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NUMERICAL SIMULATION OF HYDROGEN LEAK DETECTION AND RISK ASSESSMENT AT HYDROGEN REFUELING STATIONS

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Abstract: This study explores how Computational Fluid Dynamics (CFD) modeling predicts and mitigates safety risks from hydrogen leaks at hydrogen refueling stations (HRS). Three-dimensional simulations were performed using PHAST Standalone 9.1 software to evaluate hydrogen dispersion under wind speeds of 1, 2, and 5 m/s. The results identify critical risk factors and potential gas accumulation zones. Based on the dispersion patterns, this paper proposes strategic locations for safety equipment, including gas, acoustic, and flame detectors. This proactive modeling approach provides valuable design guidelines to enhance facility safety before real-world deployment.

Keywords: *computational fluid dynamics, hydrogen safety, leak detection, gas dispersion, risk management, preventive safety*

1. INTRODUCTION

As an alternative energy carrier, hydrogen is becoming increasingly central to the global energy transition. With over 1,200 hydrogen companies operating worldwide, the technology is gaining significant momentum. Nevertheless, hydrogen's unique physicochemical characteristics and the requirement for high-pressure systems present considerable safety challenges that must be addressed for the sustainable development of hydrogen infrastructure. The flammability, chemical reactivity, and material compatibility issues associated with hydrogen contribute to elevated risk levels. Comprehensive reviews of documented hydrogen incidents in recent years reveal that these events typically result from multiple contributing factors, including equipment failures and design flaws. Statistical data show that the two primary causes of hydrogen accidents are valve malfunctions and faulty connections (Figure 1). According to commercial loss databases, leakage accounts for approximately 25% of all hydrogen fires, with 40% of these leaks going undetected until it is too late. These figures underscore the vital importance of early detection systems and proactive maintenance strategies. Research has identified a clear link between material selection errors and subsequent failures, which can progress from initial defects to leakage and ultimately to accidents. This finding emphasizes the critical need for thorough material compatibility assessments during the design stage. Effective

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hydrogen leakage prevention demands a comprehensive strategy that addresses safety, economic, and environmental considerations simultaneously. Hydrogen's molecular characteristics, especially its extremely small molecular size and wide flammability range (4 to 75% by volume) substantially expand potential hazard zones. The fact that hydrogen is both invisible and odorless presents an additional safety challenge, as these properties can significantly delay leak detection and hinder emergency response efforts (Hydrogen Safety Panel 2020).

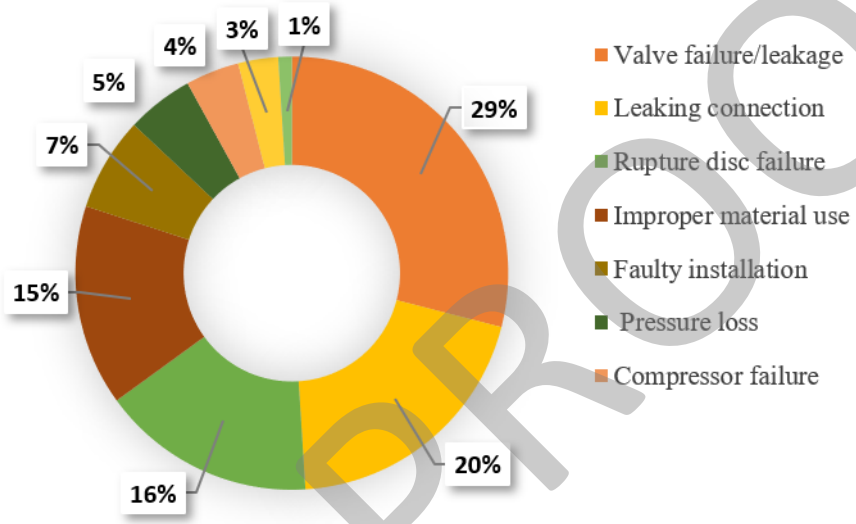


Figure 1

Distribution of causes of hydrogen accidents (Hydrogen Safety Panel 2020)

Beyond the direct costs of lost hydrogen and equipment damage, hydrogen leaks can generate substantial indirect expenses, including operational disruptions, compensation claims, and mandatory regulatory inspections, which collectively often surpass the immediate financial losses. More critically, major incidents could severely undermine public confidence in hydrogen technology, potentially slowing the transition to sustainable energy systems. Since hydrogen itself is not inherently green and demands considerable energy for production, any losses compound the overall environmental impact. With the growing emphasis on green hydrogen production, it becomes essential to minimize losses across the entire supply chain—from production through storage to distribution—to maintain the technology's long-term viability. Ensuring the safe and sustainable advancement of hydrogen infrastructure requires a comprehensive preventive strategy. This approach must incorporate sophisticated design methodologies, including Computational Fluid Dynamics (CFD) simulations and advanced risk assessment models, to proactively identify and address potential hazards before they materialize into real-world problems.

