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Performance Analysis and Safety Aspects of Hydrogen Refueling Infrastructures

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Hydrogen is assuming a pivotal role in the energy sector, intending to lead the decarbonization and overcome the fossil fuel use. In evaluating its key applications, the role of hydrogen in mobility stands out. It could transform one of the most polluting sectors, drastically reducing emissions without changing the drivers' needs. In this perspective, the focus should be placed on hydrogen refueling infrastructures, which are a key factor, along with fuel cell vehicles, for extending the hydrogen chain in the mobility sector. Given this, the study analyzes the hydrogen refueling station performance, investigating the hydrogen flow features, and estimating the evolution of pressure and temperature within the vehicle tank. An ad-hoc model for hydrogen performance analysis is used by customizing its main blocks. In addition, the main safety aspects of the hydrogen refueling stations are evaluated. The behavior of each component of the refueling infrastructure, such as hydrogen storage tanks, compressors, and cooling systems, is examined and introduced in the model, characterizing the whole system. The model is then validated by comparing its performance with experimental data. The results show the pressure, temperature, and mass flow rate between the dispenser and the vehicle tank. These findings could help boost hydrogen use in mobility since crucial aspects are investigated and important information is provided for promising integrated systems, based on the interconnection between infrastructures and vehicles.

1. Introduction

Climate change requires urgent attention and alternative energy sources are needed. Governments and industries are recognizing hydrogen as a sustainable vector, fundamental to decarbonizing hard-to-abate sectors, such as the transport sector. A joint effort of governments and industries is essential to guarantee the rollout of hydrogen systems in the transport sector. Therefore, along with the extensive fuel cell vehicle use, a widespread network of hydrogen refueling stations (HRSs) is required for an adequate and smooth transition towards zero-emission transport. HRSs are highly complex and integrated infrastructures, where numerous modules permit, according to the topology of the station, the hydrogen production, storage, compression, cooling, and dispensing. The physicochemical properties of hydrogen in ambient conditions require high compression levels (up to 70 MPa) to reach driving ranges comparable with traditional vehicles. Along with the compression, elevated mass flow rates and low temperatures are needed to achieve a fast refueling (of approximately 5 min per vehicle) and a high state of charge of the tank (over 90%) (Blazquez-Diaz, 2019).

To satisfy these requirements and guarantee suitable operations, performance, and safety aspects should be carefully considered. The aim is to perform a refueling process that satisfies the customers' needs without compromising safety. Concerning the technical performance, further technology advancements are necessary: the Clean Hydrogen Partnership (2022) reports that, at present, the HRS consumption is approximately 5

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kWh/kg for delivering hydrogen at 70 MPa and it should be almost halved by 2030, reaching 3 kWh/kg. Consequently, technological improvements move together with safety advancements, such as accurate consequence analyses, evaluations of human error, and ad-hoc inspection and maintenance strategies. In this way, the mean time between failures can be extended, going beyond another limitation cited in (Clean Hydrogen Partnership, 2022), which requires to triple this parameter, reaching a value of 168 days by 2030.

To meet this goal, simulation models are crucial tools for designing an HRS layout, sizing each component, testing the energy performance, implementing new control strategies, calculating the safety distances, and optimizing the positioning of safety barriers. In this field, the DISCHA engineering tool is a powerful and highly flexible software for investigating the thermodynamic performance of hydrogen transfer processes. DISCHA allows to analyze different configurations and investigate all the parameters of the station and vehicle, evaluating the evolution of pressure, temperature, and mass flow rate during the hydrogen transfer process. In this paper, both energy and safety aspects in HRSs are evaluated during H_2 transferring. An overview of the main elements and methods that characterize the HRS operations and performance is provided. In addition, a simplified fueling application is simulated in the DISCHA tool, highlighting the performances of the station and vehicle tank and analyzing the safety aspects.

