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Review of hydrogen safety during storage, transmission, and applications processes

Elham Abohamzeh [a], Fatemeh Salehi [b,*], Mohsen Sheikholeslami [c], Rouzbeh Abbassi [a], Faisal Khan [d]

[a] Department of Energy, Materials, and Energy Research Center (MERC), Karaj, Iran
[b] School of Engineering, Macquarie University, Australia
[c] Department of Mechanical Engineering, Babol Noshirvani University of Technology, Babol, Iran
[d] Centre for Risk, Integrity and Safety Engineering (C-RISE), Faculty of Engineering and Applied Science, Memorial University of Newfoundland, St. John's, Canada

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ABSTRACT

Hydrogen is considered an excellent clean fuel with potential applications in several fields. There are serious safety concerns associated with the hydrogen process. These concerns need to be thoroughly understood and addressed to ensure its safe operation. To better understand the safety challenges of hydrogen use, application, and process, it is essential to undertake a detailed risk analysis. This can be achieved by performing detailed consequence modellings and assessing risk using the computational fluid dynamics (CFD) approach. This study comprehensively reviews and analyses safety challenges related to hydrogen, focusing on hydrogen storage, transmission, and application processes. Range of release and dispersion scenarios are investigated to analyse associated hazards. Approaches to quantitative risk assessment are also briefly discussed.

1. Introduction

Hydrogen can be obtained from primary elements such as water, biomass, natural gas, and coal, among other sources. Hydrogen properties make it a sustainable solution to meet the long-term greenhouse gas emissions reduction targets set worldwide. It is a non-toxic, alternative energy carrier and has extensive capacity for energy storage, high energy density, and zero greenhouse gas emissions. Hydrogen production relies on two main pathways; thermochemical and electrochemical. The thermochemical process uses a fossil fuel feedstock, and it is paired with carbon capture and storage to achieve clean hydrogen. On the other hand, the electrochemical process involves splitting water into hydrogen and oxygen using an electrical current. The global hydrogen demand is currently produced through water electrolysis at 3.9%, coal gasification at 18%, naphtha or oil reforming at 30%, and natural gas steam reforming at 50%, while other sources are contributing 0.1% (Minutillo et al., 2018). Hydrogen can also be used as raw materials in different industrial processes and as a fuel in combustion processes or hydrogen fuel cells across many applications. Unlike other forms of renewable energy such as solar and wind, which cannot be stored, hydrogen can be produced and stored in different forms, including compressed gas, liquid hydrogen (LH_2), slush, solid or metallic hydrogen. Fig. 1 schematically shows different aspects of the hydrogen industry.

Despite its advantages, the flammability of hydrogen has raised public concern about hydrogen-related hazards considering catastrophic incidents, such as the hydrogen explosion at the Fukushima nuclear power plant in 2011 and the Hindenburg fire in 1937 (Itaoka et al., 2017). During the past decades, several accidents associated with handling liquid hydrogen have been reported. A 9000 gallon (34 m^3) LH_2 storage tank was exploded in 1989, as the vessel was purged with N_2 gas to boil away the LH_2 due to vent stack repair work. Even though the vacuum valve was open, the catastrophic tank rupture occurred as a result of increasing the pressure within the vacuum jacket, resulting in a catastrophic rupture where one end of the tank blew off (Verfondern, 2008). Two recent hydrogen-related incidents have happened in a chemical plant in California (Genovese et al., 2020) and in a public hydrogen refuelling station in Norway in June 2019. In these accidents, the leakage of gas led to subsequent fire and explosions. As a preventive measure, several hydrogen refuelling stations were halted for a few months, and many hydrogen-powered vehicles were called to a halt (Ustolin et al., 2020a).

While hydrogen safety issues depend on the application, they can be

* Corresponding author.
E-mail address: fatemeh.salehi@mq.edu.au (F. Salehi).

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classified into two main categories; material properties-related issues and handling-related issues. For example, the primary hazards include hydrogen release and subsequent ignition (Groth and Tchouvelev, 2014). Immediate ignition of hydrogen usually causes hydrogen jet fires, whereas delayed ignition of hydrogen leads to the explosion, which is the result of deflagration and/or detonation. There are direct and indirect impacts on humans, the environment, structures, and properties due to these accidents and their consequences, including jet fire heat flux, thermal radiation, explosion, overpressure, asphyxiation due to oxygen replacement, projectile damage due to high-pressure hydrogen from a ruptured containment vessel.

Understanding the safety aspects of hydrogen is essential to achieve reliable, safe, and effective use of hydrogen as a clean energy source. Numerous projects have worked on hydrogen safety issues, and a summary of these projects is given by the International Association for Hydrogen Safety (IA HySAFE). Some studies briefly review the risk and reliability of hydrogen storage (Moradi and Groth, 2019; Ustolina et al., 2020) and important safety issues for the transmission of hydrogen using the current natural gas piping system (Najjar, 2013; Mohammadfam and Zarei, 2015). This study aims to provide a comprehensive review of the use of hydrogen in different applications and the safety issues associated with hydrogen utilisation, transmission, and storage. It particularly aims to provide a review of the previous computational fluid dynamics (CFD) models that have been widely used to generate reliable data to potentially predict hydrogen accidents in simple and complex systems.

2. Hydrogen applications in transport

Hydrogen has been widely used in the transport sector and the energy sector for heat, power, and electricity production. Applications of hydrogen in the transport and energy sector are either in the form of fuel in the combustion process or in hydrogen fuel cells, which are briefly reviewed in this section. Hydrogen is also used as raw materials for various industrial and chemical processes, but these are beyond the scope of this study.

2.1. Hydrogen - internal combustion engines

Hydrogen combustion processes are present in internal combustion engines (ICE), including car engines and gas turbines for civil and military aviation, marine applications and electricity production. As presented in Table 1, different strategies have been developed for using hydrogen in combustion devices which are briefly discussed in this section (Arat et al., 2016).

2.1.1. Hydrogen combustion strategies

The strategies developed for hydrogen mixture in ICEs includes port fuel injection (PFI) and direct injection (DI) (Gurz et al., 2017; Deniz and Zincir, 2016). The PFI concept offers high load efficiency with ultra-low emissions but low power output. The PFI techniques transfer a gasoline spark ignition engine into H_2-ICE. On the other hand, the DI concept leads to very high efficiency with moderate emissions. H_2-ICEs have been initially proposed in the positive ignition (PI) design, where the mixture is prepared upstream of the intake valves through the PFI. Compared to gasoline engines, PFI H_2-ICEs have lower power density (Verhelst et al., 2009).

Table 1
The use of hydrogen in ICEs.

Strategies	Advantages	Limitations
Hydrogen port fuel injection (PFI)	lower NO_x emission	(1) lower power density compared to gasoline engines; (2) backfire and knock
Hydrogen direct injection (DI)	(1) limiting the fuel-air mixture to the centre of the combustion chamber; (2) conducting lean stratified mixture (3) reducing the chance of knock	–
Dual fuel direct injection	(1) better fuel conversion efficiencies compared to conventional diesel engines (2) extremely low emissions	(1) higher NO_x emissions compared to conventional diesel engines; (2) lower thermal efficiency
Blended with natural gas	(1) better combustion performance; (2) enhancing the flammability limits; (3) lowers emissions of CO_2; (4) improving the storage strategy of hydrogen	thermo-acoustic combustion instability

To improve power density and address abnormal combustion events such as backfire and knock, H_2-DI (gaseous or liquid) strategy has been suggested that significantly enhanced fuel conversion efficiencies. The concept of dual-fuel DI diesel H_2 compression ignition ICEs provides bi-fuel operation where the engine can run on diesel as well as on hydrogen. They have better fuel conversion efficiencies compared to conventional diesel engines, whereas they deliver extremely low emissions of regulated pollutants, including PM, CO, and UHC (Boretti, 2011; Salehi et al., 2017, 2020). Although the addition of hydrogen improves lean burn combustion, it increases the combustion temperature that is not favourable for NO_x reduction. Exhaust gas recirculation (EGR) techniques are commonly used to reduce NO_x emissions. Increasing both EGR rate and H_2 volume fractions enhance thermal efficiency while reduces NO_x emission. (Dimopoulos et al., 2007).

2.1.2. Natural gas blends with hydrogen

Blending hydrogen with natural gas (methane) has been suggested for vehicles (Tangöz et al., 2017; Ortenzi et al., 2008), gas turbines (Nam et al., 2019; Koç et al., 2020), and micro gas turbines (Meziane and Bentebbiche, 2019; Di Gaeta et al., 2017). Adding hydrogen to methane

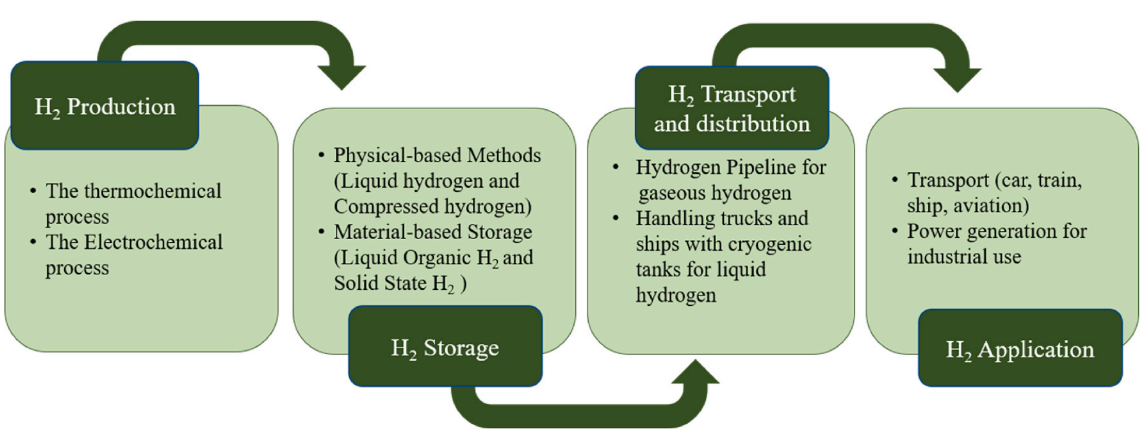

Fig. 1. Different aspects of the hydrogen industry.

extends the lean limit of natural gas, improving the combustion performance since the hydrogen burning velocity is several times higher than that of methane. It also enhances the flammability limits, and hence it increases the efficiency while lowers emissions. On the other hand, it allows for a significantly improved storage strategy since it resolves the issue of the low gravimetric storage density of compressed hydrogen. Wallner et al. (Wallner et al., 2007) demonstrated adding 5% volume fraction of methane to hydrogen increased the stored energy content by 11%.

2.1.3. Hydrogen marine engines

There is an increasing interest in the use of hydrogen in marine gas engines. It is challenging to solely use hydrogen in compression ignition engines due to its high self-ignition temperature. However, hydrogen could be an ideal fuel to combine with other fuels due to the high stoichiometric air-to-fuel ratio. A mix of liquefied natural gas (LNG) and hydrogen up to a maximum of 30% hydrogen in maritime applications works well. It is found at low-moderate engine load with the equivalence ratio between 0.4 and 0.5, NO_x has been reduced (Saravanan and Nagarajan, 2008; White et al., 2006). Hydrogen is also a sulphur-free fuel, and hence it reduces SO_x and PM emissions while its net heating value is three times larger than diesel fuel.

The use of hydrogen in ICEs, either in the form of direct injections or blended with other fuels, requires certain safety measures. The main safety issues are related to onboard hydrogen storage. These issues are common between H_2-ICEs and fuel cell electric vehicles (FCEVs) which are discussed in Section 2.2. The safety measures are also essential for testing H2-ICEs. When these engines run in a confined or semi-confined environment, it is important to identify sources where hydrogen likely accumulates. The required hydrogen is usually stored in cryogenic liquid form or in compressed form for H_2-ICEs tests where the pressure level for compressed storage is 138–414 bar. Hence, hydrogen is usually stored outdoors or in dedicated fuel canopies and then delivered to the test rig via hydrogen supply lines. This may increase the chance of hydrogen leakage from joints and pipes between hydrogen cylinders and supply manifolds.

