both release scenarios is similar. The ventilation system remains active and it is defined according to the available air speed measurements for inflow and outflow. The gas mixture in the laboratory is simulated by the individual species of air and hydrogen

3.1 Computer Model of Laboratory

The computational mesh created for the laboratory is a hybrid mesh composed mostly of hexahedral cells with some unstructured blocks (tetrahedrons and pyramids). The unstructured blocks are suitable to accommodate the very small hydrogen leak pipes into the mesh. Figure 2 shows the full model of the laboratory. A horizontal cut through the mesh is also shown at the level of the ground. Two different mesh resolutions have been employed in order to investigate the grid dependency of the simulation results. A coarser mesh with a total number of cells of about 155550 has been used for most of the simulations. A finer mesh with about 588600 cells and major refinements in the vicinity of the leak has been generated for grid-independency investigations. For both inlets and exhaust openings, the flow speeds are prescribed according to the measurements. Outflow boundary conditions are not imposed directly at the openings through which the gas is leaving the room but somewhere outside of the laboratory to allow for a more realistic and uniform pressure formation in the ventilation ducts (see Figure 2).

For both scenarios details of the leaking pipes are shown in Figure 3. The pipes themselves are meshed with structured cells, however they are embedded in unstructured blocks. This method gives flexibility if a modification of leak positions should be required. The areas from which the flow is released are shown in red. The inflow boundaries are set about ten diameters upstream of the leak to allow the flow to develop a realistic flow profile before arriving in the lab.

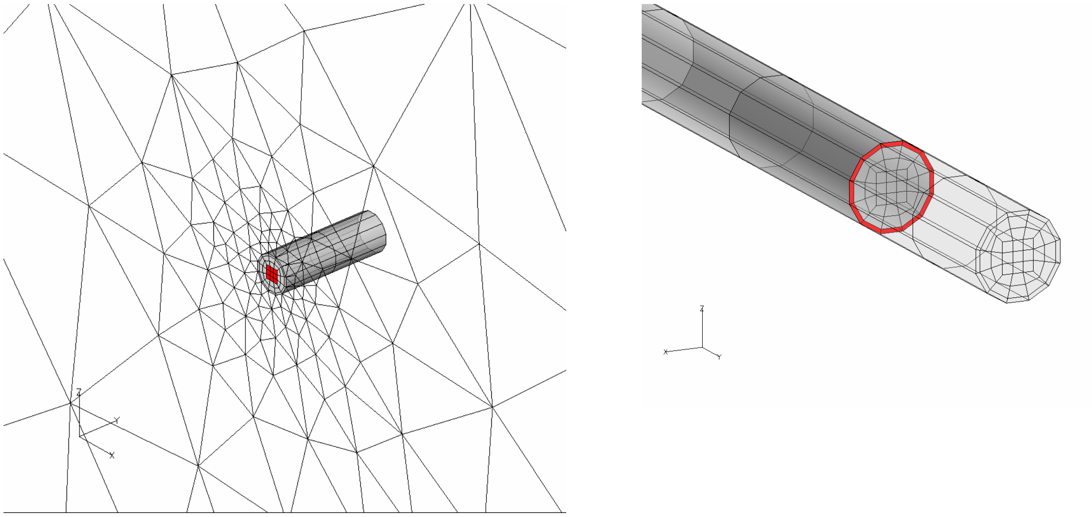

Figure 3. Details of critical (left, underneath RIG) and sub-critical release openings (underneath IVR)

3.2 CFD Simulations

Before any release simulations, the ventilated flow inside the laboratory was calculated to be in equilibrium. This was done in steady-state as well as in time dependent mode by CFX. Both simulations resulted in almost identical flow distributions in the lab. The ventilation measurements revealed that the sum of volumetric inflows is slightly different from the sum of volumetric outflows. Therefore it was decided to prescribe one exhaust opening as pressure boundary (see Figure 2, opening with cyan colour) to allow forming equilibrium between inflows and outflows. The obtained flow distributions were used as initial state for all release simulations.

For the two leak scenarios a number of simulations were carried out. Table 1 provides a summary.