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2. CFD MODELING

CFD is a numerical simulation method that models fluid and gas flow using complex mathematical equations (e.g., Navier-Stokes equations). It is widely used in hydrogen technologies to simulate and optimize flow, heat transfer, and safety scenarios across various applications, including process devices, storage systems, safety valves, tubing, flow cells, and refueling infrastructure (Korsukova et al. 2025; Bittner et al. 2024; Pusztai et al. 2021).

Modeling results show the visual spread of a hydrogen gas cloud caused by hydrogen leakage, which is affected by meteorological properties and spatial obstructions. The results are graphically presented, and the flow direction can be followed by time simulation. The unique behavior of hydrogen can be attributed to its density, which is approximately 14 times lower than that of air, allowing the gas to diffuse rapidly and ascend quickly due to its high buoyancy. The energy needed to generate hydrogen is lower than that of other common active substances. The explosion pressure is between 0,3 and 0,5 bar (humans should survive > 2-3 bar for relevant load durations).

Since hydrogen fires typically originate from leakages, the early detection of hydrogen leaks and the simulation analysis of leak scenarios are key to ensuring safe hydrogen refueling operations. CFD modeling will investigate how the geometric barriers affect gas cloud flow, which will be affected by external environmental factors and thermal uptake in addition to the specific properties of hydrogen gas. Modeling will help to identify hydrogen leak scenarios, obtain responses on which points may leak, how much of a dangerous zone might be circulating, how long it takes for critical concentrations to be achieved by the hydrogen-air mixture and what pathways hydrogen gas may flow. The modeling results can be used to determine the positions of acoustic gas leak detectors, hydrogen gas sensors, and flame detectors, while also considering the parameters specified in the manufacturer's instructions.

Simulations of gas cloud flow may also impact safety planning such as optimization of ventilation, assembly designs, and designation of safety margins. The safe and effectively cheaply reproducible software environment provided by the simulations has great advantages, which is still extensively used nowadays for initial screening validation (Tugyi et al. 2023).

3. HYDROGEN LEAK MODELING

For CFD analysis, PHAST Standalone 9.1 software was employed, a specialized tool that applies the Navier-Stokes equations to model fluid dynamics and gas dispersion behavior. This software utilizes a finite volume approach to divide the computational space into discrete elements. It incorporates a k-ε turbulence model to capture turbulent flow patterns—a crucial feature for hydrogen dispersion studies given hydrogen's exceptionally high diffusion rate. Being specifically designed for process safety engineering, the software enables comprehensive simulation of gas release scenarios, fire dynamics, and associated hazards, making it an essential tool for developing effective safety protocols. During the modeling, we simulated a mock-up

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of a possible hydrogen refueling fue (HRS), which includes the most important elements, such as a compressor, chiller, firewall, hydrogen storage tank, tube trailer and dispenser area (Figure 2). The computational domain was discretized using a structured mesh with refinement in areas of expected high velocity gradients, particularly near the leak source and around obstacles. A mesh independence study was conducted to ensure that the results were not influenced by the mesh resolution. The difference in maximum hydrogen concentration between the medium and fine meshes was less than 3%, indicating that the medium mesh resolution was sufficient for accurate predictions while maintaining computational efficiency. Validation of the CFD model against experimental data from similar hydrogen release scenarios is currently underway. Due to ongoing data reconciliation processes with experimental sources, complete validation results are not yet available. However, preliminary qualitative comparisons suggest that the model captures the essential physics of hydrogen dispersion behavior. A comprehensive validation study, including quantitative accuracy metrics, will be completed and reported in subsequent publications.