2.2. Hydrogen fuel cells

2.2.1. Hydrogen fuel cells - vehicles

In addition to thermodynamic means, there are electromechanical/electrochemical means for converting the chemical energy of the stored hydrogen to mechanical energy, aiming to generate useful work. As shown in Fig. 2, through an electrochemical reaction with oxygen, hydrogen is consumed in fuel cells to generate heat, water, and electricity. In comparison with energy generation from combustion, the efficiency of fuel cell systems is higher, they have lower emissions, and they operate without generating vibration and noise (Wang et al., 2011; Sharaf and Orhan, 2014). The major categories of fuel cells are (Kirubakaran et al., 2009) (1) Proton exchange membrane fuel cell (PEMFC); (2) Alkaline fuel cell (AFC), (3) Solid oxide fuel cells (SOFC); (4) Molten carbonate fuel cell (MCFC); (5) Direct methanol fuel cell (DMFC); (6) Phosphoric acid fuel cell (PAFC) which are briefly discussed below.

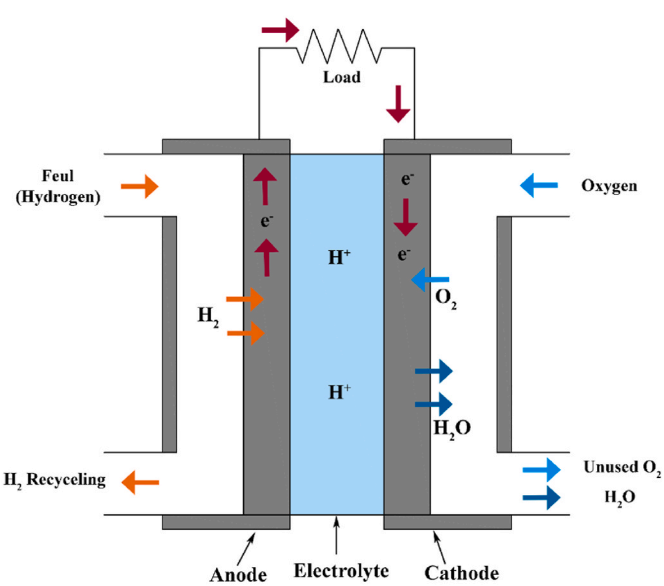

Fig. 2. Schematic diagram of hydrogen fuel cell operation.

PEMFCs include an electrode, bipolar plates, a gas diffusion layer, and a membrane (Wan et al., 2014). Its working temperature is typically 80°C, and the common sizing of the stack varies between 1 and 100 kW. This type is widely utilised due to low emissions, high efficiency, great power density, and low-temperature operation capacity. The main challenges with them include the usability of components materials, acid leaching, corrosion of materials, inadequate durability, and high-cost catalytic converter (Pei et al., 2013; Qin et al., 2016). In AFCs, an aqueous alkaline solution is utilised as an electrolyte. They are independent of high-price membrane electrolytes and have the potential for mass production at a low price. However, they face challenges, including electrode degradation and difficulties in preparing electrodes. There are health risks (Gülzow, 1996) associated with AFCs due to the use of asbestos. SOFCs use a solid electrolyte, but a liquid electrolyte is utilised in MCFCs. Both SOFC and MCFC are the most appropriate alternatives for stationary power production. The long start-up time is a disadvantage of these fuel cells associated with high operating temperatures (Zhang et al., 2015). In DMFC, methanol is directly converted into electricity with no need for an extra reformer. They possess various advantages such as ease of refuelling, long lifetime, compact size, and lightweight. Finally, PAFCs use concentrated phosphoric acid as the electrolyte. The development of PAFC has been limited because of high cost and less efficiency in comparison with the other fuel cell categories.

Different types of vehicles need various infrastructures of hydrogen. Two common pressures for dispensing hydrogen into vehicles are 350 and 700 bar. Light-duty vehicles store hydrogen gas onboard with vessels wrapped with carbon fibres with a typical 4–6 kg capacity at 700 bar pressure. The storage of hydrogen in other FCEVs, like trucks, forklifts is commonly at 350 bar pressure. The cost of vehicles that are equipped with fuel cells is higher in comparison with conventional vehicles.

2.2.2. Hydrogen fuel cells - ships and locomotives

Fuel cells have greater total efficiency and volumetric energy density compared with combustion-based energy conversion systems and other storage technics. Various studies have conducted on the use of different fuel cell technologies for marine applications (de-Troya et al., 2016; Ahn et al., 2018; Tronstad et al., 2017; Bassam et al., 2017), confirming the most promising types of fuel cells for marine applications are low- and high-temperature PEMFC and SOFC. Despite the progress, the technology of fuel cells for ships is still at the trial phase and early design. Compared with conventional diesel generators, the space occupied by fuel cells is commonly more in the context of volumetric density. It is expected that a low-temperature fuel cell which utilises liquefied hydrogen present high-density power solutions. For a broad refuelling cycle, the system size with adequate hydrogen storage can lead to a considerably higher volume. Another barrier is the hydrogen infrastructure and hence the direct use of them with fuel cells is still not possible.

There are some examples of fuel cell-powered locomotives. Vehicle Projects LLC and FuelCell Propulsion Institute studied hydrogen-powered locomotives (Dincer, 2002), showing that compared with battery locomotives, their net power was about two times more. The test of a hybrid diesel generator and passenger rail powered with hydrogen fuel cell was initiated by East Japan Railway Company. This was a fully operational passenger rail with a capacity of 65 kW. In 2016, Alstom Coradia iLint at the InnoTrans also launched a project on the train powered by a hydrogen fuel cell, which was classified as a vehicle with zero emissions. The utilisation of fuel cells to power locomotives is still associated with some challenges, such as the requirements for large storage spaces considering its low volumetric density and the high flammability of hydrogen. The onboard high pressure hydrogen storage brings new engineering safety challenges which should be addressed to avoid adverse effects of incidents/accidents involving hydrogen.

3. Hydrogen storage and transport

In hydrogen energy systems, storing the produced hydrogen is a significant aspect, particularly in large-scale hydrogen use. To define the most effective method of storing, a variety of parameters should be considered, such as the quality for kinetics of absorption and desorption, great gravimetric and volumetric capacity, the lowest possible weight and cost, high safety, and fast refuelling. Compared to fossil fuels (Salehi et al., 2015), although hydrogen posses appropriate density values per mass, its density by volume is low that causes the most critical challenge regarding storing and transport hydrogen (Roes and Patel, 2011; Khalil, 2018). The classification of different methods of hydrogen storage is schematically illustrated in Fig. 3, showing two broad classifications of hydrogen storage methods: physical storage technologies and material storage systems. The physical-base methods are classified based on storing hydrogen as a liquid, cold/cryo-compressed, and compressed gas. Two major subgroups of material storage technologies are defined as physical sorption/physisorption and chemical sorption/chemisorption (Niaz et al., 2015).

3.1. Compressed hydrogen

The compression of hydrogen is the most popular and common method for H_2 storage (Durbin and Malardier-Jugroot, 2013). A significant benefit of hydrogen storage as high-pressure gas is the great releasing ratio and rapid filling. Although this technology is simple, safety issues and the need for large spaces are its major disadvantages. Onboard vehicular, stationary, and bulk transportation are three main hydrogen storage applications that use high-pressure compressed hydrogen (von Colbe et al., 2019). Infrastructure development and public acceptance are the two main challenges of compressed hydrogen applications. The infrastructures of compression-stored hydrogen have two major difficulties; namely, low volumetric density and safety of storage system, that impose challenges in compressed H_2 storage in vehicles (Sinigaglia et al., 2017).

A significant part of hydrogen infrastructures is stationary (off-board) hydrogen storage that used for either transport applications or power generation. The facilities for storing bulk hydrogen are required in local/regional centres for the distribution of hydrogen, hydrogen production plants, as well as end-user sites, including fuel cell-based power generation plants or refuelling stations. The storage capacity requirements are different based on the application; the storage capacity ranges from 50 to 100 tons, tens of tonnes, or thousands of tonnes in distribution centres, refuelling stations, and production sites, respectively (Tzimas et al., 2003). Other requirements associated with these stationary storages include low hydrogen losses, reasonable quick recharging and delivery flow rates, appropriate long-term cycling behaviours, and manufacturing vessels with a range of storage capacity.

In bulk transportation, the utilisation of storage vessels with low weight and great capacity decreases the delivery cost. To store gaseous hydrogen, five categories of pressure vessels exist (Barthelemy et al., 2017), which are presented in Table 2. Type I vessels are the most traditional ones with the lowest cost but the heaviest, which are usually manufactured from steel or aluminium. In Type II, the structural load is shared among the composite and metal. Compared with Type I, the cost for constructing these vessels is approximately 50% more, but their weight is 30–40% less. Type III vessels use the metal liner. The composite structure carries the most structural load, and 5% of the mechanical load is shared by the metal liner. Although the cost of Type III vessels is about twice the cost of type II, their weight is approximately

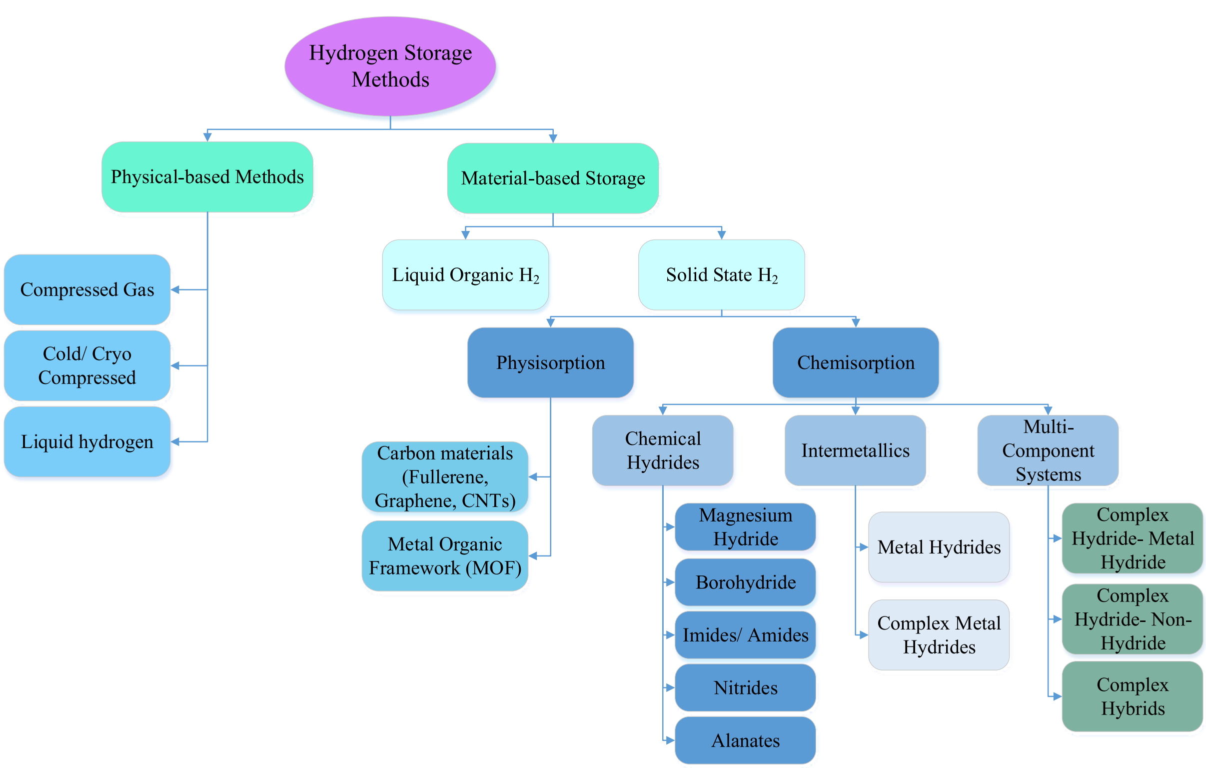

Fig. 3. Methods for storing hydrogen (Moradi and Groth, 2019; Nazir et al., 2020).

Table 2
Different types of pressure vessels for hydrogen storage.

