TOWARDS THE SIMULATION OF HYDROGEN LEAKAGE SCENARIOS IN CLOSED BUILDINGS USING CONTAINMENTFOAM

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ABSTRACT

The increase of using hydrogen as a replacement for fossil fuels in power generation and mobility is expected to witness a huge leap in the next decades. However, several safety issues arise due to the physical and chemical properties of hydrogen, especially its wide range of flammability. In case of Hydrogen leakage in confined areas, Hydrogen clouds can accumulate in the space and their concentration can build up quickly to reach the lower flammability limit (LFL) in case of not applying a proper ventilation system. As a part of the Living Lab Energy Campus (LLEC) project at Jülich Research Centre, the use of hydrogen mixed with natural gas as a fuel for the central heating system of the campus is being studied. The current research aims to investigate the release, dispersion, and formation and the spread of a hydrogen cloud inside the central utility building at the campus of Jülich Research Centre in case of hypothetical accidental leakage. Such a leakage is simulated using the open-source *containmentFoam* package base on OpenFOAM CFD code to numerically simulate the behavior of the air-hydrogen mixture. The critical locations where hydrogen concentrations can reach the LFL values are shown.

1.0 INTRODUCTION

The world nowadays witnesses a global transition from fossil fuel to more sustainable and ecological sources of energy. Despite the superb calorific values of the different fossil fuels, alternatives to this kind of fuel are being studied due to the economic, ecological, and even political implications of reliance on such a form of energy. Hydrogen has gained its reputation as an alternative to fossil fuels since its main source is water, which is available in abundance in most areas around the world [1]. The world demand for hydrogen has grown to 94 million tonnes (Mt) in 2021 with a 5% increase compared to the previous year [2]. The increase in demand for hydrogen is driven by the emerging new technologies in industry and transportation in using hydrogen as a fuel. For example, the technology of using hydrogen in the direct reduction of iron in the steel industry and the new design of automotive, maritime, and locomotive transportation units that runs on hydrogen [2]. However, the extreme physical and chemical properties of hydrogen pose a great challenge to widening its use in different applications. Therefore, this increase in using hydrogen as a fuel mandates higher safety levels to be utilized by non-trained individuals, in car refueling stations for instance [1].

Several research articles have numerically studied the leakage scenarios of different applications. For example, Qian et al. [3] performed a 3D CFD simulation of six different scenarios of gas hydrogen release in a refueling station in China. The six scenarios included different leakage locations, wind speeds, and wind directions. They have found that the closer the leakage location to the wall, the more complicated and unpredictable the flammable the hydrogen cloud is. Kim et al. [7] studied the leakage of a refueling station at different hydrogen pressures and leakage diameters. From their simulations, they managed to calculate the safety distance between hydrogen storage tanks and the nearest building to protect personnel in case of an explosion. Hwang et al. [4] also studied the dispersion of cryogenic hydrogen clouds after accidental high-pressure hydrogen leakage in a storage facility. They have found that the cloud in this case stays heavier than the air and behaves so as long as it is still in a cryogenic state. However, it starts to move upwards once its temperature increases.

For automotive applications, Choi et al. [5] studied hydrogen cloud dispersion in an underground car park due to hydrogen leakage from fuel cell vehicles (FCV). In their work, they concluded that the operation of a ventilation fan in this car park delayed the expansion of the hydrogen flammable region and hence provided a better solution to reduce the flame hazard. Hajji et al. [6] have reached the same conclusion regarding the accidental leakage of hydrogen in closed garages with natural and mechanical ventilation. In their study, they compared hydrogen concentration in a closed garage in the case of different ventilation opening shapes and in the case of using a ventilation fan. They have found also that when the aspect ratio of the vent increases, the rate of hydrogen evacuation increases. Li et al. [7] investigated the dispersion of hydrogen clouds inside a closed car park with different crossbeam heights. In addition, they have proved that the presence of ventilation openings has a significant effect on the size of the flammable region inside such a structure.

