

Review

# Hydrogen Safety Challenges: A Comprehensive Review on Production, Storage, Transport, Utilization, and CFD-Based Consequence and Risk Assessment

Marcella Calabrese <sup>1,2</sup>, Maria Portarapillo <sup>1,\*</sup>, Alessandra Di Nardo <sup>1</sup>, Virginia Venezia <sup>1,3</sup>, Maria Turco <sup>1</sup>,  
Giuseppina Luciani <sup>1</sup> and Almerinda Di Benedetto <sup>1</sup>

<sup>1</sup> Department of Chemical, Materials and Production Engineering, University of Naples Federico II, P.le Tecchio 80, 80125 Naples, Italy; marcella.calabrese2@unina.it (M.C.); alessandra.dinardo@unina.it (A.D.N.); virginia.venezia@unina.it (V.V.); maria.turco@unina.it (M.T.); luciani@unina.it (G.L.); almerinda.dibenedetto@unina.it (A.D.B.)

<sup>2</sup> Plant & Process Technology, Saipem SpA, Via Luigi Russo 5, 20138 Milan, Italy

<sup>3</sup> Department of Structures for Engineering and Architecture, University of Naples Federico II, Via Claudio 21, 80125 Naples, Italy

\* Correspondence: maria.portarapillo@unina.it

**Abstract:** This review examines the central role of hydrogen, particularly green hydrogen from renewable sources, in the global search for energy solutions that are sustainable and safe by design. Using the hydrogen square, safety measures across the hydrogen value chain—production, storage, transport, and utilisation—are discussed, thereby highlighting the need for a balanced approach to ensure a sustainable and efficient hydrogen economy. The review also underlines the challenges in safety assessments, points to past incidents, and argues for a comprehensive risk assessment that uses empirical modelling, simulation-based computational fluid dynamics (CFDs) for hydrogen dispersion, and quantitative risk assessments. It also highlights the activities carried out by our research group SaRAH (Safety, Risk Analysis, and Hydrogen) relative to a more rigorous risk assessment of hydrogen-related systems through the use of a combined approach of CFD simulations and the appropriate risk assessment tools. Our research activities are currently focused on underground hydrogen storage and hydrogen transport as hythane.

**Keywords:** hydrogen economy; safety concerns; hydrogen regulations; CFD simulations; risk assessment



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## 1. Introduction

The geopolitical and energetic crisis faced by the world in recent decades requires alternative renewable energy sources [1]. One of the issues with fossil fuels is resource availability; however, the main issue is the impact that these fuels have on ecosystems [2]. Unanimously, political forces around the world have started a campaign of investment and funding for research to aid the ecological transition and full decarbonization that are anticipated for the year 2050. Projections show that the total worldwide investment by governments, businesses, and individuals on energy and land-use systems will annually need to grow by USD 3.5 trillion per year to secure the accomplishment of net zero emissions (NZE) in 2050 [3]. The initial phase of the transition to NZE will include most of the expenses, which will be unevenly distributed among the producers of fossil fuels and emerging nations, thereby increasing the danger of disruptions in the supply of energy and price increases [4].

Hydrogen has emerged in recent years as a promising alternative energy carrier because of its potential to address the challenges of climate change, air pollution, and energy security. As a result, several prospects for accomplishing decarbonization are expected; hydrogen may be the key to reaching NZE for heavy industry and transportation [3,5]. In

particular, the interest of the scientific community is focused on green hydrogen that can be produced from the electrolysis of water with the aid of renewable energy sources such as solar, wind, and hydropower.

By 2050, the World Energy Transition Outlook predicts that 12% of total energy consumption will be covered by green hydrogen. The viability of hydrogen technology, which is projected to replace the existing fuel systems in many applications, highly depends on the costs of production, storage, and safety; moreover, despite the many benefits of green hydrogen, there are numerous challenges associated with its adoption [6].

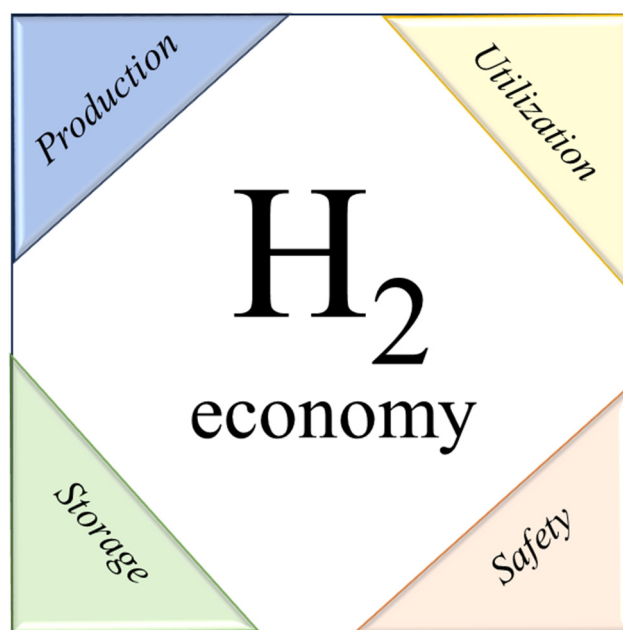
The hydrogen industry is experiencing significant growth and attention, especially as nations and industries seek to reduce carbon emissions and transition to cleaner energy sources. The market size of global hydrogen generation and utilisation is valued at USD 158.8 billion in 2023 and is estimated to reach USD 257 billion in 2028, thus growing at a compound annual growth rate of 10.2% [7].

Some key developments and safety issues in the hydrogen industry are described below as follows

1. Growth of the hydrogen economy: Many countries have announced ambitious plans to invest in hydrogen as a clean energy carrier. These include plans for the production, distribution, and utilisation of hydrogen in various sectors such as transport, industry, and power generation.
2. Advances in technology: Significant progress has been made in hydrogen production technologies, including electrolysis (both alkaline and PEM), steam methane reforming (SMR) with carbon capture and storage (CCS), the gasification of biomass, and more recently the production of green hydrogen from renewable energy sources.
3. Infrastructure development: One of the biggest challenges facing the hydrogen industry is the development of infrastructure for the production, transport, storage, and distribution of hydrogen. This includes the construction of pipelines, storage facilities, and hydrogen refuelling stations for transport.
4. Challenges in the area of safety as follows:
  - Handling hydrogen: Hydrogen is highly flammable and can easily ignite. The safe handling and storage of hydrogen requires special equipment and procedures to prevent leaks and minimise risks.
  - Hydrogen embrittlement: hydrogen can embrittle metals, which can cause problems with the structural integrity of equipment and infrastructure as well as pose a safety risk.
  - Transport safety: transporting hydrogen safely over long distances can be a challenge due to its low energy density and the need for specialised containers or pipelines.
  - Public awareness and education: in order to prevent accidents, it is important to ensure that both the public and those working in the hydrogen industry are aware of the safety risks associated with hydrogen and are trained in its proper handling.
5. Regulations framework: the development and the implementation of regulation frameworks and standards for hydrogen safety are critical for ensuring that industry practices meet safety requirements and effectively mitigate risks.
6. Research and development: continuous research and development efforts are essential to address safety issues and improve technologies for the production, storage, transport, and utilisation of hydrogen.

Overall, the hydrogen industry represents a promising path to a clean energy future, but effectively addressing safety issues is critical for the broad acceptance and success of the industry. Collaboration between governments, industry, and research institutes is essential to overcome these challenges and realise the full potential of hydrogen as a clean energy carrier.

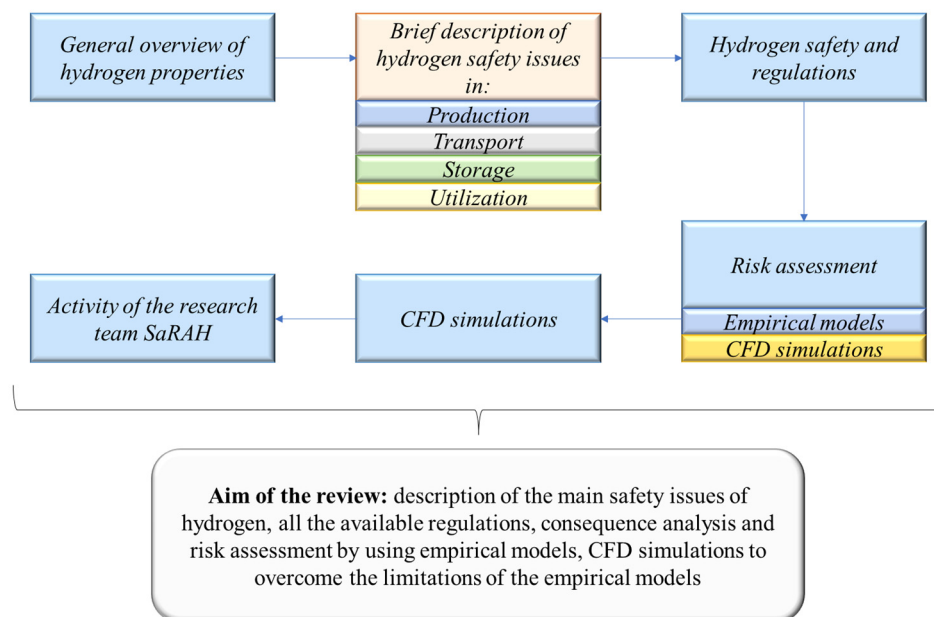
This work focuses on the balance between the safety measures required for the introduction of hydrogen as a sustainable energy source [8–10]. In this case, the hydrogen square can be used as the file rouge of this discussion (Figure 1). The hydrogen square is a conceptual framework that illustrates the different stages of the hydrogen value chain from production to end use. The four sides of the hydrogen square represent the production, storage, use, and safety of hydrogen. The goal of the hydrogen square is to ensure that these four sides are in balance to create a sustainable and efficient hydrogen economy [11]. The deployment of hydrogen as a primary energy source requires the development of robust hydrogen infrastructure that can support its production, storage, utilisation, as well as its transportation. Therefore, significant investments in research and development as well as in the construction of new facilities and infrastructure are necessary. To this aim, governments, industry, and academia need to work together to overcome the challenges associated with the deployment of hydrogen, which include cost, efficiency, and safety [12].



