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Review

Digital Twins for Cryogenic Hydrogen Safety: Integrating Computational Fluid Dynamics and Machine Learning

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Abstract

The global transition toward low-carbon energy and transportation systems positions hydrogen as a key clean and versatile energy carrier. However, ensuring the safe handling and storage of hydrogen—particularly in its liquid form LH_2)—remains a critical challenge to large-scale deployment. Accidental releases of LH_2 can lead to rapid dispersion, cryogenic hazards, and increased risks of ignition or detonation due to hydrogen's low ignition energy and wide flammability limits. This review synthesizes recent advances in the understanding and modelling of LH_2 safety scenarios, emphasizing the complementary roles of Computational Fluid Dynamics (CFD) and Machine Learning (ML). The paper first outlines the fundamental physical processes governing cryogenic hydrogen leaks, spills, and jet releases, followed by an overview of current storage and sensing technologies. Special consideration is given to safety implications arising from the differences between open and enclosed environments and the fact that existent sensing technologies present deficiencies at low temperatures. CFD-based studies are reviewed to illustrate how these methods capture complex flow and dispersion dynamics under diverse operational and environmental conditions, supported by a summary of existing experimental investigations used for model validation. The emerging role of ML is then examined, focusing on its integration with CFD simulations and sensor networks for predictive risk assessment, real-time leak detection, and the development of digital twins. Finally, integrated CFD–ML-sensor systems are discussed as a pathway toward a physics-informed, data-driven framework for advancing hydrogen safety and reliability.

Keywords: cryogenic hydrogen; safety; CFD; machine learning

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1. Introduction

The decarbonisation of energy production, driven by the urgent need to mitigate global warming, has already begun in key industrial sectors such as automotive and power generation. Among emerging alternatives, hydrogen stands out as a promising energy carrier due to its high energy efficiency, renewability, and zero-carbon combustion. However, hydrogen safety remains a critical challenge.

To maximise storage efficiency, hydrogen is often stored either as a compressed gas or a cryogenic liquid within high-pressure or thermally insulated tanks. In the case of liquid hydrogen, an accidental release—due to mechanical failure, material degradation, or impact—can result in a large, rapidly expanding spill or high-velocity jet. Hydrogen's low ignition energy and wide flammability range makes it highly prone to igniting, forming jet fires that may impinge on adjacent infrastructure, triggering cascading failures and widespread thermal damage. In confined or semi-confined spaces, there is also a non-negligible risk of deflagration or detonation, especially when ignitable mixtures accumulate over time. The extremely low temperatures of LH_2 introduce additional hazards such as material embrittlement while the dispersion of cold gaseous hydrogen significantly increases the risk of delayed ignition or detonation.

Traditionally, safety protocols and detector placement strategies have been informed by past incident records and empirical correlations [1]. However, the complexity of LH_2 release dynamics, especially under varying environmental and operational conditions, calls for more predictive and physics-informed approaches.

To that end, detailed modelling of cryo-compressed hydrogen release and dispersion is essential for improving our understanding of the governing phenomena during accidental leaks. Such studies enable better risk assessment and the optimisation of detection and mitigation strategies. Ultimately, integrating Computational Fluid Dynamics (CFD) simulations with machine learning (ML) and sensor data offers a path towards real-time monitoring through digital twins, enhancing proactive safety measures for hydrogen infrastructure.

This study provides a comprehensive review of key investigations into liquid hydrogen (LH_2) safety, with particular emphasis on the application of integrated Computational Fluid Dynamics (CFD) and Machine Learning (ML) techniques. Following a brief overview of the fundamental physical phenomena governing accidental hydrogen releases and the available sensing technologies, the review highlights how CFD simulations and experimental studies have been employed to analyse and improve representative safety scenarios. Finally, the emerging role of ML is explored, focusing on its integration with simulation and sensor data to enable risk prediction, leak detection, and real-time system monitoring. Together, these complementary approaches outline a pathway toward more predictive, data-driven, and physics-informed frameworks for enhancing hydrogen safety.

To ensure a comprehensive and systematic review of the literature, we adopted a structured search and selection strategy:

- Databases searched: Scopus, Web of Science, and Google Scholar.
- Keywords used: “hydrogen”, “hydrogen sensor,” “cryogenic hydrogen safety,” “digital twin,” “computational fluid dynamics,” “machine learning,” and combinations thereof.
- Time frame: Publications mainly from 2000 to 2025 were considered to capture both foundational and recent developments. However, articles from the last decade (2015–2025) were analysed in greater detail, as they represent the most up-to-date technological advances and safety considerations.
- Inclusion criteria: Peer-reviewed journal articles, conference proceedings, and authoritative reports that directly addressed hydrogen sensing technologies, cryogenic safety, or digital-twin/CFD–ML integration.

2. Physics of Liquid Hydrogen Jet Release and Combustion

2.1. Overview of Liquid Hydrogen Physics

Liquid hydrogen exhibits unique thermophysical properties that critically influence its behavior in both routine operation and accidental release scenarios. With a boiling point of 20.28 K at atmospheric pressure, LH_2 requires insulated containment to prevent rapid vaporization. Its very low density (approximately 70.85 kg/m^3) and high specific volume imply that even small liquid spills can generate large volumes of gaseous hydrogen upon vaporisation. The high latent heat of vaporization (around 445 kJ/kg), combined with sudden depressurization, promotes flash boiling and the formation of dense vapor clouds.

Moreover, LH_2’s extremely low viscosity and surface tension contribute to its high mobility and rapid spreading in the atmosphere and over surfaces. Although its absolute thermal conductivity is low, it remains relatively high compared to other cryogenic liquids, affecting heat transfer during spills. The gaseous hydrogen produced possesses a high specific heat capacity, allowing it to absorb substantial thermal energy that accelerates plume rise and dispersion.

The release of LH_2 through small orifices or ruptures typically generates a highly dynamic jet characterized by rapid phase change and complex fluid interactions. The fluid dynamic behavior of the jet strongly affects combustion characteristics if ignition occurs. Due to hydrogen's wide flammability range and very low ignition energy, the vapor cloud is highly susceptible to ignition. Ignition of the jet can in turn produce a turbulent jet flame or jet fire with significant momentum, resulting in elongated flames exhibiting complex dynamics and substantial radiative heat transfer. The combustion is further influenced by intermittent entrainment of ambient air and continuous vaporization of residual liquid hydrogen, sustaining combustion for extended durations. A comprehensive understanding of these coupled fluid and combustion phenomena is essential for accurate prediction of thermal hazards and the development of robust safety measures in hydrogen storage and handling.

To contextualise these risks, the key thermophysical and combustion-relevant properties of hydrogen are summarized below in Table 1, alongside those of methane (CH_4), another widely used energy carrier, for comparison. For example, from a combustion perspective, hydrogen exhibits a much wider flammability range (4–75 vol%) and a minimum ignition energy an order of magnitude lower than that of methane, making it substantially more prone to accidental ignition. Conversely, methane's higher density and narrower flammability limits result in slower dispersion and a smaller probability of detonation, though it remains a potent greenhouse gas. These contrasting properties underscore the heightened safety challenges associated with LH_2 handling and highlight the need for robust predictive modelling and monitoring strategies.

