

THE CONTRIBUTION OF NUCLEAR HYDROGEN SAFETY KNOWLEDGE TO EMERGING HYDROGEN TECHNOLOGIES

ERNST-ARNDT REINECKEÁ
PhD, Head of Department
PHD, FORSCHUNGSZENTRUM JÜLICH GMBH,
GERMANY

AHMED BENTAIB
PhD, Expert
INSTITUT DE RADIOPROTECTION ET DE SÛRETÉ
NUCLÉAIRE, FRANCEU

NABIHA CHAUMEIX
PhD, Director of Research
ICARE – CNRS ORLÉANS, FRANCES

MANUELA JOPEN
PhD
GESELLSCHAFT FUER ANLAGEN- UND
REAKTORSICHERHEIT, GERMANY

SARA BECK
Dipl.-Ing. Head of Department
GESELLSCHAFT FUER ANLAGEN- UND
REAKTORSICHERHEIT, GERMANY

THOMAS JORDAN
Prof. Dr., Head of Department KARLSRUHE
INSTITUTE OF TECHNOLOGY, GERMANY

ANDREAS FRIEDRICH
PhD, Scientist
KARLSRUHE INSTITUTE OF TECHNOLOGY,
GERMANY

SHANNON KRENZ
BSc, PhD Student

FORSCHUNGSZENTRUM JÜLICH GMBH,
GERMANY

KHALED YASSIN
PhD, Scientist
FORSCHUNGSZENTRUM JÜLICH GMBH,
GERMANY

INTRODUCTION

In the wake of the climate crisis, large parts of the world are currently rethinking the way they produce and use energy. Many countries have committed to reducing CO₂ emissions and are considering moving away from fossil fuels and making greater use of so-called renewable energy sources such as water, sun and wind. In Europe, the European Commission put forward its strategic long-term vision for a climate-neutral EU by 2050 in November 2018, which was endorsed by the European Parliament in its resolution on the European Green Deal in January 2020 [1].

However, the production of renewable energy sources is associated with high fluctuations and variable availability, which is why the availability of large energy storage systems is necessary. Hydrogen produced in times of excess electricity is considered to be a suitable candidate as it has many possible applications across industry, transport, power and buildings sectors as a feedstock, a fuel or an energy carrier. Again, the European Commission considers to install at least 40 Gigawatt of electrolyser power by 2030 and the production of up to ten million tonnes of renewable hydrogen in the EU [2].

Hydrogen is a gas with properties that vary significantly from those of other common gaseous energy carriers, such as

methane. The safety-relevant properties in particular mean that hydrogen can easily escape through leaks, has a very wide ignition range, is more flammable and is more likely to detonate due to high flame velocities. In addition, the low energy density of hydrogen means that either high pressures (up to 1000 bar) or cryogenic temperatures (-253 °C) must be used to store it, which poses further safety risks [3].

Decades of experience in the chemical industry with hydrogen as a feedstock show that it can be handled safely. However, as the hydrogen economy ramps up, numerous new companies and start-ups - many of them SMEs - are entering the market, and hydrogen is set to be used in numerous new applications, technologies and, above all, in previously unimaginable quantities. Against this backdrop, hydrogen safety will play a key role in the introduction of hydrogen as an energy carrier.

HYDROGEN SAFETY EXPERTISE WITHIN THE NUCLEAR COMMUNITY

Hydrogen safety has played an important role in the context of water-cooled nuclear power plants for decades. The reason for this is the large quantities of hydrogen that are produced in a severe accident during core degradation, which can enter the containment via the primary circuit and produce flammable gas mixtures with the oxygen present

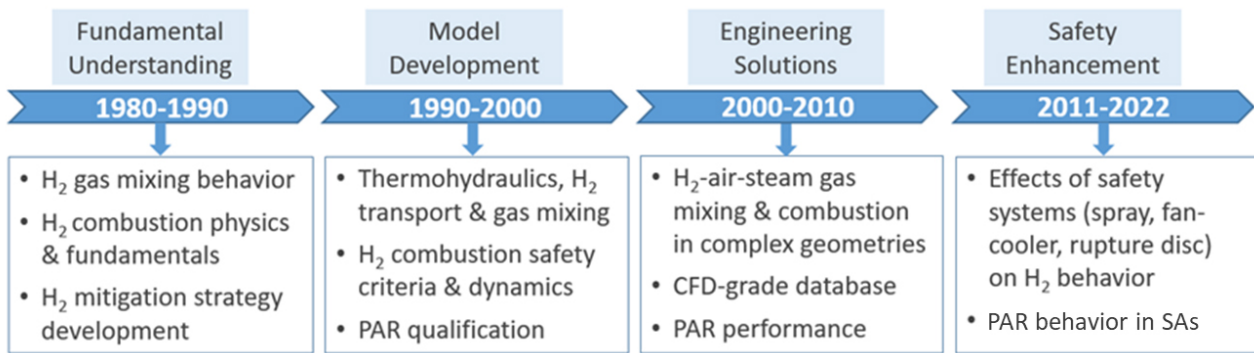


Figure 1. Evolution of hydrogen safety research in the nuclear community [5].

there. At least since the TMI-2 reactor accident in 1979, significant efforts have been made internationally in industry and research to understand the physical and chemical processes involved in such scenarios and to develop and implement suitable preventive and mitigative measures [4]. Unfortunately, the Fukushima Daiichi reactor accident has drastically confirmed the importance of such R&D activities.