**Figure 1.** Classical hydrogen square summarising production, utilisation, storage, and safety [8–10].

In this work, the safety issues in production, transportation, storage, and use are discussed, and the most dramatic incidents in recent decades are described. The risk assessment and risk analysis of hydrogen systems are discussed with a particular focus on consequence evaluation. The results obtained with empirical models are compared to those obtained with advanced models (CFDs). It is shown that empirical models may fail in predicting  $H_2$  dispersion, thus suggesting the key role of a more advanced model (CFDs). This review differs from others that are already found in the literature (e.g., [13–16]) as its aim is to comprehensively address the main safety issues at each stage of the hydrogen value chain, which is the case in other reviews, and also to discuss in detail the main regulations, standards, and guidelines on hydrogen as well as to most importantly discuss the use of empirical modelling and CFD simulations for consequences and risk analysis. Therefore, the review highlights the main safety issues that are to be addressed, the main regulatory gaps, the limitations of empirical modelling, the main potential of CFD simulations, and the current results in the literature on risk analysis that can be addressed by rigorous CFD simulations of the consequences of hydrogen.

The scheme of the review is summarised in Figure 2.



**Figure 2.** Schematization of the current review.

## 2. The Hydrogen Pyramid: Safety in Production, Transport, Storage, and Utilisation

### 2.1. Hydrogen Properties

Hydrogen has unique physical and chemical properties that make it an attractive option for energy storage, transport, and use. However, hydrogen also poses fire/explosion risks due to its high flammability. Hydrogen is a colourless, odourless, and tasteless gas that is highly flammable in air and can ignite at concentrations as low as 4%. It has the lowest density of all gases and is fourteen times lighter than air. Hydrogen occurs in nature in the form of diatomic molecules ( $H_2$ ) and can be obtained from various sources such as natural gas, water, and biomass. It has a low boiling point ( $-252.8\text{ }^\circ\text{C}$ ) and a low freezing point ( $-259.14\text{ }^\circ\text{C}$ ); therefore, it must be stored and transported at very low temperatures, which are typically below  $-253\text{ }^\circ\text{C}$ , in order to be maintained in a liquid state. In addition, hydrogen can also easily evaporate and form a flammable mixture with air, which can cause explosions if ignition occurs. Hydrogen reacts with oxygen to form water, which is a reaction that releases a significant amount of energy. This makes hydrogen an attractive option for use in fuel cells that convert hydrogen and oxygen into electricity and water without producing harmful emissions [17].

Hydrogen safety is a critical concern due to its high diffusivity and transparent flames. Hydrogen is a very light gas that diffuses rapidly in air and can easily spread over large distances. This behaviour is quite positive in terms of the risk effect since the dispersion of hydrogen in air is very effective and hydrogen can rapidly reduce its concentration. However, this poses a risk of explosion since hydrogen concentrations may reach the flammable range very close to the source point in the first moment of the gas release.

In addition, hydrogen has a very low minimum ignition energy (0.02 mJ) when compared with hydrocarbon (0.4 mJ), thereby suggesting that it can easily ignite. Conversely, the standard auto-ignition temperature of hydrogen in air starts from  $584.9\text{ }^\circ\text{C}$ , which is relatively high compared with long-molecule hydrocarbons [18]. Indeed, hydrogen does not necessarily ignite spontaneously when released under high pressure. Compression ignition, Joule–Thomson expansion, diffusion ignition, and hot surface ignition are unlikely ignition mechanisms for most accidental releases of hydrogen at ambient temperature [19]. When storing liquid hydrogen, the most important safety problem is boil-off, which is the phenomenon whereby liquid hydrogen vaporises into a gaseous state. Boil-off occurs due to various phenomena including the change in the spin isomer, heat loss, thermal stratification, sloshing, and flashing [20].

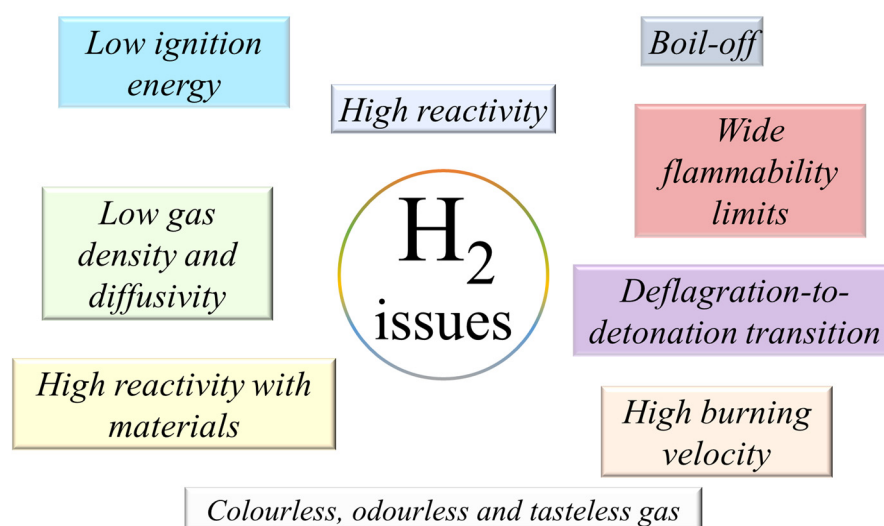
In addition, hydrogen flames are transparent and difficult to detect; therefore, it is more difficult to identify and mitigate hydrogen flames, at least in the early stages. Moreover, due to its low molecular weight, hydrogen molecules can easily penetrate materials such as metals and plastics, thus activating cracking or embrittlement phenomena which cause accidental H<sub>2</sub> release. This can pose a huge concern in terms of material choice and the safety risk if hydrogen leaks occur as it can rapidly spread and accumulate in enclosed spaces [21,22].

The laminar flame speed of hydrogen is significantly higher than that of many other fuels (3 m/s and less than 40 cm/s for hydrocarbon–air mixtures). This property makes hydrogen an excellent fuel for power generation, transportation, and industrial applications. However, the high laminar flame speed of hydrogen implies significant safety issues, leading to significant explosion severity and the possible transition from deflagration to the detonation mode of propagation (DDT) [23].

As a consequence, it is important to carefully design and implement safety measures when working with hydrogen to prevent accidents and mitigate any potential hazards.

A summary of the main safety issues of hydrogen is reported below and in Figure 3 as follows:

- Low ignition energy: one order of magnitude lower than the hydrocarbons;
- High reactivity due to its particular chemical and physical properties;
- Boil-off tendency: this can cause safety issues and economic losses;
- Wide flammability limits: 4–75% in air, being very wide with respect to methane (different ATEX category);
- Deflagration-to-detonation transition: the transition can easily occur and is often observed in the case of a high-scale system;
- High burning velocity: the laminar burning velocity is significantly higher than that of many other fuels;
- Hydrogen is colourless, odourless, and tasteless: additives cannot be easily added;
- High reactivity with materials (embrittlement): huge investments are needed on material investigation;
- Low gas density and diffusivity: particular behaviour in the case of release, and it can stratify in the upper part of confined spaces.