Table 1. Key Thermophysical Properties of Liquid Hydrogen and Liquid Methane at Boiling Point.

Property	**Symbol/Units**	**Hydrogen (LH_2)**	**Methane (LCH_4)**
Boiling Point	T_b [K]	20.3	111.7
Density (liquid)	ρ_ℓ [kg/m^3]	70.9	422.6
Density (gas at NTP)	ρ_g [kg/m^3]	0.0899	0.668
Latent Heat of Vaporization	L_v [kJ/kg]	445	510
Specific Heat Capacity (gas)	c_p [J/kg·K]	∼14,300	2220
Thermal Conductivity (liquid)	k_ℓ [W/m·K]	0.104	0.17
Viscosity (liquid)	μ_ℓ [Pa·s]	13.1×10^{-6}	160×10^{-6}
Surface Tension	σ [N/m]	2.0×10^{-3}	1.7×10^{-2}
Expansion Ratio (liquid → gas)	–	∼1:850	∼1:600
Flammability Range in Air	[% vol]	4–75	5–15
Minimum Ignition Energy	[mJ]	∼0.017	∼0.28
Autoignition Temperature	[K]	∼858	∼813

2.2. Comparison Between Liquid and Gaseous Hydrogen Releases

Compared to gaseous hydrogen, cryogenic liquid hydrogen (LH_2) introduces additional safety challenges during accidental releases. While gaseous hydrogen rapidly disperses upward due to its buoyancy, LH_2 undergoes rapid phase transitions that can initially generate dense, ground-hugging vapor clouds before sufficient heating promotes buoyant dispersion. This behaviour increases the risk of near-ground ignition and flame spread. Aspects of the differences between cryogenic and gaseous hydrogen in terms of hazards are discussed in recent publications [2].

In terms of storage, thermal stratification in storage tanks and transfer lines may also drive sudden release of large vapour masses if disturbed. Furthermore, ambient humidity can condense and freeze around cold plumes, altering jet structure, and reducing visibility during emergencies. These phenomena distinguish cryogenic releases from purely gaseous leaks and require tailored hazard assessments and mitigation strategies.

2.3. Hydrogen Storage Technologies and Safety Considerations

Hydrogen can be stored in several forms, summarised in Table 2, along with the associated challenges of each method [3–5]. Physical storage, either as compressed or cryogenic hydrogen, is currently the most established approach. Compressed hydrogen gas [6] is typically stored at pressures of 350–700 bar, where leakage may occur over time due to material fatigue, microcracks, or seal degradation. Such leaks, even if small, can accumulate to form explosive mixtures, underscoring the importance of continuous leak detection and monitoring systems. Advanced materials are being developed to improve tank integrity, but detection technology remains a critical layer of safety.

Hydrogen can also be stored in liquid form [7]. Originally developed for rocket propellants, liquid hydrogen (LH_2) requires maintaining during storage cryogenic temperatures of around 20 K. These extreme conditions introduce severe risks [8], including material embrittlement, boil-off losses, and the condensation of oxygen, all of which may lead to the unintentional formation of highly explosive environments if leaks occur. The infrastructure for LH_2 is therefore complex and costly, and safe operation depends on multi-layer insulation, pressure relief valves, and, crucially, real-time leak monitoring. Cryo-compressed storage [9], which combines cryogenic and compressed gas methods, offers higher density but is still under development, with leak prevention and detection remaining central challenges.

The second category of storage is chemical storage [10,11], where hydrogen is bound to a host material through chemical bonds. Releasing hydrogen (dehydrogenation) requires energy input, and while these carriers often offer improved safety under ambient conditions, leaks still pose risks. In particular, the release of toxic or corrosive by-products (e.g. ammonia vapours or volatile organics from LOHCs) can threaten both safety and the environment, necessitating careful leak monitoring.

Examples include porous sorbents such as Metal–Organic Frameworks (MOFs) [12], which adsorb hydrogen at low pressure and near ambient temperature. While this reduces the risk of catastrophic high-pressure failures, leaks of desorbed hydrogen still present hazards and require appropriate detection. Chemical hydrides [13] such as ammonia, formic acid, and liquid organic hydrogen carriers (LOHCs) [14] allow dense storage at ambient pressure and temperature but bring additional risks if leaks release toxic or flammable compounds. Similarly, metal hydrides [15] (e.g., magnesium- or titanium-based) store hydrogen safely in solid form with minimal leak risk under normal operation, yet thermal cycling and material degradation can still lead to unintended hydrogen release. An emerging alternative is the solidified hydrogen storage (Solid-HyStore) [16,17]. Hydrogen is encapsulated within clathrate hydrate lattices (water-based crystalline cages) under moderate temperature and pressure conditions offering high volumetric density and inherent safety but posing challenges in kinetics and stability during repeated cycles. Across all storage methods, therefore, effective leak detection and real-time monitoring remain indispensable to ensure safe deployment at scale.

Table 2. Hydrogen storage types with leakage challenges and mitigation strategies.

Storage Type	Leakage Types & Challenges	Mitigation Strategies
	Physical Storage	
Compressed Hydrogen	Permeation, embrittlement, high-pressure leaks from valve/seal, overheating during fast filling	Composite tanks, multi-stage filling, robust seals/valves, and hydrogen sensors
Cryogenic Liquid Hydrogen	Boil-off, seal failure, embrittlement	High insulation, compatible materials, pressure relief valves
Cryo-Compressed Hydrogen	Combination of cryogenic and high-pressure stress, temperature rise during fast filling	Hybrid insulated tanks, robust materials, thermal control and protocol
	Chemical Storage	
Sorbents (e.g., MOFs)	Desorption leakage, sudden release, sorbent degradation	Encapsulation, stable sorbent temp/pressure control
Chemical Hydrides	Uncontrolled reaction, by-product gas leakage	Catalyst control, sealed containment, thermal control
Metal Hydrides	Thermal desorption leakage, fatigue cracking	Durable alloys, safe desorption control, thermal management

3. Sensors

To address the growing deployment of hydrogen infrastructures and the risks of leakage in various storage methods described in the previous section, a wide range of sensor technologies for hydrogen detection has been developed. Many of these technologies originate from research in the aerospace and aviation domains, where high standards of reliability and rapid response are critical. Broadly, these sensors can be classified into five categories: thermal, electrochemical, optical, semiconductor, and acoustic. Each category relies on distinct detection principles and offers specific advantages and limitations in terms of sensitivity, selectivity, response time, durability, and cost. The most common ones currently used will be discussed in the remainder of the section, while a summary is provided in Table 3

- *Thermal sensors:* The pellistor is a thermal detector that measures a change in resistance due to the heat generated by catalytic combustion on a bead. The resulting imbalance in a Wheatstone bridge produces an output voltage proportional to the concentration of flammable gas in the air. Similarly, Thermal Conductivity Detectors (TCDs) measure differences in thermal conductivity caused by the presence of hydrogen, again using a Wheatstone bridge to detect small electrical changes linked to altered heat transfer. These sensors are robust and fast-responding but typically require high power and show limited selectivity toward hydrogen compared to other gases.
- *Electrochemical sensors:* These rely on the oxidation of hydrogen at the anode, which produces a current in an external circuit. Two main types are employed: potentiometric, which measure changes in potential and follow the Nernst equation, and amperometric, which measure current changes between the working and counter electrodes. They are low-power and highly selective, making them suitable for portable and industrial

applications. However, their performance deteriorates at low temperatures, likely due to constraints in electrode activity or redox reaction kinetics.