Han et al. [8] also studied the ventilation of the hydrogen charging platform package (HCPP), which is a mobile hydrogen charging station. They have concluded the necessity of ventilation to avoid the accumulation of hydrogen in case of leakage inside the package. Li et al. [9] have investigated the hydrogen leakage behavior in a fuel cell ship. From their simulations, they have concluded that using mechanical ventilation in fuel cell cabins is the best way to avoid hydrogen accumulation in case of leakage. Bauwens and Dorofeev [10] also simulated hydrogen leakage in a large-scale facility. After validating their CFD solver with the experiment done by Ekoto et al. [11], they simulated a storage facility with 31,200m3 volume with a fine resolution to capture the hydrogen concentrations in the facility. They have estimated that the proper ventilation rate should be 3 air changes per hour for a 1 kg/min leakage.

Despite the different research works related to hydrogen leakage as explained above, there is still no research work that simulates hydrogen leakage in facilities with complicated details. Different machines and pipes in such facilities can dramatically change the behavior of the leakage, and hence the concentrations of hydrogen in case of leakage. Therefore, the work presented in this paper provides a prototypical investigation of accidental hydrogen leakage inside the central utility building at the campus of Jülich Research Centre in case of accidental leakage. The details of all equipment inside the building were included in the 3D CAD model used in the simulations.

In the following sections, the details of the solver and the turbulence models used in the simulations are discussed. After that, validation cases and the results of the grid test are shown. The following sections show the results of the 3D building simulations in different leakage scenarios discuss the results and illustrate the conclusions from the work done.

2.0 CFD SIMULATIONS

To simulate the flow of the leaked hydrogen, it should be considered as a turbulent flow problem. As it is well known that, there is no exact solution for turbulent flow (yet). However, many turbulence models were introduced during the last few decades to approximately solve the Navier-Stokes equations of the turbulent flow. In this work, a modified version of the $k - \omega\ SST$ turbulence model is used to simulate the buoyant, turbulent hydrogen flow. Before introducing the modification applied on the $k - \omega\ SST$ the solver used in this simulation is introduced.

2.1 The *containmentFOAM* package

The *containmentFOAM* is a package of solvers and libraries that works within the OpenFOAM® CFD toolkit. Despite including numerous solvers to simulate different thermo-fluid phenomena, developing new solvers might be necessary to simulate special systems. Therefore, this package of solvers and libraries is developed and maintained by *Forschungszentrum Jülich* for nuclear reactor safety research. The aim of the development of the open-source *containmentFOAM* package was to simulate the thermo-fluid phenomena that occur in the containment building of nuclear reactors during different incident scenarios. However, the solvers and libraries in this package can also be used for hydrogen safety simulations.

2.2 Simulation of the multi-species gas mixture

Like all CFD software, OpenFOAM® numerically solves the Navier-Stokes equations for the domain to simulate the fluid flow. In this case, the conservation equations can be stated in the form:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \left(\rho \vec{U}\right) = 0 \quad (1)$$

$$\frac{\partial \rho \vec{U}}{\partial t} + \nabla \cdot (\rho \vec{U} \otimes \vec{U}) = -\nabla \mathrm{p} + \nabla \cdot \tau + \rho \vec{g} \quad (2)$$

$$\frac{\partial \rho \mathrm{h}}{\partial t} + \nabla \cdot (\rho \vec{U} h) + \frac{\partial \rho \mathrm{K}}{\partial t} + \nabla \cdot (\rho \vec{U} K) = \vec{U} \cdot \rho \vec{g} + \frac{\partial p}{\partial t} + \nabla \cdot \left(\vec{U} \cdot \tau\right) - \nabla \cdot \vec{q}'' - \nabla \cdot \vec{q}''_{rad} \quad (3)$$

where equations 1, 2, and 3 are the mass, momentum, and energy conservation equations respectively. The shear stress tensor (τ) in Eq. 2 is calculated from the equation:

$$\tau = \rho \left(v + v_t\right) \left[\nabla \vec{U} + \left(\nabla \vec{U}\right)^T - \frac{2}{3} \delta \nabla \cdot \vec{U}\right] \quad (4)$$