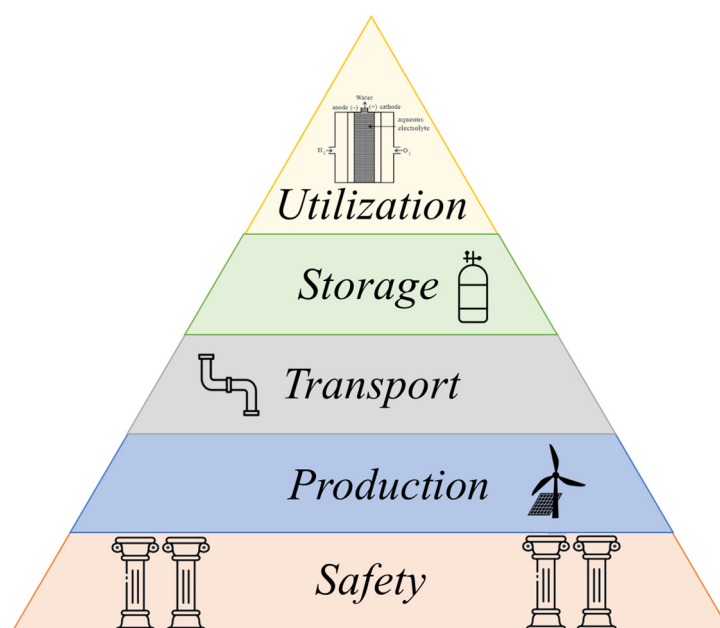


**Figure 3.** Summary of the main hydrogen-related safety issues.

As a result, hydrogen production, storage, transportation, and utilisation facilities must be designed to prevent, detect, and mitigate hydrogen release. Safety systems, such as gas detection and emergency shutdown systems, must be designed ad hoc and installed in all hydrogen production/transport/storage/utilisation facilities. By ensuring these safety measures and by providing safety training and protocols to workers involved in

hydrogen production, storage, transport, and use, the risks associated with hydrogen can be minimised to achieve the safe use of hydrogen.

In this review, we decided to consider as a mantra an evolution of the hydrogen square, the hydrogen pyramid, including hydrogen transport as well since it plays a key role in the hydrogen value chain (Figure 4). In the classic hydrogen square [8–10], the transition to a hydrogen economy is proposed as the resolution of a square whose vertices contain production, storage, utilisation, and safety. In our view, safety must take a primary role and should therefore be considered at the base of all other sectors. The other layers of the pyramid are arranged in a row, with the typical work chain in mind as follows: production, transport, storage, and finally the safe use of the hydrogen produced for various purposes. Indeed, safety is a hub activity which has to be ensured and studied for all technologies involving H<sub>2</sub>.



**Figure 4.** Evolution of the hydrogen square: hydrogen pyramid as an expression of the research team.

## 2.2. Safety Issues in Production

Hydrogen production involves several safety issues that need to be addressed to ensure safe processes for workers and environment. Traditional methods of hydrogen production, such as steam methane reforming ones, require the handling of high-pressure gases and hazardous chemicals. This can increase the risk of accidents if safety protocols are not followed. On the other hand, innovative methods of hydrogen production such as electrolysis can also present safety challenges, including the handling of high-voltage equipment and the potential for the release of hazardous gases (Table 1).

**Table 1.** Main safety issues concerning blue and green hydrogen.

| Blue Hydrogen  | Green Hydrogen  |
|--|---|
| <p><u>Release of hydrogen</u>: large quantities of hydrogen are handled during production, posing the risk of accidental release that leads to a flammable atmosphere.</p>       | <p><u>Release of hydrogen</u>: similarly to the production of blue hydrogen, the production of green hydrogen also involves the handling of significant quantities of hydrogen, thereby leading to potential release hazards.</p> |
| <p><u>Carbon capture and storage</u>: the transport and storage of captured carbon dioxide (CO<sub>2</sub>) raises concerns about leaks and potential environmental impacts.</p> | <p><u>Electrical hazard</u>: high electrical currents are used during electrolysis, creating a risk of electric shocks, short circuits, and fires.</p>  |

Table 1. Cont.

| Blue Hydrogen   | Green Hydrogen  |
|---|---|
| High temperatures and pressures: the reforming processes take place at high temperatures and pressures, thereby requiring robust equipment and safety measures. | Chemical exposure: electrolysis uses electrolytes that can result in chemical exposure.   |
| Typical accidents: hydrogen release and ignition, with CO <sub>2</sub> release having an impact on the environment  | Typical accidents: fire in chlorine electrolyser cells [24,25], hydrogen explosion, hydrogen–oxygen explosion, explosion during the operation of a HP WE, membrane perforation in a PEM-FC cell, destruction of a PEM FC short stack, deflagration of H <sub>2</sub> /O <sub>2</sub> with a short circuit, fire, hydrogen gas holder exploded due to a malfunction in the electrolyser. |

Several accidents have occurred during hydrogen production in recent years, highlighting the importance of safety measures. In 1996, a pipe rupture occurred in a steam methane reformer (SMR). The rupture occurred in a 24-inch diameter stainless steel pipe that was used to direct the process gas flow past the high-temperature shift converter (HTS) during start-up. When the pipe ruptured, the process gas located in the process equipment both upstream and downstream of the rupture flowed into the SMR plant yard. The escaping process gas was a mixture of hydrogen, carbon monoxide, carbon dioxide, steam, and methane at a pressure of 550 psig and at 650 °F. The escaping high-pressure gas caused an energy release and subsequent fire. In 2001, a hydrogen production plant (using electrolysis) experienced a fire and significant damage due to a concussive combustion that started in a high-pressure hydrogen supply line. The primary explosion in the high-pressure hydrogen feed lines caused welds and joints on the storage banks to fail, thus releasing hydrogen gas in large quantities. The escaping hydrogen self-ignited resulted in a secondary explosion and fire. The cause of the initial explosions was the spontaneous ignition of an explosive hydrogen–oxygen mixture in the high-pressure feed pipes. It was concluded that the oxygen from the hydrogen cells entered the system [26,27].

Several accidents have also occurred in green hydrogen production. A hydrogen tank explosion happened at a pilot plant for alkaline water electrolysis in Gangneung19, South Korea, on 23 May 2019; it killed two people and injured six. The investigation found that the hydrogen separator exploded due to an oxygen spillover at a low load and human error. The ignition was caused by static electricity as there were no proper earthing connections. Another incident occurred on 5 April 1975 at Laporte Industries Ltd., Ilford, the United Kingdom. An operator died from severe skin burns with hot electrolytes (30% KOH) after the oxygen lysis separator exploded due to a membrane rupture. The cause was that of the corrosion of the nets and damage to the cell seals due to clogging with sludge. This led to a hydrogen leak into the oxygen–gas–liquid separator [26,27].

To address these safety issues, safety protocols and regulations have been put in place for hydrogen production. These regulations require the use of safety equipment and training for workers, as well as the monitoring and reporting of safety incidents. Additionally, research is being conducted to develop safer methods of hydrogen production such as the use of renewable energy sources.

### 2.3. Safety Issues in Transportation

Hydrogen transportation involves several safety issues that need to be addressed to ensure a safe process for workers and the public. Hydrogen gas is highly flammable and can easily ignite, thus leading to potential accidents and explosions. Additionally, hydrogen transportation involves the use of high-pressure containers and pipelines, which can pose safety risks if they are not properly maintained. Hythane, which is a mixture

of hydrogen and natural gas, is another form of hydrogen fuel that is being explored for transportation. While hythane has a lower risk of explosion compared with pure hydrogen, it still presents safety challenges due to the use of high-pressure containers and pipelines.

Several hydrogen transport accidents have occurred in recent years, highlighting the importance of safety measures [27]. In 2003, a hydrogen leak and subsequent explosion occurred when the fasteners on a hydrogen transport trailer securing the hydrogen cylinder packs failed. The failure of the fasteners caused the hydrogen cylinder packs to fall from the trailer, and some cylinders containing compressed hydrogen gas at a pressure of 200 bar to be thrown onto the roadway. A spark or other local heat source (e.g., from a nearby vehicle engine) ignited the leaking hydrogen and caused a deflagration/explosion that damaged a car following the trailer and smashed the windows in a nearby house. In 2004, while transporting hydrogen to a commercial facility, a plume of hydrogen gas leaked from the unloading valve of a liquid hydrogen delivery truck. The gas plume ignited, causing a lightning flash and shaking that was loud enough to be heard in the nearby building and to set off the building seismic detectors. A small amount of hydrogen gas continued to leak from the trailer tank and burn until a company specialist arrived to manually close a critical valve nearly eight hours later. The actual cause of this incident appears to have primarily been driver error. Several steps required by the standard safety procedure were either incorrectly applied or omitted altogether [26,27].

Attention to proper procedures could have prevented these accidents. These accidents also highlight the need for thorough training on the properties and behaviour of hydrogen, not only for refuelling operators but also for emergency responders and the public. The physical and chemical properties of hydrogen are different from those of fossil fuels and must be communicated, understood, and considered when handling and using hydrogen. Consequently, to address these safety issues, safety regulations and guidelines have been put in place for hydrogen transportation. These regulations require the use of safety equipment and training for workers, as well as regular inspections and maintenance of hydrogen transportation infrastructure. Additionally, research is being conducted to develop safer methods of hydrogen transportation such as the use of safer storage materials and the development of better leak detection technologies.