- *Optical sensors:* Optical detectors have demonstrated high precision in hydrogen detection but are often expensive or complex and, in many cases, remain at the research or laboratory development stage. Nevertheless, they are among the most promising options for cryogenic systems owing to the stability and robustness of their sensing materials under low-temperature conditions. Raman spectroscopy, a subclass of optical detection, measures frequency shifts in scattered light to identify the unique spectral fingerprint of hydrogen molecules. Other detectors based on absorption and emission principles exploit the interaction of hydrogen gas with infrared (IR) or ultraviolet (UV) radiation. A particularly well-established approach is the optical fiber sensor, which detects variations in light transmission or reflection induced by the presence of hydrogen. Numerous subcategories of optical fiber sensors exist, including the Fiber Bragg Grating (FBG), which employs periodic microstructures along the fiber to filter specific wavelengths. Another important class is surface plasmon resonance (SPR) sensors, which utilize metallic films—often palladium layers—that interact with hydrogen to modify the propagation of light. Several optical sensing concepts have been adapted for cryogenic environments. For example, Bévenot et al. [18] developed an optical fiber sensor capable of detecting hydrogen leaks in cryogenic rocket engines. The sensor, designed to operate between -196 °C and 23 °C, features a palladium-coated fiber tip that exploits the metal's strong hydrogen absorption properties. The experimental setup combined the coated optical fiber with a laser source to monitor changes in reflectivity as an indicator of hydrogen presence. Although the tests were primarily performed at room temperature, the results demonstrated effective operation at low temperatures, aided by optical heating from the laser. Overall, optical sensors—particularly those employing palladium-based coatings—show strong potential for cryogenic hydrogen applications due to their high sensitivity, electromagnetic immunity, and suitability for harsh operating environments without requiring electrical power at the sensing point.
- *Semiconductor sensors:* A common example is the Metal Oxide Semiconductor (MOS) detector, which relies on changes in conductivity of a sensing material when exposed to hydrogen. The gas reacts with absorbed oxygen at the material surface, releasing electrons and thereby increasing conductivity. The resulting change in resistance is correlated with the hydrogen concentration. These sensors are compact and inexpensive, but they can suffer from cross-sensitivity to other gases and typically require regular calibration to ensure reliable long-term performance.
- *Acoustic sensors:* These devices rely on piezoelectric materials that generate an electrical charge when deformed by an acoustic wave. The adsorption of hydrogen molecules on the sensing surface alters the resonance frequency of the device. This frequency shift can result from mechanisms such as mass loading, catalytic oxidation (temperature change induced by reaction), or variations in gas concentration that modify the propagation velocity of the acoustic wave. Acoustic sensors can achieve high sensitivity, however, their performance is often affected by environmental conditions such as humidity and temperature. Among the most common designs are Surface Acoustic Wave (SAW) sensors [19], which employ substrates such as Pd, metal oxides, or polymers to absorb hydrogen molecules and therefore influence the acoustic wave traversing the surface. Another technology is the Quartz Crystal Microbalance (QCM), which measures frequency changes arising from hydrogen absorption in the sensing layer.

Table 3. Summary table of hydrogen sensor types. It gathers the five main categories of detectors and their principles.

Type of Sensor	Principle	Advantages	Limitations
Thermal	Heat transfer or combustion causes changes in temperature or resistance	Robust, fast response	High power, not selective
Electrochemical	Chemical reactions generate electrical signals such as current, voltage, conductivity, or impedance	Sensitive, low power, selective	Lifespan, sensitive to environment
Optical	Interaction with hydrogen changes light absorption, reflection, or emission	Highly precise, fast response	Expensive, complex
Semiconductor	Hydrogen adsorption on the sensing layer changes electrical resistance	Cheap, compact	Low selectivity, humidity sensitive
Acoustic	Hydrogen presence changes the resonance frequency of piezoelectric materials	Highly sensitive, fast response	Fragile, temperature sensitive

Sensors for Cryogenic Hydrogen

While the sensor technologies described above have been successfully applied in conventional hydrogen safety applications, their use under cryogenic conditions poses significant challenges. In Table 4 and overview of the performance of different sensors in presented and the Temperature range is highlighted. At very low temperatures, thermal and electrochemical sensors often suffer from reduced sensitivity or even operational failure due to limitations in catalytic activity, electrolyte stability, or electrode kinetics. Semiconductor sensors may also become unreliable, as their surface reactions and conductivity strongly depend on temperature. Acoustic sensors, on the contrary, may offer more promise in cryogenic environments, since their resonance-based mechanism is less directly affected by temperature extremes, although calibration against cryogenic-specific effects such as frost formation and material contraction is still required. Overall, while none of the existing sensor families is inherently designed for cryogenic hydrogen detection, some (e.g., acoustic or specially engineered semiconductor sensors) could potentially be adapted, provided careful material selection, surface engineering, and calibration strategies are employed.

Table 4. Evaluation of the performance of different hydrogen sensors. The table presents only broad operational ranges [20–22] for the sensors discussed earlier. Determining precise values is challenging, as they depend strongly on the specific sensing materials used. For example, even within MOS sensors, numerous subcategories exhibit significantly different properties. Consequently, it is challenging to provide a single representative value for an entire category of sensors. Additionally, response time is influenced by temperature, further complicating generalization.

Sensor Type	Detection (ppm)	Response Time	Temp. (°C)	Application
Pellistor	1–1000 ppm	<10 s	[−20;50]	Leak detection, industrial and mining with explosive gases
TCD	500–40,000 ppm	<4 s	[−20;90]	Leak detection, industrial, home safety devices
Potentio	100 ppm	10–90 s	[0;100]	Leak detection, industrial
Ampero	~ 10 ppm	20–50 s	[−20;80]	R&D
Raman	500 ppm	s–min	[20;30]	Research, Lab
Absor/Emi	1–100 ppm	s/min	[20;30]	Industrial hydrogen leak detection
FBG	0.15–10 ppm	1–5 s	[−30;80]	Leak detection
SPR	40,000 ppm	<1 s	[−20;60]	Hydrogen leak detection in industrial
MOS	100 ppm	<5 s	[80;400]	Safety devices
SAW	10 ppm	<5 s	[−20;80]	Automotive, wireless sensing devices
QCM	10 ppm	<5 s	Room Tempe.	Leak detection

These challenges have also been confirmed experimentally. Latka et al. [23] investigated hydrogen sensors for monitoring cryogenic storage tanks and demonstrated their limitations at low temperatures. In particular, palladium-based sensors, which are widely used due to Pd's strong affinity for hydrogen, were found to become ineffective below $T = -85\ ^\circ\mathrm{C}$. At such cryogenic temperatures, Pd loses its ability to absorb hydrogen and undergo the associated lattice expansion, thereby preventing reliable signal generation and detection. This finding highlights a key bottleneck in applying conventional hydrogen sensors to extreme environments. In parallel, Pijolat et al. [24] developed a tin dioxide (SnO_2)-based semiconductor sensor designed for cryogenic motors in space applications. Since SnO_2 detectors typically require elevated operating temperatures, the authors integrated a local heating structure to maintain sensor performance while shielding it from the surrounding cryogenic environment. The device achieved real-time monitoring with good sensitivity and response times, although calibration and maintenance under such conditions remained demanding. The work ultimately enabled the deployment of a larger-scale sensor network, illustrating both the feasibility and the complexity of hydrogen detection in cryogenic systems.