Here c_p is the heat capacity at constant pressure and $\rho \vec{U}. \vec{g}$ is the potential energy. Based on the simple gradient diffusion hypothesis (SGDH), Schmidt and Prandtl numbers take the values:

$$Sc_t = Pr_t = 0.9 \quad (5)$$

Additionally, the species transport equation takes the form:

$$\frac{\partial \rho Y_i}{\partial t} + \nabla \cdot (\rho \vec{U} Y_i) = \nabla \left[\rho \left(D_{i,m} + \frac{v_i}{Sc_i}\right) \nabla Y_i\right] \quad (6)$$

Where Y_i and $D_{i,m}$ is the mass fraction of species (i) and its diffusion coefficient with the mixture respectively.

2.3 Turbulence modeling

The $k - \omega$ SST model is used in many research and industrial applications as a reliable turbulence mode for many wall-bounded problems. This is reliability comes from its unique treatment for the wall and boundary layer. Since the complexity of the problem that is discussed in this work comes from the presence of different structures, like pipes and machines, inside the domain, the $k - \omega$ SST turbulence model should be a candidate for such simulations. According to Menter and Esch [12], the $k - \omega$ SST takes the form:

$$\frac{\partial(\rho k)}{\partial t} + \frac{\partial(\rho \vec{U} k)}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\left(\mu + \sigma_k \mu_t\right)\frac{\partial k}{\partial x_j}\right) + \tilde{P}_k - \rho \beta^* \omega k + P_{k,b} \quad (7)$$

$$\frac{\partial(\rho \omega)}{\partial t} + \frac{\partial(\rho \vec{U_j} \omega)}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\left(\mu + \sigma_{\omega 3} \mu_t\right)\frac{\partial \omega}{\partial x_j}\right) + \frac{\gamma}{\nu_t} P_k - \rho \beta \omega^2 + 2(1 - F_1)\frac{\rho \sigma_{\omega 2}}{\omega}\frac{\partial k}{\partial x_j}\frac{\partial \omega}{\partial x_j} + P_{\omega,b} \quad (8)$$

The variables in equations 7 and 8 are explained in the work of Menter and Esch [15]. However, the $k - \omega\ SST$ turbulence models in this form cannot be used to simulate buoyant gas clouds without the addition of a source term that simulates buoyancy. Therefore, the SGDH defines the production terms in equations 7 and 8, namely $P_{k,b}$ and $P_{\omega,b}$ as:

$$P_{k,b} = -\frac{\nu_t}{\sigma_t} g_i \frac{\partial \rho}{\partial x_i} \quad (9)$$

$$P_{\omega,b} = \nu_t \left((\gamma + 1)\, C_3 \cdot \max\left(P_{k,b}\, , 0\right) - P_{k,b} \right) \quad (10)$$

Where $\sigma_\rho = 1$ and C_3 is the turbulent dissipation coefficient and in this case was taken to equal 1.