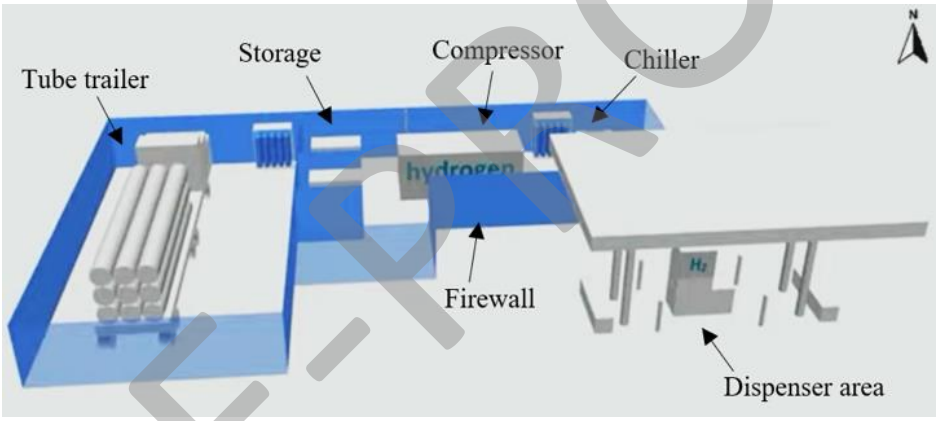


Figure 2
Hydrogen refueling station (HRS) model components

In the numerical simulation, hydrogen leakage can be tested under different environmental conditions, considering the unique physical properties of hydrogen, such as its extremely low density and rapid diffusion capacity.

Critical Ranges of Hydrogen Emission Rate Based on Safety Considerations:

- Natural leakage range (0.001-0.01 kg/s): Due to the molecular structure of hydrogen, micro-sized diffusion losses must be expected even with the best seals. This is an accepted level in industrial practice that can be managed with routine maintenance.
- Detectable but non-critical leakage (0.01-0.1 kg/s): A quantity that can already be detected by sensors, does not require immediate intervention, but justifies scheduled maintenance. In open spaces, flammable mixtures generally do not form (4-75 vol.% hydrogen in air).

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- Medium-risk leakage (0.1-1 kg/s): In enclosed or semi-enclosed spaces, explosive zones may develop locally. Requires immediate intervention, area closure, and identification of the source of the leak. This is the range where the placement of detectors is crucial for leak detection.

Critical leakage range (1-10 kg/s): Falls into a very dangerous scenario (e.g., high-pressure pipeline crack, compressor seal failure). This enables precise mapping of potential hazard zones and worst-case scenario analysis. Catastrophic leakage (>10 kg/s): Mass outflow (e.g., tank rupture), in which case evacuation and automatic activation of safety protocols are the primary responses. While the 1 kg/s hydrogen emission rate used in our modeling falls within the critical leakage range, it represents a conservative scenario rather than the most common leak situation. In real-world conditions, smaller leaks (0.01-0.1 kg/s) are more likely to occur. However, we chose to model the higher flow rate to establish safety margins that would encompass worst-case scenarios. For comparison, a typical small leak from a fitting might be in the range of 0.001-0.01 kg/s, while a medium-sized leak from a damaged connection might be 0.1-0.5 kg/s. Future work will include simulations with lower, more commonly occurring leak rates to provide a comprehensive risk assessment across different scenarios. The 1 kg/s hydrogen emission rate used in the modeling, which falls within the critical leakage range, represents a realistic leakage scenario enabling precise delineation of potential hazard zones. The three-dimensional dynamic visualization is used to monitor the spatial and temporal spread of the flammable gas cloud (yellow gas cloud) providing essential information for optimal placement of the safety plug. In Hungary, the annual average wind speed is typically between 2–4 m/s, which makes our country a moderately windy area. Wind speed, as an environmental parameter, has a significant impact on the dispersion pattern of hydrogen gas clouds. During the modeling, I examined the dispersion direction and distribution of gas clouds at wind speeds of 1, 2 and 5 m/s, as these values represent the most common and critical meteorological conditions in Hungary.

