SIMULATION OF THE EFFICIENCY OF HYDROGEN RECOMBINERS AS SAFETY DEVICES

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ABSTRACT

Passive auto-catalytic recombiners (PARs) are used as safety devices in the containments of nuclear power plants (NPPs) for the removal of hydrogen that may be generated during specific reactor accident scenarios. In the presented study, it was investigated whether a PAR designed for hydrogen removal inside a NPP containment would perform principally inside a typical surrounding of hydrogen or fuel cell applications. For this purpose, a hydrogen release scenario inside a garage – based on experiments performed by CEA in the GARAGE facility (France) – has been simulated with and without PAR installation. For modeling the operational behavior of the PAR, the in-house code REKO-DIREKT was implemented in the CFD code ANSYS-CFX. The study was performed in three steps: First, a helium release scenario was simulated and validated against experimental data. Second, helium was replaced by hydrogen in the simulation. This step served as a reference case for the unmitigated scenario. Finally, the numerical garage setup was enhanced with a commercial PAR model. The study shows that the PAR works efficiently by removing hydrogen and promoting mixing inside the garage. The hot exhaust plume promotes the formation of a thermal stratification that pushes the initial hydrogen rich gas downwards and in direction of the PAR inlet. The paper describes the code implementation and simulation results.

1.0 INTRODUCTION

The use of hydrogen in confined spaces is accompanied by the risk of unintended releases due to leaks or component failures. Various safety measures or devices may be applied to detect and/or avoid hazardous hydrogen/air mixtures. The project InsHyde – within the framework of the European HySafe network [1] – has investigated realistic small-medium indoor hydrogen leaks and provided recommendations for the safe use/storage of indoor hydrogen systems [2]. Protection measures according to the principles prevention, detection, protection, and intervention have been summarized. Safety measures such as avoiding a leak, limiting a leak's magnitude and hydrogen quantity to be released, detecting a leak or a fire, interrupting a leak, avoiding hydrogen accumulation and ignition or explosion, and finally limiting the damages in a case of an ignition or explosion have been discussed in a public report [3].

As a measure avoiding hydrogen accumulation, passive auto-catalytic recombiners (PARs) are used in the containments of nuclear power plants (NPP) for the removal of hydrogen that may be generated during specific reactor accident scenarios [4]. Due to their ability to convert hydrogen and oxygen into water already at low (ambient) temperature, PARs provide a hydrogen sink even in situations where dilution and venting is limited or impossible.

The principle of a PAR is illustrated in Fig. 1. Inside the open bottom part of a steel housing, catalyst sheets form a set of parallel vertical flow channels. On the catalyst surface, hydrogen entering the PAR is converted with oxygen to water. Due to the exothermal reaction, a buoyancy-driven flow is induced inside the chimney part which ensures a continuous gaseous flow through the PAR. PARs are passive safety devices without the need of external power supply. Different designs aim at performance optimization in terms of hydrogen conversion rate, avoiding ignition, and protection of the catalyst against poisoning and related deactivation effects. In order to assess the efficiency of PAR applications, substantial efforts have been spent on developing model strategies [6].

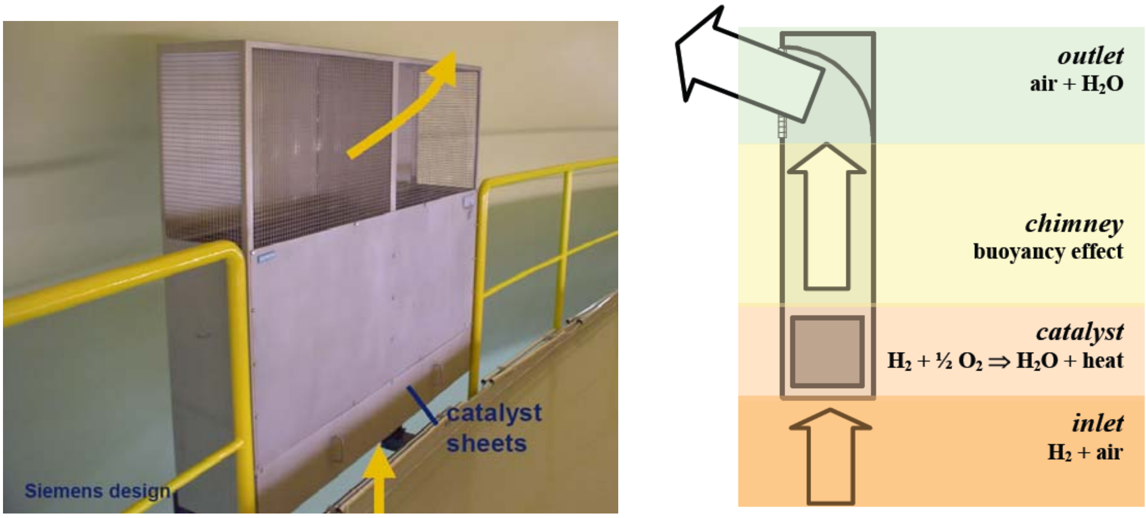

Figure 1. PAR installed inside a nuclear power plant (left), principle of a PAR (right) [5].