Figure 1 gives an overview of the broad expertise related to hydrogen safety, which was developed in the nuclear community since the 1980s [5]. The focus was on the areas of hydrogen distribution, hydrogen combustion and suitable countermeasures.

In the field of hydrogen distribution behaviour inside the containment, code development involved initially lumped-parameter and system codes, such as GOTHIC and MELCOR (USA), COCOSYS (Germany) and ASTEC (France). Since the late 1990s, more detailed codes, e.g. GASFLOW (Germany) – still with large nodalization – and increasingly the commercial CFD codes (computational fluid dynamics) ANSYS-CFX and FLUENT were qualified to allow a better resolution of the computational domain. More recently, the open source tool containmentFOAM (Germany) is under development to allow tailored containment analysis. Over these decades, code development has been supported by large scale experiments, such as PANDA (Switzerland), MISTRA (France), THAI (Germany) and experimental programs in the framework of OECD/NEA, for example ISP-29, ISP-47, SETH, and HYMERES.

Understanding the conditions for flame acceleration and deflagration-to-detonation-transition as well as the consequences for the containment integrity was in the focus of hydrogen combustion research. Combustion codes, such as COM3D, made use of hydrogen distribution simulations to obtain the initial conditions for the computation. Due to the complex nature of the combustion phenomena, high-resolution computational tools are increasingly applied. Relevant early large-scale experiments on hydrogen detonations were provided by the RUT facility (Russia), complemented by numerous shock tube experiments, such as ENACCEF/ENACCEF2 (France) and international benchmarks, e.g. OECD/NEA ISP-49.

Supported by increasing knowledge of hydrogen behaviour, mitigation strategies were developed and implemented in European PWRs since the late 1990s. Passive auto-catalytic recombiners (PARs) provided by Siemens (Germany, today

Framatome), AECL (Canada, today CNL), NIS (Germany, today Westinghouse) and partially igniters were retrofitted after extensive testing and qualification programs. Throughout the last two decades, numerous national and international research programs, e.g. OECD/NEA THAI and the EU project AMHYCO, involving experimental facilities, such as BMC (Germany), KALI and H2PAR (France), as well as THAI and the REKO platform (Germany), have deepened the understanding of PAR performance under severe accident conditions. The large database enabled the development of robust numerical PAR models, which are today available in all relevant codes to assess the performance of mitigation measures in severe accident scenarios [4].

PROJECTS ADVANCING THE SAFETY OF HYDROGEN TECHNOLOGIES

Expertise from the nuclear community is in demand when hydrogen safety needs to be ensured. This is reflected by the key participation of institutions with originally nuclear background in safety-related projects. The following examples give an overview of selected projects involving hydrogen safety expertise from the nuclear community.

Living Lab Energy Campus (LLEC)

As part of the "Living Lab Energy Campus" (LLEC) project, the campus of Forschungszentrum Jülich, Germany (FZJ) with its more than 7,000 employees is currently becoming a real laboratory where electrical, thermal and chemical energy flows in the plant network will be linked via a new intelligent IT system. Interactions between technology, energy sources and consumers will be scientifically investigated with a view to optimizing the interaction between humans and technology [6].

Hydrogen technologies are an important component and are being scientifically investigated along the entire value chain. In the field of hydrogen production, a test platform is available for investigating electrolysis stacks with proton exchange membranes (PEM technology for short). This means that stacks up to max. 400 kW from FZJ's own development but also from other manufacturers can be tested with regard to their performance in the LLEC network. One usage option is to transport the hydrogen via pipeline to the research center's central utility building (WVZ), where hydrogen is blended into natural gas for heat generation. In addition, storage in Liquid Organic Hydrogen Carriers (LOHC) is also being investigated.

As part of the LLEC's activities, the "Hydrogen Safety" team studies new safety aspects arising from the coupling of different hydrogen technologies. In this context, the team is investigating accident scenarios assessing the effects of possible hydrogen leakages. The knowledge in the field of hydrogen distribution and mitigation from nuclear safety research supported by dispersion calculations using containmentFOAM [7] are used to analyse hydrogen leakage scenarios in large scale installations.