Types of pressure vessels	Weight	Cost	Pressure
Type I: Full metal pressure vessels	Heaviest	the lowest cost	up to 200 bar
Type II: Steel vessel with a glass-fibre composite layer added around the steel	30–40% lighter than Type I	50% more than Type I	300 bar
Type III: Fully- wrapped vessels with composite and metal liner	70% lighter than Type I	about twice the cost of Type II	350–700 bar
Type IV: Full composite	80% lighter than Type I	Higher cost than Type I - III	up to 1000 bar
Type V: linerless fully composite pressure vessel	85% lighter than Type I	–	–

50% lower. Further improvements were made in Type IV, where the structural load is carried by carbon-glass composites or carbon fibre, and usually, a polymer is utilised as a liner. Their cost is yet extremely high. There is also a so-called Type V vessel, a linerless fully composite pressure vessel, which is still pre-commercial (LeGault, 2012).

3.2. Liquid hydrogen (LH_2)

It is possible to store H_2 at the liquid state, which is non-corrosive and colourless. The liquified H_2 tanks can store 0.07 kg per litre, which is higher than compressed hydrogen tanks that store 0.03 kg per litre (Niaz et al., 2015). Hydrogen liquefication is carried out at extremely low (<- 253°C) temperature, and the most critical challenge of cryogenic H_2 storage is keeping hydrogen under such a low temperature. Liquidifying hydrogen is an expensive and time-consuming process. The energy loss during this process is about 40%, while the energy loss in compressed H_2 storage is approximately 10% (Barthelemy et al., 2017). Besides, a proportion of stored liquid hydrogen is lost (about 0.2% in large and 2–3% in smaller containers daily), which is due to evaporation (known as the boil-off). Liquid storage systems also require continuous consumption to avoid pressure buildup and ultimately blowoff of hydrogen. The materials also turn to be brittle under low temperatures, increasing the risk for vessels' failure. This technology is commonly applied for average to large-scale storing and supply, like intercontinental shipping as well as truck delivery. Generally, 5000 kg of H_2 can be carried by a cryogenic tanker, and this is approximately five times more than that of compressed hydrogen tube trailers.

3.3. Cryo-compressed H_2 storage

Aceves et al. (2010) presented cryo-compressed H_2 storage technology for the first time, which is a supercritical cryogenic gas. In this method, the compression of gaseous H_2 happens under approximately −233 °C without any liquefaction. Because of the vacuum enclosure, this method has high levels of safety. Moreover, great storage density, fast and effective refuelling are advantages of cryo-compressed storage. Nevertheless, this technology is still in the development phase since the availability and price of infrastructures are still the most important challenges of this technology (Moradi and Groth, 2019).

3.4. Hydrogen transmission

Hydrogen can be transmitted in the form of liquid, gas, and metal hydrides through the ocean, road, and pipelines. For hydrogen at low pressure, which is stored in metal hydrides, the transmission is only possible in short distances and small amounts, while large quantities of liquid hydrogen are transmitted and distributed using pipelines. The pipeline's length varies between 1 km to hundreds of kilometres, and operational pressures are 10–30 bar. This can be achieved by employing available natural gas pipelines, which have several advantages, including (1) broad geographic extent, (2) interconnectivity, (3) high capacity, (4) well-developed maintenance and control structure, (5) well-established safety procedures, grid management and operational strategies, and (6) broad public acceptance. However, considerable modifications might be required for adopting natural gas pipelines to carry pure hydrogen (Cerniauskas et al., 2020).

As shown in Fig. 4, a natural gas supply chain contains different transmission lines and process sections to provide natural gas for both large volume customers and local customers. Interactions between pipe materials and hydrogen under high working pressure are not still fully realised, in particular with the consideration of pressure cycling. Materials durability is also affected by high pressures and pressure cycling. Transmission lines are mainly made of steel and polyethylene that require to be utilised for the addition of hydrogen. New coatings are particularly needed to be developed to avoid steel pipeline embrittlement (Reddi et al., 2016). Adaptation of end-use systems is also required at higher hydrogen blend levels. For local costumers, hydrogen concentrations of up to 28% may safely be used with existing domestic appliances, however, for large-volume costumers, particularly industrial combustion applications case by case studies are required.

4. Hydrogen safety aspects

While combustion properties of hydrogen, such as its wide range of flammability (Cashdollar et al., 2000), low minimum ignition energy, and high burning velocity, make it an excellent alternative fuel, due to these properties, there are various safety aspects in hydrogen utilisation and storage (Molnarne and Schroeder, 2019; Royle and Willoughby, 2011). As shown in Table 3, hydrogen has a very low boiling point, and density, and a relatively low ignition temperature of 585 °C (Najjar, 2013), whereas its diffusion coefficient in the air is high. Furthermore, hydrogen has low ignition energy of 0.017 MJ and high latent heat of combustion of 141.6 MJ/kg (HuangL.X et al., 2015). The detonation of hydrogen can occur at a volumetric concentration ratio of hydrogen to air as low as 4% and as high as 75% (Ball and Weeda, 2015). On the other hand, hydrogen has a high permeability through many materials. These properties make safety measures to be very important for hydrogen. Accurate hydrogen detection techniques are critical to measuring hydrogen concentration, particularly in accidental leakage events, since hydrogen is a colourless, odourless, and tasteless, flammable gas that cannot be noticed by human senses (Dutta, 2014).

As schematically shown in Fig. 5, the hazardous issues encountered in hydrogen applications and facilities can be classified as (i) material properties-related issues and (ii) hydrogen handling-related issues.

Both experimental and computational fluid dynamics (CFD) techniques have been employed to understand these risk components associated with hydrogen handling and applications. Some previous experimental works on hydrogen safety are reviewed in Table 4. While experimental measurements provided valuable insights, they are limited, expensive, and even impossible, particularly for more realistic large scale accidents. On the other hand, CFD models have been effectively used as predictive tools to analyse the impact of influencing parameters and to give insight into physical phenomena encountered in hydrogen risk components.

CFD simulations of such flows require proper real gas models (compressibility effects) turbulence models, combustion models, and heat transfer models. In the case of liquid hydrogen, two-phase models that can address the complexity of phase change (both evaporation and condensation) are also needed (Tolias et al., 2019). Over previous years, various codes have been developed with customised solvers. CFD simulations for hydrogen safety applications, particularly handling-related issues, have been conducted in both Reynolds-averaged Navier–Stokes (RANS) and large eddy simulations (LES) using commercial software such as ANSYS Fluent, ANSYS CFX, FLACS, in-house codes such as ADREA-HF, and open-source codes such as Fires Dynamics Simulator (FDS) and OpenFOAM. Table 5 gives the most used submodels for

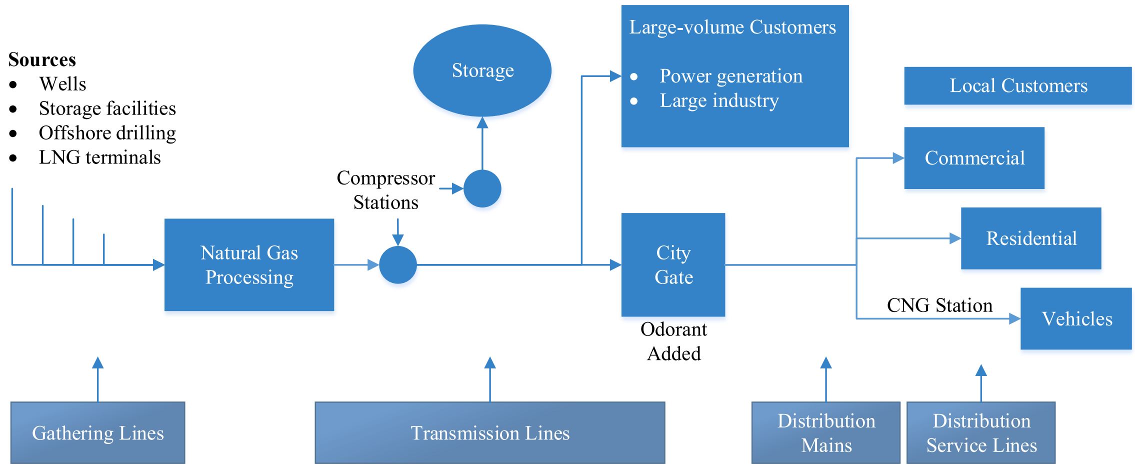

Fig. 4. Natural gas supply chain (Gillette and Kolpa, 2008b).

Table 3
Properties of hydrogen.

Properties	Values	
	Liquid	Gaseous
density	708 kg/m^3 (−253 °C)	0.0899 kg/m^3 (0 °C)
Molecular weight		2.01594 g/mol
Boiling temperature	−252.76 °C	–
diffusion coefficient	–	0.61 cm^2/s
flammable range	–	4–75% concentration in air
heat of combustion	–	142 kJ/g
Heat of vaporisation	447 kJ/kg (−253 °C)	–
Thermal conductivity	–	0.019 kJ/kg (25 °C)
Minimum ignition energy	–	0.017 MJ
Ignition temperature	–	585 °C
Heat capacity (Cp)	14.3 kJ/kg °C (25 °C)	8.1 kJ/kg °C (−256 °C)

hydrogen safety applications whereas Table 6 shows a summary of selected CFD studies for gaseous and liquid hydrogen cases, aiming to understand the physical phenomena associated with the hydrogen risk components, which are further discussed in this section.

4.1. *Material properties-related safety aspects*

4.1.1. *Hydrogen embrittlement*

Hydrogen embrittlement (HE) happens when metals are exposed to hydrogen, leading to degradation of metals' mechanical properties, failure, and leaks. The process commonly gains importance when it results in cracking, particularly for hydrogen storage and transmission pipelines. This occurs by applying sufficient stress on the object, which is embrittled with hydrogen. Both applied service and residual stresses generated during fabrication operations can cause such sufficient stress states. Embrittlement is a complicated phenomenon and dependent on metal purity, surface conditions, exposure time to H_2, and environmental pressure and temperature. With enhancing hydrogen purity, the vulnerability of steel to embrittlement increases. The influence of partial pressure of hydrogen on embrittlement was investigated in the study of Barthélémy (2007). They conducted tests of disk rapture on AISI 321 steel and observed that the highest embrittlement happens in the partial pressure range of 20–100 bar. Furthermore, the investigation of X100, X65, and X52 steel behaviour under a high-pressure hydrogen gas environment revealed that increasing alloy strength and hydrogen pressure results in larger embrittlement. The stress concentration in crack and notch roots decreases when yield strength is lower. A key issue regarding hydrogen embrittlement is the dependency of this phenomenon on the exposure time which should be considered in the test procedures. For instance, the test for measuring the threshold of hydrogen embrittlement for steel (ASTM F1624) is conducted for 30 h or less (Murakami et al., 2010).

4.1.2. *Hydrogen permeation*

Permeability is one of the material considerations within the usage of hydrogen. Due to the small size of hydrogen molecules, hydrogen can migrate through permeable materials or embrittle them over time. Within the framework of compressed gaseous hydrogen storage systems, permeation can be determined as the rate of hydrogen flux passing through the walls or gaps of tanks, interface materials, or piping. It is a current safety issue in standardisation and regulatory activities. Permeation increases with increasing material ageing, temperature, and storage pressure. The permeation rate in the pressure vessels of Type I, II, and III is insignificant. Losses of hydrogen might happen within several years, and it does not cause any safety matter for daily applications. Nevertheless, it is a safety issue for pressure vessels with non-metallic (polymer) liners (pressure vessels of Type IV), which have higher rates of hydrogen permeation (Friedrich et al., 2004). Approaches were developed to calculate an upper limit for hydrogen permeation in automotive applications by investigating the hydrogen behaviour during the release. Several issues such as level of safety, environmental scenarios, vehicle scenarios, and hydrogen dispersion behaviour should be considered to estimate the allowable rate. The permeation rate is considerably restricted in new containers by the carbon fibre overwrap, while in the containers that are reaching the end of their lives, the substantial micro-cracking affects the resin/carbon fibre matrix, allowing the rise in the permeation of hydrogen. The allowable hydrogen permeation rates presented in some standards and regulations are given in Table 7 (Adams et al., 2011).