The goal of the presented study was to investigate whether a PAR designed for hydrogen removal inside a NPP containment would operate efficiently inside a realistic environment for hydrogen or fuel cell applications. Inside NPP containments, the thermal hydraulic conditions for PAR operation are dominated by large natural convection loops due to large temperature and density gradients in large geometries (20,000-70,000 m^3 containment volume, typical length scales 5-50 m). However, typical surroundings of hydrogen or fuel cell applications – e.g. service rooms or car garages – are of significant smaller scale and different thermal hydraulic conditions.

As a suitable scenario, a release scenario inside a car garage was selected. Experimental data on helium dispersion experiments performed in the GARAGE facility operated by CEA/Saclay in France [7] were available from the HySafe standard benchmark exercise problem SBEP-21 [8].

2.0 NUMERICAL APPROACH

From a physical point of view, the modeling of the operational behavior of a PAR is a complex task, as the relevant phenomena include the interaction of heterogeneous catalysis and buoyancy driven flows. Due to the heating of the gas in the catalyst section, the buoyancy driven flow is induced inside the chimney. However, the flow velocity is influencing the mass transfer controlled catalytic reaction which in turn represents the heat source. The modeling of the interaction of both sections is considered essential for the accurate description of the PAR operational behavior.

Furthermore, modeling of PARs encompasses a large variety of scales, from micrometers (thickness of the catalysts) up to meters (size of the confinement). A CFD calculation resolving all these scales would be much too expensive [6]. However, the transport processes occurring on small scales define important parameters, e.g. the efficiency and heat source of the PAR, and need to be considered carefully in order to perform a reliable analysis on PAR performance in accident scenarios.

At Forschungszentrum Jülich, a coupled approach has been developed: REKO-DIREKT [9], a 2D mechanistic PAR model, has been coupled with ANSYS-CFX [10]. 3D atmospheric flows are simulated by means of the CFD code, while PARs are considered as black-boxes represented by means of inlet and outlet boundary conditions. The characteristic physical phenomena inside the PAR are modeled by means of REKO-DIREKT, which provides the boundary conditions for the CFD calculation.

Besides the geometrical information for the catalyst sheets and the PAR box, a REKO-DIREKT run needs information on the gas temperature and gas composition at the PAR inlet and the total pressure. Based on this input, REKO-DIREKT calculates (Fig. 2)

- the catalyst temperature distribution,
- the change of the gas composition along the catalyst sheets (i.e. hydrogen depletion),
- the mass flow through the PAR, induced by buoyancy,
- the outlet gas temperature, and
- the outlet gas composition.

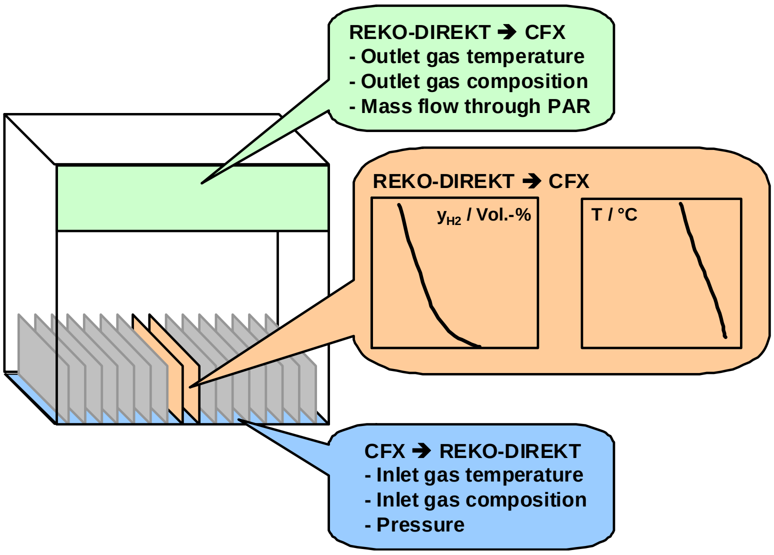

Figure 2. REKO-DIREKT input and output data.

Data handling between REKO-DIREKT and CFX is performed by means of the CFX Memory Management System (MMS), which can be accessed by both codes. The coupling is performed on a master-slave base, i.e. the REKO-DIREKT execution is fully controlled by CFX. All variable fields are stored in the MMS and read out as an initialization for the next REKO-DIREKT start.

The coupling of REKO-DIREKT and CFX is performed by means of two types of user routines: junction box routines which are program flow controlled (i.e. executed at certain steps in CFX program flow) and user functions which are data controlled (i.e. executed if data is requested). All input parameters for REKO-DIREKT, such as PAR geometry or grid resolution are supplied by the CFX definition file. Fig. 3 shows the data management between REKO-DIREKT and CFX. Blue dashed lines mark reading from MMS, red dashed lines writing to MMS.

At the start of the CFX run, the junction box routine ‘createinput’ initializes data arrays and saves the input parameters to the MMS. These parameters are the gas composition, temperature, and absolute pressure, as well as all the initialization values and parameters necessary for the REKO-DIREKT run. The junction box routine ‘rekodirekt’ contains the main program and is called once at the beginning of each CFX time step. It reads out the REKO-DIREKT variable fields and input values, performs one REKO-DIREKT run, and writes the updated variable fields and output parameters back to the MMS.