These insights underscore the critical role of predictive modelling and digital twin technology in cryogenic hydrogen infrastructures. By integrating sensor behaviour, material limitations, and environmental conditions into a digital twin, it becomes possible to anticipate sensor failures, optimize placement, and simulate safety scenarios in real time, ultimately enhancing the reliability and resilience of cryogenic hydrogen systems.

4. Safety Consideration Open and Enclosed Environments

In open environments, such as outdoor storage facilities or refuelling stations, a liquid hydrogen (LH_2) leak typically results in rapid vaporization upon contact with ambient conditions, leading to the formation of a cold, dense gas cloud. In the initial stages of the release, the sudden depressurisation creates a superheated cryogenic fluid, which is highly prone to flash boiling, further accelerating the vaporisation process. The resulting hydrogen vapor initially remains near the ground due to thermal stratification, but as it warms and becomes less dense than air, it transitions to a buoyant plume and disperses vertically into the atmosphere. While natural ventilation in open settings aids in the dilution of the hydrogen cloud, it also introduces complexity in predicting concentration fields, which evolve rapidly in response to changing wind conditions and turbulence. Consequently, early leak detection becomes critically dependent on strategic sensor placement and the fast response of detection systems. Technologies such as infrared imaging, hydrogen-specific gas sensors, and acoustic leak detectors are commonly employed, but they must be calibrated to perform reliably under variable environmental conditions. The main safety hazard in open environments arises from delayed ignition, where an initially undetected accumulation of flammable hydrogen may encounter an ignition source before it has fully dispersed, potentially resulting in a jet fire or localized explosion.

In contrast, closed or semi-enclosed environments such as indoor experimental facilities, or vehicle or aeroplane compartments, pose additional safety and detection challenges. The limited ventilation and confined geometry can lead to the accumulation of hydrogen vapors, especially in ceiling areas due to hydrogen's buoyancy. The cold gas cloud resulting from LH_2 vaporization may initially remain stratified, but over time can mix and reach flammable concentrations. Detection systems in such settings must account for spatial stratification, the potential for localized hotspots, and the risk of pressurization or deflagration in the event of ignition. Distributed sensor networks, coupled with real-time data analytics or ML-based leak localization algorithms, are critical in this case for identifying leaks before hazardous thresholds are reached. Additionally, in enclosed environments there is higher requirement for cryogenic-compatible sensors, redundancy in detection pathways, and integration with automated ventilation and isolation systems. Understanding the contrasting leak behaviors between open and closed settings is essential for designing robust, scenario-specific hydrogen safety strategies.

5. Experimental Investigations of Hydrogen Dispersion

Experimental campaigns related to hydrogen application safety are either conducted for releases in open or closed environments, with the latter often at a laboratory scale.

Over the years, studies have investigated controlled hydrogen releases in open environments. These studies aim to replicate unintentional hydrogen leaks from storage systems and assess the associated safety hazards. For example, NASA [25] conducted hydrogen vapour cloud dispersion experiments to obtain information regarding the physical phenomena governing the dispersion of flammable clouds formed as the result of spills of large quantities of liquid hydrogen. The experiments consisted of ground spills of up to 5.7 m^3 of liquid hydrogen, with spill duration around 35 s, where temperature, hydrogen concentration and turbulence levels were measured while the hydrogen cloud drifted downwind. These results showed the role of thermal and momentum-induced turbulence in dispersing the cloud to safe concentration level, with a buoyant nature present before the mixing, due to normal atmospheric turbulence. Furthermore, an adiabatic mixing model was developed to deduce hydrogen-air mixture ratios for temperature measurements obtained within the cloud formed.

In an additional study [26] four LH_2 spill experiments were conducted. The focus was on the liquid pool formed by the spill, either on solid or liquid ground. They measured both the vaporisation and spreading of the pool, as well as the ice layer formation when LH_2 was spilled on water. Compared to other cryogenic pools, the LH_2 one showed higher vaporisation on smaller area. Other experimental investigations of spills in open environment were undertaken by Royle et al. [27] and Hall et al. [28] at the Health and Safety Laboratory. Initially, assessments were conducted on a spillage scenario involving LH_2 at a discharge rate of 60 lt/min, both without [27] and subsequently with ignition [28]. The experiments encompassed measurements of hydrogen concentration in the surrounding air, thermal gradients within the concrete substrate, formation of liquid pools, and temperatures within these pools for the unignited case. For the ignited case the focus shifted to parameters such as flammability limits of a LH_2 vapour cloud, flame propagation speeds through such a cloud, and ensuing radiative heat and over-pressures post-ignition. The studies revealed the behaviour of released LH_2, showing an initial flash upon contact with the ground followed by the formation of a liquid pool. The shape and spread of this pool depend on the release orientation, and the release can generate a flammable mixture extending at least nine meters downwind from the release point. Furthermore, the deposit from the air solidification can trap liquid hydrogen within its matrix producing a potentially hazardous mixture. When shifting the focus on the ignition, four separate regimes have been found to occur: an initial deflagration of the cloud back to source, travelling at speeds up to 50 m/s; a possible secondary explosion emanating from the solid deposit generated after the initial deflagration of the release cloud due to oxygen enrichment; a buoyancy driven jet-fire when wind conditions are minimal, and a momentum dominated jet-fire when wind conditions are high.

Kawasaki Heavy Industries conducted experimental investigation [29] to examine the dispersion characteristics of liquefied hydrogen and liquefied natural gas (LNG). Providing insights into the contrasting behaviours of these substances upon spillage, they showed that LH_2 immediately dispersed upward compared to LNG, as the horizontal diffusion distance of LH_2 is smaller than that of LNG and the liquefied hydrogen promptly evaporates and diffuses upward. Furthermore, the flammability limit of low temperature hydrogen gas was narrower than the range at normal temperature.

Kobayashi et al. [30] performed experimental investigation of hydrogen ignition for high-pressure applications in fuel cell vehicle stations. In particular, pressurized cryogenic hydrogen (up to 90 MPa, 50–300 K) was released through pinhole nozzles, and the resulting blast pressure and flame length were measured. The results demonstrated that flame length and blast pressure correlate with the leakage flow rate, with cryogenic hydrogen flames extending up to 30% longer than those at ambient conditions.

The aforementioned experiments offer valuable insights into hydrogen cloud penetration and the potential ignition under hazard-relevant conditions, serving as robust benchmarks for numerical validation. However, the data are subject to uncertainties arising from factors such as sensor placement, environmental fluctuations (e.g., wind speed and direction), measurement errors, and variability in ground material properties (e.g., conductivity, humidity, and heat capacity). Furthermore, fundamental processes like mixing, warming, and the influence of turbulence remain poorly understood due to the wide scope and variability inherent in these large-scale studies.