While the basic properties of hydrogen are obviously the same in both nuclear and non-nuclear contexts, the boundary conditions of hydrogen dispersion differ considerably. The existing model for simulating accident-related hydrogen dispersion was therefore evaluated on the basis of the scenarios to be simulated and the need for further development was identified. In particular, turbulent dispersion under buoyant flow or jet-like release in variable flow conditions (especially for external flows and wind fields) had to be considered. In addition, there is a need for models of technical components (e.g. active ventilation systems) which, in addition to direct implementation in containmentFOAM, also include a connection to the open-source simulation package 'OpenModelica', which already contains a broad library for the simulation of dynamic technical systems [8]. Hence, a prototypical coupling with the open-source package OpenModelica was developed based on an explicit coupling scheme. For the first time, component models written in Modelica, for example to describe the operating

behaviour of catalytic recombiners, can be implemented into the CFD simulation as a 'Functional Mockup Unit' (FMU).

A three-dimensional CAD model of the building (Figure 2) was created to simulate potential hydrogen releases within the WWZ [9]. This CAD model was used to generate the numerical grid to simulate various scenarios of hydrogen leakages in the hydrogen piping system (Figure 3). The simulations show the rapid accumulation of hydrogen near the ceiling at the corners located far from the ventilation windows. 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.

The simulation results allow comparing the effects of both natural and forced ventilation. As mechanical ventilation is considered to be triggered by sensors located inside the building, the locations of these sensors could be optimized by the simulation results. Additionally, the different mechanical ventilation rates recommended in standards and codes could be considered to check if these values are adequate to prevent the ignition of hydrogen.

Towards safe storage and transportation of cryogenic hydrogen (STACY)

Hydrogen in liquefied form is considered to be the most economical way for long-distance transportation. However, storage and transportation of liquid hydrogen at large scales is connected with significant hazards connected with leakages

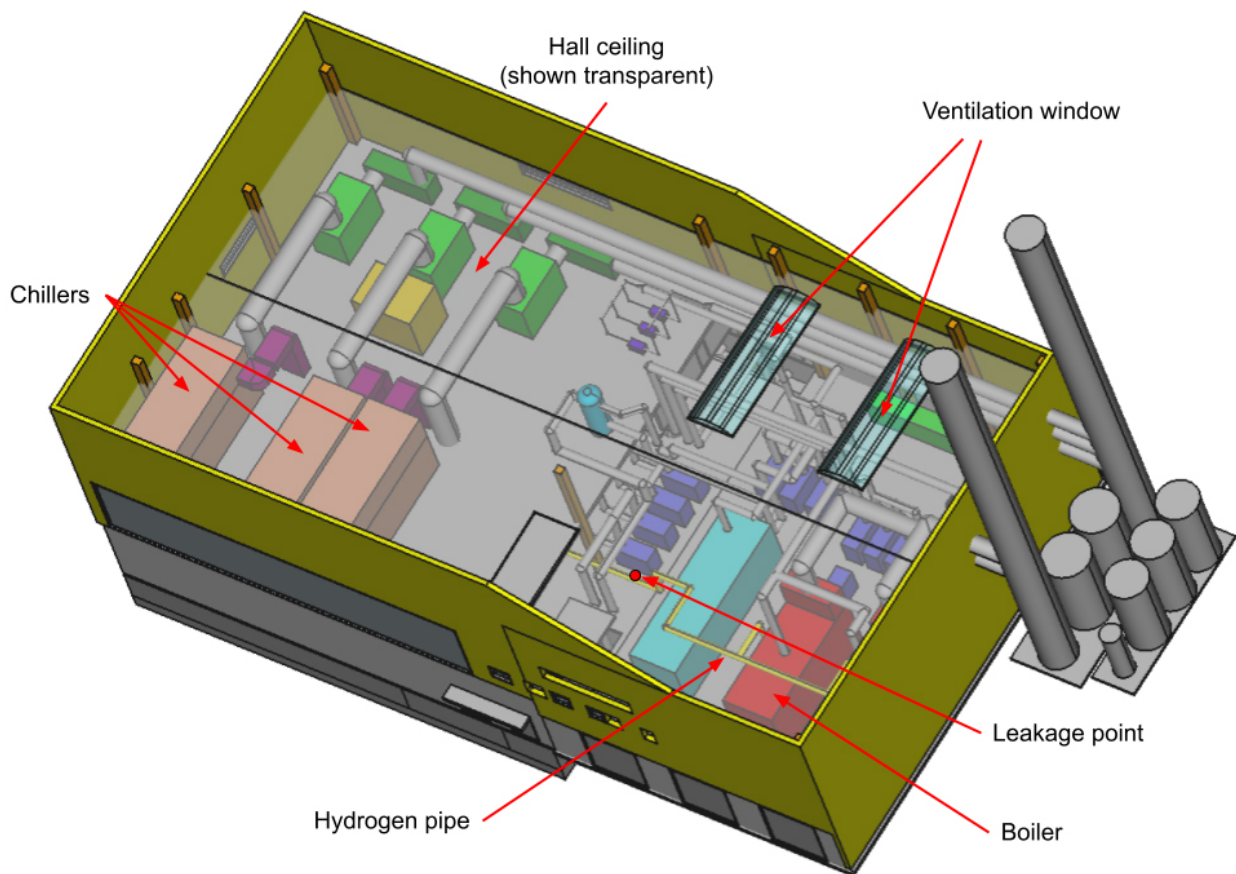


Figure 2. 3D CAD model of the central utility building at FZJ [9].