#### 2.4. Safety Issues in Storage

There are several methods of hydrogen storage including compressed gas storage, liquid hydrogen storage, and solid-state storage. To increase the storage density, hydrogen gas may be compressed and stored in high-pressure tanks (350–750 bar). Liquid hydrogen storage consists of cooling hydrogen gas to a very low temperature ( $-253\text{ }^{\circ}\text{C}$ ) and storing it in insulated tanks. Moreover, cryocompressed hydrogen ( $\text{CcH}_2$ ) storage refers to the storage of  $\text{H}_2$  at cryogenic temperatures in a container that can be pressurised (nominally to 250–350 atm) as opposed to the current cryogenic containers that store liquid hydrogen ( $\text{LH}_2$ ) at a near-ambient pressure. In solid-state storage, hydrogen is physically or chemically stored in solid materials such as carbon nanotubes or metal hydrides, while the use of liquid organic carriers consists of a chemical cycle of hydrogenation and dehydrogenation steps. In both the liquid and solid chemical storage systems, heat is required for the dehydrogenation step, and the typical reaction conditions for the exothermic hydrogenation are a high pressure (1 to 5 MPa) and temperatures from 373 to 523 K [28]. The aforementioned systems are considered to be safe and practical because hydrogen can be stored and transported as a liquid or solid, eliminating the safety and storage problems associated with gaseous hydrogen. However, most of the materials used are themselves flammable and/or toxic, with this posing safety problems in any case; moreover, in some cases, the inherent danger is exacerbated by the presence of hydrogen due to the synergistic effects that are associated with it in the discharge phase [29]. All these technologies combine severe operating conditions (high temperature and/or high pressure and/or flammable solid particles) with an intrinsically hazardous gas  $\text{H}_2$ , thus resulting in high-risk systems (Table 2).



**Table 2.** Main safety issues concerning hydrogen storage.

| Storage                  | Safety Issues  |
|--------------------------|--|
| Compressed hydrogen      | High pressure, strong interaction with materials, high frequency of occurrence of release.   |
| Cryogenic hydrogen       | Low temperature, strong interaction with materials, difficult thermal management, blow-out, ground release for the high density, freezer burns, complex phenomena close to the release point.  |
| Cryo-compressed hydrogen | High pressure, low temperature, strong interaction with materials, difficult thermal management, blow-out, ground release for the high density, freezer burns, complex phenomena close to the release point.   |
| LOHC                     | <u>Formic acid</u> : corrosive chemical that causes severe burns to the skin and eyes.<br><u>DBT</u> : low flammability, and toxicity is not well defined since it is a mixture of different regioisomers.   |
| Chemical storage         | <u>Methanol</u> : toxic (ingestion of 56.2 g per person and for inhalation a concentration of 4000–13,000 ppm), low FP, low BP.<br><u>Ammonia</u> : toxic (the lethal dose after 10 min of exposure is already estimated to be 2700 ppm, with severe irritation already estimated to be 220 ppm. The lethal dose of ammonia after 8 h of exposure can be as low as 390 ppm) and flammable. |

Several accidents involving hydrogen storage have occurred in the past, highlighting the importance of safety measures [16]. In 1999, a fire occurred in a hydrogen storage facility. The fire was reported by an employee after he had adjusted the valves on the hydrogen storage tank in preparation for the commissioning of the hydrogen injection system. The employee was uninjured as he was wearing fire-retardant protective clothing and was able to quickly climb over a three-metre-high fence surrounding the hydrogen area. The local fire brigade fought the fire with external support until the hydrogen supply was exhausted, and the fire was declared extinguished about six hours later. In 1969, an explosion occurred in a spherical vessel for hydrogen storage. The sphere was divided into two hemispheres by a neoprene membrane placed around the equator. Hydrogen was stored under the membrane, while the upper hemisphere contained air. In the upper part of the sphere was an explosion-proof fan that provided a slight overpressure on the top of the membrane. When the plant was shut down for a local holiday, the fan on the top of the hydrogen sphere was also switched off. When the plant was started up two days later, the sphere shell was ripped into many pieces by an explosion, some of which were thrown up to 1200 feet. Some of these pieces hit flammable liquid storage tanks and tore into the roofs of adjacent buildings. Most of the windows of the surrounding buildings were shattered by the blast wave. Fortunately, there were no serious injuries [26,27]. Inadequate maintenance, system monitoring, and oversight of the upkeep of this equipment can contribute to the ignition of a fire that is difficult to extinguish and poses a high level of danger to emergency personnel. Proper maintenance, monitoring, and supervision measures of hydrogen storage equipment can minimise the risk of a fire or explosion.

### 2.5. Safety Issues in Utilisation

Hydrogen utilisation involves the use of hydrogen as a fuel source in various applications [30] including fuel cell vehicles [31,32], power generation, and chemical production. While hydrogen is a clean and efficient fuel source, safety concerns must be addressed to ensure that the hydrogen utilisation technology is safe. One potential safety concern in hydrogen utilisation is that of refuelling hydrogen fuel cell vehicles. Hydrogen refuelling

stations must be designed and operated safely to prevent accidents and ensure the safety of drivers and station personnel. Accidents [27] have occurred in the past, such as a fire at a hydrogen refuelling station in Norway in 2019, which was caused by a leak in the high-pressure storage tanks. In 2012, a pressure-relief device valve failed on a high-pressure storage pipe at a hydrogen filling station, releasing about 300 kg of hydrogen gas. The gas ignited at the outlet of the vent pipe and burned for two and a half hours until technicians from the local fire brigade were able to enter the filling station and stop the gas flow. During the incident, firefighters evacuated nearby businesses and a primary school, closed off adjacent roads, and instructed a high school to take shelter [26,27].

Another safety concern in hydrogen utilisation is the use of hydrogen fuel cells. While fuel cells are generally safe, there is a risk of explosion and/or fire if hydrogen leaks from the fuel cell stack or storage tanks. The fuel cell vehicle accident reinforced the need for training of drivers, supervisors, and emergency response personnel. In 2011, during the refuelling of the hydrogen tank of a fuel cell-powered forklift truck, a significant hydrogen leak occurred while it was completely empty. The shut-off solenoid valve in the tank had recently been replaced, and this was the first refuelling operation after the replacement. The fuel zone access panel was removed to allow for continuous visual leak testing with leak detection fluid. The incident occurred during the final pressure test of the repaired system when an O-ring failed at approximately 4500 psi and the entire contents of the hydrogen tank were released in approximately 10 min [27].

Finally, safety concerns also exist in the production of chemicals using hydrogen as a feedstock. Hydrogen is a key ingredient in many chemical production processes, but it can be dangerous if not handled properly. In 2006, during the restart of an ammonia production plant, syngas (50% hydrogen mixed with methane, ammonia, and nitrogen) ignited and leaked from a flange directly behind the synthesis reactor. The plant had been shut down for about 90 min due to a technical problem. The incident was caused by inappropriate tightening the torque on the bolts of the leaking flange, which was not adapted to the exceptional operating conditions at the time of the incident (i.e., a high difference in the temperature between the bolts and the flange due to the relatively short shutdown time) [27]. In 2006, a hydrogen leak on the flange of a 6-inch synthesis turbocharger valve in an ammonia production plant ignited and exploded. Hydrogen detectors and the fire alarm alerted the control room, which immediately shut the plant down, whereupon the fire was quickly extinguished. The escaping gas was 70% hydrogen and had a flow rate of 15,000 cubic metres per hour.

To address these safety concerns, safety regulations and guidelines have been put in place for hydrogen utilisation. These regulations require the use of safety equipment and training for workers, as well as regular inspections and maintenance of hydrogen utilisation infrastructure. Additionally, research is being conducted to develop safer methods of hydrogen utilisation, such as the use of safer materials in fuel cells and the development of better hydrogen leak detection systems.

### 3. Hydrogen Safety and Regulations

Generally, poor attention is spent regarding safety system design and the improvement of hydrogen systems. Indeed, in large green hydrogen Capex projects, only 0.2% of the spending is related to safety [33]. The implementation of the regulations and their constant updating must first and foremost lead to the elimination of the main causes of hydrogen-related accidents. According to the European Industrial Gas Association (EIGA) database [34], there have been 208 major accidents related to the production, storage, transportation, and use of hydrogen since 1976, of which around 21 have occurred in the last ten years. About 20% of these accidents were caused by valve malfunctions or leaks, including at connection points (16%) (Figure 5). On the other hand, almost 26% of accidents are due to human error, whereas accidents due to contamination, e.g., with air, and material incompatibilities are less common (Figure 6).

The standardisation of safety requirements is ensured by codes and standards for the safe design, maintenance, and operation of equipment, systems, and installations. These guidelines provide local inspectors and safety officers with the information that they need to authorise installations. The main safety standards and codes operating across the hydrogen value chain in Europe are reported in Table 3 [34–41].