To address these knowledge gaps, experimental campaigns have been undertaken at the laboratory scale, focusing on elucidating the influence of specific parameters and the role of fundamental phenomena. For instance, Li et al. [31] conducted experimental studies on the decay behaviour of subsonic and sonic vertical releases and dispersion of helium and hydrogen. They employed a planar laser Rayleigh scattering system to measure mean concentration fields in a series of subsonic and under-expanded jets. The experimental data were then compared with a reduced-order jet model for under-expanded jets, with certain key model parameters calibrated based on comparisons with the experimental results. These laboratory-scale investigations provide valuable insights into fundamental processes and help refine models for predicting the behaviour of hydrogen releases in various scenarios.

Other experimental campaigns investigated the influence of buoyancy and turbulence on H_2 release [32–34]. Pure hydrogen is released into air at standard conditions from a 1.91 mm was investigated at three different exit velocities, with Reynolds numbers (Re) ranging from transitional and fully turbulent flow conditions. While buoyancy is found to have a negligible effect on centreline velocity fluctuation intensities, the maximum H_2 mass fraction fluctuation intensity increases nearly 70% in the buoyant regime and the peak value shifts from the mixing region to the jet centreline.

In the experimental campaign of Hecht and Panda [35], the focus was on the temperature and concentration measurements, i.e., in the mixing and warming, of the release hydrogen from cryogenic storage tanks, to mimic the leak from a cryogenic hydrogen storage system, such as a hydrogen fuel cell vehicle fuelling station. The reservoir temperature was in the range of 50–61 K and the reservoir pressure was 2–5 bar. Two nozzle diameters were tested, 1 mm and 1.25 mm. The main goal of their work was to provide a series of data at controlled release conditions for the validation of quantitative model for releases at temperatures below 80 K [1,36].

Further investigations on low temperature releases were presented by Gong et al. [37]. They measured low-temperature hydrogen releases (200–300 K) at 0.5 MPa through pinhole nozzles. The results showed that axial concentration increases with lower storage temperature and larger nozzle diameter, and inverse concentration distributions were derived.

Han et al. [38] instead examined hydrogen dispersion from small-hole leaks under high-pressure conditions (100–400 bar, nozzle diameters 0.5–1.0 mm) to support the definition of safety distances at refueling stations. The large Froude numbers associated with these releases imply negligible buoyancy effects, a finding confirmed by laser-based flow visualization. Centerline concentration measurements further showed that actual values are consistently lower than isentropic predictions.

An additional area of interest is the sensitivity of the dynamics of hydrogen jets to the release orifices which are characterised by high-aspect ratio. This effect was investigated in ref. [39]. Release of cryogenic hydrogen jets (50–64 K) from high aspect ratio nozzles have been measured for storage condition of 3 and 5 bar_{abs}. They showed that, at the pressures investigated, when comparing the results with equivalent round nozzles, minimal differences in concentration observed along the major and minor axes. centreline concentration decay and temperature increase are similar to round jets when normalized. Nevertheless, increasing the pressures at range of applicability to cryo-compressed hydrogen systems phenomena as two dimensional flow regions of non-Gaussian profiles along the major and minor axes, and centreline decay rates that are higher than round nozzles of the same effective diameter can be observed.

6. CFD Tools and Their Predictive Capabilities

Computational Fluid Dynamics (CFD) is a numerical approach for solving the governing equations of fluid motion to predict flow behaviour, heat transfer, and species transport in complex geometries. At its core, CFD solves discretised forms of the Navier–Stokes equations. In practice, the CFD process involves (i) defining the problem geometry, (ii) generating a computational mesh, (iii) specifying boundary and initial conditions, and (iv) solving the governing equations iteratively until convergence.

CFD has become an indispensable tool for analyzing complex hydrogen safety scenarios, offering detailed insights into fluid flow, heat transfer, and chemical reactions during leak and dispersion events. This section reviews the current state-of-the-art CFD tools commonly employed in hydrogen safety research, focusing on their ability to accurately predict critical phenomena such as vaporization dynamics, turbulent mixing, and ignition risks. Emphasis is placed on model fidelity, numerical methods, and computational efficiency, as well as the challenges associated with simulating multiphase cryogenic flows and reactive mixtures. The predictive capabilities of these tools are evaluated through comparison with experimental data and case studies, highlighting their role in informing design and risk mitigation strategies.

Table 5 compiles these different case studies, providing a description of the experiments and their main results. It offers a general overview of the physical behavior of hydrogen release, as well as the performance of CFD methods, which are discussed in the following sections.

6.1. Dispersion

One key advantage of CFD simulations in dispersion scenarios lies in their ability to capture the complex interactions between the released hydrogen cloud and the surrounding environment, including atmospheric conditions. However, the large spatial and temporal scales involved in dispersion phenomena necessitate the use of advanced sub-modeling approaches—particularly for turbulence—to achieve accurate and computationally feasible predictions.

A further complication arises from the fact that turbulence in cryogenic hydrogen releases differs significantly from standard atmospheric or high-temperature turbulence. Strong density gradients, rapid phase change, and intense thermal stratification alter the energy cascade and mixing processes, challenging the assumptions embedded in conventional turbulence models such as k–ϵ or LES sub-grid closures. As a result, models specifically tuned or adapted for cryogenic releases are required to account for buoyancy-driven instabilities, variable thermophysical properties, and phase-transition dynamics.

Without such refinements, simulations risk misrepresenting plume rise, dispersion rates, and ignition potential, limiting their reliability for safety-critical applications.

For flammable fuels like hydrogen, sudden releases in open environments pose a risk because the dispersed gas can travel significant distances while remaining within its wide flammability limits. In confined spaces, accumulation of hydrogen can lead to potentially explosive conditions. Therefore, accurate prediction of hydrogen dispersion is essential not only to define safe separation distances but also to optimize safety strategies such as detector placement and emergency response protocols. A summary of relevant CFD applications for both high-pressure gaseous and liquid hydrogen dispersion is provided in Table 5.

Several studies have addressed both LH_2 spills and high-pressure hydrogen gas releases. For instance, Giannissi et al. [40] simulated LH_2 spill experiments on flat ground, demonstrating the influence of atmospheric humidity on vapor dispersion and, in particular, on the buoyancy-driven behavior of the vapor cloud. In contrast, Jin et al. [41] characterized LH_2 vapour dispersion into three stages: an initial rapid spread, a quasi-steady dispersion, and a final disappearance phase. Their results showed that vapour cloud composition and wind conditions significantly affect cloud fluctuations during diffusion.

Regarding high-pressure gaseous hydrogen dispersion, Choi et al. [42] modelled hydrogen leaks from an FCV in an underground parking garage, analyzing how ventilation systems influence the expansion of flammable regions. Their findings indicated that mechanical fans can delay the growth of hazardous hydrogen concentrations. A related study by Dadashzadeh et al. [43] further investigated the effectiveness of both mechanical and natural ventilation in mitigating hydrogen accumulation in confined spaces, emphasizing ventilation's critical role in dispersion control.