2. Modeling of hydrogen transferring

Hydrogen refueling stations have a crucial role in the development of a hydrogen-based transport sector with low environmental impact. HRSs are highly complex systems, composed of different devices, depending on the configuration considered, and thoroughly controlled to respect the protocols during refueling processes (Genovese and Fragiacomo, 2023). Regarding the complexity of the infrastructure, an HRS can be divided into three different macro-areas: production-supply, compression-storage, and cooling-dispensing. The production-supply section depends on the hydrogen supply method. If the hydrogen is produced within the HRS, through electrolyzers or steam methane reforming plants, it is referred to as on-site HRSs. On the contrary, in the off-site HRSs, the hydrogen is produced in external plants and delivered to the station by tube trailers or pipelines. The compression-storage section plays multiple roles. It includes the storage systems, composed of several hydrogen storage tanks, and employs compressors at medium or high pressure (up to 30 and 100 MPa, respectively), depending on the dispensing process. In detail, two different dispensing methods can be considered:

- Cascade process, if the refueling is achieved through the pressure difference between the station tank and the vehicle tank without using a compressor;
- Direct process, where a compressor allows the refueling, following the users' requests.

Finally, the cooling-dispensing stage performs the last phases of the refueling process. It cools down the hydrogen flow at different temperatures (ranging from 0 °C to -40 °C). This step allows for avoiding thermal issues in the vehicle tank such as overheating and compromising the safety of the tank (Zhao B., 2022). The last process concerns the refueling of the vehicle at different pressure levels (the most used are 35 MPa and 70 MPa), according to the tank typology.

The high complexity of the HRS is also due to the control strategy, which permits proper refueling. During this process, different variables, above all pressure, temperature, and mass flow rate, are continuously measured and controlled to guarantee safe operations, while reaching a high state of charge of the tank in a reasonable time. Instructions, conditions, and values of several parameters are collected and reported in codes and protocols. The SAE J2601 (SAE, 2020) is the most used protocol. It classifies the HRSs according to the cooling temperature and provides numerous operative lookup tables depending on the initial conditions and the features of the HRS and vehicle tank. An average pressure ramp rate is imposed for a suitable refueling in a proper time. If these specific instructions are not respected, the refueling process is aborted.

Starting from these considerations, several models have been implemented to investigate HRSs' performances. Reddi et al. (2014) presented H2SCOPE, a tool for evaluating the technical and economic performances of an HRS and testing the operations with different fueling profiles. Kavadias et al. (2018) developed an optimization sizing tool for HRS design, considering the refueling of a scooter fleet composed of 263 units. Riedl (2020) implemented and validated a mathematical model for HRS performance analysis, reaching an overall error below 0.5% compared to real data. In (Schäfer and Klein, 2019), a Matlab-based model for HRS with liquid storage is built, evaluating the main performance parameters, and obtaining a maximum consumption of the heat exchanger of 0.4 kWh/kg. Piraino et al. (2021) modeled a techno-economical tool for an integrated system composed of refueling infrastructure and a hydrogen hybrid fuel cell train. They demonstrated the feasibility and benefits of this technology, with a fuel cell efficiency higher than 47% and a facility efficiency of over 50%. In (Blazquez-Diaz, 2019), an HRS model capable of finding an optimal design from an economical point of view and optimizing the state of charge of the vehicle tank and the configuration of the banks, was built in a Matlab environment.

3. Safety of hydrogen refueling stations

The development of an extensive refueling infrastructure for fuel cell vehicles depends on the design of reliable components, the operational safety of the refueling process, and the public perception regarding this technology. Despite the relatively low market penetration of HRSs, tens incidents and accidents involved these infrastructures. Hydrogen leaks from pipes, fittings, compressors, and dispensers can occur and result in fire and explosions if not promptly detected (Campari et al., 2023a). A major leak from a high-pressure storage tank occurred in 2019 at the refueling station in Kjørbo (Norway) due to untightened bolts. This incident not only caused a significant financial loss for the company involved but also determined the loss of trust of the public regarding the safe use of hydrogen technologies. Hence, the risk associated with HRSs should be kept as low as reasonably practicable by designing ad-hoc safety barriers to prevent leakages or mitigate the consequences of potential unintended releases.

The hazards faced by operators and equipment are related to the unique hydrogen properties in terms of low ignition energy, broad flammability range, and capability of permeating and embrittling most structural materials. The operational safety of the hydrogen refueling infrastructure can be ensured by defining the hazards, guaranteeing components' integrity, providing proper ventilation of enclosed spaces, ensuring leak detection and isolation, and properly training the operators. The risk of fire, detonation, deflagration, overpressure, and exposure to extremely low temperatures can be effectively mitigated through risk assessment techniques (Vereš et al., 2022). This process, summarized in Figure 1, includes risk identification, evaluation of probabilities and consequences of the undesired events, risk evaluation, and eventually the implementation of mitigation measures if the risk level is deemed unacceptable.