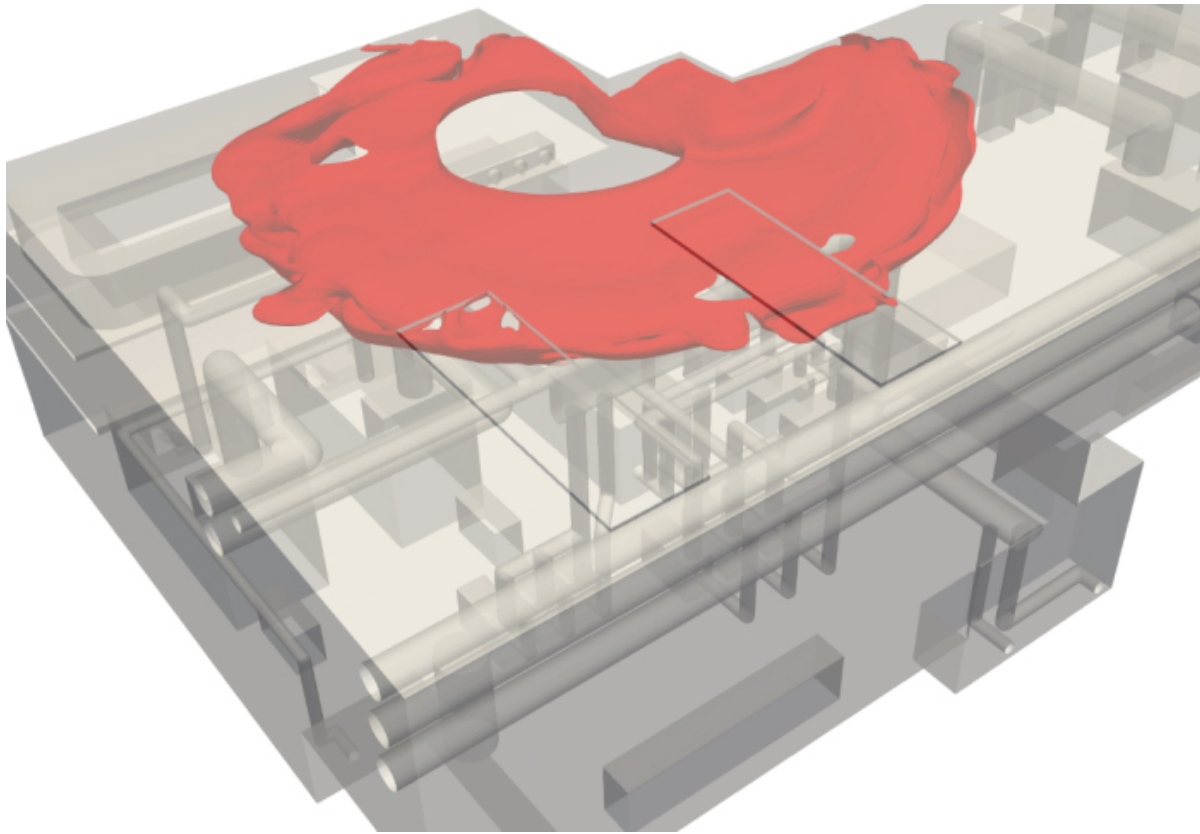


Figure 3. Contour surface of the lower flammability limit of hydrogen (4% vol.) After leakage inside the central utility building.

and evaporation of the cryogenic liquid (~ 20 K). Specifically in maritime transportation, several similarities with the severe accident-related hydrogen risk in nuclear power plants exist: The hydrogen releases could be massive and occur inside large and complex structures involving enclosed and semi-enclosed volumes [10]. Furthermore, the remote passage of a hydrogen carrier ship requires safety solutions that can be operated without external intervention. Hence, hydrogen safety experience gained over decades in reactor safety research is well suited to contribute to the safe long-distance transportation of cryogenic hydrogen.

The consortium of the STACY project involves institutions with a long tradition in nuclear safety research [11]. IRSN (France) holds substantial knowledge in the field of hydrogen risk in nuclear power plants and was involved in the development of related safety assessment methodologies and the corresponding risk prevention procedures. FZJ (Germany) performed long-term activities in studying the operational behaviour of PARs under severe accident conditions. The consortium is complemented by CNRS-ICARE (France) with expertise in flame and explosion dynamics with an emphasis on explosions safety, while KGU (Japan) holds expertise in catalyst development, specifically from the automotive sector. In order to enable knowledge exchange between nuclear and non-nuclear experts and stakeholders, the industrial advisory board of the project involves nuclear players, e.g. JAEA, and non-nuclear players such as Air Liquide, Kawasaki Heavy Industries and Daihatsu Motor Company.