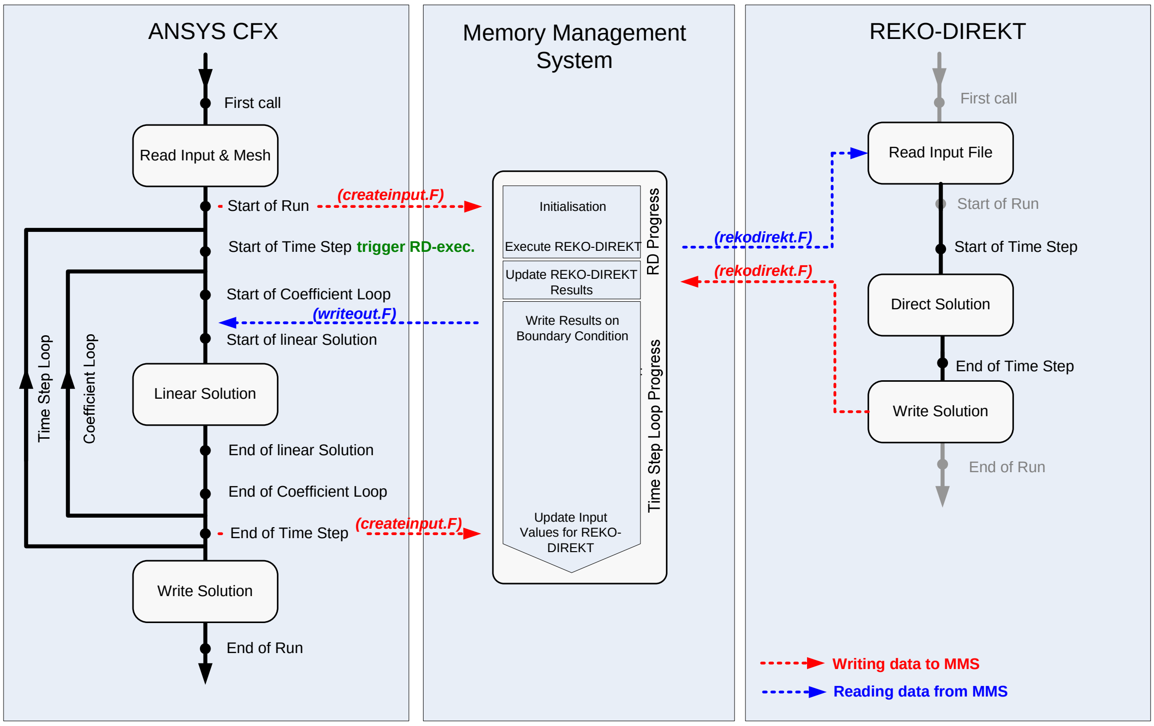

Figure 3. Data management for a coupled REKO-DIREKT-CFX run.

While the CFX 'coefficient loops' are performed, the REKO-DIREKT results are requested several times and read out by the data controlled user function ‘writeout’, which returns PAR mass flow, outlet concentrations and temperature to CFX. At the end of each CFX time step, the REKO-DIREKT input values within the MMS are updated by means of the 'createinput' routine.

The transient coupling of both codes is clarified in Fig. 4. At the beginning of a time step, REKO-DIREKT provides a solution based on initial input values or values from the previous time step to CFX (1). CFX uses these values and performs a time step loop (2). At the end, the input values for REKO-DIREKT are updated (3) and used to calculate new REKO-DIREKT output values (4). These are provided to CFX (1) at the next time step.

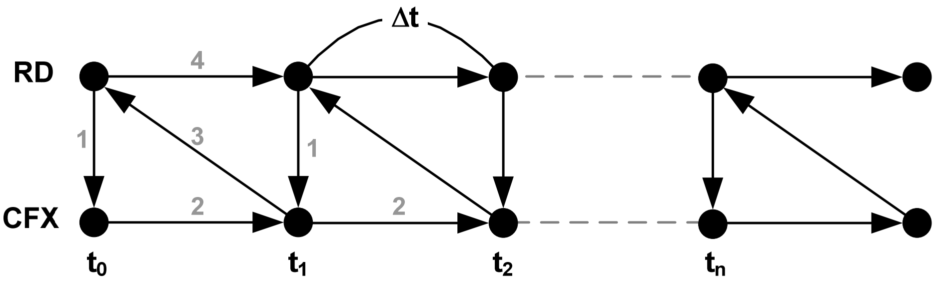

Figure 4. REKO-DIREKT-CFX transient coupling: explicit scheme.

In this manner the transient coupling is performed explicitly, i.e. the REKO-DIREKT solution of each time step is based only on the input values of the previous CFX time step, not the current one. By doing so the REKO-DIREKT runtime is reduced to a single run (~70 ms) per time step. Additionally, the coupling is more stable as the boundary conditions don't change within a time step loop. From a physical point of view the error induced by this explicit coupling is marginal because PAR response on changing inlet conditions is quite slow compared to the atmospheric flow, which is due to thermal inertia of the PAR structures.

3.0 SIMULATION RESULTS

The simulation of PAR efficiency as a mitigation measure inside a garage is performed in three steps:

1) Simulation of the GARAGE Test-1 – which was performed with helium – in order to validate the dispersion and mixing model.

2) Simulation of the same scenario, but with hydrogen instead of helium. This step addresses two aspects. First, a comparison with the helium-injection scenario allows a further check of the model. Second, differences between helium and hydrogen are addressed. In the context of the last step, this calculation also serves as an “unmitigated” reference case.

3) Inclusion of a PAR and simulation of the mitigated scenario in order to investigate the feasibility and efficiency of such a measure.