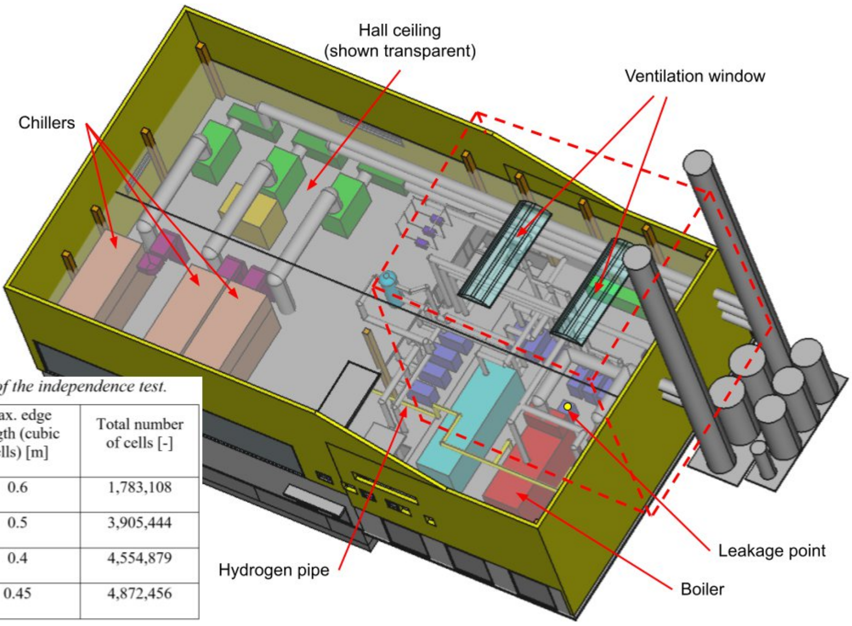
Extensive verification and validation work was carried out to ensure the accuracy of using the above-described turbulence models in the simulations of buoyant gas releases. The validation cases are explained in detail in many published literature [13-15]. The next section shows how the above-shown turbulence model is applied to our simulations to simulate hydrogen leakage scenarios.

3.0 NUMERICAL SETUP

The correct application of the modified $k - \omega\ SST$ requires the generation of a proper computational grid and the usage of the different numerical solvers and schemes and boundary and initial conditions. The following describe the 3D geometry used for the simulation of the industrial facility. Also, the generated grid for this study and the used schemes, solvers, boundary conditions, and initial conditions are explained. After that, a detailed grid dependence study is shown.

3.1 Facility geometry

The geometry of the facility selected for simulation is the actual 3D building of the central utility building at Jülich research center including the 3D shapes of the different equipment and pipes of the building. The 3D model and the different equipment are shown in Fig. 1. In this figure and for the sake of clarity, the roof of the building is shown as transparent to show the different components inside the building. In this work, only a part of the building surrounding the hydrogen release, as marked in Fig. 1, is simulated. This part was selected to minimize the computational effort needed to perform such simulations and also because the lateral spread of the hydrogen cloud is not expected to be extended beyond this part. This 3D model is then used to generate the computational grid that represents the void inside the building in which the hydrogen can flow.



Grid sizes of the independence test.

Grid No.	Max. edge length (cubic cells) [m]	Total number of cells [-]
1	0.6	1,783,108
2	0.5	3,905,444
3	0.4	4,554,879
4	0.45	4,872,456

Figure 1: 3D CAD model of the central utility building at Jülich research center.

The main machine hall of the building has two parts: one part with double-height area and the other part consists of two single-height areas. The focus of this study is on a part of the double-height area where the boilers, which operate with mixed natural gas and hydrogen, are located. In addition, two skylights are located on the ceiling of this area. These two skylights act as a natural outlet in case of fire to vent out the smoke or to vent out hydrogen in case of leakage. Additionally, the hall is provided with other mechanical ventilation equipment that their effect is not in the scope of this work

3.2 Grid and numerical setup

Using the 3D CAD model described in the last section, the computational grid is generated using cfMesh software [16]. In the present work, the grids used are Cartesian hex-dominated grids with a fine first cell layer near all walls. Special refinement around the walls (construction walls, pipes, equipment…etc.) was applied to ensure accurate simulation of the flow. Furthermore, additional refinement was added to the grid 1.8m below the ceiling of the equipment hall to ensure adequate spatial resolution of the space and hence accurate simulation of the hydrogen cloud as recommended by Tolias et al. [17]. Since the outlet for the hydrogen cloud is the two openings of the roof of the building as shown in Fig. 1, the final computational grid was extended about 15m above the roof to ensure that the hydrogen cloud will flow with pure buoyancy without being affected by any boundary conditions. Such an approach was applied in many research works like Giannissi et al. [18] and Matsuura et al. [19]. Additionally, this approach complies with the best practice guidelines (BPG) of applying boundary conditions away from the area of interest. A section in the final grid and the locations of the measuring points, marked in red, used during simulations are shown in Fig. 2. As shown in the figure, the measuring points are selected to be located close to the ceiling to measure the cloud concentration. However, the measuring points are not too close to the ceiling to be influenced by the boundary condition of the ceiling.