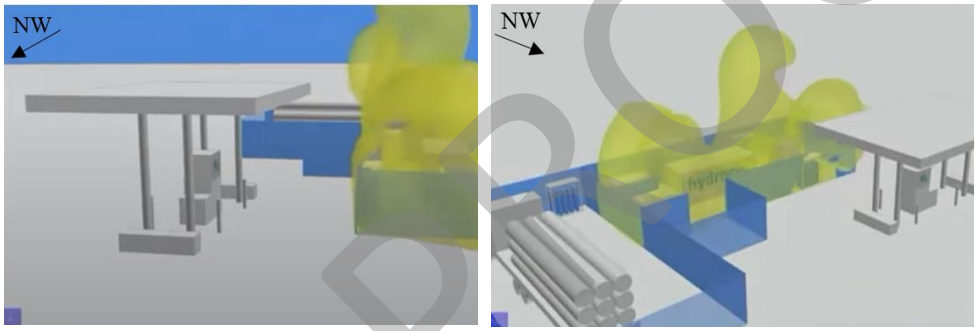
- 1 m/s: light wind: extremely calm weather conditions, creating ideal circumstances for upward gas cloud rise, where hydrogen's natural buoyancy dominates. Characteristic air movement in closed or semi-closed spaces and dangerous because the gas cloud concentration can remain locally high.
- 2 m/s: moderate wind: the most frequently occurring range (~80% frequency), typical average wind speed in urban environments in Hungary, balance between buoyancy and wind-induced dilution. Turbulence around buildings already has a significant impact. Most real incidents can occur under such weather conditions, which align with the official regional meteorological datasets (Wind conditions of Hungary, 2020).
- 5 m/s: fresh wind: results in strong dilution and rapid dispersion. Turbulent mixing dominates the dispersion, characteristic of daytime wind speed in open areas. The gas cloud disperses over a larger area but at lower concentrations at lower levels. These wind speeds cover the safety-critical range.

The prevailing wind direction in Hungary is from the northwest. This direction develops because of the westerly wind system characteristic of the temperate zone,

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along with the influence of cyclones originating from the Atlantic Ocean and Mediterranean Sea.

In all simulations, the wind direction was from the northwest, consistent with the prevailing wind direction in Hungary. This direction was chosen to represent the most common meteorological condition that would affect a hydrogen facility in the region. The figures clearly show the wind flowing from the northwest corner of the computational domain, carrying the hydrogen cloud toward the southeast. In the northwest edge simulation of 1 m/s, it is observed that the flammable gas cloud will spread rapidly around the equipment, but that as a passive safety element, not only in the event of fire, but also in the restriction of the spread of hydrogen gas (Figure 3). The combination of the mild wind speed and the natural uptake force of hydrogen results in a vertical spreading component, thereby an upward movement of the gas cloud.



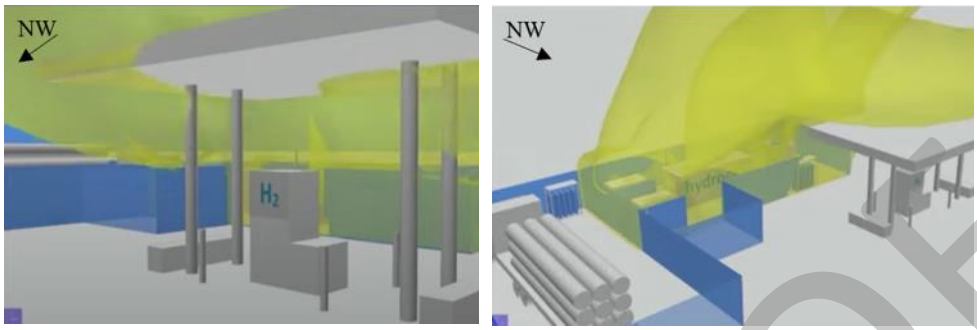
(a) (b)

Figure 3

Hydrogen gas cloud dispersion at a wind speed of 1 m/s: (a) isometric view focused on the dispenser area, (b) top-down perspective of the facility layout

When increasing the wind speed to 2 m/s, modeling showed that the environment of the equipment is significantly exposed to the flammable hydrogen gas cloud, a critical safety issue (Figure 4). The simulation revealed that the gas cloud also leaks and accumulates under the top structure above the hydrogen fill point, which may lead to a particularly dangerous situation in closed or partially closed spaces. This phenomenon highlights the importance of proper ventilation systems and open-air development.