The GARAGE facility (Fig. 5) represents a single prototypical vehicle storage place with the geometric dimensions 5.8 m x 3.0 m x 2.4 m (L x W x H). The volume of the garage is about 41 m³. The helium injection is controlled by a mass flow controller. The facility is equipped with 64 helium sensors (‘mini-katharometers’) in order to obtain a detailed picture of the gas distribution. Due to safety reasons, helium gas is used to simulate the hydrogen dispersion characteristics [7].

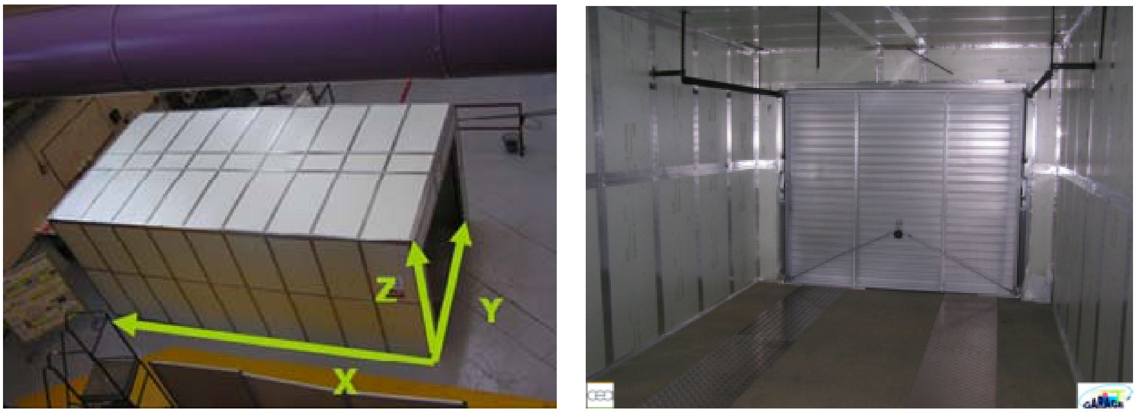

Figure 5. Garage facility: top view (left), inside (right) [8].

3.1 Helium distribution

The GARAGE Test-1 scenario is characterized by a short term release of around 240 g helium with high injection momentum and flow rate (1.99 g/s). Fig. 6 shows the numerical setup of the CFD simulation.

The helium injection pipe is located in the center of the rectangular domain. The numerical domain has been bisected and a symmetry assumption has been applied in order to reduce the computational effort. The injection is modeled by means of an inlet boundary condition with a prescribed mass flow rate and a turbulence degree of 5%. Helium is injected upwards at a constant rate of 1.99 g/s over a period of 121 s. In order to describe the thermal hydraulics and the species transport within the

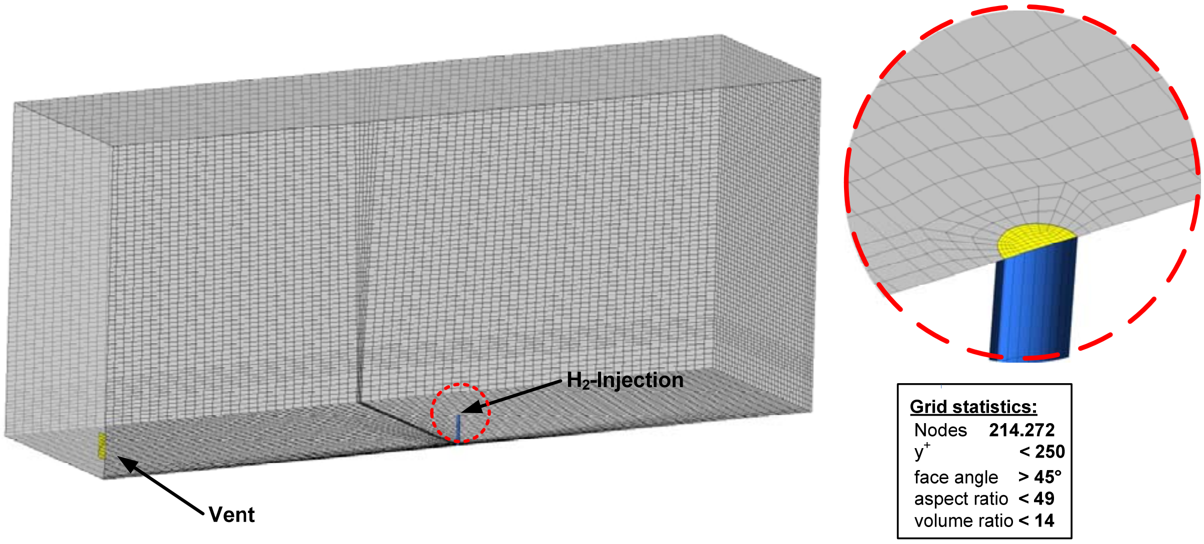

Figure 6. Numerical setup for the helium release and dispersion scenario.

GARAGE facility, a system of Reynolds and Favre averaged Navier Stokes equations and an additional transport equation for helium closed by ideal gas equations of state and the SAS-SST turbulence model [10] is solved. The latter contains additional terms in order to describe turbulence production and dissipation due to buoyancy. Buoyancy is modeled by means of the full-buoyancy model based on density differences. In the present case of the pure dispersion scenario an isothermal calculation is performed. The vent located close to the bottom at the rear side of the facility is modeled as an opening, which allows in and out flow in both directions.