4.1.3. *Changes in material properties at cryogenic temperatures*

The most important considerations for materials behaviour at low temperatures are the transition from ductile to brittle, certain unusual modes of plastic deformation, and the effect of phase transformations in the crystalline structure on the elastic and mechanical properties of materials. Materials used in liquid hydrogen services are exposed to cryogenic temperatures, so in particular, for selecting the materials to be used in these services, these changes in the material properties should be taken into account. The most important thermal characteristics for hydrogen services at cryogenic temperatures are low-temperature thermal contraction and low-temperature embrittlement. Various materials show the transition from ductile to brittle at low temperatures, which might result in the storage tank or pipe failure, leading to an accident (Rigas and Amyotte, 2012). Such an accident due to low-temperature embrittlement took place in 1994 for a tank containing

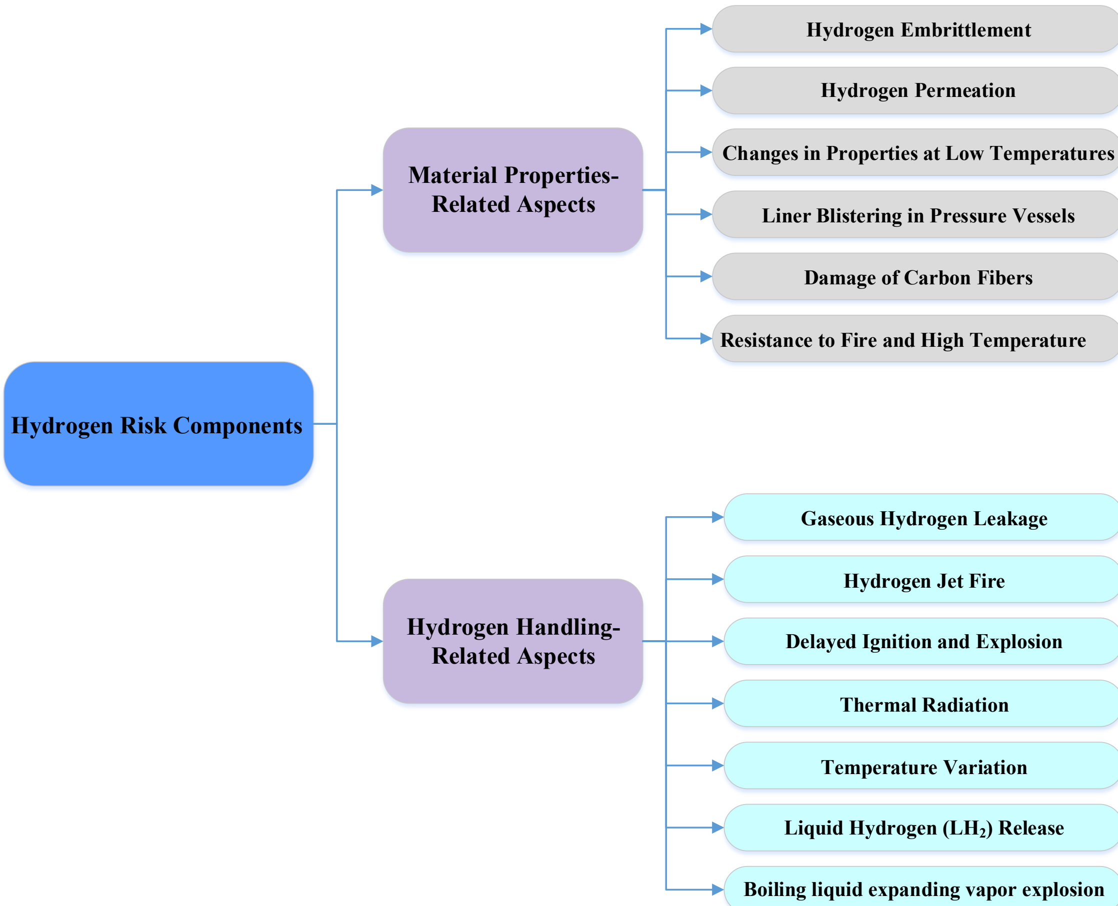

Fig. 5. Safety issues concerning the application of hydrogen.

liquid natural gas in Cleveland, U.S. state of Ohio where a nearby tank collapsed that caused 200 to 400 injuries, 128 deaths, and huge property damage. Generally, most metals have room-temperature to liquefaction temperature of H_2, showing less than 1% contraction, while this value is between 1 and 2.5% for the most common structural plastic (Guy, 2000).

4.1.4. Liner blistering in pressure vessels

Pressure vessels of Type VI consist of carbon fibre composites overwrap, a polymer as the liner for sealing purposes, and at least one boss. Under high pressures, hydrogen gas is absorbed by a plastic liner, and if the depressurisation rate becomes higher than the rate of escaping the absorbed gas by diffusion, plastic liner blistering occurs (Moradi and Groth, 2019). A model for the prediction of blistering in the hydrogen storage tank of Type IV has been developed by Yersak et al. (2017). Their study provided showed a good agreement with the experimental data, so the prediction of the blistering as a function of depressurisation rate and liner thickness was presented through performing a parametric investigation. The required number of experiments can be decreased by the presented pre-selection approach for liner materials and designs in this model, resulting in reducing the expenses for developing hydrogen storage systems. A test rig was built by Pépin et al. (2018) to replicate liner blistering that allowed the detection of the liner failure. Both liner deformation and composite cracks were observed with the tomographic monitoring on collapsed samples. Based on their observations, the collapses happen at the interface of liner/composite in regions that are not efficiently bonded. It was found blistering in the hydrogen tank of Type IV depends on working conditions such as including dwell time at residual pressure level before emptying initial filling pressure, the emptying rate, and initial filling pressure. The main collapse after the decompression test resulted in a void of 1.54 mm high. After seven days, this amount decreased to 0.51 mm (Pépin et al., 2018).

Pressured hydrogen vessels are equipped with a thermally activated pressure relief device (TPRD) that empties the vessels in case of elevated temperatures to reduce the chance of burst/explosion (Ng and Lee, 2008; Li et al., 2019). The opening diameter in the case of TPRD activation has a significant impact on the safety release of hydrogen and, consequently, the hydrogen flame length (Ruban et al., 2012). Although the installation of TPRD is necessary for preventing the catastrophic rupture of vehicular high-pressure hydrogen vessels, there is a risk of fire hazards for drivers as a result of the intended release of hydrogen from TPRD. The mitigation measures for the reduction of hydrogen fire risks caused by TPRD have been developed in the study of Li and Sun (2020). The new design of TPRD, which was rotatable, provided the opportunity of adjusting the release direction of H_2 for the system, leading to minimising the hydrogen fire risks.

Regarding safety issues, verifying the activation of TPRD to release H_2 from the cylinder is required. A method for TPRD activation was developed in the study conducted by Yamazaki and Tamura (2017). For the development of an uncomplicated approach to verify the activation of TPRD at post-fire accident sites, they performed an investigation on a verifying method based on measuring the concentration of hydrogen at the gas release port of TPRD, utilising an H_2 densitometer. They reported that in the case of using a catalytic combustion H_2 densitometer, it is possible to continuously measure the concentrations of hydrogen above 3000 ppm for approximately 24 h for cylinders of Type IV and approximately a month for cylinders of Type III.

Table 4
Previous experimental studies on hydrogen safety assessment.

Risk category	Ref	Work topic	Main findings
Hydrogen dispersion and explosion	Tanaka et al. (2007)	Hydrogen explosions in a full-scale hydrogen filling station model	Based on the dispersion experiments, the produced hydrogen concentration was remarkably affected by the room ventilation characteristics, the volume of hydrogen released, and leak diameter. For hydrogen concentration up to 15%, the size of the resulting hazardous area is found to be negligible for the explosions. However, for the concentration of 30%, the tolerable limit of overpressures is exceeded in the whole filling station for an explosion. This study reveals the importance of hydrogen leakage detection and isolating the supply before the concentration of hydrogen exceeds 15% in enclosed spaces.
Hydrogen leakage diffusion	Kobayashi et al. (2018)	Cryo-compressed hydrogen leakage diffusion	With the decrease of supply temperature, the risk degree for hydrogen increases. For an 820 bar cryogenic pump system, a separation distance of 9.22 m is required. The concentration distance is in proportion to the flow rate of the leakage to the 0.5th power.
Hydrogen embrittlement	Nanninga et al. (2012)	Hydrogen embrittlement in three types of steel pipelines in high-pressure gaseous hydrogen environments	The comparison of the embrittlement behaviour for X100, X65, and X52 steel under a high-pressure hydrogen gas environment revealed that the increase of alloy strength and hydrogen pressure results in increasing hydrogen embrittlement.
Thermal radiation	Kuroki et al. (2018a)	Temperature rise of hydrogen storage cylinders by thermal radiation from fire at hydrogen-gasoline hybrid refuelling stations.	The radiative heat flux from a fire near the storage vessels can be significantly reduced by using container walls around above-ground hydrogen storage tanks
Hydrogen jet fire	Schefer et al. (2007)	Characterization of high-pressure hydrogen-jet flames	The radiative and dimensional characteristics of hydrogen jet flames are measured. These hydrogen jet flames' radiative heat flux properties are observed to obey scaling laws developed for low-pressure flames with smaller scales and many fuels. The results for the length of flames reveals that lower-pressure correlations and the Froude number can be used for releasing up to 413 bar.
Hydrogen ignition	Wang et al. (2020)	the pressure and flame characteristics induced by high-pressure hydrogen spontaneous ignition	The effects of the size of the tube and hydrogen release pressure are studied. The self-ignition of hydrogen with high pressure was characterised. This study elucidated the process from self-ignition to the jet fire, also defined the critical factors needed for spontaneous ignition.
High-pressure hydrogen leakage	Weiyang et al. (2019)	Spontaneous combustion of high-pressure hydrogen leakage to form jet fire	At a constant length of the pipeline, when the initial pressure for hydrogen release is low, no spontaneous combustion occurs. Considering a constant length for the pipeline, the propagation of the shock would be faster, and the position of hydrogen self-ignition within the pipe would be closer to the rupture disc when the initial release pressure is higher. The length of flame augments first and decreases gradually afterwards as time passes.
Cryogenic hydrogen releases	Panda and Hecht (2017)	Ignition and flame characteristics of cryogenic hydrogen releases	For cryogenic hydrogen jets, radiative heat flux and ignition distance are measured. The normalized length of flame is in proportion to the Reynolds number of the jet. For cryogenic jet flames, radiative heat flux and flame length are greater. This study proposed a correlation based on power law for predicting the radiation fraction.

4.1.5. *Damage of carbon fibres*

The structures of composite pressure vessels are complicated, and their characteristics are dependent on several parameters. Designing a reliable pressure vessel that meets the safety considerations requires comprehensive knowledge on the physical basis of matrix cracking, delamination, fibre breaks, the influence of dome geometry on the composite vessel burst pressure, and the resistance mechanism against various kinds of impact. Wu et al. (2017) numerically and experimentally analysed the damage mechanisms of carbon fibre. Further studies focused on the influence of repetitive and single impacts on burst pressure of glass fibre reinforced vessels (Demir et al., 2015), reporting a 47% reduction in burst pressure. However, the properties of composite materials change remarkably by fibre density, stacking procedure, and so forth. Thus, probabilistic approaches for the prediction of fibre failures can be an acceptable path forward (Ramirez et al., 2015).

4.1.6. *Resistance to fire and high temperature in storage vessels*

Polymers and resins are considerably more susceptible to high temperatures compared to metallic materials. Thus the maximum operating temperature is a safety concern for their use. Consequently, evaluation of the composite behaviour in fire and the fire protection mechanism is extremely important, in particular, for onboard applications. A bone-fire test was conducted by Ruban et al. (2012) on fully composite vessels, showing the pressure increase before leakage or bursting was small (up to 12.7%), and the bursting delay was between 6 and 12 min, which was not acceptable. Saldi and Wen (2017) applied a combined CFD and finite element method (FEM) module for the simulation of a Type IV pressure vessel response to fire and succeeded in the accurate prediction of the bursting delay.