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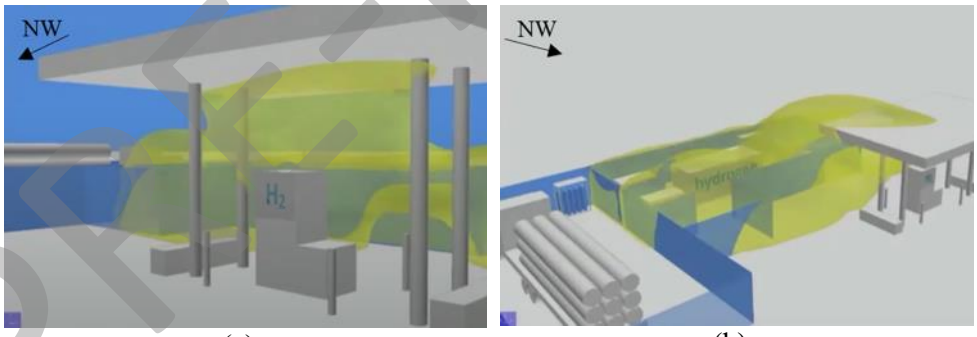


(a) (b)

Figure 4

Hydrogen gas cloud dispersion at a wind speed of 2 m/s: (a) view of gas accumulation under the dispenser canopy, (b) overall plume development over the equipment compound

Simulations at a wind rate of 5 m/s showed substantially different spread patterns. Higher wind rates make the hydrogen gas cloud flow less upward and take up a more horizontal, flatter spread profile instead (Figure 5). These results in a lower level of the gas cloud, even at flammable concentrations, affecting soil levels, which poses an increased risk to the staff located there and to the sources of ignition on the ground. The results of CFD modeling clearly show that it is preferable to position the hydrogen filling point several meters away from storage equipment, as this spatial separation may greatly reduce the risk in high wind speeds when the horizontal spread predominates.



(a) (b)

Figure 5

Hydrogen gas cloud dispersion at a wind speed of 5 m/s: (a) low-level horizontal spreading profile, (b) side view of the flattened gas plume

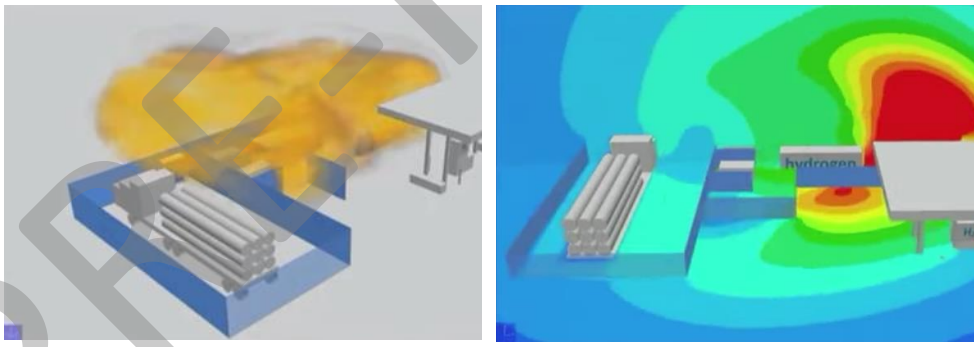
While the current simulations were focused on wind speed variations, other weather conditions can significantly impact hydrogen dispersion patterns. For instance, atmospheric stability conditions (stable, neutral, or unstable) affect vertical mixing and dispersion. Temperature inversions can trap hydrogen near the ground,

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while precipitation can influence dispersion patterns through increased turbulence. Humidity levels may also affect the behavior of hydrogen-air mixtures. Future work will incorporate these additional weather parameters to provide a more comprehensive understanding of hydrogen dispersion under various environmental conditions. CFD modeling provides a complex multivariate analysis that considers the interaction of leakage rate, meteorological conditions, and assembly design and equipment placement. This Holistic approach is essential for the development of effective safety strategies and the safe operations of hydrogen infrastructure.

4. EXACERBATION SIMULATION

One of the most critical uses of CFD modeling is simulation of scenarios that allow preliminary analysis of potential impact events and quantification of expected outcomes before the actual event occurs. Numerical simulations allow for extensive evaluation of the spatial distribution of the flammable hydrogen-air mixture, the extent of the gas cloud and the identification of accumulation zones, which provide critical information to determine the potential strength of the hazards. During the calibration simulation it can be concluded that the volume of the flammable gas cloud resulting from hydrogen leakage directly affects the intensity of the vapor (Figure 6). Modeling results show that at a volume of 2.240 m^3, an overflow of 0.5 bar can cause damage to buildings, both equipment and building structures, and can pose a serious threat to people. This pressure is considerably greater than the structural capacity of most industrial facilities, which stresses the primary importance of prevention.