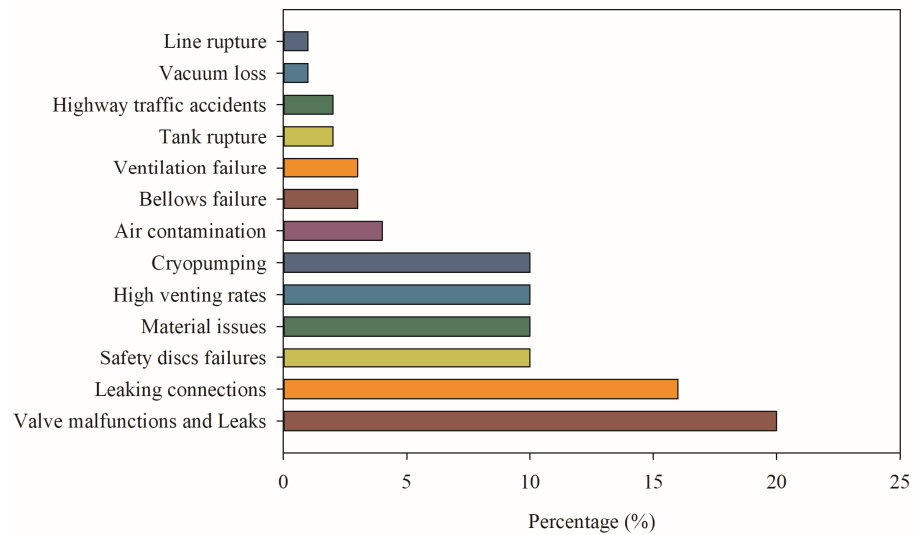


Figure 5. Main initiating events causing hydrogen releases [34].

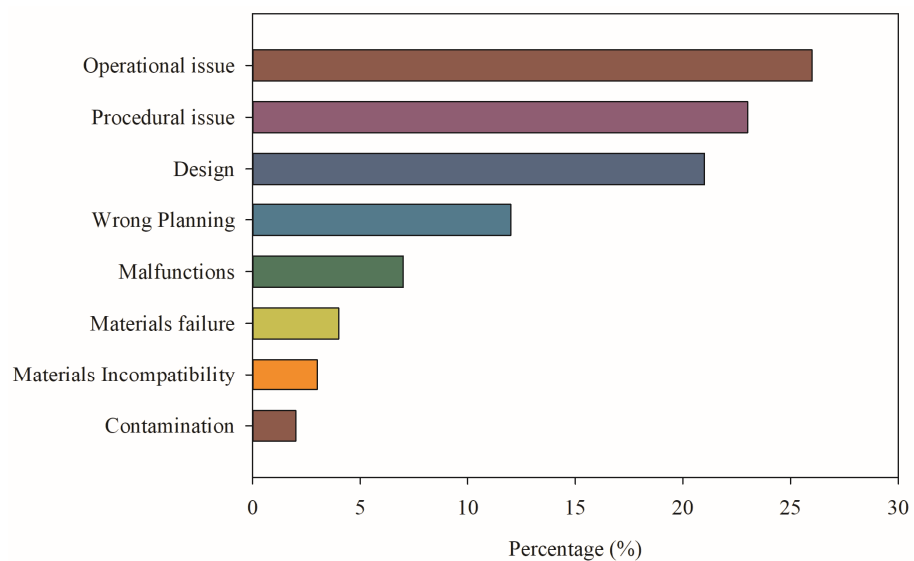


Figure 6. Main causes of hydrogen releases [34].

Table 3. Main standards and codes used for different applications in the hydrogen value chain in Europe and US.

| Hydrogen Value Chain Step | Operation                   | European Standards    | US Standards |
|---------------------------|-----------------------------|-----------------------|--------------|
| Production                | Electrolysis                | CEN-CENELEC [36]      | UL [38]      |
|                           | Traditional steam reforming | ISO [37]<br>NFPA [35] | CSA [39]     |
| Conditioning              | Compression                 | ISO [37]              | NFPA [35]    |
|                           | Liquification               | NFPA [35]             |              |

Table 3. Cont.

| Hydrogen Value Chain Step | Operation            | European Standards  | US Standards                     |
|---------------------------|----------------------|---|----------------------------------|
| Storage and transport     | Pipeline             | ISO [37]  | ASME [41]                        |
|                           | Storage              | EIGA [34]<br>SAE [40]   | CSA [39]<br>NFPA [35]            |
|                           | Cryogenic tank       | NFPA [35]   |                                  |
| End use                   | Fuel cell mobility   | ISO [37]<br>SAE [40]<br>CEN-CENELEC [36]                          | UL [38]<br>SAE [40]              |
|                           | Refuelling           | ISO [37]<br>SAE [40]<br>CEN-CENELEC [36]<br>NFPA [35]             | UL [38]<br>SAE [40]<br>NFPA [35] |
| Process control           | Sensor and detectors | IEC [36]<br>SAE [40]<br>CEN-CENELEC [36]<br>ISO [37]<br>NFPA [35] | UL [38]<br>NFPA [35]             |

It is important to note that there is a clear distinction in the codes and standards between recommendations (characterised by “should”) and requirements (characterised by “shall”). The recommendations are mainly derived from NRTL standards and technical reports, industry peers, and experiences, and they are general instructions that primarily consider cost rather than the rigorous assessment of hazards and risks. In general, the recommendations indicate what to undertake but not how undertake it, and violations may have an impact on a company’s legal situation in the event of an accident. The requirements arise from recommendations and are derived primarily from national and federal codes, industrial peers, and government. They are enriched based on historical events and accidents and require adaptation by workers in terms of training, certification, and hazard and risk analysis updates. In general, the consequences related to noncompliance with the requirements are warnings, fines, and facility shutdowns. Generally, hydrogen safety professionals are urged to review all industry codes and standards with the relevant references to the fire, flame, and gas systems. Regarding fires, there are two main international fire codes, the International Fire Code (IFC) and ISO/TS 19880-1:2020 [42,43]. The IFC establishes the minimum requirements for fire prevention and protection systems using prescriptive and performance-related provisions. The code is very similar to the requirements included in NFPA 72 and is updated with new applications for energy transition and hydrogen utilisation [42]. ISO/TS 19880-1:2020 includes several recommendations about the minimum design characteristics for the safety and for performance of fuelling stations that dispense gaseous hydrogen to light-duty land vehicles. Additional requirements are reported for detection systems and risk assessments to set the appropriate response to alarms [43]. Regarding primary European and USA regulatory codes, NFPA 2:2023, NFPA 55:2023, and NFPA 853:2020 are the most used ones in the case of hydrogen [44–46]. The summary of the most important scopes and sections of these NFPA standards are reported in Table 4.

All the recommendations about how to carry out, design, and use specific hydrogen-based systems are generally contained in technical reports and guidelines. One of the most used ones is the ISA TR 84.00.07:2018, which is a technical report that is useful as a guide for the evaluation of fire, combustible, and toxic gas system effectiveness [47].

The main scopes of this guidelines consist of the following:

- Providing example scenarios to demonstrate the application of performance-based concepts for analysing and designing fire and gas systems (FGS);
- Providing a performance-based methodology for the allocation of fire and gas detectors. The methodology provides considerations for more effective hazard detection and detector placement in cases where fusible plugs (fire) may be required;
- Defining a methodology that addresses the design and effectiveness of FGS mitigation features that are consistent with the underlying principles used to design and evaluate the effectiveness of preventive features.

**Table 4.** Main NFPA hydrogen-related standards with scopes and brief descriptions of the main sections.

| Standard | General Scope   | Main Sections                          | Section Indications   |
|----------|---|--|---|
| NFPA 2   | Fundamental safeguards for the generation, installation, storage, piping, use, and handling of hydrogen in a compressed gas (GH <sub>2</sub> ) form or a cryogenic liquid (LH <sub>2</sub> ) form; fuelling stations. | 6. General H <sub>2</sub> requirements | Appropriate design for gas detection, maintenance, and control; inspection; calibration; testing.   |
|          |   | 7. GH <sub>2</sub> supply and storage  | <ul style="list-style-type: none"> <li>• Cylinders, containers, and tanks: DOT, Transport Canada [48], or ASME Boiler and Pressure Vessel Code [41].</li> <li>• Pressure-relief devices: CGA Standards [49].</li> <li>• Stationary containers: NFPA 704 [35].</li> <li>• Piping systems: ASME A13.1 [41].</li> <li>• Hazard identification and area warning signs posted.</li> <li>• Areas must be secured and guard posts installed to prevent physical damage.</li> <li>• Valve is provided—for bulk storage or tube trailers—but is not needed for individual cylinders.</li> <li>• General separation requirements—combustibles, sources of ignition, temperature extremes.</li> <li>• Unauthorized use is prohibited.</li> <li>• Containers exposed to fire, leaking, or damaged containers are removed from use.</li> </ul> |
|          |   | 8. LH <sub>2</sub> bulk storage        | <ul style="list-style-type: none"> <li>• Hydrogen higher than 39.7 gals (150 L).</li> <li>• Provided with pressure-relief devices, with the aim of preventing freezing, arranged to discharge in an unobstructed manner.</li> <li>• Venting: CGA 5–5 [49].</li> <li>• Piping: ASME B31.12 [41].</li> <li>• Containers larger than 2000 gallons equipped with automatic emergency shutoff.</li> <li>• Connections for the points of filling must meet the separation distance requirements.</li> <li>• Stationary containers not installed in enclosed courts.</li> </ul>  |