A further study conducted by Zheng et al. (2012b) applied a three-dimensional CFD model to evaluate the characteristics of heat transfer in 700 bar hydrogen composite vessels exposed to localised fire. They observed that during 600 s exposure to the localised fire, the rise in pressure and temperature is slow. The intensity of convective heat transfer in the internal hydrogen is higher than conductive heat transfer in the walls of vessels when the area of flame impingement is far from the pressure relief device (PRD). Furthermore, the heat transfer in Type III vessels is faster compared to Type IV vessels. In another study (Zheng et al., 2013), a Type III vessel was experimentally and numerically studied to understand the air and hydrogen effect in the filling media. They developed a three-dimensional model of the whole process of localised fire test and observed that with extending the time of exposure to the localised fire, the activation time of PRD increases.

4.2. *Hydrogen handling-related safety aspects*

The major handling hazards issues that can happen to liquid hydrogen and compressed hydrogen storage tanks during operations, often result in a loss of containment (LOC). A LOC is an uncontrolled or unplanned release of materials from primary containment. Therefore, LOCs involve both spills and leakages. Table 8 presents a summary of the possible accident scenarios upon loss of containment for gaseous and liquid hydrogen (Delvosalle et al., 2006) which are more discussed in this section.

Table 5
A summary of models for different phenomena occurring in hydrogen safety applications.

Phenomena	Models

Turbulence	• laminar model for rejoins where the flow is not laminar
	• RANS
	  • Realizable k-ε model
	  • Renormalization group k-ε model
	  • Shear stress transport k-ω model
	• LES

High-pressure hydrogen release (expansion shocks)	• Birch (Birch et al., 1987), Schefer (Schefer et al., 2007) approaches • Notional nozzle models based on mass, momentum, and energy conservation (Xiao et al., 2011) • Abel-Noble Equation of State (EoS) with the conservation of mass and energy (Molkov, 2012)
Self-ignition of sudden hydrogen release	• A physicochemical model involving gas-dynamic transport of a viscous gas, hydrogen oxidation kinetics, heat exchange, and multi-component diffusion (Golub et al., 2007, 2008, 2009)
Flashing (liquid hydrogen release)	Models based on enthalpic or isentropic expansion
Two-phase models (liquid hydrogen)	• Models based on thermodynamic and hydrodynamic equilibrium • Models based on an additional conservation equation for the vapour mass fraction (Jin et al., 2017)
Cryogenic hydrogen releases	• Models for condensation and/or freezing of the ambient humidity and the nitrogen and oxygen component of air
Cryogenic hydrogen releases near ground/water	• 1D conduction heat transfer models in the ground (or water)
Thermodynamic	• Ideal gas approximation for atmospheric condition • Cubic Redlich-Kwong-Mathias-Copema EoS for high pressures and low temperature
Ignition and jet fire (combustion)	• Expensive models that handle shocks, small scale turbulent mixing, and shock wave/vortex interactions • Eddy Break-Up (EBU) • Eddy Dissipation Model (EDM) • flamelet model • Eddy dissipation concept (EDC)
Deflagration	• Models that account for Rayleigh-Taylor instability and potentially, flame-acoustic interactions • Porosity Distributed Resistant (PDR) for RANS (Hansen et al., 2005., Tieszen)

4.2.1. Gaseous hydrogen leakage

Hydrogen's small molecular weight causes a high tendency leaking issue through pipelines or storage, which is a key safety issue. The hydrogen release may be due to damaged piping, loose-fitting, or a valve on the system. Hence, any small cracks or deformities within the vessel result in the rapid ejection of hydrogen gas. As a result, mixtures of hydrogen gas with atmospheric oxygen are formed over a wide range of concentrations in the range 4.0–75% v/v, resulting in the combustible mixture and 18–59% v/v causing explosive mixtures. Hydrogen release is followed by immediate ignition causing jet fires or a delayed ignition resulting in the explosion (Ehrhart, 2018). The consequences of these events have a direct or indirect impact on humans, the environment, structures, and properties (Cashdollar et al., 2000).

The hydrogen release without fire accidents is still a hazard issue, particularly in confined spaces, since it causes asphyxiation. This is because H_2, which is a non-toxic gas, replaces O_2, and hence oxygen concentration reduces below 19.5% by volume. The accumulation of hydrogen into closed spaces adjacent to the source then poses an asphyxiation hazard for the people being there. Recently, the CFD modelling of hydrogen dispersion within closed facilities was conducted by Giannissi et al. (2020) to simulate the accumulation of helium (as a surrogate for H_2) within an enclosure representing a garage with real-scale under a low rate of release. Because of the studied flow nature, different turbulence modelling methods (LES and RANS), as well as the laminar one, were investigated. Despite the gas release in low Reynolds, the formation of turbulent flow was observed. The results confirmed that the LES and RANS methods were able to provide the most accurate data for the distribution of gas within the facility, whereas more increased stratification was predicted by the laminar method at the phase of release.

Hussein et al. (2020) applied CFD simulation to study the release and dispersion of un-ignited hydrogen from onboard storage with the pressure of 700 bar within a closed car park, which is ventilated naturally. The effect of leak direction angle and leak diameter on forming flammable clouds and the consequences for car park ventilation, first responders, and vehicle passengers are discussed. The study considered a parking space with two opposing vents. The comparison between the release from three TPRD having different diameters of 0.50, 2.00, and 3.34 mm was conducted to understand the dispersion of gas, particularly the envelope formation dynamics for 4%, 2%, and 1% hydrogen volume. Based on their results, the TPRD release angle was revealed to possess consequences for the egress of passengers, showing the TPRD with a diameter of 0.5 mm was safer for 700 bar storage.

4.2.2. Hydrogen jet fire

A possible scenario that happens after the release of hydrogen is immediate ignition that leads to a jet fire. A jet fire is a high-velocity turbulent flame that results from the combustion of fuel releasing in a certain direction with substantial momentum. For stored gaseous hydrogen in pressurised vessels, the pressure difference between the ambient environment and conditions within the vessel causes the high momentum of released fuel that quickly mixes with the turbulent ambient air. The ignition can be initiated by several sources such as sparks from electrical equipment and/or rapidly closing valves, electrostatic discharges, etc. Gaseous hydrogen store tanks for hydrogen fuel cell vehicles are pressurised between 350 and 700 bar (Folkson, 2014), whereas other fuels such as Liquefied petroleum gas (LPG) store tanks in similar gas-powered vehicles are pressurised between 2.5 and 21 bar (Martyr and Plint, 2012). Therefore, the risk of an accident or collision involving a hydrogen fuel cell vehicle may be catastrophic. This risk is further ameliorated in hydrogen fuel cell buses, which can carry up to 50 kg of hydrogen on board, as opposed to a hydrogen fuel cell car, which can carry up to 4 kg of hydrogen.

It is worth noting that a hydrogen fire burns clean with minimal smoke and soot yield, and hence a hydrogen flame may not be detectable or visible to the naked eye. Considering hydrogen flames have high velocity and high heat release rate, this presents an increased risk of fire growth and exposure to occupants as humans. Hence, the North American National Fire Protection Association (NFPA) has awarded hydrogen with a flammability rating of 4, the highest rating on the NFPA 704 flammability scale (National Fire Protection, 2007).

Brennan et al. (2009) modelled hydrogen jet fire with high pressure applying a laminar flamelet technique and LES approach and compared the results with the experimental test of large-scale vertical jet fire (Schefer et al., 2007). The LES sensitivity analysis imposing at the nozzle exit showed that for 0–20% turbulence intensity, a restricted influence on the width and length of the flame was observed. Above 20%, increasing in turbulence intensity resulted in a reduction in the length of the flame and increasing the width of the flame. The most accurate results compared to experimental tests were obtained for a turbulence length scale of 7% equivalent diameter and a turbulence intensity equal to 25% for a finer grid.

Jang et al. (2015) performed a CFD study to determine the outcomes of hydrogen jet fires produced at pipelines of high-pressure hydrogen at a pipe rack structure in a processing plant. Using the Kameleon FireEx (KFX) code, they computed radiant heat, jet fire temperature, and heat

Table 6
A summary of major CFD studies of hydrogen safety issues.

Risk category	Ref	Work topic	Modelling framework	CFD code	Main findings
Hydrogen dispersion	Wilkening and Baraldi (2007)	Accidental methane and hydrogen release from pipelines	LES	CFD-ACE	The flammable mixture amount would be greater for hydrogen release due to the wider range of flammability. If an explosion occurs, the flame acceleration can be raised when there exist obstacles near the ground.
Hydrogen dispersion	Giannissi et al. (2020)	Hydrogen dispersion at low-Reynolds number release in a closed facility	Laminar model, RANS, LES	ANSYS CFX, ADREA-HF and ANSYS Fluent	RANS and LES approaches reproduce well the gas distribution inside the facility, while the laminar approach predicts more enhanced stratification at the release phase. For releases within closed facilities, narrower acceptable ranges were proposed in comparison with a release in open areas.
Hydrogen dispersion	Hussein et al. (2020)	Dispersion of hydrogen release in a naturally ventilated covered car park	RANS	ANSYS Fluent	The TPRD release angle was revealed to possess consequences for the egress of passengers. Among three different TPRD with different diameters of 0.50, 2.00, and 3.34 mm, the TPRD with a diameter of 0.5 mm was safer for 700 bar storage.
Hydrogen dispersion	Papanikolaou et al. (2010)	Hydrogen release and dispersion	RANS	ADREA-HF, FLACS, ANSYS Fluent	The study determined the ventilation requirements for parking hydrogen-fuelled vehicles in residential garages. The turbulence model and boundary conditions have important effects on the results.
Hydrogen jet fire	Gu et al. (2020)	Hydrogen jet fire in tunnels under different conditions	LES	FDS	The overall temperature in the tunnel can be efficiently reduced by longitudinal ventilation. However, the layer with a high temperature would be lowered under the safe height. For controlling hazards, enough transverse and longitudinal ventilation is required within the tunnel.
Hydrogen jet fire	Brennan et al. (2009)	hydrogen jet fire	LES	ANSYS Fluent	Compared to experimental tests, the most accurate results were obtained for a turbulence length scale of 7% equivalent diameter and a turbulence intensity equal to 25% for a finer grid. Based on this study, the influence of grid resolution on the width and length of the flame was more compared to turbulent boundary conditions.
Hydrogen jet fire	Jang et al. (2015)	fire damage analysis of jet fire on hydrogen pipeline	RANS	Kameleon FireEx	An analysis was conducted to study the damaging effect on surrounding pipes by the temperature and radiant heat. In the pipe rack structure, severe damages were observed resulting from a high-pressure jet fire, and also, many equipment and facilities were melted and collapsed.
Hydrogen pool fire	Knechtel et al. (2015)	properties of an LH2 pool fire	SAS-SST	ANSYS CFX	Large fire scenarios with liquid hydrogen were modelled with a focus on the simulation of jet and pool fire. For pool fires, the maximum flame temperature was defined to be about 2300 K, while it was around 2100 K for jet fires. The specific emissions (SEP) were determined to calculate thermal safety distances, and then appropriate position factors were selected to define reliable safety distances. With the help of virtual radiometers, the irradiance was determined as a function of the relative distance from the pool edge and the limit of the adverse effect.
Liquid hydrogen release	Giannissi and Venetsanos (2018)	Liquid hydrogen release and dispersion in an open environment	RANS	ADREA-HF	The non-homogeneous equilibrium model that considers the wind variability, the slip impacts among phases, and the humidity and oxygen and nitrogen phase change provide more accurate results with a satisfactory agreement with the experiment.
Liquid hydrogen releases	Ichard et al. (2012)	Liquid hydrogen releases	RANS	FLACS	The results of the sensitivity study demonstrated the negligible impact of air condensation on the flow field. The temperature time series showed the incapability of the model for predicting the hydrogen presence at different sensor locations in both tests.
Liquid hydrogen release	Giannissi et al. (2014)	Liquid hydrogen dispersion under cryogenic release conditions	RANS	ADREA-HF	The simulation, which considered humidity and used slip model (humid-slip), provided more accurate data with a great agreement with the data from the experimental tests compared to the other cases (dry, humid-no-slip) in terms of peak and time-averaged concentrations.
Liquid hydrogen releases	Jin et al. (2017)	Liquid hydrogen releases in the open environment	RANS	ANSYS Fluent	The ground-plume thermal interaction significantly affects the LH_2 release. With increasing the ground temperature, the spreading range and duration for