(a) (b)

Figure 6

Simulation of hydrogen gas cloud accumulation and consequences: (a) 3D representation of the flammable cloud volume, (b) overpressure distribution contour map during a potential deflagration event

CFD simulations provide particularly valuable information on the spatial distribution and time development of loads. Modeling is able to predict the rate at which the flame front propagates from a distant ignition source through the flammable hydrogen-air mixture, the resulting overpressure at various distances, and where the

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highest fatality or lethality rates are expected. The spread of pressure waves during deflagration burns and the possibility of a possible Deflagration to Detonation Transition (DDT) can also be modeled, which is critical for determining safety distances. Regarding an accident scenario where hydrogen leaks from the connections of high-pressure hydrogen facilities or the tubing of hydrogen vapor, it is assumed that hydrogen may be lit by static electricity or a flame outside the base (Kikukawa 2008). The results of the explosion consequence simulation identify critical zones where gas accumulation is most likely to occur and where the highest level of structural damage is expected. This allows for the targeted use of safety measures such as optimal placement of pressure-relieving surfaces, tamper-proof structures, and barriers. Modeling will also help to identify the minimum necessary safety distances from dwelling areas, traffic routes and other critical personnel, ensuring protection of the surrounding compartment. CFD-based research analysis, therefore, is an essential tool for the overall risk assessment of hydrogen compounds, which enables preliminary investigation of worst-case scenarios and the planning of effective risk mitigation measures, thereby contributing to the safe development and operation of the hydrogen infrastructure.

5. CONCLUSIONS BASED ON MODELING RESULTS

Increasing the spatial distance between hydrogen filling points and storage equipment significantly reduces the risk, especially at high wind rates. The open design and adequate natural ventilation are critical to prevent gas accumulation. They and other passive safety elements are effective in limiting the gas spread but are not sufficient to guarantee safety on their own. CFD modeling provides precise guidance for optimal placement of hydrogen gas, auditory leakage detectors and flame detectors. Based on the simulated dispersion behavior, detector placement at multiple heights is recommended to address different risks: detectors at 3 m capture the buoyant, rising plumes under low wind conditions (1 m/s), while sensors at 0.5 m and 1.5 m monitor the horizontal, ground-level dispersion and breathing zones dominant during higher wind speeds (5 m/s). This multi-level configuration is proposed as a cautious approach to ensure comprehensive coverage across varying meteorological scenarios. Additional detectors are placed at the perimeter of the equipment compound, particularly on the southeast side. Acoustic detectors are installed near high-pressure components such as compressors and storage connections. Flame detectors with line-of-sight coverage of the entire facility (Figure 7). This multi-level detection system would provide comprehensive coverage for both the buoyant hydrogen plumes that form under low wind conditions and the ground-level dispersions that occur during higher wind speeds.

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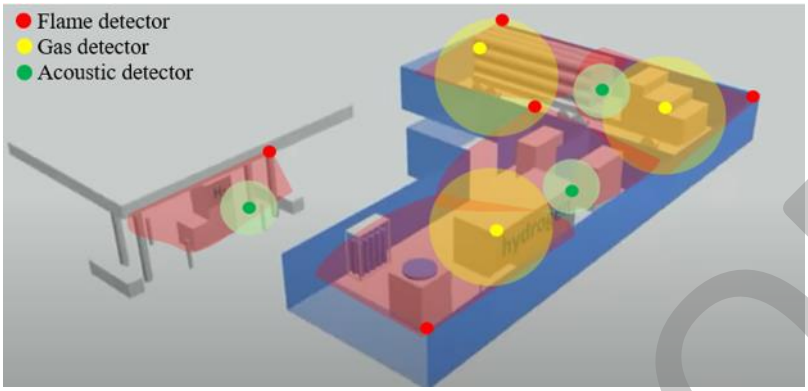