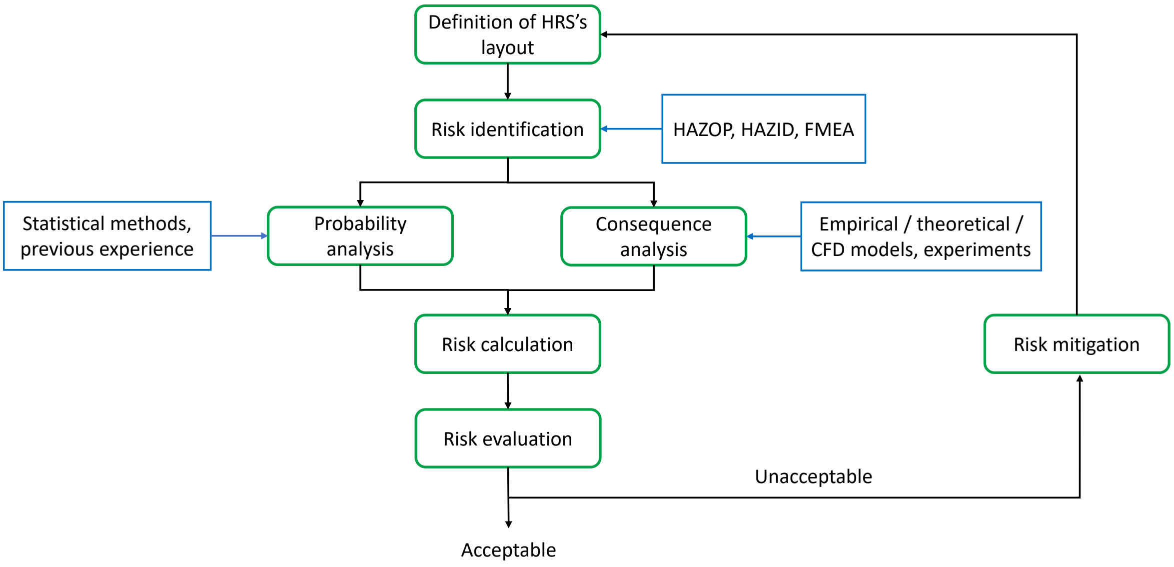

Figure 1: Typical risk assessment for a hydrogen refueling station (abbreviations: HAZID: HAZard IDentification; HAZOP: HAZard and OPerability study; FMEA: Failure Mode and Effects Analysis)

The risk identification allows one to foresee any accident scenario likely to occur in the HRS. This step relies on structured and systematic techniques for identifying potential hazards in the systems, such as the Hazards and Operability Analysis (HAZOP), Hazard Identification Study (HAZID), and Failure Mode and Effects Analysis (FMEA). Then, the probabilities of any undesired event should be estimated through statistical methods and incident and accident databases such as HIAD 2.0 or H_2Tools (Campari et al., 2023a). The consequences of each credible scenario can be evaluated through empirical and theoretical models. CFD tools allow the analysis of the physical properties of the release but have high computational costs. Robust source models for the leakage (e.g. DISCHA, see Section 4) are paramount to assessing the consequences of jet fires, flash fires, vapor cloud explosions, etc. All these computational models should be validated by test results. The risk can be calculated by combining the frequencies and consequences of each undesired event. Hence, this value should be compared with predefined thresholds based on expert judgments or safety guidelines. If the risk is deemed unacceptable, the layout of the HRS should be integrated with safety barriers to reduce the likelihood of undesired events and mitigate their consequences. The selection of hydrogen-compatible materials can reduce the risk of hydrogen embrittlement. Austenitic steels and high-strength composite materials are commonly used for high-pressure equipment since their mechanical properties are slightly affected by hydrogen. Together with an inherently safe component design (e.g., the installation of emergency breakaway couplings), the probability of failure can be dramatically reduced by operational measures, such as inspection and maintenance activities (Campari et al., 2024). If leakages occur, it is critical to mitigate them. Concentration sensors can identify any unintended release before reaching the lower flammability limit and allow the emergency shutdown of the HRS. Ultrasonic leak detectors are a promising option for outdoor areas where hydrogen gas is handled and stored at high-pressures (Campari et al., 2023b). Finally, a proper training of the operators can dramatically reduce the occurrence of human errors during normal operations and maintenance activities.