Table 1. Summary of simulations performed

	Scenario A **Low speed release (position IVR)**	**Scenario B** **Critical release (position RIG)**
Flow speed	100 m/s, 500 m/s	critical
Outlet pressure option	1 bar	50 bar, 100 bar
Mesh resolution	coarse (155550)	coarse (155550), fine (588605)

A parametric study has been carried out in order to investigate the effects of factors on the simulations such as the flow speed for the subsonic case and the outlet pressure for the sonic case. Moreover the effect of the mesh resolution on the results has been investigated in the sonic case.

3.2.1 Subcritical Hydrogen Release (scenario A)

The low speed release through a defected junction is believed to occur over a distributed area rather than over the pipe cross section. The release source is defined as a ring of 1 mm thickness with an outer diameter of 10 mm (Figure 3, right). The simulations were carried out with release speeds according to Table 1 (100 m/s and 500 m/s). In Figure 4 the flammable mass history is shown for both cases, being the flammable range defined between 4% and 75% by volume. Within 20 s the inflow of hydrogen is balanced by the losses through the ventilation system, producing an almost steady amount of flammable hydrogen. The maximum flammable mass is just above 1 gram for the 500 m/s case and above 0.1 gram for 100 m/s. As the maximum flammable mass is small, it appears that further investigations are not necessary.

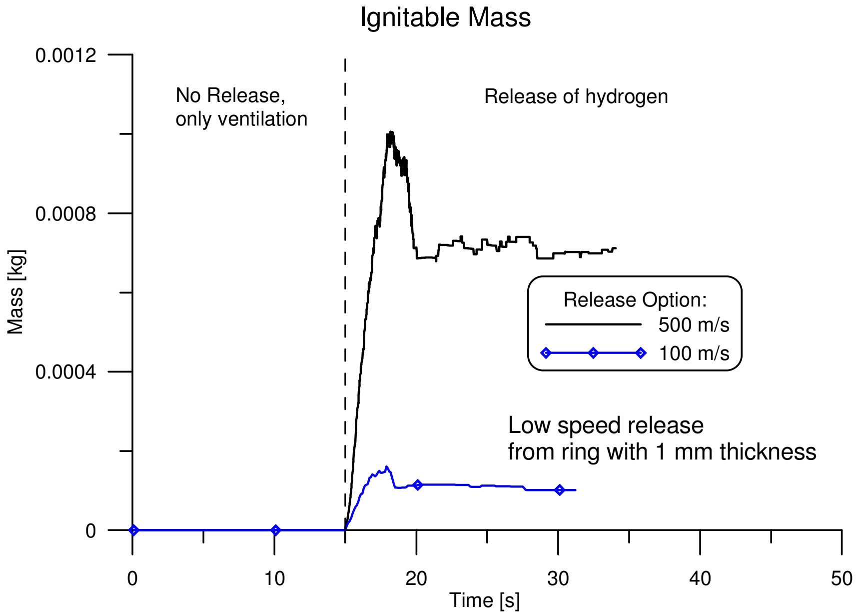

Figure 4. Flammable mass history (>4% hydrogen mol fraction) with subsonic speed hydrogen releases

3.2.2 Critical Hydrogen Release (scenario B)

Two different pressures have been considered at the leakage opening for the choked flow conditions: 50 and 100 bar. The pressure at the exit was assumed to be constant for the whole duration of the release. This assumption is conservative since the pressure at the exit in reality decreases with time. The duration of the release is limited by the total amount of hydrogen in the system, which is 1.2 kg. For the 100 bar case, the injection duration is 9 s while for the 50 bar case it is 20 s.

