



Hydrogen Component Leak Rate Quantification for System Risk and Reliability Assessment through QRA and PHM Frameworks

Preprint

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HYDROGEN COMPONENT LEAK RATE QUANTIFICATION FOR SYSTEM RISK AND RELIABILITY ASSESSMENT THROUGH QRA AND PHM FRAMEWORKS

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ABSTRACT

The National Renewable Energy Laboratory's (NREL) Hydrogen Safety Research and Development (HSR&D) program in collaboration with the University of Maryland's Systems Risk and Reliability Analysis Laboratory (SyRRA) are working to improve reliability and reduce risk in hydrogen systems. This approach strives to use quantitative data on component leaks and failures, together with Prognosis and Health Management (PHM), and Quantitative Risk Assessment (QRA) to identify at-risk components, reduce component failures and downtime, and predict when components require maintenance.

Hydrogen component failures increase facility maintenance cost, facility downtime, and reduce public acceptance of hydrogen technologies, ultimately increasing facility size and cost because of conservative design requirements. Leaks are a predominant failure mode for hydrogen components. However, uncertainties in the amount of hydrogen emitted from leaking components and the frequency of those failure events limit the understanding of the risks that they present under real-world operational conditions. NREL has deployed a test fixture, the Leak Rate Quantification Apparatus (LRQA), to quantify the mass flow rate of leaking gases from medium and high-pressure components that have failed while in service. Quantitative hydrogen leak rate data from this system could ultimately be used to better inform risk assessment and Regulation Codes and Standards (RCS).

Parallel activity explores the use of PHM and QRA techniques to assess and reduce risk, thereby improving safety and reliability of hydrogen systems. The results of QRAs could further provide a systematic and science-based foundation for the design and implementation of RCS, as in the latest versions of the NFPA 2 code for gaseous hydrogen stations. Alternatively, data-driven techniques of PHM could provide new damage diagnosis and health-state prognosis tools. This research will help end users, station owners and operators, and regulatory bodies move towards risk-informed preventative maintenance versus emergency corrective maintenance, reducing cost and improving reliability. Predictive modelling of failures could improve safety and affect RCS requirements such as setback distances at liquid hydrogen fueling sites. The combination of leak rate quantification research, PHM, and QRA can lead to better informed models enabling data-based decision to be made for hydrogen system safety improvements.

1. INTRODUCTION

The worldwide use of hydrogen as a green energy storage mechanism is increasing. This multiuse chemical can be used in transportation, industrial processes, integrate with the natural gas infrastructure, and support the electrical grid. The US Department of Energy's H2@Scale initiative captures the potential uses and widespread impact of hydrogen [1]. Regulation codes and standards (RCS) and safety research must continue to be developed and modernized to enable technology adoption and the growth of the hydrogen economy. Advanced methods of risk and reliability analysis are needed to support the growth and expanding adoption of hydrogen technologies [2]. The National Renewable Energy Laboratory (NREL) in collaboration with the University of Maryland (UMD) are establishing a scientific basis for risk and reliability analysis through integrated work with data collection, model development and stakeholder engagement.

Quantitative Risk Assessment (QRA) frameworks provide a systematic and science-based foundation for the design and implementation of RCS and have been used in key hydrogen RCS including multiple aspects of both the U.S. National Fire Protection Association NFPA 2 code for gaseous hydrogen (GH₂) stations and the international standard ISO 19880-1 [3], [4]. Currently, the limited availability of reliability and safety data for liquid hydrogen systems represent a barrier to fully employ risk-informed tools such as QRA. NREL has designed a test system for leak rate quantification measurements to ultimately allow risk reduction credits through Quantitative Risk Assessment (QRA) in RCS. Although extensive modelling and analytic studies have been completed for hydrogen leaks in fueling applications, the corpus of experimental studies specific to hydrogen fueling stations is still limited [5]–[7]. This leaves models to depend on experimental data collected in different conditions, often in the fossil fuel or aerospace industries. The characterization of the leaks of actual failed gaseous hydrogen components looks to begin to fill that gap while providing risk information that can be leveraged by QRA.