To study the proper grid resolution, different Cartesian-dominated grids are generated to fill the air domain inside the geometry and locally refined in critical regions like around and above the leakage point. In this work, four different grids with different numbers of cells are used and the concentrations of hydrogen at different locations near the ceiling of the space are compared. The table in Fig. 1 shows the different grid sizes in this grid independence studies and the locations of the measuring points are shown in Fig. 2. From the grid independence study, it is concluded that Grid 2 shows the closest behavior compared to the finest grid, Grid 4 in this case. Accordingly, grid characteristics and resolution of Grid 2, grid refinement locations, for instance, are used to generate the grid of the domain for the simulations in this work. The difference between the aforementioned Grid 2 and the final grid is that the final one has a 15 m extension above the ventilation windows for the reasons explained earlier in this section.

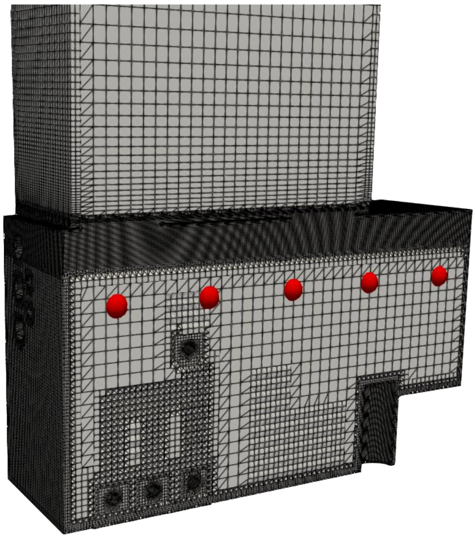


Figure 2: Section in the computational grid with measuring points marked in red

For the boundary conditions, all solid boundaries inside the building are treated as walls with non-slip conditions for velocity and zero-gradient for pressure and fixed temperature. On the other hand, the external sides of the extended region are considered as zero-gradient in case of outlet flow and with a fixed zero value in case of inlet flow. It should be noticed that an additional inlet patch was added to an external wall of the building. This addition aims to ensure an inflow of pure air to the building to enhance the buoyancy of the hydrogen cloud and compensate for the exhausted gases from the roof openings. Since the hydrogen pipe is equipped with different pressure and flow rate sensors to detect any damage in the pipe, it is thought that the worst-case scenario (WCS) is that the leakage will last for 20 s before the detection of any high flow-rate leakage and hence cutting the hydrogen flow from the source. Accordingly, the final simulations are carried out for 20 s after the start of the leakage.

4.0 SIMULATION RESULTS AND DISCUSSION

In this case, the hydrogen flow rate was taken to be equivalent to the leakage from a 40 mm diameter hole, which corresponds to the jet-to-plume transition diameter, in a 10 bar pipe. By using the jet model explained by Molkov [20], the given leakage characteristics lead to a flow rate of 0.984 kg/m^3. To avoid running the simulations at excessively low CFL numbers, the hydrogen flow is assumed to be flowing through an inlet patch with a larger area than the area of the 40 mm hole. Despite this might lead to inaccurate results near the inlet due to the changed velocity, it is proven that it has a minor effect on the hydrogen cloud shape near the ceiling.

The preliminary results of the simulations show the hydrogen cloud distribution inside the building near the ceiling of the hall and the exit of the hydrogen cloud from the ceiling openings. Fig. 3 shows the contour surface of hydrogen volumetric concentration at 4%, the lower flammability limit (LFL) of hydrogen. This figure shows that the hydrogen layer shows maximum depth at the corners of the building away from the ventilation openings. Such behavior is expected since the current simulations show only the distribution in the case of natural ventilation. Additionally, the figure shows that the overhead piping enhances the distribution of the cloud as the hydrogen flows toward the ceiling and is forced to flow around the pipes. Such piping can hinder the natural flow of hydrogen when it is located in the track of the flow to the ventilation openings in the ceiling.