6.2. Jet Fires

High-pressure releases of liquids, gases, or vapors through small orifices or size-limited openings—such as leaks in vessels or pipelines—can give rise to jet fires. Due to the combination of a restricted opening and elevated pressures, the escaping fluid can reach very high velocities. When ignited, these high-velocity jets produce flames with characteristic trajectories and intense momentum-driven behavior. The associated hazards primarily involve localized, severe heat fluxes that threaten nearby personnel and equipment. Direct flame impingement on storage tanks or pipelines can rapidly degrade containment integrity, potentially triggering catastrophic failures or a domino effect of cascading incidents.

Understanding the geometry, dynamics, and radiative heat transfer of jet fires is therefore critical for industrial safety. Several CFD studies have been dedicated to investigating this phenomenon. For example, Wang et al. [44] analyzed the radiant fraction of high-pressure hydrogen jet flames, demonstrating that the flame length increases with discharge pressure but decreases with larger nozzle diameters and greater temperature differences between the hydrogen and the environment. Similarly, Cirrone et al. [45,46] employed Reynolds-Averaged Navier-Stokes (RANS) simulations to assess the thermal hazards of cryogenic hydrogen jet fires, quantifying radiative heat fluxes at various positions relevant to automotive hydrogen storage and thermal pressure relief scenarios.

A summary of key CFD investigations into hydrogen jet fires is provided in Table 5. Generally, these studies confirm that CFD simulations effectively predict jet fire flame length, radiative heat transfer, and thermal load distribution. CFD models also enable the assessment of how factors like wind, leak location, surrounding obstacles, and jet orientation influence thermal loads. This capability is vital for optimizing passive fire protection (PFP) strategies, helping to prevent secondary incidents during firefighting operations and mitigate the overall impact of jet fire events.

Table 5. Collection of different numerical studies regarding H_2 release.

Reference	Case of Study	Brief Description	Main Results
		Jet Fire: Geometry, Dynamics and Heat Transfer	
[45]	Cryogenic hydrogen fires from storage with pressure up to 5 bar abs and temperature between 48 and 82 K	RANS ($\kappa - \epsilon$), combustion: EDC; radiation: DO (Discrete Ordinates) model in ANSYS FLUENT.	Flame length and radiative heat flux for cryogenic jet fires.
[46]	Sudden release from a 25 L tank at initial pressure of 930 bar through 2 mm orifice	RANS ($\kappa - \epsilon$), combustion: EDC; radiation: DO model in ANSYS FLUENT.	Dynamics of radiative heat transfer and flame length for under-expanded hydrogen jet fire (900 bar).
[44]	Six cases of under-expanded hydrogen and hydrogen/methane jet fires (horizontal/vertical); nozzle diameters 5.08–20.9 mm; tank pressures 33–105 bar; varying ground reflectance	LES turbulence; combustion: modified EDM; radiative transfer: fvDOM in FireFOAM.	Flame length and radiation characteristics of hydrogen and hydrogen/methane jet fires.
[47]	PRD activation of cylindrical Al-carbon fiber/epoxy composite vessel (900 mm length, 400 mm diameter); discharge pressures 10–40 MPa; barrier inclinations	SST $\kappa - \omega$ turbulence; finite-rate/EDM combustion in SIMPLE.	Characteristics of hydrogen jet fires from Pressure Relief Devices (PRD).
		Liquid Hydrogen (LH_2) Dispersion	
[40]	Spill diameter 26.6 mm; two horizontal and one vertical releases; spill rate 60 L/min; fluctuating wind direction	Simulations with ANDREA-HF code.	LH_2 spill experiments on flat concrete pad in open environment (HSL data).
[48]	Horizontal open area 0.5×0.5 m^2; mass flow 9.52 kg/s; effects of wind velocity, temperature	Unsteady RANS with realizable $\kappa - \epsilon$ model, enhanced wall treatment, ANSYS FLUENT.	LH_2 spill dynamics on the ground, including vaporization and dispersion.
[41]	Two-phase jet, horizontal cross-section 0.5×0.5 m; mass flow 9.52 kg/s; varying vapor cloud compositions	Mixture multiphase model with realizable $\kappa - \epsilon$ turbulence and gas transport in ANSYS FLUENT.	Evolution and flow fields of flammable vapor cloud formed by LH_2 spills.
		High-Pressure Hydrogen Gas Dispersion	
[43]	Parking compartment $6.4 \times 3.7 \times 2.8$ m; hydrogen release 6.7×10^{-4} kg/s; multiple ventilation scenarios	$\kappa - \epsilon$ turbulence model in FDS.	Dispersion of hydrogen gas in confined/semi-confined spaces from Fuel Cell Vehicle (FCV).
[42]	Underground parking garage with 12 slots; hydrogen leak from FCV corner; leakage area 5 cm square; leakage rates 131–1310 L/min; fan air volumes 20–60 m^3/min	$\kappa - \epsilon$ turbulence in STAR-CCM+.	Dispersion process of hydrogen leak in underground parking garage.

7. Machine Learning for Hydrogen Safety

Machine Learning (ML) has emerged as a powerful approach to enhance hydrogen safety by enabling rapid analysis and predictive capabilities that complement traditional physics-based models. The complexity and variability inherent in hydrogen release, dispersion, and combustion phenomena often challenge conventional simulation methods, especially under uncertain or dynamic conditions. ML techniques—ranging from supervised learning to deep neural networks—offer the potential to extract meaningful patterns from large experimental and simulation datasets, facilitating improved leak detection, risk assessment, and real-time monitoring. This section provides an overview of current ML applications in hydrogen safety, highlighting how these data-driven methods contribute to early warning systems, predictive maintenance, and optimized safety protocols, thereby supporting safer deployment of hydrogen technologies. Table 6 provides a collection of the classical and Deep Learning Methods principles and applications discussed below.

In Zhao et al. [49], a hydrogen leak localization system was developed using machine learning on experimental concentration data. A scaled parking garage model simulated fuel cell vehicle leaks with helium as a safe hydrogen surrogate. Twelve ceiling-mounted sensors recorded concentrations at varied leak positions to generate a dataset for training an artificial neural network (ANN) and a K-DTW algorithm. The ANN predicted unseen leak locations with 78.4 % accuracy, while the K-DTW algorithm classified unknown leaks by assigning them to the nearest known location, achieving 87.5% accuracy.

El-Amin [50] employed various machine learning techniques—including artificial neural networks, random forests, gradient boosting regression, and decision trees—to predict the atmospheric dispersion of hydrogen leaks. The training dataset was generated using a hybrid empirical-analytical-numerical model, enabling comprehensive coverage of relevant physical scenarios. The study included detailed investigations into dataset preparation, feature importance, correlation analysis, and hyperparameter tuning. Model performance was evaluated using multiple error metrics alongside the coefficient of determination (R^2) to assess prediction accuracy. Among the tested methods, the random forest (RF) algorithm demonstrated superior effectiveness in forecasting hydrogen leak dispersion, offering a promising data-driven approach for hydrogen safety applications.