The project aims at providing new experimental data on two aspects relevant for the safety assessment of LH2 transportation. First, fundamental combustion parameters,

which are required to assess the risk in hazardous situations, are determined at CNRS-ICARE combustion lab. These experiments are being performed to determine parameters such as the laminar flame speed under cryogenic conditions. Second, the performance of PARs under conditions of maritime LH2 transportation is studied in the FZJ hydrogen lab. In nuclear power plants, PARs are supposed to operate during a severe accident at elevated temperatures and pressures under highly humid atmosphere. On the liquid hydrogen carrier, cold evaporated hydrogen is supposed to mix with air atmospheric pressure. Hence, existing simulation tools need to be enhanced towards these conditions.

Experiments are performed to characterize the performance of commercial PARs under these conditions. **Figure 4** shows the installation of a catalytic recombiner inside the REKO-4 test vessel. Furthermore, catalysts with specific properties related to the operation under maritime transport conditions developed at KGU are qualified. Data are used to develop and validate enhanced PAR models.

The adaptation to the new boundary conditions represents a first-time application of catalytic recombiners in cold environment, and provides pre-requisite to safe hydrogen storage expected to be transferred to other hydrogen applications such as e.g. underground storage.

Nuclear Powered Hydrogen Cogeneration (NPHyCo)

In NPHyCo, the feasibility of hydrogen generation near a nuclear power plant will be investigated. In this project, GRS is working on the licensing requirements and safety-related impacts of hydrogen cogeneration. In addition, GRS is investigating the effects of a possible explosion pressure

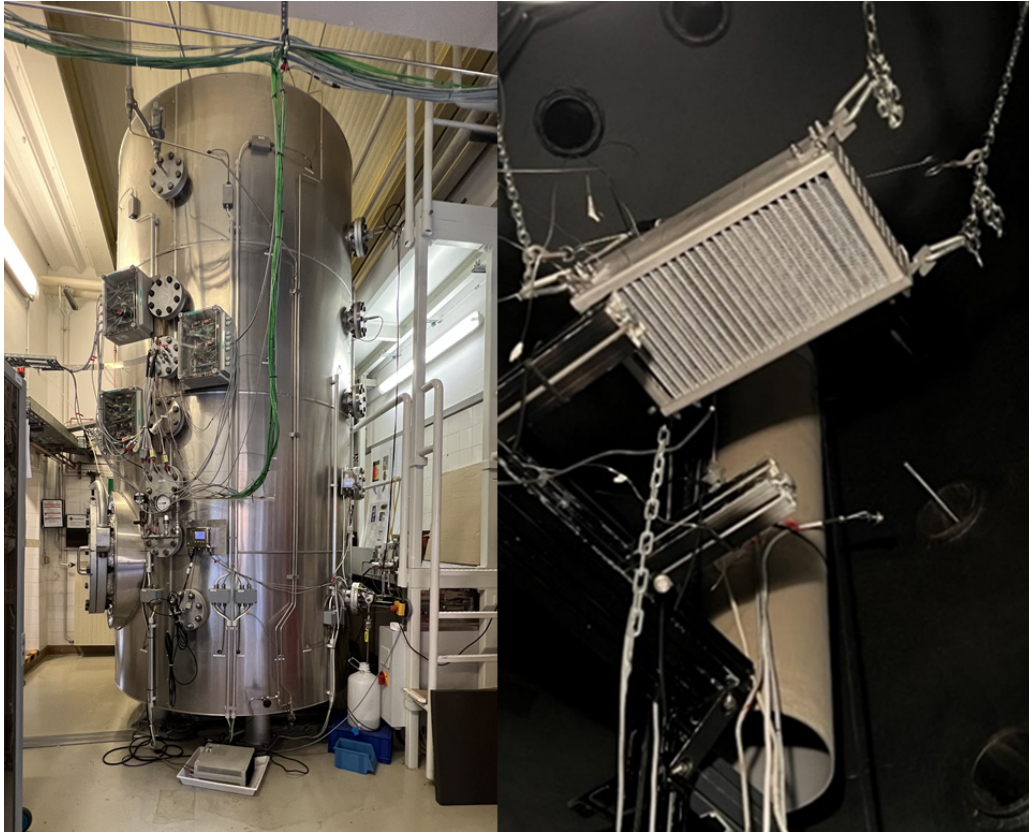


Figure 4. REKO-4 facility (left), PAR installation next to the mixing fan (right) [12].

wave on the immediate vicinity of the electrolyser.