Fig. 7 gives an impression of the calculated flow and concentration field within the GARAGE facility and the location of the helium sensors. For this qualitative illustration, a picture of a calculation performed with hydrogen is used. In order to enhance the visibility of the different concentration levels, the color scheme is limited to 10 vol.%. The helium plume is rising from the injection and

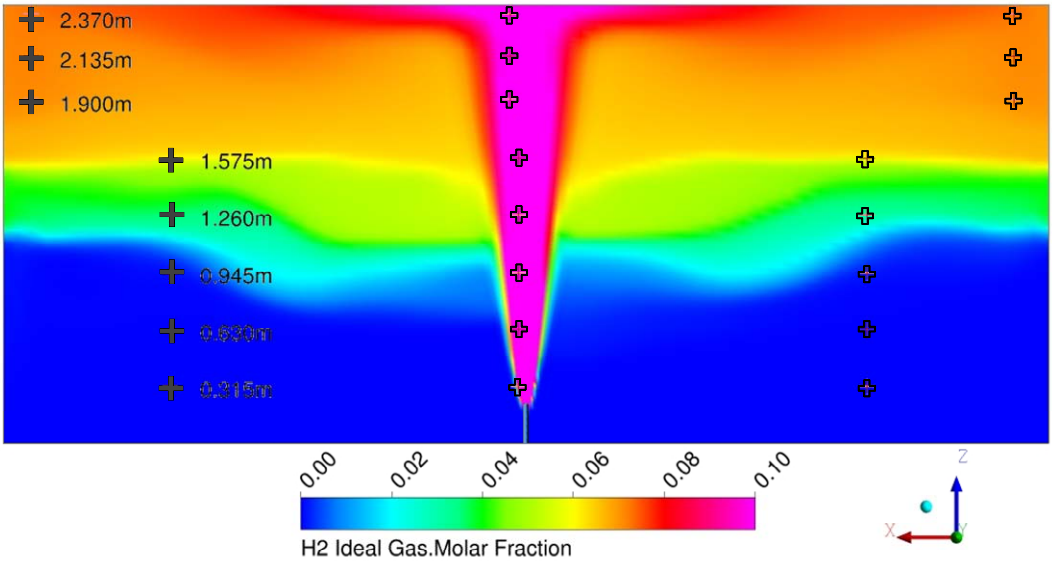

Figure 7. Qualitative impression of the release scenario and measurement locations.

forming a stable ceiling layer. After a time of 121 s, the helium injection is stopped and the situation changes into a diffusion controlled scenario, characterized by slow decrease in concentrations. Fig. 8 quantitatively compares the predicted helium concentration profiles by means of average values for a layer equal to the z-values of the measurement points (to be identified in Fig. 7) at several times during the injection phase. The experimental results are predicted quite well; however a slight over prediction of the mixing process near the layer interface becomes obvious.

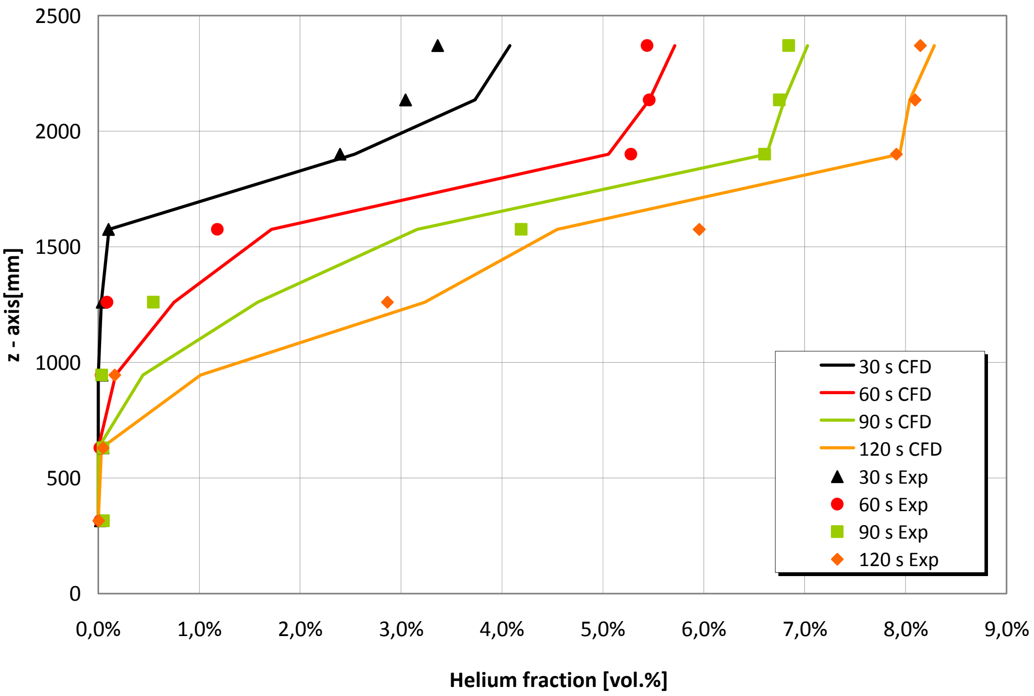

Figure 8. Quantitative comparison of the helium concentration profiles.