Ustolin et al. [51] applied machine learning to experimental data from liquid hydrogen (LH_2) release tests to predict oxygen condensation and solidification during accidental releases. The study developed a supervised classification model using TensorFlow to determine (i) whether LH_2 releases induce liquefaction or solidification of air components and (ii) whether hydrogen concentrations exceed the lower flammability limit (LFL). The model was trained and validated on outdoor leakage experiments conducted by the Norwegian Defence Research Establishment (FFI) [52]. These tests aimed to understand LH_2 behavior in maritime fuel applications and included both outdoor leakage experiments and studies in confined spaces with ventilation masts, providing accurate predictions to guide safety measures such as water deluge systems.

Following this work, Alfarizi et al. [53] employed the Random Forest (RF) algorithm to predict two critical outcomes during LH_2 leakage events: (i) oxygen phase changes (condensation or solidification) and (ii) whether hydrogen concentrations exceed the lower flammability limit (LFL). Using three databases derived from experimental tests conducted by the Norwegian Defence Research Establishment [52], the study demonstrated that RF models can effectively forecast oxygen phase transitions and hydrogen flammability, offering actionable insights to improve safety measures and prevent hazardous incidents during LH_2 releases.

Yang et al. [54] developed a comprehensive approach to assess the safety of hydrogen refueling stations using multiple machine learning algorithms, including multi-source data association prediction, random gradient descent, and deep neural network optimization. These methods analyzed operational data to detect correlations, dependencies, and patterns, enabling accurate assessment of equipment safety. Real-time sensor data were compared with model predictions to optimize control strategies. For example, the model predicted equipment operating temperatures, enabling the formulation of control actions to maintain safe temperature ranges and ensure operational safety. Gradient decision tree regression identified key features affecting safety, and a 70:30 training-testing split validated the model. Simulated predictions closely matched actual measurements, confirming high predictive accuracy.

Patil et al. [55] review the application of machine learning to enhance safety in hydrogen systems, evaluating Artificial Neural Networks (ANNs), Computer Vision (CV), other ML algorithms, data diffusion techniques, and wireless sensor networks. They demonstrated that ANNs can predict leaks when trained on datasets including pressure, temperature, concentration, and flow, providing early warnings before alarms trigger. CV approaches are promising for real-time leak detection and optical analysis, leveraging video and motion data to locate leaks. The study further highlights the strong potential of AI-driven safety systems while noting challenges related to data scarcity.

He et al. [56] proposed a Physics-informed Convolutional Long Short-Term Memory Network (PI-ConvLSTM), trained on FLACS-simulated leakage data, to predict hydrogen concentration distributions in real time. By incorporating physical constraints into the neural network's loss function, the model significantly improves accuracy at gas cloud boundaries while enabling rapid consequence prediction.

Lee et al. [57] evaluated several ML models enhanced by Genetic Algorithms (GA) to predict hydrogen dispersion in typical leakage scenarios, using a comprehensive dataset of 6561 PHAST-simulated leakage scenarios. By optimizing hyperparameters and validating performance with k-fold cross validation and statistical metrics, the study identified a GA-optimized deep neural network as the most effective model.

Zhang et al. [58] introduced a physics-informed graph neural network (Physics_GNN) trained on sparse sensor data and validated on experimental jet data. By incorporating spatial dependencies and governing physical laws directly into the network architecture, the model could predict leak characteristics (concentration and velocity axial profiles) with a higher accuracy (1000 times greater) than conventional physics-informed neural networks (PINNs), and with a substantial speedup (100 times faster) than conventional CFD simulations.

ML-Transformer Architecture

The Transformer is a deep learning architecture initially developed for natural language processing (NLP) and later extended to time-series forecasting and other predictive tasks. Its core innovation is the self-attention mechanism, which enables the model to weigh the relative importance of each input element, capturing contextual dependencies without relying on recurrence. Today, the most widely known Transformer-based models are large language models, such as GPT. Beyond NLP, the Transformer architecture offers significant potential for fast and accurate forecasting in safety-critical applications. For instance, H_2-Informer, a Transformer-based model, leverages this architecture to predict hydrogen diffusion and leak propagation at refueling stations. By integrating sparse sensor data with environmental factors like wind speed, direction, and height, H_2-Informer provides rapid, high-accuracy predictions that allow timely mitigation measures, demonstrating how Transformer models can directly enhance the safety and operational management of hydrogen infrastructures.

Martvall et al. [59] present an innovative method to increase the response time of an optical plasmonic hydrogen sensor by using machine learning. The authors use a hybrid deep learning method, the Long Short-term Transformer (LSTR), to predict hydrogen concentration change faster than the physical sensor. LSTR is specifically used because the situation requires short-term memory to capture recent and complex patterns, while capturing long-term trends. Even if the model does not use LSTM layers, it relies on the idea of long short-term memory and implements it in a Transformer architecture. Based on these models, the authors developed the LEMAS (Long Short-term Transformer Ensemble Model for Accelerated Sensing) framework. It showed an increase of 40 in the response time of the sensor in an enclosed inert environment. This technology highlights the potential of deep learning, especially the Transformer architecture, in enhancing safety systems for hydrogen infrastructure.

Q. Wu et al. [60] developed H_2-Informer, a Transformer-based deep learning model specifically designed to predict hydrogen diffusion at refueling stations. The model builds on the Informer architecture, which optimizes the classical self-attention mechanism by focusing only on the most relevant sequence positions, thereby reducing computational cost while maintaining high accuracy. H_2-Informer integrates sparse sensor concentration data along with wind speed, wind direction, and height information to predict two-dimensional planar hydrogen diffusion distributions over multiple future time points, including vertical evolution at different heights. Following hyperparameter tuning, the model achieved high predictive accuracy with an inference time of just 1.5 s, significantly faster than conventional CFD simulations. Compared with standard Transformer models, H_2-Informer demonstrated superior long-term prediction accuracy and efficiency, enabling timely hazard detection and response in hydrogen refuelling stations.

Table 6. Supervised Learning: Classical ML and Deep Learning Methods.

Category	Methods	Principle and Applications
Classical ML	Decision Trees (DT)	Tree-based model. Predictions of dispersion of hydrogen.
	Random Forests (RF)	Ensemble of decision trees. Predictions of oxygen phase changes and hydrogen concentrations.
	Gradient Boosting (GBR)	Ensemble of learning algorithms. Predictions of dispersion of hydrogen.
	Genetic Algorithms (GA)	Computing technique for optimization. Predictions of hydrogen dispersion.
Deep Learning	Artificial Neural Networks (ANN)	General neural network. Predictions of leak locations
	Deep Neural Networks (DNN)	Multi-layer ANNs for complex representations. Predictions of leaks with pressure, temperature, or concentration.
	Convolutional Neural Networks (CNN, CV)	Specialized ANN for Computer Vision tasks.
	Recurrent Neural Networks (RNN, LSTM)	Sequential/time-series modeling. Predictions of hydrogen concentration.
	Graph Neural Networks (GNN)	Learning from graph-structured data. Predictions of leak characteristics.
	Transformers	Self-attention mechanism, mainly used in NLP (Natural Language Processing). Predictions of hydrogen diffusion

8. Conceptual Framework for Digital Twins in Cryogenic Hydrogen Systems

In the context of hydrogen safety, a digital twin can be envisioned as a virtual replica of a physical system (e.g., storage tanks, pipelines, or release scenarios) that continuously interacts with real-world data to predict, diagnose, and prevent hazardous events. Its architecture could integrate three main components: (i) sensor data streams, which provide real-time measurements of pressure, temperature, hydrogen concentration, and environmental conditions; (ii) CFD-based simulation models, which can be used both to provide synthetic data as well as capturing the detailed physics of hydrogen dispersion and cryogenic effects; and (iii) machine learning modules, which can act as add ons to conventional sesors enabling real-time prediction and adaptive control by learning from both sensor inputs and CFD outputs.