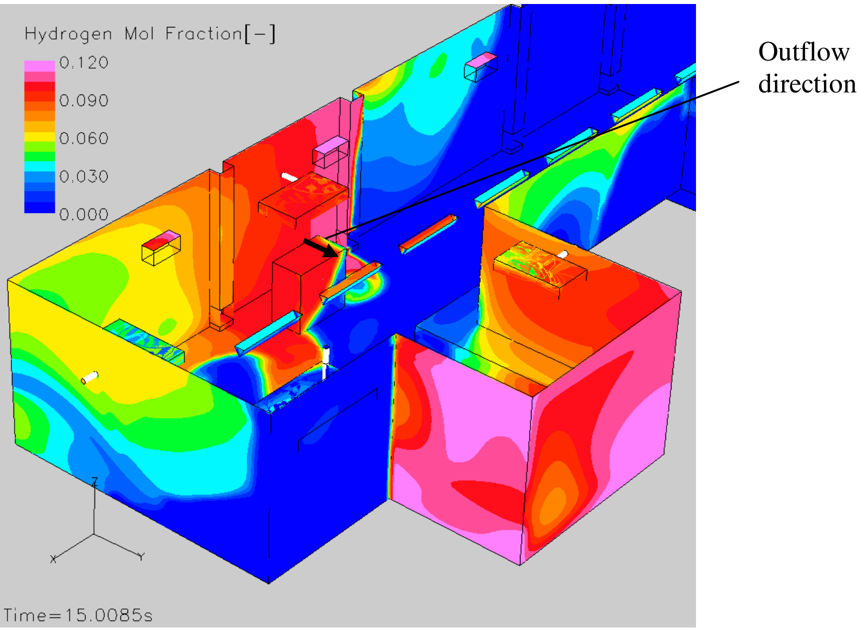

Figure 5. Hydrogen concentration in the lab at the end of release. Exit pressure equal to 100 bar.

In Figure 5 the hydrogen concentration on the walls is illustrated at the end of the release for the case with the exit pressure equal to 100 bar. The full analysis of the 3-D results shows that the highest concentrations are found in the regions along the jet axis and in the regions of the laboratory opposite to the leak source.

In Figure 6 the history of the flammable mass is shown for both pressures. The maximum flammable mass is slightly larger and it occurs earlier in time for the 100 bar case than for the 50 bar case. Since experimental investigations by Swain and his co-workers showed that hydrogen mixtures between 4 and 10% are not easy to ignite with ignition sources from electrical appliances [8], in Figure 6 the range of hydrogen-air mixture between 10% and 75% is also plotted. This additional information shows that a significant amount of flammable mass is between 4% and 10% that is the less reactive flammable range. Similar considerations can be done also for the flammable volumes, as shown in Figure 7.

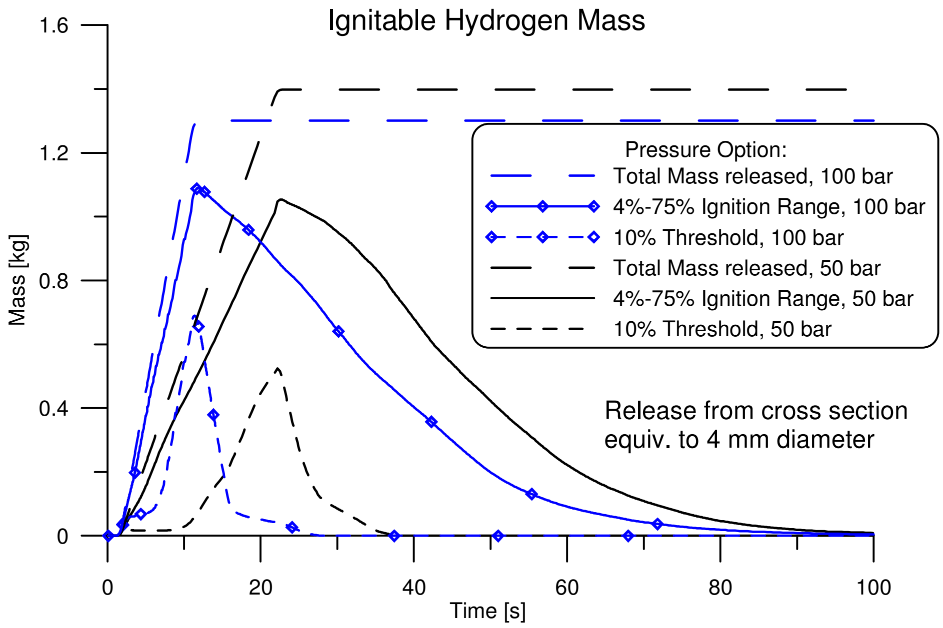

Figure 6. History of flammable mass for 50 and 100 bar release pressure.