(*continued on next page*)

Table 6 (*continued*)

Risk category	Ref	Work topic	Modelling framework	CFD code	Main findings
					the LH_2 reduce. The downwind distance of the flammable cloud is expanded as the wind speed increases.
Delayed ignition and explosion	(Vyazmina and Jallais, 2016)	Influences of the ignition position on the overpressure originated from a delayed ignition of high-pressure releases of hydrogen	The turbulence model, The combustion model	FLACS	The hydrogen concentration of about 65% provides the highest overpressure. A new methodology for the prediction of explosion strength from delayed ignition releases of high-pressure hydrogen was presented.
Delayed ignition and explosion	(Vyazmina and Jallais, 2017)	A benchmark study for evaluation of CFD modelling for the jet dispersion and a delayed explosion	RANS	FLACS P^2REMICS	The results of CFD data for dispersion modelling was accurate compared to experimental data, although P^2REMICS overestimated the concentration. The results of explosion simulations for both codes were in close agreement with experiments. However, the positive impulse was underestimated in 2D simulation compared to 3D (FLACS). The results of this benchmark study prove the more accuracy of 3D CFD modelling for the delayed explosion of hydrogen high-pressure jets.
Delayed ignition and explosion	(Vyazmina and Jallais, 2017)	Effects of obstacles on a delayed deflagration of hydrogen jets in a highly obstructed geometry	RANS	FLACS	CFD code was used to reproduce the empirical data. At different monitoring points, the calculated signals of overpressure are compared with the results of experiments, and considering the reasonable agreement with these data, CFD code can be applied for overpressure prediction where pressure detectors are saturated. Moreover, a new approach of an equivalent mixture of air/hydrogen to a stoichiometric mixture of air/methane is proposed for homogenous stationary clouds
Hydrogen jet fire	Zheng et al. (2012a)	The investigation of the hydrogen jet flames resulted from the activation of PRD	RANS	SIMPLE	The jet flame length decreases with the increase of nozzle diameter and the temperature difference between the environment temperature and the filling hydrogen temperature, but this length increases with augmenting discharge pressure. The safety performance of a barrier structure of 45° is better than that of 60° and 90° structures.
Hydrogen jet fire	Cirrone et al. (2019)	The simulation of flame length and radiative heat flux for cryogenic hydrogen jet fires	RANS	ANSYS Fluent	Among the evaluated turbulence models, the realizable k-ε model can provide the most accurate data when compared to experimental test data. The simulated radiative heat flux is revealed to be considerably affected by humidity in the air and angular divisions' refinement for the radiation model based on the sensitivity analysis. The turbulent Schmidt number, the absorption coefficient and hydrogen inlet turbulence parameters have significant influences on radiative quantities
Hydrogen jet fire	Rajendram et al. (2015)	Flame height and radiative heat flux from the natural gas jet fires	LES	FDS 6.0.1	These fire scenarios were investigated with two approaches of fire modelling; CFD modelling and solid flame model. More realistic results were obtained using CFD modelling compared to the solid flame model, so CFD can be suggested for risk modelling of offshore fire.
Temperature variation	Kim et al. (2010)	Investigation of the thermal characteristics of type IV vessel during the hydrogen fueling process	RANS	ANSYS Fluent	When the initial gas pressure is higher, the CFD results are closer to the experimental data. The temperature of the upper gas is higher because of the buoyancy effects in the cylinder. When the tank is pressurised from 10 bar to 350 bar, the maximum temperature of the gas exceeds that the allowed value in the ISO safety code (85 C).
Temperature variation	Galassi et al. (2012)	Prediction of the temperature distribution in the vessel during the hydrogen fueling process	RANS	ANSYS CFX	CFD code was used to define temperature distribution in vessel Type IV under different working conditions during the filling to 700 bar in 245 s. An increase of about 70 C was noticed for the maximum average temperature of hydrogen and also, it was observed that a significant parameter in the thermodynamics of the process is the heat transfer to the solid structure. Pre-cooling of hydrogen was revealed to have a good influence on lowering the temperature of both the tank and the inside gas, keeping the temperature within the allowed temperature by international standards.

Table 7
Allowable hydrogen permeation rate from different sources (Adams et al., 2011).

Source	Justification Reference	New or simulated end of life container	Minimum testing temperature (°C)	Maximum allowable rate for hydrogen permeation (Nml/hr/L water capacity-except where indicated)
SAE J2579: 01 2009	–	Simulated end of life	55	150 NmL/min per standard vehicle
ACEA for EC Hydrogen Regulation	LLNL (Mitlitsky et al., 2000)	New	20 ± 10	10
JARI for UN ECE HFCV GTR	–	–	15	5
ISO/TS15869:2009 Option ii) Test E5	–	Simulated end of life	20	75 Nml/min per container
ISO/TS15869:2009 Option i) Test B16	JARI (2004) (Institute, 2004)	New	Ambient	20@350 bar & 2.8@700 bar
HySafe Proposal (Adams et al., 2011)	–	New	15 20	4.6 6.0

Table 8
Accident scenarios upon loss of containment (Ustolina et al., 2020; Delvosalle et al., 2006; Brown et al., 2005).

	Consequences
Compressed H_2 storage	Fireball Overpressure generation Missile ejection Jet fire Flashfire Vapour cloud explosion (VCE) Gas puff (ignited) Gas dispersion Gas jet (ignited) Fire
Liquid hydrogen (LH_2)	Fireball Overpressure generation Missile ejection Jet fire Flashfire Vapour cloud explosion (VCE) Gas puff (ignited) Gas dispersion Gas jet (ignited) Fire Aerosol puff ignited Aerosol puff Two-phase jet Pool dispersion Pool ignited Pool formation

flux distribution upon the complicated pipe rack structure configuration. They also analysed the consequence of thermal damages and presented the fire damages from large-scale jet fires at pipe rack structures. Gu et al. (2020) performed CFD numerical studies on the hydrogen jet fire from a hydrogen-powered car within a tunnel. Various parameters, including the leakage location, the tunnel volume, transverse ventilation, longitudinal ventilation, leakage area, and the rate of hydrogen leakage, were studied. With increasing the rate of H_2 release, the rate of hydrogen diffusion and temperature rise increased within the tunnel. On the other hand, further hydrogen diffusion within the tunnel was inhibited with the excessive rate of leakage. With increasing the cross-sectional tunnel area, the rate of hydrogen diffusion decreased. The overall temperature in the tunnel can be efficiently reduced by longitudinal ventilation. However, the layer with a high temperature would be lowered under the safe height. Enough transverse and longitudinal ventilation is required within the tunnel for controlling hazards and avoiding the consequent disaster of the H2 jet fire.

4.2.3. Delayed ignition and explosion

Another possible scenario after the release of hydrogen is a delay between release and ignition, which may cause an explosion. In this case, the hydrogen has sufficient time to be mixed with air before being ignited, and the consequence would be a flash fire or a vapour cloud explosion (VCE). The delayed ignition probability significantly differs from the release conditions (Zhang et al., 2020). The hazardous effects of the continuous and instantaneous release of liquid hydrogen were studied by Li et al. (2012). They concluded that for both cases, VCE has the highest harmful effects and can be considered as a basis for the determination of the safety distances from liquid hydrogen vessels since it is more destructive than jet fire and flash fire. In the study of Daubech et al. (2015) for the nozzle diameter of 12 mm and the pressure of 36 bar, the ignition of the flammable cloud was on the centreline of the jet at a position downstream of the releasing point where the mixture of air/hydrogen having a 30% volume of H_2. They measured the explosion overpressure at different positions and concluded that the highest overpressure was defined at a distance of 2.5 m and perpendicular to the point of ignition, which was equal to 0.08 bar. Vyazmina et al. (Vyazmina and Jallais, 2016) performed a numerical study to determine the worst-case ignition position of hydrogen jets with high pressure; 260 g/s at 36 bar (Daubech et al., 2015), and 1000 and 8000 g/s at a pressure of 70 bar (Miller et al., 2015). They conducted a parametric investigation for identifying the position of ignition in proportion to the case with the highest overpressure (the worst scenario), leading to the development of a new methodology for the prediction of explosion strength from delayed ignition releases of high-pressure hydrogen.

4.2.4. Thermal radiation and thermal hazards

There are risks of damage for equipment and structures exposed to thermal radiation and direct flames. A summary of the types of damage for different thermal radiation intensities is presented in Table 9. Thermal radiation from hydrogen has no significant effect on equipment and structures. However, exposure to thermal radiation from hydrogen fires can be extremely destructive. Hydrogen is flammable, and hence there is a risk of fire. Escaping hydrogen gas from the leak can lead to creating a jet flame, and thermal radiation from this flame might be substantial. Based on reports, several hydrogen failures in the delivery phase caused injuries, damage the neighbourhood's properties, and led

Table 9
Possible damages for structure exposed to thermal radiation (LaChance et al., 2011).

Thermal Radiation Intensity (kW/m2)	Type of damage
4	Glass breakage (30 min exposure)
12.5–15	Piloted ignition of wood, melting of plastics (>30 min exposure)
18–20	Cable insulation degrades (>30 min exposure)
10 or 20	Ignition of fuel oil (120 or 40 s, respectively)
25–32	Unpiloted ignition of wood, steel deformation (>30 min exposure)
35–37.5	Process equipment and structural damage (including storage tanks) (>30 min exposure)
100	Steel structure collapse (>30 min exposure)

to negative effects on human life (Dagdougui et al., 2010).

As previously mentioned, the storage of hydrogen is in the liquid state at moderate pressure and low temperature or in the gaseous state at normal temperature and high pressure. In both cases, a substantial possible risk exists for the explosion of vessels containing hydrogen in the case of their exposure to thermal radiation or high temperature. The exposure of hydrogen vessels to high thermal radiation may result in a considerable hazard potential for mechanical explosion. Commonly, the main sources of ignition can be neighbouring fires or electrostatic sparks caused by discharging of the content. These circumstances are recognised as domino effects because a primary coincidence creates other accidents making an accident's chain with intensified effects on the surroundings, leading to increasing temperature in the shell of the vessel and its content. As a result, the vessel explodes, and its content commonly ignited and burns in the fireball or jet fire form (Dincer, 2002; Schulte et al., 2004). Unlike storage tanks of gaseous hydrogen with high pressure, the operation of the ones containing liquid hydrogen is at low to moderate pressures lower than 20 bar. Consequently, the design of the wall is sensible to be based on less pressure resistance compared with the design for gaseous hydrogen. The engulfing of the container in the fire resulted in heating the metal and losing mechanical strength.

Compared with the liquid phases, which absorb considerable quantities of heat, the specific heat capacity of vapours is much lower, leading to the rise of the local temperature of the wall in the container part with vapour phase as a result of supplied heat, which makes its metal to weaken (Kumar, 1994). The overheating of vessels in the case of the storage of liquid hydrogen cause interior temperatures to become more than the content boiling point, leading to the superheating of the liquid. The occurrence is noticed in the case of the existence of a nucleation site shortage in the liquid bulk. Nevertheless, above a specified temperature limit, the remaining fluid in the liquid phase is not possible any longer (superheat limit temperature or homogeneous nucleation limit). The fluctuations of random molecular density at that limit in the liquid bulk generate hole-like areas with molecular dimensions that might perform as bubbles. This finally results in the liquid explosive flash in the company of a severe shock wave propagating across the fluid and rupturing the vessel and the spill of the content. The travel of ruptured walls' missiles up to a hundred meters is probable, while a sphere (fireball) is formed by the flammable content to burn from the outer to inner layers (Rigas and Sklavounos, 2005).