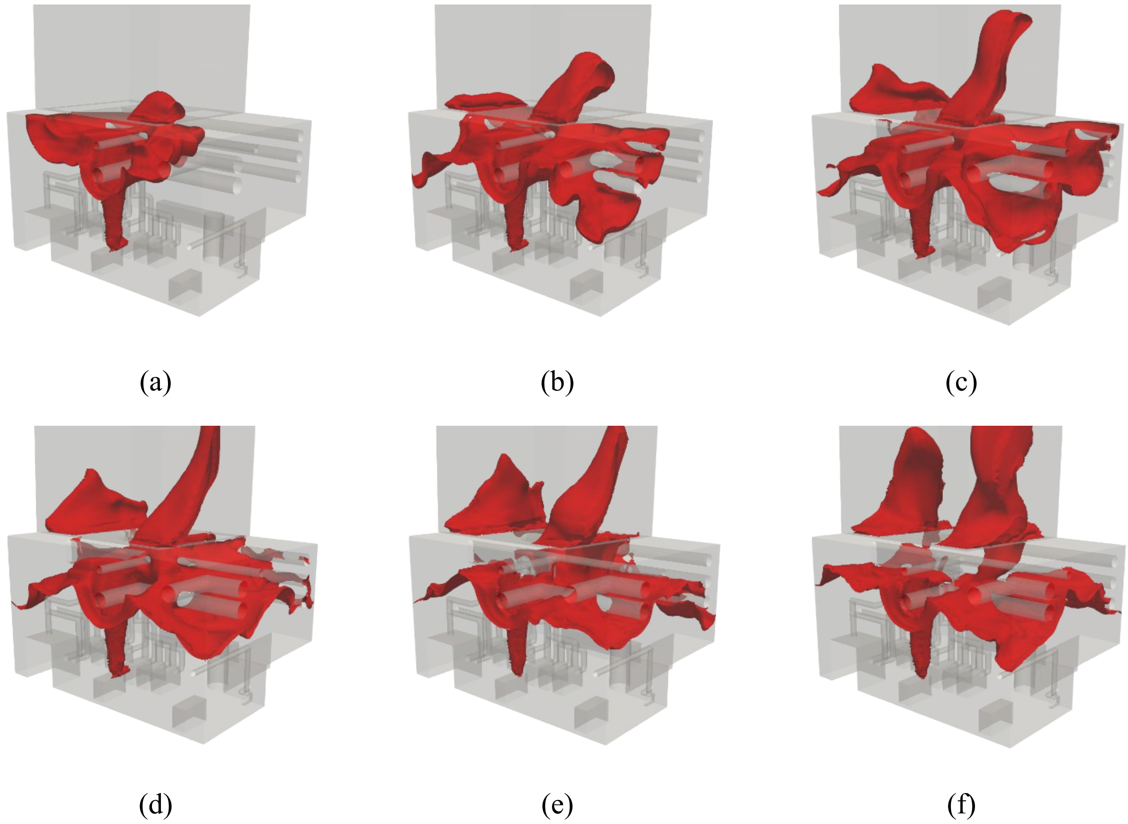


Figure 3: Contour surface of hydrogen cloud at LFL concentration after (a) 3 s, (b) 6 s, (c) 9 s, (d) 12 s, (e) 15 s, and (f) 18 s from the leakage start.

Fig. 4 depicts the development of hydrogen concentrations at the different sensors shown in Fig. 2. From this figure, it can be seen that the concentrations near the ceiling have almost zero values from the start of the leakage to around 4 seconds. After this period, the concentrations jump to levels higher than the LFL after about 9 seconds and keep increasing. This jump and increase represent the accumulation of the hydrogen cloud near the ceiling. This accumulation represents the real risk behind such a leakage since any location inside the building with concentrations higher than the LFL represents a potential ignition point of the cloud.