Work Package 2 of NPHyCo aims to assess the technical feasibility of integrating a hydrogen production plant (HPP) within a nuclear power plant (NPP) site for hydrogen cogeneration. GRS has conducted calculations using a selected electrolyser facility and evaluated the impacts of external hazards from the HPP on the NPP structures based on worst-case scenarios.

Hydrogen explosions, while rare, can cause extensive damage over large distances. Therefore, the impact assessment focused on hydrogen vapour cloud explosions (VCE) due to their potential for widespread damage. Worst-case accident scenarios considered the specific conditions required for hydrogen vapour clouds to form and ignite. These scenarios were used to analyse 'minimum separation distances' between the HPP and NPP structures to prevent impacts from hydrogen explosions at the HPP on the NPP structures.

As part of the project, COCOSYS simulations were conducted to assess the risk of hydrogen explosions for two HPP enclosure solutions: a smaller HPP container with a volume of about 100 m³ and a larger HPP building with more than 4000 m³. The analysis included the dispersion of hydrogen and the composition of gas clouds within the HPP container for three hydrogen leak scenarios. These COCOSYS calculations were performed without considering hydrogen combustion and flame front propagation processes.

The current state of science and technology involves using analysis software to study the propagation of pressure waves

in complex topographies. GRS applied the hydrocode ANSYS AUTODYN to the facilities selected in the NPHyCo project. This involved using the TNT equivalence method, where the detonation of a TNT charge in air is explicitly modelled. In this context catastrophic failure of a hydrogen storage was considered to represent the most critical scenario and chosen for the determination of a TNT equivalent mass. TNT is represented by the Jones-Lee-Wilkins equation of state (JWL-EOS) and the properties of air are represented by the ideal-gas EOS. The fluid parts of the model are discretized by the multi-material Euler solver, while the topography is represented by the Lagrange solver of ANSYS AUTODYN (**Figure 5**). Coupling of Eulerian and Lagrangian domains automatically accounts for shielding and reflection effects in pressure wave propagation problems. Pressures are evaluated at selected locations of building structures and compared to simulation results neglecting topographical features.

The results of the analysis showed that in principle, ANSYS AUTODYN simulations can account for the reflection and shielding of pressure waves caused by the geometric features of a complex structure.

ANSYS AUTODYN can be used to:

- Assess the negative effects of reflections on blast loads for a specific layout.
- Evaluate the positive effects of shielding measures, such as protective walls, on blast loads.
- Determine minimum safety distances for a particular layout.

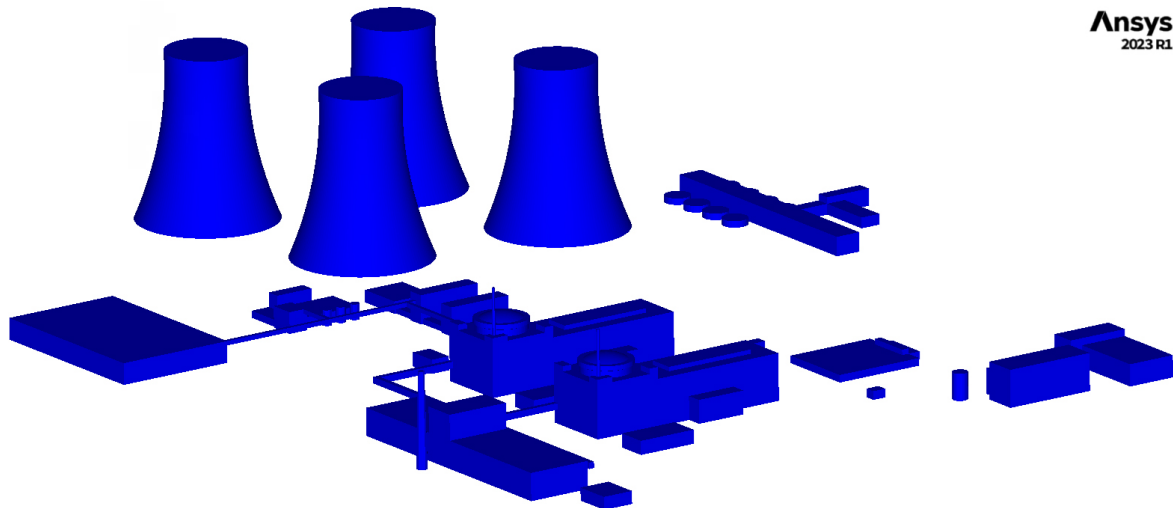


Figure 5. Isometric view of generic NPP site topography used in AUTODYN 3D simulations.

Combustion of hydrogen-air mixtures in semi confined geometries

At KIT-ITES the combustion behaviour of hydrogen-air-mixtures in semi-confined geometries, with and without hydrogen concentration gradients was investigated together with the SME Pro-Science GmbH (PS). Such mixtures might form in a NPP after severe reactor accidents with core meltdown, but are also conceivable for accident scenarios in semi-confined public spaces, as e.g., traffic accidents with hydrogen powered vehicles in tunnels or parking decks.