3.2 Hydrogen distribution

In order to assess the efficiency of PAR operation in this scenario, an “unmitigated” reference case was calculated. For this purpose, the same simulation as described above has been performed with a hydrogen/oxygen/nitrogen mixture instead of a helium-air mixture. Fig. 9 compares concentration profiles between the helium and hydrogen cases for various times during the injection phase. Due to the lower density of hydrogen the gradients are slightly steeper but, apart from that fact, comparable.

This simulation shows the formation of a hydrogen rich ceiling layer with concentrations above the ignition limit. Due to the slow diffusive mixing process there is the risk of ignition/combustion if there is no sufficient venting available.

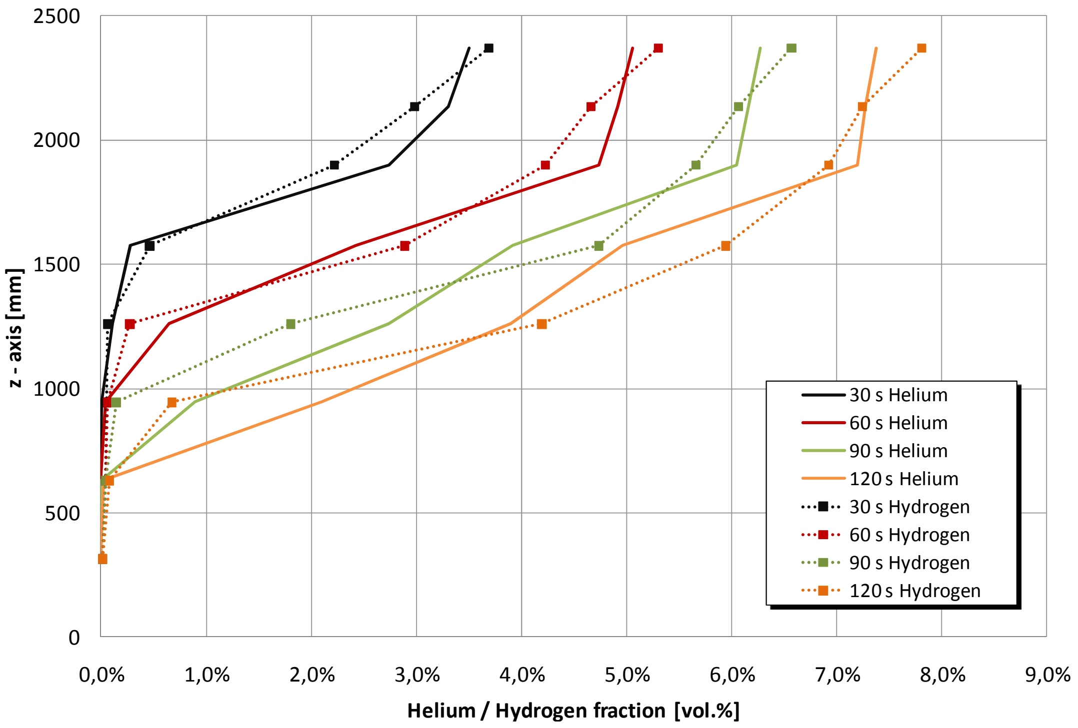

Figure 9. Comparison of calculated helium and hydrogen concentration profiles.

3.3 PAR performance and efficiency

For the final step of the study, the implementation of a commercial PAR unit (AREVA FR90-150) inside the garage is assumed in order to avoid or at least mitigate the consequences of hydrogen combustion. The PAR box has a cross section of approx. 20 cm x 17 cm and a height of 1 m. This

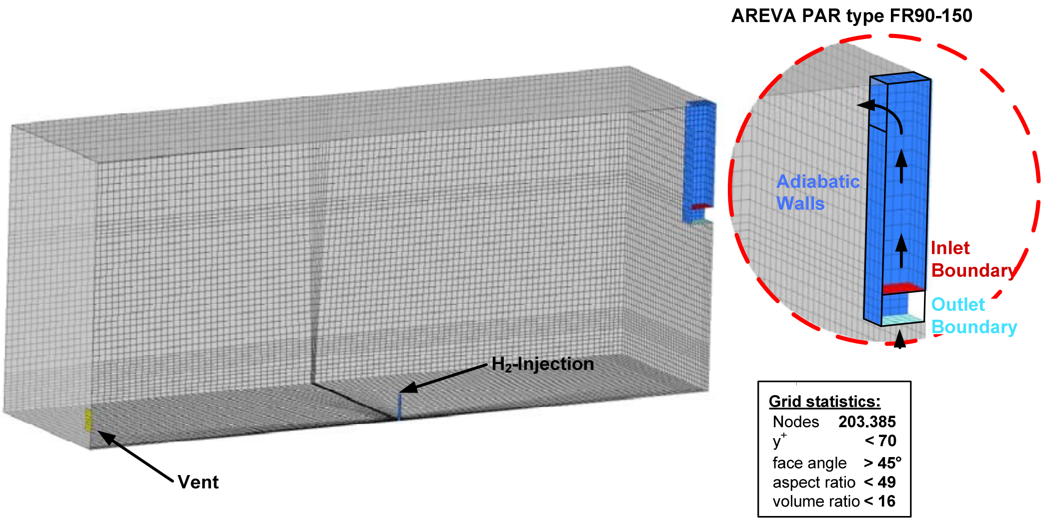

Figure 10. Numerical setup for the PAR mitigation scenario.