4. DISCHA Engineering tool

Different models have been developed to simulate and optimize the operations of hydrogen refueling stations, as reported in Section 2. Among them, an innovative tool named DISCHA is presented. The potential of this tool for investigating hydrogen refueling processes is the main goal of this paper. DISCHA is a highly powerful and flexible tool, based on Fortran language with a Python interface. It can perform different tasks, such as:

- Characterize the thermodynamic state of different substances, such as H_2, para-H_2, CH_4, H_2O, CO_2, and NH_3, defining the physical properties in gaseous, liquid, supercritical, or two-phase conditions, using different equations of state (e.g., the Helmholtz free energy one);
- Investigate the discharge process from a storage tank (gaseous or two-phase) through an offloading line, both in steady state and transient conditions;
- Analyze the evolution of the fluid conditions during a tank-to-tank transfer;
- Evaluate the conditions of fictitious nozzles for fluid releases.

The main inputs concerning the initial thermodynamic conditions and the geometric specifications that can be inserted in DISCHA are listed in Table 1.

Table 1: Parameters used as input in DISCHA

Input types	Parameters
Thermodynamic	Pressure, temperature, density, vapor quality, enthalpy, entropy
Geometric	Volume, length, diameter

The DISCHA tool is continuously upgraded to enhance the accuracy of the simulation for increasingly complex applications. Firstly, it was used to estimate the hydrogen release conditions, simulating the depressurization process between stagnation and bubbly flow regimes (Venetsanos, 2018). In this study, the model was validated considering the NASA hydrogen critical flow experiments, achieving a 10% maximum overestimation of the throat mass fluxes and a 50% maximum underestimation of the throat-to-stagnation pressure ratios. In (Venetsanos, 2019), the DISCHA tool analyzed all the main thermodynamic parameters during a steady state two-phase choked flow of liquefied hydrogen through a discharge line with a variable cross-section. In (Venetsanos et al., 2021a) and (Venetsanos et al., 2021b), this tool was used to model the flow features during the discharge phase and the blowdown in a simplified hydrogen system based on tanks and lines, considering experimental data collected during the PRESLHY project. Regarding the blowdown scenario, the results obtained were in line with the experimental data and can be considered acceptable for the application tested, even if the tank pressure and temperature were underestimated. In the discharge scenario, three two-phase models were tested, and the Homogeneous Equilibrium Mixture model showed satisfactory results with a mass flow rate error between -3.3% and 9.6%. Future implementations of the DISCHA tool will concern the transfer of liquid hydrogen, within the ELVHYS project, which aims to enhance the safety of liquid hydrogen transfer technologies for mobile applications (Ustolin et al., 2023).

4.1 Example of H_2 transfer simulation

A simplified refueling process is presented as a case study. The simplified system is composed of a supply tank and a receiver tank, connected by a pipe. The initial conditions and the technical characteristics of the components are reported in Table 2. The simulation time is 300 s, in line with a standard refueling period. The results obtained are shown in Figure 2. Given its large size, the supply tank slightly decreases its pressure, reaching approximately 80 MPa (Figure 2(a)). A total of 3.88 kg of hydrogen is transferred from the supply tank to the receiver one, accounting only for 2% of the hydrogen contained in the tank. The mass flow rate is quite variable (Figure 2(b)), reaching the maximum value during the first phase of the refueling process (almost 18 g/s), decreasing smoothly over time, and arriving at a value near 0 g/s at the end of the process.

Regarding the receiver tank, its pressure (Figure 2(c)) varies in a wide interval, reaching approximately 80 MPa; while the temperature within the tank is subjected to some oscillations, ranging between 350 K and 370 K (Figure 2(d)).