The most destructive consequences of a hydrogen release can be expected when the combustion reaches the regime of a detonation, where the reaction front, coupled with a shock-wave, propagates with supersonic velocity through the mixture. Prerequisite for a Deflagration-to-Detonation-Transition (DDT) is that the flame accelerates to sonic speed (FA). So, the conditions leading to FA or DDT events are of fundamental importance for safety analyses of incidents with hydrogen releases in confined spaces.

Currently, such events in large geometries cannot be described numerically, as the relevant physical processes take place on much smaller time and length scales, which cannot be resolved accurately enough in current simulations. Therefore, at KIT empirical criteria for the onset of FA and DDT in completely confined homogeneous H₂-air-mixtures were initially derived from experiments in different length-scales [13]. These criteria allow the simulation software to assess, whether and when FA or DDT is possible in a given scenario, but they might overestimate the risk associated with the hydrogen release, since in most accident scenarios predominantly stratified mixtures with only partial confinement occur. In semi-confined geometries vent openings lead to losses of burned and unburned gas that may mitigate flame acceleration and help avoiding detonations, while mixture gradients are responsible for a position dependent energy production and more complex flame development.

To investigate these phenomena KIT/PS commissioned a test facility in the hydrogen test site HYKA that allows performing large-scale hydrogen combustion experiments in a semi-confined geometry (Figure 6). The facility consists of a

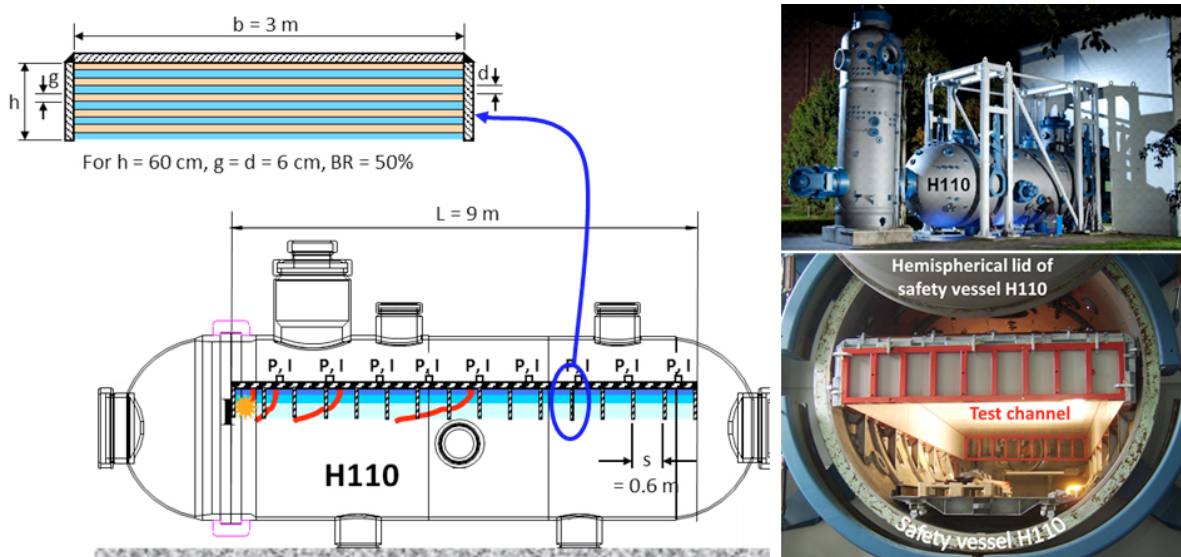


Figure 6. Semi-confined combustion channel at KIT-HYKA.

rectangular channel with open ground face and rear end with the dimensions 9 x 3 x 0.6 m (length x width x height). Initially this facility was filled with homogeneous hydrogen-air-mixtures of defined concentration that were ignited at one channel end.

Using the records of pressure sensors, photodiodes and ionisation probes distributed along the channel ceiling, the combustion regimes in the experiments could be identified and criteria for FA and DDT in homogeneous hydrogen-air-mixtures in a semi-confined geometry were derived. These criteria were formulated in the form of dimensionless expressions in dependency of the geometrical properties of the facility and the thermodynamic properties of the mixture [14]. These criteria were then extended to mixtures with pre-defined vertical hydrogen concentration gradients and different gradient slopes that were generated inside the same facility [15, 16]. These experiments showed that the maximum hydrogen concentration in the gradient and the layer thickness of the combustible mixture are the main properties that govern the hazard potential of such mixtures. It was shown experimentally that inhomogeneous mixtures with a given maximum concentration show similar flame velocities and combustion overpressures as homogeneous mixtures of the same concentration and similar layer thickness, i.e. with larger hydrogen mass in the flammable cloud. Concerning flame velocity, inhomogeneous mixtures turned out to be even slightly more reactive.