PAR type was investigated in the German ThAI facility operated by Becker Technologies in Eschborn [11]. Data from these experiments served for the validation of the REKO-DIREKT code [9].

The PAR is placed directly below the ceiling, i.e. within the ceiling layer (Fig. 10). It is located directly at the symmetry plane, thus representing a PAR of twice the size. In order to simulate the hydrogen recombination, the energy equation and additional transport equations for the species H_2, O_2 and H_2O are included. For the sake of simplification, heat losses through the isolated garage walls, radiative heat exchange between the PAR and the garage walls, and conductive heat transport through the PAR housing are neglected. The PAR itself is modeled by means of inlet and outlet boundary conditions, which are delivered by the REKO-DIREKT-CFX interface.

Figure 11 compares the scenario with and without mitigation by means of the hydrogen concentration field in the symmetry plane at three times (120 s, 240 s, 800 s). Again, the color scheme is limited to 10 vol.% in order to enhance the visibility of the different concentration levels. At the beginning of the injection phase, the scenario is quite similar for both cases as the hydrogen rich layer doesn’t reach the PAR inlet located 1 m below the ceiling. After a time of ~60 s, an inlet concentration of approx. 1.5 vol.% is reached and PAR operation slowly starts. The hot exhaust gas plume of the PAR is lighter than the cold hydrogen-air mixture and thus forms a thermal stratification above the hydrogen layer. With continuing recombination, the thermal stratification expands downwards and thus pushes the hydrogen rich layer down to the PAR inlet. After around 600 s, the maximum hydrogen concentration in the mitigated scenario falls below the ignition limit of 4 vol.% while in the pure release and dispersion scenario, only slow diffusive dilution of the ceiling layer occurs.

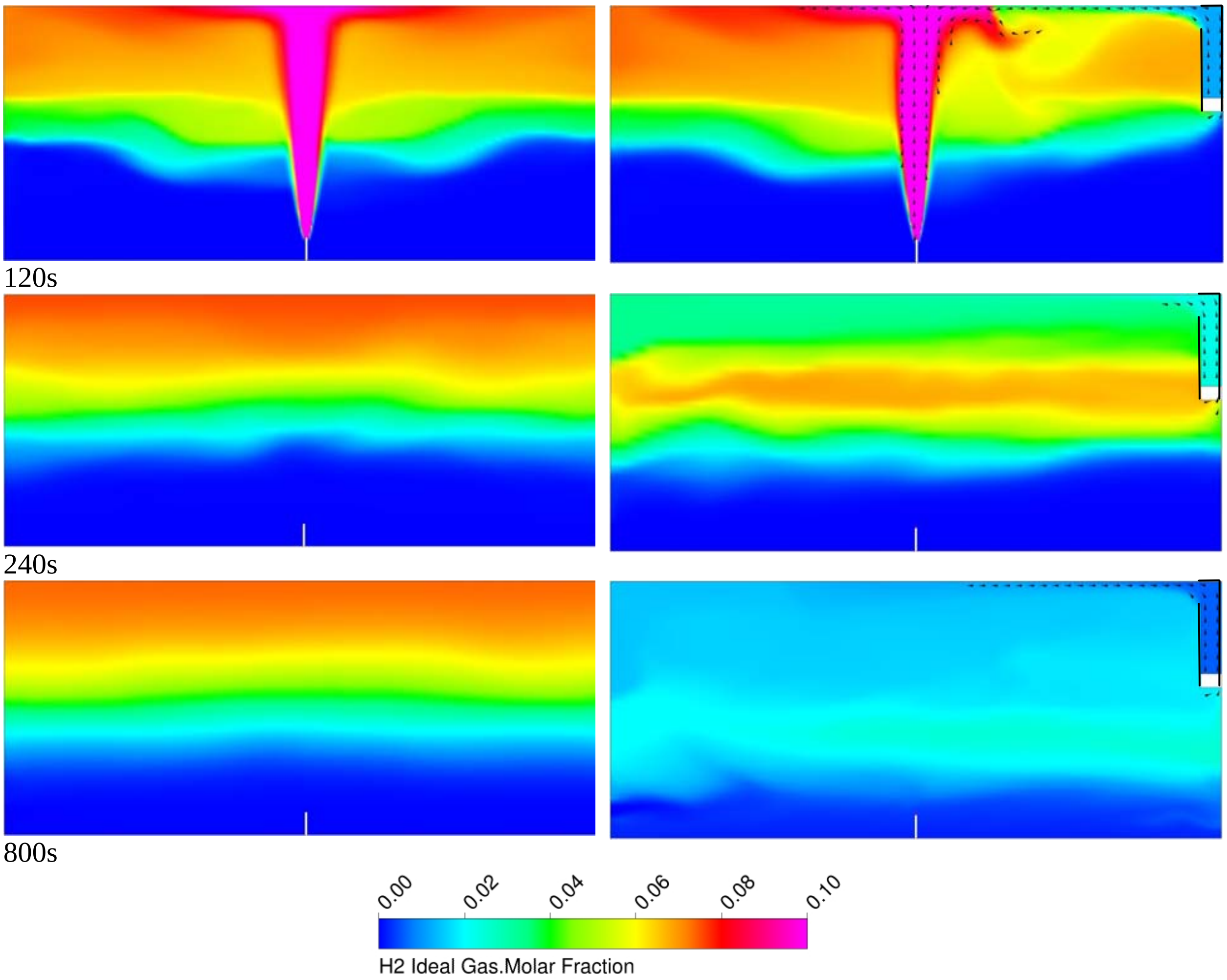

Figure 11. Hydrogen concentration field for unmitigated (left) and mitigated scenario (right).