Table 2: Initial conditions of the case study analyzed

	Supply tank	Vehicle tank	Pipe
Volume (m^3)	4.0	0.1	-
Initial mass (kg)	178.00	0.08	-
Initial pressure (MPa)	85	1	-
Length (m)	-	-	20
Diameter (mm)	-	-	2.5

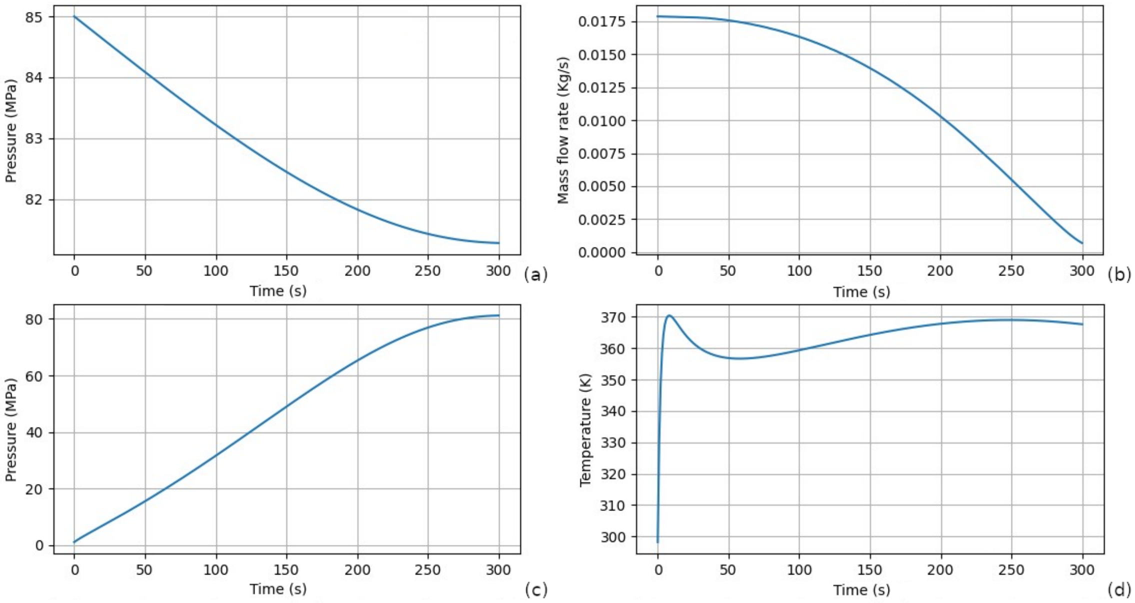

Figure 2: Simulation results: (a) Supply tank pressure; (b) H2 mass flow rate; (c) Receiver tank pressure; (d) Receiver tank temperature

It should be underlined that this example refers to a gaseous hydrogen transfer between two tanks, which is quite far from modeling a refueling process since fundamental components, such as a cooling system and controlled pressure valves, are neglected and the detailed flow rate control is not performed. For this reason, the mass flow rate has an inappropriate trend and the temperature is excessively elevated for standard refueling, according to the existing protocols. In fact, the temperature must be kept below 85 °C and the average pressure ramp rate should be around 1.5 MPa/s for standard ambient conditions to respect the safety limits and suitable refueling times (SAE, 2020).

5. Conclusion

In this paper, the performance and safety aspects of hydrogen refueling infrastructures were analyzed, evaluating the station components, highlighting the potential of modeling for consequence analyses, and testing a hydrogen transfer between station and vehicle through the DISCHA software. Critical aspects, in terms of thermodynamics and safety, were highlighted to improve HRS operations. Through the DISCHA tool, energy parameters were analyzed, such as pressure, temperature, and mass flow rate. The refueling simulation was performed with 3.88 kg of hydrogen in 300 s, reaching a vehicle tank's pressure of approximately 80 MPa. However, the simplified configuration, which did not consider the cooling system and the valves to control the mass flow rate, reached an elevated temperature, beyond 85 °C. This value is above the limit imposed by the HRS protocols. The results achieved show the promising features of DISCHA software, as a flexible and versatile tool for energy and safety analysis. It should be highlighted that DISCHA is under development, and new features are going to be implemented. In addition, a validation process with real data from HRS experimental tests is necessary. For these reasons, future works will concern further tests on new configurations with other components present in a hydrogen infrastructure.

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