The new criteria for FA and DDT contribute to more realistic evaluations of the hazard potential of hydrogen-air-mixtures with concentration gradients in semi-confined geometries by preventing too conservative classifications concerning FA and DDT. The criteria can be used for safety analyses of postulated accidents in NPPs as well as in non-nuclear applications and are suitable for both, Lumped Parameter and CFD codes.

CONCLUSIONS AND OUTLOOK

Hydrogen safety will play a key role in the introduction of hydrogen as an energy carrier in the future. As hydrogen safety has been one of the priority research topics in connection with water-cooled nuclear power plants for decades, the nuclear community's expertise is in demand when it comes to ensuring hydrogen safety.

This article has given examples of projects in which hydrogen safety expertise from nuclear safety research is being used. This short list is far from complete and only gives a small insight into the large number of national and international projects. In view of the growing interest in hydrogen technologies and the associated safety challenges, significantly more projects with nuclear involvement can be expected. In addition, national hydrogen safety partnerships with nuclear experts as relevant partners are currently being formed in Canada, Germany and France, for example. The synergies that can be achieved in this way can also be expected to have a fruitful feedback effect on nuclear safety research.

REFERENCIAS

- [1] European Commission, Resolution on the European Green Deal, 2019/2956(RSP), 2020.
- [2] European Commission, Questions and answers: A Hydrogen Strategy for a climate neutral Europe, Brussels, 8 July 2020.
- [3] A. Kotchourko and T. Jordan (Eds.), Hydrogen Safety for Energy Applications – Engineering Design, Risk Assessment, and Codes and Standards, ISBN 978-0-12-820492-4, Elsevier, 2002.
- [4] Z. Liang, M. Sonnenkalb, A. Bentaib and M. Sangiorgi, Status report on hydrogen management and related computer codes", NEA/CSNI/R(2014)8.
- [5] Z. Liang, E. Studer, N. Chaumeix, E.-A. Reinecke, S. Gupta, S. Kelm, A. Bentaib, L. Gardner, Hydrogen Behavior and Mitigation Measures: State of Knowledge and Database from Nuclear Community, Proc. 10th International Conference on Hydrogen Safety (ICHS 2023), Québec, Canada, September 19-21, 2023
- [6] https://www.fz-juelich.de/en/llec_subsite.
- [7] K. Yassin, S. Kelm, M. Kampili, E.-A. Reinecke, Validation and verification of containmentFOAM CFD simulations in hydrogen safety, *Energies* 16 (2023) 5993.
- [8] <https://openmodelica.org/>
- [9] K. Yassin, S. Kelm, E.-A. Reinecke, Towards the simulation of hydrogen leakage scenarios in closed buildings using containmentFOAM, Proc. 10th International Conference on Hydrogen Safety (ICHS 2023), Québec, Canada, September 19-21, 2023.
- [10] S. Kelm, J. Baggemann, E.-A. Reinecke, K. Verfondern, S. Kamiya, Simulation of hydrogen mixing and PAR operation during accidental release in an LH2 carrier machine room, Proc. 9th International Conference on Hydrogen Safety (ICHS 2021), Edinburgh, Scotland, September 21-24, 2021.
- [11] <https://www.stacy-project.eu/en>
- [12] S.R. Krenz, E.-A. Reinecke, H. Tanaka, A. Bentaib, N. Chaumeix, Experimental characterization of the operational behavior of a catalytic recombiner for hydrogen mitigation, Proc. 10th International Conference on Hydrogen Safety (ICHS 2023), Québec, Canada, September 19-21, 2023.
- [13] S.B. Dorofeev, M.S. Kuznetsov, V.I. Alekseev, A.A. Efimenko, W. Breitung, Evaluation of limits for effective flame acceleration in hydrogen mixtures, *J. Loss Prev. Proc. Ind.* 14 (2001) 583-589.
- [14] M. Kuznetsov, J. Grune, A. Friedrich, K. Sempert, W. Breitung, T. Jordan, Hydrogen-air deflagrations and detonations in a semi-confined flat layer, In: D. Bradley, G. Makhviladze, V. Molkov (Eds.) *Fire and Explosion Hazards – Proc. 6th Int. Seminar* (2011) 125-136.
- [15] A. Friedrich, J. Grune, G. Necker, K. Sempert, G. Stern, A. Vesper, A., Criteria for flame acceleration and deflagration-to-detonation transition in hydrogen-air-mixtures with concentration gradients and partial inclusion, Final report nuclear safety project 1501346, Pro-Science GmbH, Ettlingen, January 2011.
- [16] J. Grune, K. Sempert, M. Kuznetsov, T. Jordan, Experimental investigation of fast flame propagation in stratified hydrogen-air mixtures in semi-confined flat layers, *Journal of Loss Prevention in the Process Industries* 26 (2013) 1442-1452.