Table 4. Cont.

| Standard | General Scope   | Main Sections                               | Section Indications  |
|----------|---|---|--|
| NFPA 2   | Fundamental safeguards for the generation, installation, storage, piping, use, and handling of hydrogen in a compressed gas (GH <sub>2</sub> ) form or a cryogenic liquid (LH <sub>2</sub> ) form; fuelling stations. | 10. Gaseous hydrogen fuelling systems       | <ul style="list-style-type: none"> <li>• Dispensing facilities must be certified as meeting the code requirements.</li> <li>• Hazard analysis must be conducted.</li> <li>• System components must be listed or approved.</li> <li>• Hydrogen safety panel is developing a hydrogen equipment certification guide [50].</li> <li>• Hose-to-hose connections are compatible with hydrogen.</li> <li>• Maintenance in accordance with manufacturer instructions.</li> <li>• Station operator develop the management of the change system.</li> <li>• Dispenser integrity checks required prior to fuelling events.</li> <li>• Dispensers using communication protocol stop fuelling in the event of a communication failure.</li> <li>• Stop fuel automatically when system pressure is reached or there is the activation of overpressure.</li> <li>• Sources of ignition not allowed within 10 ft of any filling connection during transfer.</li> <li>• Fuelling nozzles: SAE J2600 [40].</li> </ul> |
| NFPA 55  | Protection from over-pressurisation, explosive, and flammability hazards associated with compressed gases and cryogenic fluids.   | 10. Gaseous hydrogen systems                | Strong references to NFPA 2 [44].  |
|          |   | 11. Liquid hydrogen systems                 | Strong references to NFPA 2 [44].  |
| NFPA 853 | Fire prevention and protection requirements for safeguarding life and physical property associated with buildings or facilities that employ stationary fuel cell systems of all sizes.                                | 6. Fuel supplies and storage arrangements   | Storage following NFPA 55 [45].  |
|          |   | 8. Fire protection                          | In the case of hydrogen, the position and detection range are suggested.   |
|          |   | 9. Fuel cell power systems of 50 kW or less | Requirements about indoor and outdoor installation, ventilation, and fire protection.  |

#### 4. Risk Assessment and Consequence Analysis of Hydrogen Systems: Criticism of Empirical Models

The evaluation of risk requires the knowledge of the probability of the occurrence of an outcome and the quantification of the consequence [51,52]. The evaluation of the likelihood of incidents mainly relies on the statistical analysis of past accidents through empirical models. However, the low number of hydrogen accidents and the high number of uncertainties associated with the available data make it challenging to accurately predict risks. Additionally, the empirical models may not consider all the potential failure scenarios or human errors that could lead to accidents. Therefore, more comprehensive and reliable risk assessment methods that consider all the possible scenarios and factors are necessary. These may include probabilistic risk assessments and fault tree analyses, which can provide a more accurate picture of the risks associated with hydrogen systems [53].

In the case of orifice generation, the exiting mass flow rate in the case of high-pressure hydrogen jets can be calculated using different models based on notional nozzles. A notional nozzle can be used instead of an actual one as a fictitious nozzle or a pseudo-

nozzle that occupies a higher area but has the same flow rate as that of the real nozzle at an ambient pressure and a uniform speed. The existing models differ from each other for the different hypothesis related to the conservation of mass [54,55], the conservation of momentum, jet temperature [56], expansion type, the use of different equations of the state for the calculation of real gas properties instead of the ideal gas law, the conservation of energy, and the position of the notional nozzle as a function of the Mach number [57,58].

Regarding the evaluation of the consequences, the empirical models that are available in the literature and widely used have been criticized for their applicability to hydrogen systems. In particular, the quantification of the dispersion is typically performed using empirical models assuming that the gas behaves as a passive fluid (Pasquill-Gifford model) and quickly disperses in the event of a leak or release [51]. Hydrogen has a very low density and then disperses with a positive buoyancy. This behaviour is not accounted for in many empirical models, which can lead to an underestimation of the risks associated with hydrogen. To address this issue, more sophisticated models that consider the behaviour of buoyant gases are needed. Houf and Winters (2013) formulated a model that is able to capture the high-pressure liquid and gaseous hydrogen release [59–61]. In particular, the release and dispersion are discretized into different zones of accelerating flow due to the momentum action, the under-expanded flow, the initial entrainment of oxygen and nitrogen and heating, and the full development of the flow. It should be noted that in the case of cryogenic hydrogen, it is difficult to calculate the properties in the near-flow region where oxygen and nitrogen may condense from the entrained air due to the extremely low temperatures [59–61]. Briggs (1984) proposed a general equation for the trajectory of a plume assumed to be initially upward and considering the combination of momentum and positive buoyancy [62].

In addition to criticism of their applicability to buoyant gases, empirical models for the risk assessment of hydrogen systems have also been criticized for their treatment of hydrogen's high diffusivity. Because hydrogen is highly diffusive, it can rapidly mix with air in the event of a release or leak, thereby leading to the formation of flammable or explosive mixtures. Empirical models may not fully capture the rapid mixing and dispersion of hydrogen in the environment, leading to an underestimation of the risks associated with hydrogen systems. To address this issue, more advanced modelling approaches that incorporate the transport and mixing of hydrogen at the molecular scale may be needed. These could include molecular dynamic simulations and computational fluid dynamic (CFD) simulations that explicitly model the behaviour of individual hydrogen molecules.

In addition to the models for H<sub>2</sub> dispersion, there is also the concern of the quantification of the effect of H<sub>2</sub> fires and/or explosions.

In the case of the continuous release of gaseous (or flashing hydrogen) and immediate ignition, a jet fire may occur. In this case, the model proposed by Houf and Schefer (2007) can compute the heat radiation generated by a straight, turbulent jet flame in the case of different kinds of high-pressure hydrogen releases [63]. However, recent measurements of the heat flux of two horizontally aligned hydrogen flames on a high scale have shown that current methods underestimate the radiation portion of the flame by 40% or more. More recently, to consider the buoyancy effects that can cause this underestimation, Ekoto et al. (2014) developed a model of the radiation flame, which was also validated by two high-scale hydrogen jet fires with compressed hydrogen gas released at a nominal stagnation pressure of 60 bar [64].

There are several methods for predicting the strength of the blast wave generated by an unconfined vapour cloud explosion (UVCE) as a function of the distance to the vapour cloud. Recent work uses the TNT model, the TNO model, the Baker–Strehlow–Tang (BST) model, and the Dorofeev model to predict the strength of the explosion of an unconfined hydrogen cloud. The results show that the TNT model predicts higher explosion overpressures at the same distance as the others [65–68].

Regarding harm and loss models, LaChance et al. (2011) tried to unify uniform the harm criteria for use in the quantitative risk analysis of the hydrogen infrastructure [69]. In

the case of thermal harm, several probit models are available to assess the thermal radiation [70–72]. Among them, LaChance et al. (2011) recommend using both the Eisenberg and the Tsao and Perry probit models for hydrogen-related applications. In the case of overpressure harm, among all the available probit models [52,73–75], LaChance et al. (2011) recommend the use of the TNO probit models and pointed out that the indirect effects of overpressure events were of the highest concern to people. In fact, the overpressures required to cause fatal lung damage are much higher than the levels required to hurl a person against obstacles or create missiles that can penetrate skin. Furthermore, a person inside a building would be more likely to be killed by the collapse of the structure than by lung damage. All the main empirical model used for the simplified consequence analysis of hydrogen-based systems are summarised in Table 5.