4.2.5. *Temperature variation*

A fast-filling is required in the compressed gas filling process to achieve a satisfactory refuelling duration, close to that of conventional vehicles, which results in high gas temperature due to compressor work on gas for increasing its pressure. On the other hand, for fueling the gas inside the vessel, the process of discharging is a cooling process. The mechanical characteristics of carbon fibres and epoxy resin would be seriously affected by temperature variations. At low temperatures, the fracture toughness of the epoxy resin matrices reduces dramatically, whereas, at high temperatures, composites interlaminar shear strength reduces seriously. Moreover, considerable thermal stresses are created in the composite layer and aluminium liner of the vessel (Pei et al., 2013). The structural integrity of the storage system might be jeopardised due to high temperatures (Melideo et al., 2014), and in the long term, temperature variations of gas and tank have negative effects on the storage vessel's lifetime (Moradi and Groth, 2019). Three thermodynamic phenomena attribute to this issue. The first phenomenon is transforming the hydrogen kinetic energy generated by a higher pressured tank into internal energy. The second phenomenon is increasing gas temperature due to passing the hydrogen through the dispenser throttling device, and the third phenomenon is continuous gas compression within the cylinder throughout the filling process when the gas with higher pressure enters from the fuelling station. Although some parts of the heat inside the cylinder transfer to the ambient, some amount of this heat is stored in the cylinder material (Kuroki et al., 2018b).

Temperature rise in the filling process has been investigated in previous studies, showing both properties of tanks and filling conditions can affect the temperature increase. Type III pressure vessels reach lower temperatures during the refuelling process compared to Type IV (Hirotani et al., 2007) and when the diameter of the hydrogen dispenser or nozzle is smaller, the maximum temperature is lower, and gas temperatures distribute more uniformly within the tank (Terada et al., 2008). Moreover, the increase in gas temperatures within the tank decreases by reducing the length to diameter ratio of the vessel (Li et al., 2012). Regarding the filling conditions parameters, if the starting pressure in the refuelling process increases, the maximum temperature of the gas in the vessel decreases (Kim et al., 2010; Zhao et al., 2010; Liu et al., 2010). Various studies showed that lower flow rate (Zhao et al., 2010; Liu et al., 2010; Cebolla et al., 2014), ambient temperature (Pei et al., 2013; Melideo et al., 2014; Zhao et al., 2010; Liu et al., 2010; Cebolla et al., 2014), and inlet gas temperature (Melideo et al., 2014) result in a lower maximum temperature of the gas. There are still some doubts regarding the heat exchange between the tank solid components and the inside gas in the process of hydrogen vessels' on-road services (refuelling, and holding under pressure). Furthermore, locations of temperature measurement points in onboard vessels have not still been specified in the available regulations and standards for hydrogen-fuelled cars.

4.2.6. *Liquid hydrogen (LH_2) release*

Storage and transportation of hydrogen as a cryogenic liquid (or LH_2) is common since it enhances the volumetric density and hence requires significantly less volume for the same mass of hydrogen fuel compared to gaseous hydrogen (Ichard et al., 2012). The LH_2 can be achieved under extremely low temperature (−251.35 C) and low pressure (a few bars above atmospheric) (Giannissi and Venetsanos, 2018) that can be used in ICE, particularly ship engines. One of the main concerns is the accidental release of LH_2 from pressurised and non-pressurised tanks. The LH_2 release involves two-phase flow jet dispersion with the subsequent spreading of the LH_2 on the ground or water surface (Middha et al., 2011), followed by vaporisation and formation of a potentially dense hazardous gas cloud that may cause damage to equipment and structure and/or harm to people. The main physical phenomena involved in an accidental LH_2 leak can be classified as (i) flash evaporation, (ii) partial or full vaporisation, (iii) cryogenic boiling pool formation, and (iv) air components condensation and freezing. The pressure change from the storage to the atmospheric pressure results in instantaneous vaporisation of saturated liquid hydrogen at the orifice that causes the occurrence of flash inside the tank or pipelines. Due to the temperate difference between LH_2 and atmospheric temperature, the released fuel evaporates and mixes with the air. However, in the case of partial vaporisation, the cryogenic pool forms on the ground surface that absorbs heat from the atmosphere and the ground, creating a boiling film while causing freezing of the solid ground. Finally, due to the extremely low prevailing temperatures, the nitrogen, oxygen of the air, and ambient humidity may condense and or freeze, creating liquid or solid particles. During air and humidity phase change, the mixture density increases due to the formation of liquid and solid phase that enhances the cloud's dense behaviour, which has negative buoyancy effects. On the other hand, the heat release from the phase change results in a positive buoyancy effect. These conflicting phenomena affect the formation and dispersion of the flammable cloud. The standards related to LH_2 safety are presented in Table 10.

CFD models have been extensively applied to study the release and spread of LH_2 (Liu et al., 2021). Giannissi et al. (Giannissi and Venetsanos, 2018) used CFD modelling for the simulation of LH_2 dispersion based on experimental tests performed by the Health Safety Laboratory (HSL). Modelling air components (oxygen and nitrogen), ambient humidity condensation, and impose of transient wind profile were investigated in this study. The numerical studies that modelled the wind variability, the slip impacts among phases, and the humidity and oxygen

Table 10
The standards related to liquid hydrogen.

Standard	Title	Notes
CGA H-5-2014	Installation Standard for Bulk Hydrogen Supply Systems	This standard covers requirements for gaseous and liquid hydrogen bulk supply systems
CGA P-12-2017	Safe handling of cryogenic liquids	This standard presents information on the characteristics, transport, storing, safe handling, and utilisation of the cryogenic liquids commonly utilised in institutions and industry.
CGA PS-17-2004	CGA position statement on the underground installation of liquid hydrogen storage tanks	This standard presents information on minimum criteria and the design of underground installation of LH_2 storage vessels.
CGA H-3-2019	Standard for cryogenic Hydrogen Storage	This standard includes the proposed minimum design and performance requirements of vacuum-insulated, shop-fabricated cryogenic tanks intended for above-ground storage of liquid hydrogen.
ISO 13985:2006	Liquid hydrogen - Land vehicle fuel tanks	This standard defines the construction criteria for liquid hydrogen fuel vessels used in land vehicles and also testing procedures needed for ensuring an acceptable degree of safety against loss of life and property due to explosion and fire.
NFPA-2-2020	Hydrogen Technologies Code	This standard presents safety requirements for the production, piping, storage, installation, utilisation, and handling of hydrogen in all cryogenic liquid or compressed gas forms.
ISO 13984:1999	Liquid hydrogen - Land vehicle fuelling system interface	This standard defines the features of liquid hydrogen dispensing and refuelling systems for all types of land vehicles for reducing risks of explosion and fire during the refuelling process and thereby providing an acceptable degree of protection against loss of property and life.
CGA G-5.4-2019	Standard for hydrogen piping systems at user locations	This standard provides the recommendations of general principles and specifications for piping systems for liquid or gaseous hydrogen.
NFPA 55	Compressed gases and cryogenic fluids code	It presents standards for the handling, use, and storage of cryogenic fluids and compressed gases in portable and stationary tanks, cylinders, and containers
NFPA 50B	Liquefied Hydrogen Systems at Consumer Sites	This standard covers the standards recommended for the use of liquid hydrogen for consumer use.

ISO: Organization for Standardization
CGA: Compressed Gas Association
NFPA: National Fire Protection Association

and nitrogen phase change provided more accurate results with a satisfactory agreement.

Ichard et al. (2012) have simulated two experiments, Test-06 and Test-07 that consider a vertical downward jet with a distance of 0.1 m above the ground and a horizontal release of liquid hydrogen with a distance of 860 mm above the ground. For defining the source term impacts on the flow field, a sensitivity study was carried out. An upward velocity is generated by nitrogen and oxygen condensation through energy release, leading to bringing cold hydrogen gas to upper heights in comparison with when there is no air condensation. The temperature time series showed that the incapability of the CFD model for predicting the hydrogen presence at different sensor locations in both tests.

In another study (Giannissi et al., 2014), the CFD code, ADREA-HF, was adopted to model three experimental studies on the LH_2 spill experiments performed by HSL in 2010. It was found that the humidity existence in the atmosphere and fluctuating wind direction had important influences on the vapour dispersion. Both hydrodynamic and non-hydrodynamic equilibrium models were considered. Similar to the hydrodynamic equilibrium model, the non-hydrodynamic equilibrium model (slip model) assumed that there is thermodynamic equilibrium between two phases but it allows that the phases to achieve dissimilar speeds utilising additional slip terms in the equation of conservation. They found the slip effect and humidity greatly influenced the cloud buoyancy, where the model used the slip model (humid-slip) provided more accurate data.

4.2.7. Boiling liquid expanding vapour explosion (BLEVE)

A possible event scenario for the LH_2 technology is boiling liquid expanding vapour explosion (BLEVE). This accident scenario is an explosion caused by the rupture of tanks containing LH_2 at atmospheric pressure and under temperatures above the boiling point because of the expansion of both the liquid and vapour phases. BLEVE is caused by quick phase change and expansion, not by chemical reactions, so it can be considered a physical explosion. Pressure waves, a fireball in case of flammable materials and presence of ignition sources, and fragment projection are the consequences of BLEVE. The generation of pressure waves as a result of the explosion is the first consequence of BLEVE. Depending on the intensity of the blast wave, overpressure, injury and death of humans, and various forms of structural damages can be caused (Baker et al., 2012).

Fragments (also referred to as projectiles or missiles) are a consequence of BLEVE involving the tear of the vessel and throwing away its debris and is caused by part of the mechanical energy released by the explosion. In the case of the flammability of the stored material and the presence of an ignition source, the occurrence of a fireball is probable. An actual fireball does not occur in some cases. Instead, following the loss of containment, a fire initiates on the ground, which can represent the third type of consequence for BLEVE. These event circumstances were studied by Bader et al. (1971). They defined the rocket propellant's critical mass above which the fireball is formed and lift off. Ustolin et al. (2020b) evaluated all the consequence typologies (fireball, fragments, and pressure wave) for LH_2 BLEVEs, for both mid-scale and small-scale tests applying analytical and theoretical models. The experimental data from BMW safety tests were used to validate the models, and then the most appropriate approaches were chosen for conducting the blind prediction study of the forthcoming liquid hydrogen BLEVE experimental studies of the Safe Hydrogen fuel handling and Use for Efficient Implementation (SH_2IFT) project. They also highlighted the shortcomings of the models, as well as the uncertainties and information gap in liquid hydrogen physical explosions.

Ustolin et al. (Ustolin et al., 2020) estimated the consequences of both supercritical and subcritical LH_2 BLEVE applying real and ideal gas behavior models. At a fixed distance from the tank, they calculated the blast wave overpressure and the generated mechanical energy by the explosion. To perform comparative hazard assessments, similar estimations were performed for methane and liquefied propane tanks. However, there is still a lack of knowledge in the literature for the LH_2 BLEVE phenomenon, and further experimental tests and studies are required.

5. Hydrogen risk assessment

Hydrogen risk analysis creates a reliable connection between scientific knowledge from numerical analysis, experimental data, theoretical models, and industry practices (Crowl and Jo, 2007). Identification of key risk drivers, the establishment of mitigation strategies, and the prevention of potential accidents are some of the outcomes of hydrogen risk assessment (LaChance, 2009). Risk assessment has been performed to form the basis of regulations, codes, and standards (RCS) (Groth and Tchouvelev, 2014; Groth et al., 2012). Measures of a preventive and protective nature based on this RCS are applied to limit the quantity of hydrogen release, reducing its frequency of occurrence, and reducing the intensity of the impact and the probability of exposure of the subsequent hazard to different targets, including people and structures (Molnarne and Schroeder, 2019). The outcomes of hydrogen risk assessment can be used as a reference for hydrogen system operation and system failure analysis (Rusin and Stolecka, 2015).

Fig. 6 illustrates hazard identification and risk assessment procedure with the left image presenting a generalized procedure (Crowl and Jo, 2007) and the right image showing a general hydrogen quantitative risk assessment (QRA) procedure (San Marchi et al., 2017). When the hydrogen system is comprehensively described, identification of the condition that has the potential for causing damage to targets and characterisation of the occurrence that result in an accident is straightforward. Decisions making on whether to build, operate, or modify a hydrogen application system is easier once the total risk is determined and the subsequent risk acceptance procedure is performed. With the total risk determined, the risk acceptance procedure is applied, facilitating in decisions making on whether to build, operate, or modify the hydrogen application system (Shen et al., 2018).