Figure 7
Location and coverage of gas detectors and flame detectors at the HRS

Consideration of different meteorological scenarios is essential to ensure complete sensory coverage. The use of multi-level sensor systems is recommended, considering both vertical and horizontal spread patterns. The preventive approach using CFD modeling during the design phase is more efficient than reactive safety measures. The unique properties of hydrogen are characterized by a wide flammability range and low ignition energy, necessitating a safety approach that differs fundamentally from conventional hydrocarbon infrastructures (Kislinger et al. 2025). Historical incidents highlight the risks associated with hydrogen infrastructure, particularly as these facilities are increasingly deployed in close proximity to the general public. Demonstrating safety and transparent risk management is essential to build social responsibility. Communication of CFD modeling results may contribute to the understanding and acceptance of the safety of hydrogen technology. The CFD modeling results provide specific guidance for hydrogen facility design and safety system implementation. Key recommendations include: A safe distance must be maintained between hydrogen dispensers and storage equipment. Implementing strategic placement of gas detectors at multiple heights to account for different dispersion patterns. Designing ventilation systems that can effectively manage hydrogen accumulation under various wind conditions. Establishing safety protocols specific to different weather scenarios. These recommendations are directly derived from the simulation results and provide actionable guidance for hydrogen facility designers and operators. The methodology demonstrated in this study can be applied to site-specific analyses, allowing for customized safety measures based on local conditions and facility layouts.

CFD modeling enables a complex multivariate analysis that considers the interaction of leakage rate, meteorological conditions, and assembly design and equipment placement. This Holistic approach is essential for the development of effective safety strategies and the safe operation of hydrogen infrastructure. The results of this study clearly demonstrate that the use of numerical simulation during the design phase can substantially reduce the risk of accidents, optimize the placement of safety systems, and contribute to the safe and sustained development of hydrogen-based

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mobility. As a guide for future research, it is recommended that a systematic comparison of different settings, the integration of real-time sensor data and CFD models, as well as the development of predictive safety systems based on artificial intelligence, be performed. Only continuous innovation and a scientifically sound safety approach can ensure that hydrogen technology achieves a safety level comparable to current conventional gas infrastructure, thereby facilitating the green energy transition and supporting a sustainable future.

When evaluating and positioning gas and flame detection systems based on numerical simulations, internationally recognized engineering practices must be integrated into the risk assessment framework. Due to the high flame propagation velocity, low ignition energy, and invisible nature of hydrogen flames, conventional detection methods are insufficient. Therefore, the design and layout of the proposed multi-level sensor system should align with the technical requirements of the IEC 60079-29 series for gas detectors and ISO 26142:2010 for hydrogen detection apparatus. Furthermore, overall mitigation strategies and facility layout optimization should consider the safety and functional safety guidelines outlined in ISO 19880-1:2020, IEC 61508 (Parts 1–3), and ANSI/FM 3260. Integrating these standards ensures that the simulation-derived safety distances and detector locations provide robust, reliable, and standardized protection for hydrogen refueling infrastructures.

6. CONCLUSIONS

This research examined the safety challenges associated with HRS and explored how CFD modeling can contribute to preventing and managing hydrogen leaks. Our findings clearly demonstrate that numerical simulation serves as a vital tool for both the design and operational phases of hydrogen infrastructure. Global experience from over 1,200 hydrogen facilities indicates that many accidents could have been avoided through comprehensive planning and thorough risk assessment. Statistical evidence reveals that leakage is responsible for approximately 25% of all hydrogen fires. Common failure modes—such as valve malfunctions, connection leaks, and monitoring system failures—represent areas where proactive CFD modeling can provide effective analysis and risk mitigation strategies. Our three-dimensional simulations using PHAST Standalone 9.1 software revealed that environmental conditions, particularly wind velocity, significantly influence hydrogen gas cloud dispersion patterns. Simulations conducted at a release rate of 1 kg/s showed distinct behaviors across different wind conditions. Under low wind conditions (1 m/s), hydrogen's natural buoyancy dominates, causing the gas cloud to rise vertically while passive safety barriers effectively contain lateral spread. From a safety perspective, this represents the most favorable scenario, as hydrogen rapidly ascends and dilutes in the atmosphere. At moderate wind speeds (2 m/s), the area surrounding the equipment becomes significantly exposed to flammable gas concentrations, with the potential for gas accumulation beneath overhead structures.

This condition presents the greatest hazard, particularly in enclosed or semi-enclosed environments where natural ventilation proves inadequate for maintaining safe concentration levels. Under high wind conditions (5 m/s), horizontal dispersion

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becomes dominant, causing the gas cloud to adopt a flatter profile that remains closer to ground level. This behavior increases risks to personnel and potential ignition sources at grade. These findings emphasize the critical importance of maintaining adequate separation distances between dispensing areas and storage facilities.

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