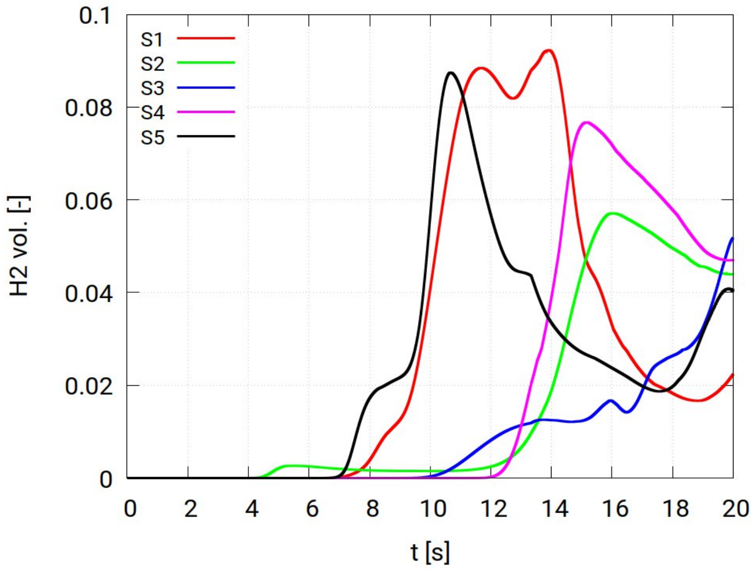


Figure 4: Hydrogen vol. concentrations development in the building at three different locations shown in Fig. 2.

In general, it can be concluded that the hydrogen concentration can build up inside the building rapidly. Accordingly, there is a need for careful study of the ventilation process during hydrogen leakage to avoid flammable locations inside the buildings. In addition, different ventilation strategies such as mechanical ventilation or local ventilation in critical areas should be considered in such a study to enable the extraction of hydrogen from the space as soon as possible to avoid ignition. To trigger such a ventilation, a sensors concept should be designed based on flow analysis to study the proper locations and the time lag between the start of the leakage and the start of the ventilation system.

5.0 CONCLUSIONS AND FUTURE WORK

In this work, the hydrogen leakage inside an industrial building is simulated. The details of the building, such as different equipment and pipes, were included in this study to analyze their effects on the hydrogen concentrations. To simulate such a case, the open-source package *containmentFOAM* was used in this simulation. The preliminary simulations shows the rapid accumulation of hydrogen cloud near the ceiling of the machine hall at the corners located far from the ceiling openings. These locations are potential ignition locations and should be ventilated. Also, the overhead pipes near the leakage location play a very important role in distributing the hydrogen concentration to wider areas of the ceiling and partially blocking the natural flow of hydrogen.

From the preliminary simulations, it can be concluded that natural ventilation of hydrogen cloud is only effective if the hydrogen source is located close to the ventilation openings. Otherwise, the hydrogen cloud can accumulate rapidly. In addition, it should be considered to locate such sources away from the walls to delay the accumulation of hydrogen near the walls and in the corners. A good alternative for natural ventilation is to use mechanical ventilation near the hydrogen sources to extract hydrogen from the space safely and rapidly. Such a mechanical ventilation should be triggered by sensors located inside the building to detect hydrogen leakage. The locations of these sensors should be carefully studied using flow analysis to decrease the response time of the ventilation system and hence to remove the hydrogen before its accumulation.

Such mechanical ventilation systems will be considered in future work of this research. Additionally, the whole building should be considered in such simulations to check the extents of the distribution of hydrogen below the ceiling. However, this represents a challenge due to the high computational effort needed to simulate the whole building for a time period long enough to see the full effects of all parameters. Additionally, the different mechanical ventilation rates recommended in standards and codes should be considered to check if these values are adequate to prevent the ignition of hydrogen.

ACKNOWLEDGMENT

The Living Lab Energy Campus (LLEC) project is funded by the German Federal Ministry of Education and Research (BMBF) project No.:03SF0573. The simulations are carried out on the JURECA supercomputer at Jülich Supercomputer Center (JSC) under the project *cfrun* grant No. 26701.

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