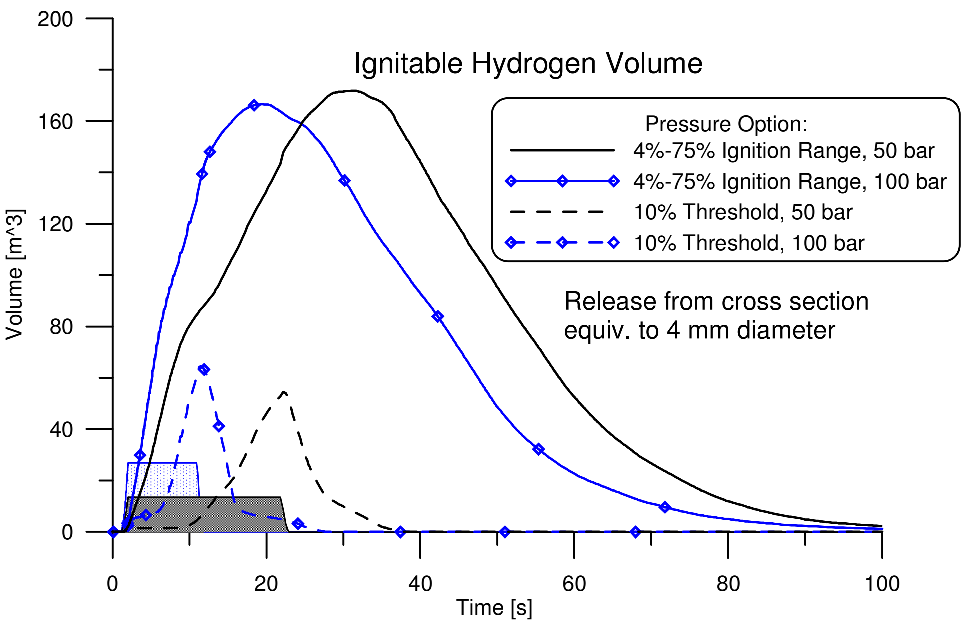

Figure 7. History of flammable volume for 50 and 100 bar pressure. The two shaded regions on the left bottom corner indicate the duration of the hydrogen release for both pressures (blue colour for 100 bar and black colour for 50 bar)

In terms of the maximum of flammable mass and volume, it appears that the results are very similar for 50 bar and 100 bar. The pressure does not affect significantly the value of the maximum flammable mass and volume.

Additional simulations have been performed in order to investigate the influence of mesh resolution on the results of the calculations. In Figure 8, as example of this investigation, flammable volume histories calculated with a coarse and a fine computational mesh are compared in the case of 50 bar release pressure. It is shown that results do not change significantly between the two meshes.