The envisioned workflow begins with sensors feeding high-frequency data into the digital twin. These data are processed and compared against CFD predictions, with ML algorithms serving as intermediaries to bridge computational gaps, accelerate inference, and capture nonlinear correlations that may be difficult to model directly. Over time, the digital twin improves through continuous learning, combining historical CFD simulations, synthetic datasets, and real-world sensor measurements. A schematic of the conceptual framework for digital twins in cryogenic hydrogen systems can be seen in Figure 1.

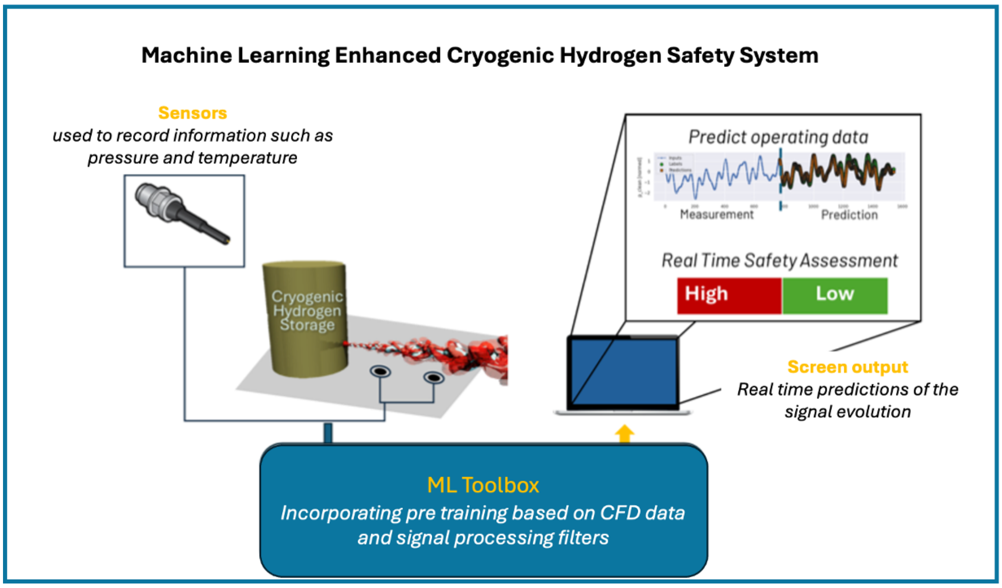

Figure 1. Conceptual Framework for Digital Twins in Cryogenic Hydrogen Systems.

One critical aspect of this process is signal cleaning, which ensures that the data entering the Digital Twin are accurate, consistent, and free from artefacts. Raw sensor data often contain noise, bias, or missing values caused by environmental interference, calibration drift, or sensor degradation—issues that can severely compromise model reliability if left uncorrected. The cleaning process typically involves several stages. For example, noise filtering using techniques such as moving averages, Fast Fourier transforms, or Kalman filters is employed to smooth high-frequency fluctuations while preserving meaningful physical trends. As discussed in our previous publication [61], signal cleaning is also critical for improving the performance of machine learning approaches. Despite this, very limited literature currently exists regarding the optimal signal cleaning strategies for cryogenic hydrogen applications.

9. Conclusions and Discussion

Digital Twins, such as those described in the previous section that integrate machine learning, computational fluid dynamics, and real-life sensor data, hold significant potential to advance cryogenic hydrogen safety. By enabling accurate, real-time analysis and prediction of complex phenomena—including leak detection, vapor dispersion, phase changes, and combustion risks—they provide a powerful framework for safety assessment. The capability of ML models to learn from a wide range of experimental and simulation datasets representing both point and field information can substantially enhance prediction accuracy and enable rapid identification of hazardous conditions that traditional (low-order) methods may struggle to capture efficiently. Applications presented in the previous sections ranging from leak location to continuous safety monitoring illustrate how ML-driven Digital Twins can strengthen early warning systems and support proactive safety management across hydrogen infrastructures.

Our review also indicates that although advances in hydrogen sensors, computational fluid dynamics, and machine learning have each been significant, achieving their seamless integration for real-time safety management still presents several challenges.

One of the key barriers to the effective application of machine learning in hydrogen safety is the scarcity of diverse and high-quality datasets. Several strategies can help mitigate this challenge. Physics-informed machine learning approaches reduce reliance on large empirical datasets by embedding conservation laws and safety constraints directly into model training. Furthermore, with increasing computational power and the wider availability of High-Performance Computing facilities, synthetic data generated through high-fidelity CFD simulations—such as Direct Numerical Simulations (DNS) and Large Eddy Simulations—can be used to augment limited experimental data, although currently DNS remains mostly applicable to simplified geometries. Transfer learning [62], a deep learning approach in which a model trained for one task is used as a starting point for a model that performs a similar task, offers another promising route. It can help leverage models trained in related domains, such as combustion or cryogenics, potentially for different fluids and adapting them to hydrogen-specific conditions. Finally, hybrid digital twin frameworks that integrate sensor data with simulation outputs enable continuous data enrichment during operation. Establishing collaborative open datasets within the hydrogen safety community would further accelerate progress by enhancing reproducibility and providing a broader foundation for robust model development.

A second important challenge is data interoperability issues, as sensor data, CFD simulations, and ML models often operate at different timescales and formats. For example, hydrogen sensors may produce high-frequency time-series data in the millisecond range, while CFD simulations often generate outputs at coarser temporal intervals (seconds to minutes) and at a spatial resolution dependent on the computational mesh. ML models, on the other hand, require input data that are pre-processed into consistent feature sets, often necessitating resampling, dimensionality reduction, or feature engineering to align with available training data.

Addressing these challenges will require interdisciplinary collaboration. Below is a summary of suggestions for moving forward.

- Dedicated test beds that combine sensing, modelling, and control, enabling future systems to move toward reliable real-time hydrogen safety management.
- In the computational front, one important area of research should be the development of surrogate models and reduced-order approaches specifically tailored for cryogenic conditions that can help speed up the prediction and monitoring process.
- Development of standardised data exchange protocols, metadata frameworks, and intermediate data layers that can translate between different sources. Recent advances in semantic data models and ontologies for engineering systems, along with cloud-based platforms for real-time data fusion, offer promising pathways to overcome these interoperability barriers.
- Moreover, real-time digital twins must incorporate robust methods for uncertainty quantification to ensure trustworthiness in safety-critical decisions.

- Cyber-physical integration further demands secure and fault-tolerant digital infrastructures. Addressing these challenges will require more enhanced interdisciplinary research.

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