**Table 5.** Summary of the main empirical models used for the simplified consequence analysis of hydrogen-based systems.

| Model Name                                     | Safety Issues   | Limitations  | References |
|--|---|--|------------|
| Notional nozzle                                | Mass flow rate in the case of high-pressure hydrogen jets | Highly dependent on jet temperature, expansion type, real gas properties, the conservation of energy, and the position of the notional nozzle as a function of the Mach number | [54–58]    |
| Pasquill-Gifford                               | Dispersion in the atmosphere                              | Model developed for passive dispersion, with the density of the substance being similar to that of air   | [51]       |
| Houf and Winters (2013)                        | Dispersion in the atmosphere                              | No consideration for positive buoyancy in the case of gas and not applicable in the near-field zone in the case of cryogenic hydrogen  | [59–61]    |
| Briggs (1984)                                  | Dispersion in the atmosphere                              | Combination of momentum and positive buoyancy  | [62]       |
| Houf and Schefer                               | Jet fire  | Underestimation of the radiation portion of the flame by 40% or more   | [63]       |
| Ekoto et al. (2014)                            | Jet fire with buoyancy effects                            | Applicable for hydrogen gas stored at 60 bar   | [64]       |
| TNT model                                      | Overpressure of an unconfined vapour cloud explosion      | Overestimation in most cases   | [65–68]    |
| TNO model                                      | Overpressure of an unconfined vapour cloud explosion      | Underestimation in most cases  | [65–68]    |
| Baker–Strehlow–Tang (BST) model                | Overpressure of an unconfined vapour cloud explosion      | Underestimation in most cases  | [65–68]    |
| Dorofeev model                                 | Overpressure of an unconfined vapour cloud explosion      | Underestimation in most cases  | [65–68]    |
| Eisenberg and the Tsao and Perry probit models | Thermal harm  | Generic probit but the most applicable one for hydrogen  | [70–72]    |
| TNO probit models                              | Overpressure harm   | Generic probit but the most applicable one for hydrogen  | [52,73–75] |

## 5. CFD Simulations of Hydrogen Dispersion and the Consequences and Risk Assessment

To overcome the limitations related to the empirical models, more advanced models based on coupling among the momentum, mass, and energy balance equations are required (computational fluid dynamics, CFDs) [76,77].

These models are a powerful tool for simulating the behaviour of hydrogen dispersion in complex geometries and flow conditions. A great deal of research has been carried out



on this topic, with varying degrees of complexity in the models, the geometry, and the assumptions [16].

In general, the works focused on CFD models of gaseous hydrogen dispersion to investigate the release inside the confined spaces. This is because, as a result of the properties described above, hydrogen tends to dilute easily in an open atmosphere and to accumulate and stratify in the upper part of enclosed spaces, thereby leading to major fire and explosion risks. This behaviour cannot be captured with empirical models. For this reason, there are fewer studies on releases in the atmosphere [78] such as from the generation of holes in pipes [79], and there are more frequent studies on releases in tunnels, garages, fuel cell rooms [32], and enclosed spaces in general [80–86]. The models found in the literature mainly differ in terms of the equation solution approach, the geometry, the boundary conditions, the turbulence of the sub-model, and the CFD code used.

The literature results show that Reynolds-averaged Navier–Stokes (RANS) and Large-Eddy Simulation (LES) models do not significantly differ in terms of the prediction of the motion field and concentration in the case of hydrogen [87].

In CFD modelling of jet fires, the LES approach is generally used to better capture the interactions of the (at least large) vortices with the flame front. This interaction cannot be captured through the use of empirical models, even the most accurate ones. In these models, the evaluation of the radiation heat flux is also modelled. The results of the literature mainly comprise temperature and heat flux maps to eventually calculate damages to the buildings and people in adjacent areas [88–91]. The effect of ventilation on the direction of the flash fire and the inclination of the flame are often considered. The effect of protective devices such as sprinklers can also be evaluated through CFD simulations to design protective systems or verify their appropriate design [92].

In the case of the evaluation of the consequences coming from the accidental release of liquid hydrogen stored in cryogenic conditions, the model equations are more complex. After release, the hydrogen almost completely deflagrates, but due to the very low temperatures, a pool of liquid hydrogen can form in the immediate vicinity of the release site, which also contains liquid nitrogen and oxygen. For this reason, in the event of an immediate ignition, a mixed scenario may result that lies somewhere between a jet fire and a pool fire [52,93]. For liquid hydrogen release and dispersion, the CFD models that are currently available in the literature use the RANS approach [94–97]. Some of the most important factors influencing dispersion that are analysed in these simulations are wind speed, wind temperature, and ground temperature. In a recent work, Sun et al. (2023) investigated the effect of air condensation on the formation of a soil pool [98]. The results showed that the condensed air fraction increased once the release finished since the turbulence induced by the momentum favoured the thermal exchange with air. However, the papers still point out the difficulty in accurately capturing the behaviour of the cloud in the near-field zone even when refining the computational grid. To overcome this issue, Kangwanpongpan et al. (2024) presented LES model of two-phase (liquid-gas) hydrogen behaviour during pressurized tank venting [99]. The LES model predicts physical phenomena during the depressurization of the LH2 storage tank, including pressure recovery as well as the dynamics of the LH2 level and temperature in the tank [99].

The papers related to the investigation of ignited liquid hydrogen are still scarce. The modelling of the flame is always carried out with the LES approach, and some of the most frequently investigated parameters are the temperature and the release pressure [100,101]. In these cases, the validation of the results is one of the most complex steps. In the case of the origin of a pool fire, a very recent work shows the functioning of appropriately designed sprinklers to be protective measures and their efficiency with varying droplet sizes [102].

The delayed explosion of an accidental release of hydrogen under high pressure is an important risk scenario for safety studies of production plants, transport lines, and charging lines for fuel cell vehicles. Vyazmina et al. (2016) proposed a numerical study by means of the CFD commercial code FLACS to identify the worst-case ignition position

of high-pressure jets of hydrogen [103,104]. FLACS uses the RANS approach for fluid mechanics and the  $k-\epsilon$  model to model the eddy viscosity. The results showed that the maximum overpressure is obtained for ignition at the location corresponding to a 65% concentration and were used to propose a new methodology for determining blast strength using the TNO multi-energy model with the strength index as a function of the mass flow rate [103,104]. Middha and Hansen (2009) developed a CFD simulation study to predict the quantitative explosion risk for hydrogen vehicles in tunnels for two different tunnel layouts and a number of longitudinal ventilation conditions, which was in support of the HyTunnel project [105–107]. The results showed that the maximum possible pressure load was about 0.1–0.3 barg for the analysed tunnels configurations, which represents a limited human fatality risk, and that the ventilation velocity only plays a small role in pressure reduction.

CFD simulations are an essential tool for studying hydrogen safety and for the design of safety measures. Many studies have been conducted on CFD simulations of hydrogen release, but less work has been carried out on hythane release. Many experimental studies have been conducted to capture the effect of the addition of hydrogen on the explosibility of methane [108–110], and some CFD simulations of hythane release were also carried out [111,112]. Risk evaluations in terms of accident frequency were performed for methane alone in underground pipelines [113]. Overall, these studies suggest that hythane has different explosion features compared with those of pure hydrogen and that the concentration of methane in the blend plays an important role in determining the explosion behaviour. However, a complete risk assessment of this hydrogen transport system was never carried out [114]. All the main CFD simulation results of hydrogen dispersion and the consequences are summarised in Table 6.

**Table 6.** Summary of the main CFD simulations of hydrogen dispersion and consequences.

| Model               | Aim and Results   | References |
|---------------------|---|------------|
| Hydrogen dispersion | Validation of the CFD tool FLACS–HYDROGEN ( <a href="https://www.gexcon.com/software/flacs-cfd/">https://www.gexcon.com/software/flacs-cfd/</a> ) and next (RANS approach) in the case of GH2 and LH2 dispersion. Reasonable agreement was seen for many different kinds of release conditions.   | [78]       |
| Hydrogen dispersion | Two-dimensional CFD modelling of accidental hydrogen release from pipelines using CFD-ACE (RANS approach). The hydrogen clouds are further away from the ground or buildings than the methane clouds, so the probability of ignition is reduced and flame acceleration is reduced due to obstacles in the event of ignition.  | [79]       |
| Hydrogen dispersion | Hydrogen dispersion from tube fittings on fuel cell vehicles under the effect of ambient wind using FLACS (RANS approach). In the case of a crosswind, the flammable region becomes far away from the car in 20 s.  | [32]       |
| Hydrogen dispersion | Hydrogen dispersion in enclosed spaces like a residential garage, fuel cell room, covered car park, and large enclosures. Simulations were carried out with FLACS-Hydrogen and validated against experimental data. The results are highly dependent on the used geometry.  | [80–86]    |
| Jet fires           | CFD simulations of a vertical and horizontal high-pressure jet fire, mainly using the LES approach and Ansys Fluent ( <a href="https://www.ansys.com/products/fluids/ansys-fluent">https://www.ansys.com/products/fluids/ansys-fluent</a> ) and next but also Kameleon FireEx (KFX) ( <a href="https://www.dnv.co.kr/services/cfd-simulation-kameleon-fireex-kfx-110598">https://www.dnv.co.kr/services/cfd-simulation-kameleon-fireex-kfx-110598</a> ) with the RANS approach. All the results were validated against experimental data. | [88–91]    |

Table 6. Cont.