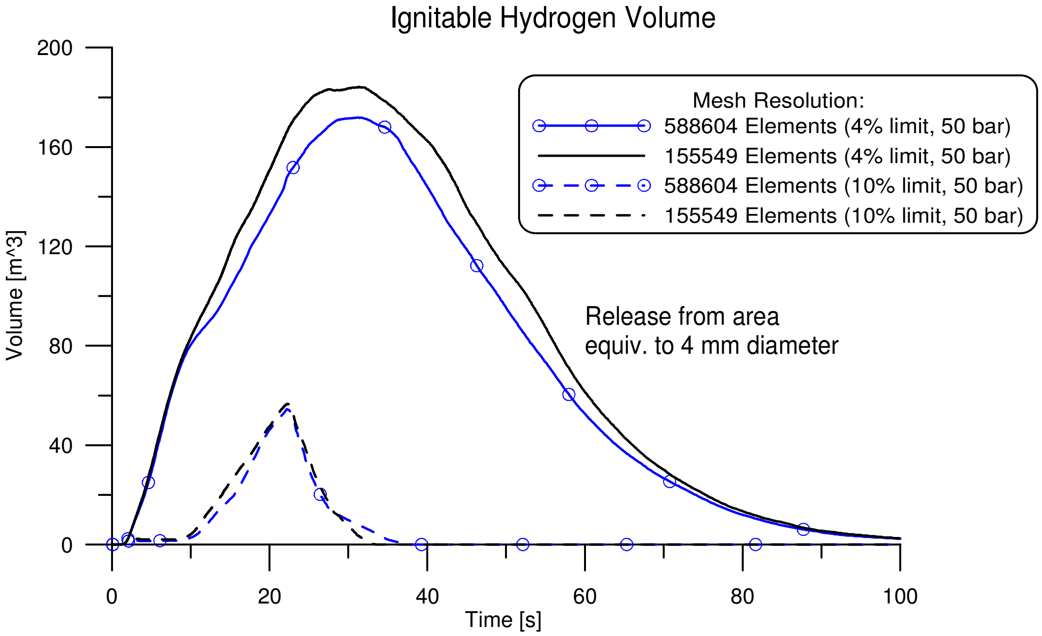

Figure 8. Influence of mesh resolution on size of flammable cloud in lab

In Figure 9, the history of hydrogen molar fraction at two different sensor locations is given. The two sensors are located under two fume hoods: the RIG hood that is just above the leak and the AMC hood that is located on the opposite side of the lab, as shown in Figure 2. Due to the horizontal high momentum jet release, hydrogen is detected first by the AMC sensor and only later by the RIG sensor which is located closer to the release source. In any case, since the alarm threshold of the sensors is very low (0.4%), both sensors are capable of detecting the leak within some seconds.

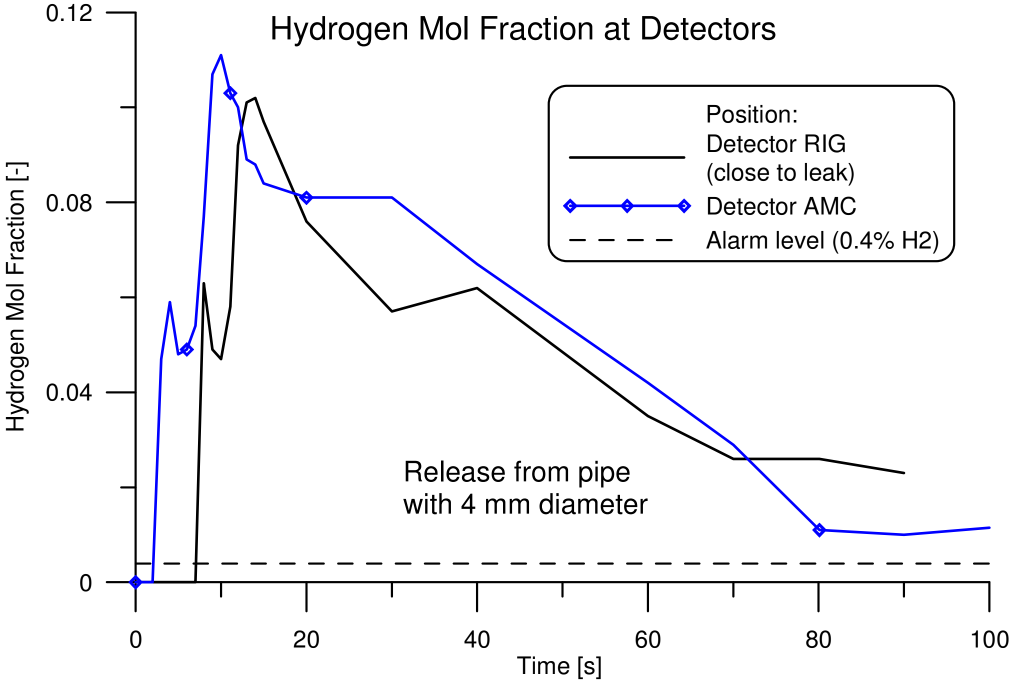

Figure 9. Hydrogen build-up at detector locations underneath fume hoods RIG and AMC

4.0 CONCLUSIONS

Numerical simulations of accidental leakage from high-pressure hydrogen system in a real laboratory were performed with the CFD code CFX. It was assumed that the mitigation measures are not available at the time of the accidental releases in order to consider a worst case scenario.
Two different release scenarios were selected: a sub-sonic release and a critical (sonic) release. In the sub-sonic case a very small amount of flammable mixture in the order of few grams is formed in the lab. In this case equilibrium is reached between leak flow and sinks of hydrogen within 20 seconds due to the operating ventilation system. In the critical speed case a flammable cloud in the order of one kilogram is observed for a short time. It must be emphasized that a significant fraction of the flammable mass is in the range between 4% and 10%, which is the least reactive range. The ventilation system of the lab is able to remove the hydrogen almost completely about 80 s after the release has finished.

Mesh dependency investigations were performed in order to demonstrate that the simulations results are almost grid independent.

The results of the numerical simulations will be used to identify critical positions for the installation of additional safety sensors.

As a future work, additional release scenarios will be taken into account, e.g., the hydrogen supply system will be included in the simulation. A further area of investigation will be a combustion scenario based on the dispersion calculations.

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