In order to demonstrate the efficiency of the PAR, Fig. 12 compares the flammable cloud volume histories for both cases. In the unmitigated case, after the end of injection nearly 50% of the garage volume is filled with a flammable mixture. Dilution is very slow due to the slow diffusion process. In the mitigated case, approx. 120 s after the start of the hydrogen injection the first significant effect of the starting PAR operation becomes visible. For about 50 s, the volume of the flammable mixture further increases, due to the fact that the depleted outlet gas leaving the PAR at the top is mixing with the hydrogen rich layer without diluting it below the flammability limit. As a consequence, the volume of the flammable mixture increases although hydrogen is consumed. Approx. 175 s after the start of the hydrogen injection, the PAR efficiently removes the flammable gas mixture at a rate of about 2.4 m³/min. In addition, the induced mixing process leads to a further mobilization and dilution of the flammable cloud much faster than a pure diffusion driven process.

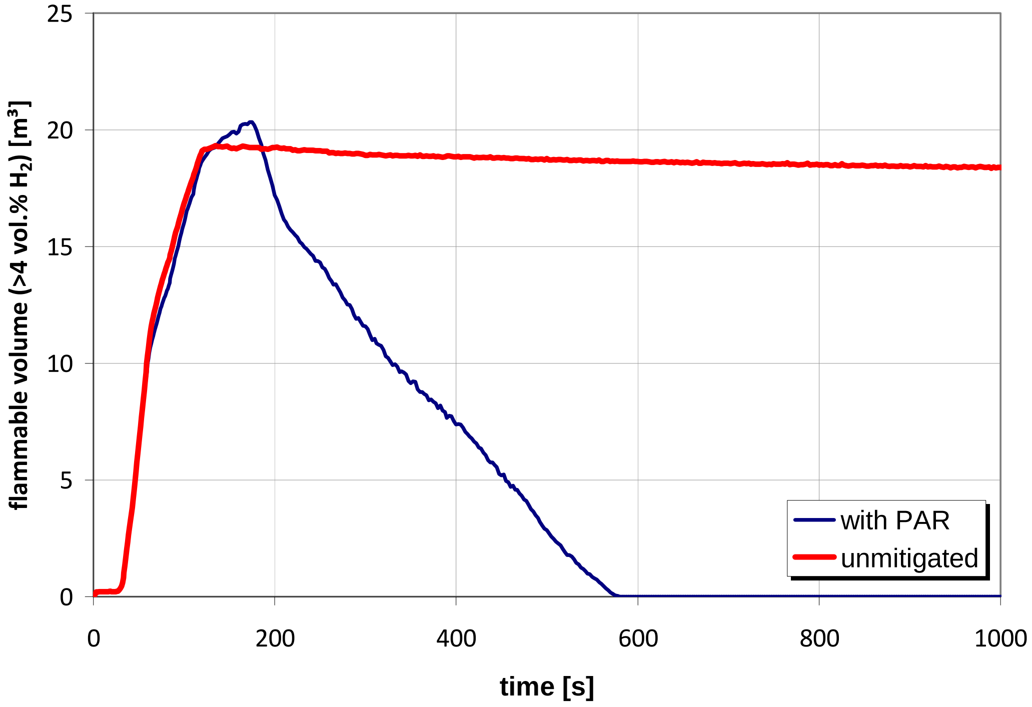

Figure 12. Flammable cloud volume histories for the mitigated and unmitigated scenario.

The predicted mixing scenario is beneficial for PAR operation as the depleted hot exhaust gas can build a layer above the hydrogen and thus mobilize and transport the hydrogen to the PAR inlet. If this is also the case for releases of higher amounts of hydrogen remains to be studied. Future work will cover different hydrogen release conditions (injection rate, location, and direction), different PAR designs and numbers, and different geometries of the enclosure.

4.0 CONCLUSIONS

The efficiency of the application of a PAR inside a car garage for hydrogen removal from a small leak has been studied. The goal was to estimate whether a PAR designed for operation under the thermal hydraulic conditions inside a NPP containment would operate efficiently inside a realistic environment for hydrogen or fuel cell applications. The study was performed with the CFD code ANSYS-CFX. For the modeling of the operational behavior of the PAR, the in-house code REKO-DIREKT was implemented.

The simulation results show that the PAR works efficiently by removing hydrogen and promoting mixing inside the garage. In the selected scenario with a total injection of approx. 1.5 m³ hydrogen, the PAR eliminates the flammable cloud within 10 min of the injection. The hot exhaust plume promotes the formation of a thermal stratification that pushes the initial hydrogen rich gas downwards and in the direction of the PAR inlet.

The study will be continued with the variation of several parameters such as hydrogen release (injection rate, location, and direction), PAR design and number, and geometry of the enclosure. Important specific attention will have to be paid to potential scenarios where the PAR may ignite the hydrogen/air mixture or where airborne substances may poison the catalyst. The results may help assess the efficiency of PAR application for plant design and safety considerations within conventional power plants, e.g hydrogen cooled generators and hydrogen processing plants, as well as stationary storage facilities, e.g. fuel stations.

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