| Model                                  | Aim and Results   | References |
|--|---|------------|
| Jet fires                              | Suppression of hydrogen jet fires on hydrogen fuel cell ships using a fine water mist with a Fire Dynamics Simulator (FDS) (LES approach). Water mist with a spray velocity of 30 m/s and average droplet size of 30 $\mu\text{m}$ can effectively reduce the fire field temperature of hydrogen jet fires and prevent the fire from developing further.  | [92]       |
| Liquid hydrogen release and dispersion | Release and dispersion in an open environment was always simulated with the RANS approach using FLACS, Ansys Fluent, or ADREA-HF ( <a href="http://www2.ipta.demokritos.gr/pages/ADREA-HF.html">http://www2.ipta.demokritos.gr/pages/ADREA-HF.html</a> ), and the effect of the influence of ground temperature, wind speed, wind temperature, and both air liquefaction and solidification was investigated. The results were generally validated against NASA data and/or experimental results. | [94–97]    |
| Liquid hydrogen release and dispersion | Flash-boiling and pressure recovery phenomena during release from high-scale pressurized liquid hydrogen storage tank with the LES approach.  | [99]       |
| Liquid hydrogen fires                  | CFD simulations (LES approach) and novel empirical models were proposed to capture the features of the phenomenon. The effect of pressure and temperature was considered, and the results were validated against experimental data.   | [100,101]  |
| Liquid hydrogen fires                  | Extinguishing the action of sprinklers in a hydrogen pool fire using the Fire Dynamics Simulator (FDS). A higher spray velocity and a smaller droplet size enhanced the extinguishing efficiency, and the number of sprinklers required to suppress hydrogen pool fire was optimized.   | [102]      |
| Vapor cloud explosions                 | Blast wave predictions performed using FLACS-Hydrogen, with a focus on the dynamic effects in the near- and far-field zones, time-dependent pressure loads, reflection, and blast waves.  | [103–107]  |
| Hythane                                | Methane–hydrogen explosion in the gas compartment in utility tunnels using FLACS. The results show that higher overpressures were seen with methane compared with hythane.  | [111,112]  |

The literature results discussed above suggest that the quantitative risk assessment of systems used for hydrogen production, transport, storage, and utilisation should be performed by advanced models such as CFDs. However, full examples of rigorous CFD-based quantitative risk assessment (QRA) are scarce in the literature. Middha and Hansen (2009) proposed a CFD-based explosion risk assessment methodology for hydrogen systems [78,105,106]. This methodology consists of three different steps, with an increasing degree of complexity as follows:

1. Worst-case assessment, with the stoichiometric cloud covering the entire geometry;
2. “Realistic worst-case” assessment, where releases are simulated with ventilation and the worst case of a “realistic” flammable cloud is estimated;
3. Probabilistic risk assessment, where a range of release and ventilation conditions is simulated, the cloud size distribution is established, and explosions with various cloud sizes are simulated.

Based on possible release scenarios, the methodology enables us to accurately estimate the overall risk of a given system in terms of probable explosion pressure exposure and the frequency of occurrence. Therefore, it is recommended that such approaches are actively used and relied upon in the development of regulations, rules, and standards for hydrogen applications. Kashkarov et al. (2022) also proposed a quantitative risk assessment methodology for a hydrogen tank rupture in a tunnel fire, where the consequence analysis

of the effects of a generated blast wave was performed using a dimensionless correlation developed and improved thanks to experimental data and CFD simulations [115,116].

In most cases, CFD simulations are used for consequence analysis or only to model the hydrogen dispersion, and the results are used to establish guidelines and recommendations to increase the intrinsic safety of the system. For instance, Guan et al. (2023) developed a CFD model to analyse the hydrogen dispersion behaviour and concentration distributions in the hydrogen fuel cell room based on the ship's parameters. The results were used to appropriately design the layout of hydrogen detectors and the hydrogen gas supply system [82]. Wang et al. (2023) developed a CFD model of hydrogen leakage and the diffusion of a hydrogen production container. The equivalent TNT method was then used to evaluate the hazard degree of hydrogen leakage, comparing the obtained overpressures with the level of concern that is typical of direct damages and indirectly harms human beings [117]. Lin et al. (2023) performed a numerical simulation and the consequence analysis of accidental hydrogen fires in a conceptual offshore hydrogen production platform. The different hazardous areas were only classified as a function of the temperature [118].

## 6. Our Activity with the Combination of Risk Assessments and CFDs

The aim of our research group named SaRAH (Safety, Risk Analysis, and Hydrogen) is to develop a comprehensive approach for the quantitative risk assessment (QRA) of hydrogen release events. To achieve this, we are currently working on combining CFD simulations of hydrogen releases and its consequences with advanced QRA techniques. Our aim is to make more accurate and reliable predictions of the possible consequences of hydrogen releases and thus support the development of safety measures for hydrogen systems. By integrating CFD simulations into QRA methods, we can better understand the complex physical and chemical phenomena that occur during a hydrogen release and more effectively assess the associated risks. This complete and rigorous approach is rarely used in the literature. In most cases, CFD simulations are only performed to assess the impact of accidents and not for a full quantitative risk assessment, and when a risk assessment is performed, the impact analysis is often performed using empirical modelling. This combined approach has the potential to significantly enhance the safety of hydrogen systems and to facilitate the widespread adoption of hydrogen as a clean energy source.

We are currently working to develop CFD models for hydrogen dispersion after a release coming from the full-bore rupture of a pipe connecting the ground with a salt cavern used for underground hydrogen storage. The results will be coupled with the consequences analysis performed both with empirical and CFD models and frequency analysis also to compare the risk map with that obtained in a recent work of our research team. CFD simulations will also be interesting when capturing the possible demixing of the gaseous species present in the released current together with hydrogen if the bacteria metabolism and the generation of methane and hydrogen sulphide are considered. In the framework of this project, which is carried out in collaboration with Energy System Research, RSE S.p.A., we are also approaching the possibility of including the simulation of the consequences in terms of fires and explosions instead of the use of empirical models. We started working on this topic in 2021 [119] when we performed a quantitative risk assessment developing an appropriate bow-tie diagram and also using empirical models for dispersion. The results showed that an UVCE is the most frequent outcome, but its effect zone decreases with time due to hydrogen contamination and the higher contents of methane and hydrogen sulphide.

In the framework of the National Recovery and Resilience Plan (PNRR) within the RETURN Extended Partnership, we are performing CFD simulations in the case of hole generation or a full-bore rupture and the consequent release of hydrogen from on-ground pipelines, and we are also performing a natural hazard triggering technological disasters (NaTECH) risk analysis of the hydrogen transport infrastructure. Preliminary results, which have been achieved by locating a pipeline in Northern Italy, show that flooding does not result in a loss of containment while a seismic event may cause atmospheric dispersion, a

vapour cloud explosion (VCE), and jet fire. This last outcome is the only one that can occur with a relevant probability in the event of a lightning strike.

It is worth mentioning that in the framework of the National Recovery and Resilience Plan (PNRR) within the MOST—Sustainable Mobility National Research Center, we are performing CFD simulations of fuel cell systems in order to optimize their performances and are working on the design of integrated systems including hydrogen production systems from alcohols, oxidative steam reforming, and ammonia cracking together with high-temperature fuel cells used for railway transport.

## 7. Conclusions

The increasing use of hydrogen in various sectors in recent years underlines the absolute need for a relentless commitment to improving operational safety. The key role that safety aspects play in promoting public acceptance cannot be overemphasized. In this review, the multifaceted landscape of hydrogen applications in the transport and energy sectors has been examined in detail, highlighting critical aspects such as storage, transmission, and, most importantly, safety. The focus is on predicting potential hazards, establishing relevant standards to delineate permissible areas of operation, and providing foolproof equipment and guidelines as cornerstones for the safe use of hydrogen technology.

Just as an example, in the production of green hydrogen, one of the main challenges is that of reducing the number of accidents, which are mainly related to electrical risk and oxygen contamination of hydrogen. To facilitate this, the development of regulations and guidelines would be necessary not only in relation to the basic requirements for the designation of green hydrogen but also throughout the value chain, taking into account the specific features of the production process compared with conventional methods. In addition to the inherent safety issues of hydrogen, which are mainly related to its wide flammability range, its easy ignitability, and the fact that it can detonate quickly and easily, one of the main issues is that it is difficult to perform experimental measures for each type of production process, storage, transport, and use. For this and other reasons, CFD simulations currently seem to play a key role in the transition to hydrogen with a safety-by-design approach.

Within this safety framework, computational fluid dynamics (CFDs) have proven to be a particularly robust tool for predicting hazard scenarios in hydrogen applications and to perform corrections and improvements to the standard that is currently active in the hydrogen field. This paper provides an overview of the recent studies using CFD techniques for modelling gaseous and liquid hydrogen release, dispersion, fires, and explosions. Despite the huge push of the authors towards this direction, only a few works rigorously discuss the risk assessment of hydrogen-based systems. For this reason, the SaRAH research group is working on this topic in different research projects.

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