As the hydrogen industry grows, various data-driven approach methods have been studied to risk inform on operational and design requirements of hydrogen systems, providing a baseline for the guidelines for the hydrogen systems design and operational parameters. The CFD simulations of different accidental scenarios provide a comprehensive understanding of hydrogen physics, which is required for the development of RCS. These codes are based on the hazards such as the dispersion of hydrogen and understanding the consequences of events like the heat-flux of hydrogen flame discussed in Section 4.

While most hydrogen QRAs follow the steps shown in Fig. 6, they adopt different models for each step and the integration between the steps. Modelling root causes can be conducted by (i) traditional QRA models such as event trees, fault trees, and parts counts (LaChance, 2009), (ii) extended QRA techniques by adopting Bayesian Networks (Haugom and Friis-Hansen, 2011), and (iii) advanced QRA approaches, which are based on dynamic probabilistic safety assessment (PSA) including Discrete Dynamic Event Trees, Event Sequence Diagrams, various sampling and simulation-based QRA and PSA models (Ham et al., 2011; Hansen and Middha, 2008).

LaChance (2009) applied QRA methods to assess the minimum distances separating different targets, including facilities, structure, and people, from the consequences of potential accidents related to the operation of a hydrogen refuelling facility. They found that the key influencing parameters for selecting distances are the availability of mitigation features (e.g., leakage detection), isolation features, and operating conditions such as volume and pressure. Their findings affected the development of guidance for the siting of hydrogen fueling stations in the United States, which was established in the National Fire Protection Agency's Hydrogen Technologies Code (NFPA 2). This becomes more challenging for hydrogen as a transportation fuel due to the involvement of oil and gas and nuclear power industries. Groth et al. (2012) used experimental data set and CFD simulation results for a QRA to understand the safety of indoor gaseous hydrogen fuelling of HFCV. Their findings indicated that the proper application of systematic QRA would lead to the seldom occurrence of fatalities within the HFCV industry.

Gye et al. (2019) proposed a QRA for H_2 refuelling stations within urban areas with high congestion between the equipment and instruments. The major hazards were leakages from the dispenser and tube-trailer and the possible tube-trailer explosion based on their investigations. To enhance safety, more mitigation scenarios, including the addition of more safety barrier systems, must be applied on the dispenser and compressor to prevent continuing accidental hydrogen release. Jafari et al. (2012) conducted a QRA to analyse risks of the hydrogen production process imposed on the neighbourhood, applying validated instrumentation and techniques. Based on the obtained

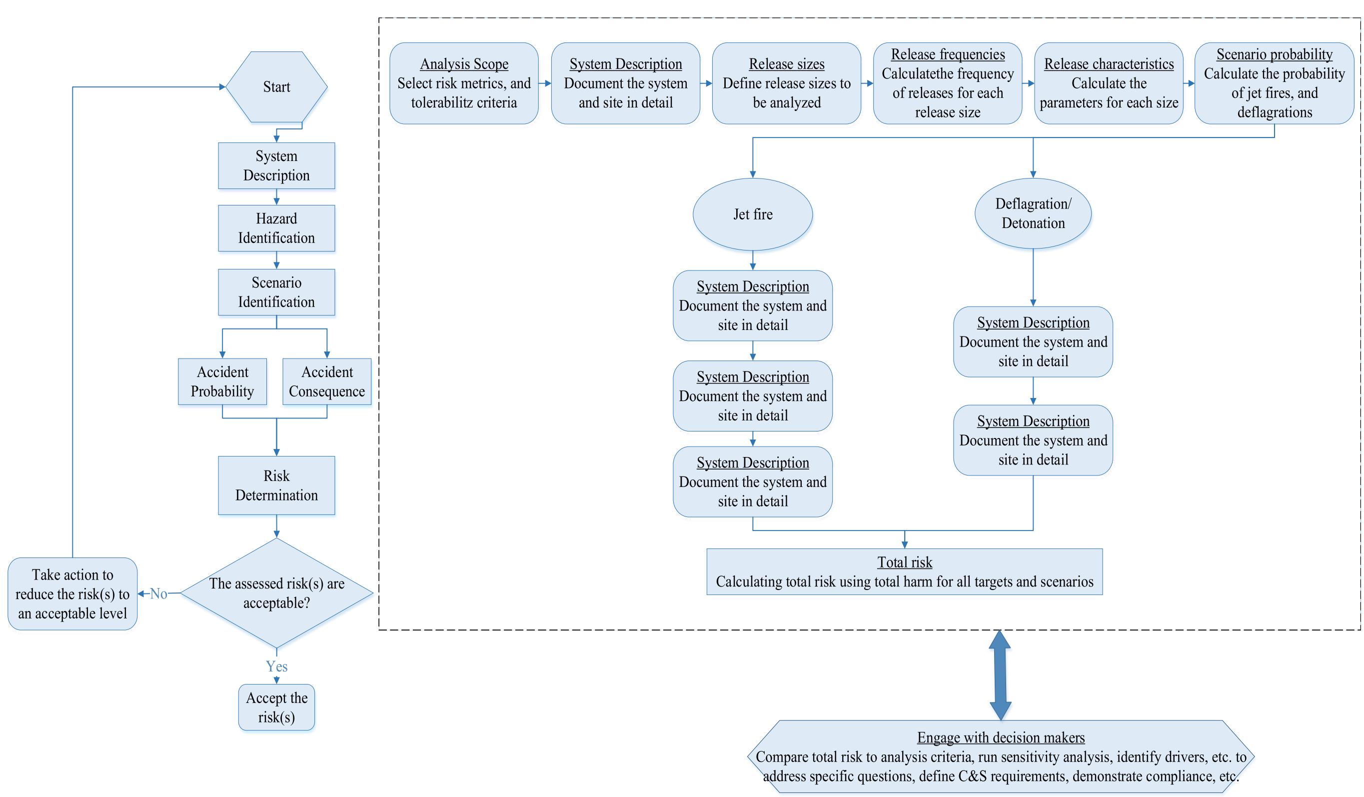

Fig. 6. The hazard identification and risk assessment procedure (Crowl and Jo, 2007) and QRA procedure for decision support in hydrogen applications (San Marchi et al., 2017).

results, the maximum fatality (26 persons) was reported for jet fire result from a rupture in Desulphurization reactors, which affected the highest zone of 5102 m^2. The safe distance, maximum radiation, and lethality radius from this occurrence were 225 m, 370 kW/m^2, and 140 m, respectively. The most hazardous flash fire resulted from a full bore rupture in Reformer. The social risks of hydrogen purification absorbers, reformer and desulphurization reactor and the individual risks of the heat exchanger and reformer were revealed to be undesirable (Shi et al., 2020). A QRA on onboard hydrogen storage subjected to fire was performed by Dadashzadeh et al. (2018). They assessed the fatality risk of a vehicle per year for hydrogen fuel cell cars. They also calculated the risk concerning cost per accident. Based on their survey, increasing the storage vessel's resistance rate against fire was revealed to remarkably decrease the acceptable level of risk.

5.1. The inherent safety of hydrogen storage systems

The safe performance of hydrogen-related technologies can be evaluated by a promising approach which is analyzing the embedded hazards using the inherent safety guidewords of "simplification", "moderation", "substitution", and "minimization" (Landucci et al., 2008). Inherent safety assessment has been identified as an appropriate indicator for the evaluation of the possible effects on health during the design of the energy systems since the selection of process conditions and conversion technologies can be classified based on their intrinsic characteristics (Landucci et al., 2010). Tugnoli et al. (2009) developed a new quantitative methodology for assessing the inherent safety of process flow diagrams in the early stages of design. Based on a series of key performance indicators (KPIs), a metric is presented as the output for quantifying the process scheme's inherent safety fingerprint. The objective of each KPI is the assessment of a particular aspect of the inherent safety fingerprint of the system. The suggested KPIs make it possible to score the inherent safety values of limitation, simplification, attenuation, substitution, and minimization of effects (Khan and Amyotte, 2003; Kletz, 2003). For quantifying the hazards associated with process conditions, materials, and equipment characteristics, they used physical parameters. The analysis focuses on identifying and modelling possible incidence consequences for equipment and humans. A clear and accurate image from the inherent safety performance can be provided by adopting tangible factors based on consequence modelling.

The anticipated inherent safety performance for technologies of hydrogen storage was investigated by Landucci et al. (2008). They considered different sizes for storage, associated with several industrial applications. According to the results of the comparative analysis, the novel hydrogen storage technologies always have lower potential hazards. This is mostly due to the employment of concepts underlying the inherent safety guideword "substitution" because hydrogen was stored as a hydride with fewer hazards in these replacement technologies. Furthermore, compared to conventional technologies, the operative conditions for storage systems of complex hydrides and metal hydrides containment structures are less severe, underlying the inherent safety "substitution" guideword. However, in the case of considering credit parameters of loss of containment (LOC) incidents, lower safety performances are exhibited by novel technologies, especially by metal hydrides storage in comparison with conventional storage processes, according to the standard equipment reliability data. They also developed an innovative consequence-based methodology for assessing the inherent safety of the envisaged hydrogen production, transport, and application systems for vehicle purposes (Landucci et al., 2010). They assessed different scenarios for the hydrogen system chain from production on a large scale to end utilisation. In their analysis, the transport and delivery of hydrogen were also considered. A set of KPIs was used to quantify the inherent safety fingerprint of every system. They also conducted comparisons with proposed technologies for the utilisation of other fuels like natural gas and LPG. The hazards of compressed hydrogen-powered cars were similar, but reference new hydrogen technologies showed a possibly greater level of safety. As a result, moving toward inherently safer technologies can have a significant effect on the safety improvement of hydrogen cars, leading to a considerable increase in the entire hydrogen system safety performance.

The conceptual design of distributed energy systems was investigated by Fonseca et al. (2021) using a multi-objective optimisation strategy for addressing the social, environmental, and economic aspects in the design of energy systems. They first considered and evaluated the inherent safety indicators and the water consumption with two single-objective optimisation problems for enhancing the evaluation of the social and environmental dimensions of sustainability. To conduct the multi-objective analysis, they utilised a framework containing inherent safety index, grid dependence, water consumption, CO_2 emissions annualized cost. They suggested four optimisation cases involving various sustainability indicator combinations for conducting a comprehensive and thorough analysis. They identified a compromise between the objective functions and explored the obtained Based on the results, values between 27.8 and 70.2 m^3 H_2O/GWh for water consumption, 10.6 and 68.5 $kgCO_2$/MWh for the CO_2 emissions, 0.37 and 0.63 €/kWh for the energy cost were obtained.

6. Conclusions

In recent years, the use of hydrogen in different sectors has increased. However, for further development of hydrogen technology and reaching the increased public acceptance, increasing operational safety is one of the crucial parameters that has drawn the attention of the ones who are active in this field. In this regard, it is extremely important to predict the potential hazards, develop relevant standards to determine the allowable operating ranges, and provide risk-free equipment and guidelines aiming to achieve very safe operation.

This paper provided a comprehensive review on applications of hydrogen in the transport and energy sector, its storage and transmission, and safety aspects of hydrogen handling with a special focus on CFD modelling as a suitable method for predicting hazardous scenarios in hydrogen applications. Recent studies in which the CFD techniques were applied for modelling hydrogen dispersion, jet fires, explosions, and other safety areas have been summarised and presented. With the advancement of CFD tools and research in this area, the role of CFD modelling in consequence analyses, hazard predictions, safe design, planning for mitigation measures, and risk assessments has become more prominent. Despite some limitations, the possibility of simulating complicated geometries and regenerating real-world boundary conditions of various problems, and eliminating high experimental costs, especially the possibility of simulating phenomena for which there are limitations in experimental testing, make CFD modelling a promising method in the field of hydrogen safety research. Finally, in the problems related to hydrogen safety, the connection between experimental, theoretical, and numerical analyses and industry practices can be reliably provided by risk analysis, which was also discussed in this study.

Author contribution

The authors contributed equally to this review paper.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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