Recent research trends in Prognosis and Health Management (PHM) and data monitoring analysis have focused on proactive asset management, as well as operation and maintenance scheduling optimization in complex systems based on the use of sensor and condition-monitoring data [8]. Given the wide variety of PHM applications in complex engineering systems, these frameworks could provide valuable tools for expanding available risk and reliability analysis for hydrogen systems. This work presents the identified opportunities for condition-monitoring data collection for fault diagnosis in these systems.

The structure of this paper is as follows. Section 2 details NREL’s Leak Rate Quantification Apparatus (LRQA) including design parameters, system validation, and results from initial testing of failed hydrogen components. Section 3 presents the identified data needs for both QRA and PHM applications in liquid hydrogen systems. Section 4 discusses the planned integration of these efforts. Section 5 presents the main conclusions of this work.

2. HYDROGEN COMPONENT LEAK RATE QUANTIFICATION

The LRQA has been deployed for testing at NREL to capture quantitative data on the failures of hydrogen components to ultimately allow risk reduction credits through QRA in RCS. The risk associated with leaks and the actual behaviour of a real leak has the potential to inform risk assessment work (PHM and QRA), and better inform the safety community providing quantitative inputs to modelling and analysis work [9], [10]. The LRQA takes components that have failed (are leaking) and redeploy these components into a system to measure the mass flow rate of the leak. When hydrogen components fail a leak is detected via system level monitoring (e.g., pressure sensors), wide area monitoring by hydrogen sensors, audible or ultrasonic detection, and or operator inspection with handheld hydrogen detectors or soap bubble leak detection. Once a leak is detected action must be taken to monitor and repair the failure. Common component failure scenarios have been identified but the actual flow rate of a variety of different leaks is not as well understood [3], [10]. Some of guiding questions of the experimental research with the LRQA is what is the mass flow rate of a leak? What is the hazard that is created? Is this leak likely to change in size based on system pressure, based on temperature, based on component lifetime? Do these leaks behave as expected or assumed for the purpose of leak modelling?

2.1. LRQA System Description

The LRQA is designed to measure the mass flow rate of a leak from a failed gaseous hydrogen component. The failed component will be referred to as the device under test (DUT). Critical components on the LRQA are double block and bleed isolation valves, a 1.15 L pressure vessel rated up to 89.63 MPa, and a pressure transducer and thermocouple located at the pressure vessel and near the DUT. As shown in Fig. 1, the DUT is deployed on top of a shielded tower. Pressurized gas is provided to the system either from high pressure hydrogen storage or gas cylinders connected to a small gas booster. As a stop gap measure, during system upgrades to enable heavy duty vehicle fueling

research at the Hydrogen Infrastructure Testing and Research Facility (HITRF), the LRQA apparatus has had two deployment locations (<https://www.nrel.gov/hydrogen/hitrf.html>) [11]. The original deployment location was designed for testing with hydrogen gas. The current temporary location, in which the gas booster is used for pressurization, can only use inert gas (nitrogen and helium) for testing. The LRQA will be returned to the hydrogen station pad following construction for future testing with hydrogen gas.



Figure 1. LRQA in its original deployment location. Photo by K. Hartmann (NREL)

The standard test sequence begins with pressurizing the small pressure vessel on the LRQA. The volume of the pressure vessel is known, and the pressure and temperature of the gas are measured with calibrated transducers. The mass of gas in the system is calculated using the equations of state that are built into EES [12]–[15]. After allowing the pressure and temperature of the pressure vessel to stabilize, a pneumatic valve is opened, allowing gas to flow to the DUT. The pressure and temperature are measured near the DUT and at the pressure vessel and a mass flow rate is calculated at each timestep at each location. The mass flow rate can be related to an equivalent orifice diameter using the standard equations from ISO 9300: *Measurement of Gas Flow by Means of Critical Flow Venturi Nozzles* [16]. For leaks where the geometry is unknown, all components except calibration orifices, the discharge coefficient was assumed to be 0.9 based on typical values that are listed in ISO 9300. This assumption is used to convert the $C'_d * A$ values that are calculated from the mass flow rate into equivalent nozzle diameters that are more easily conceptualized by experts. To incorporate these data into models, the $C'_d * A$ values can be used directly to estimate mass flow rates at various conditions rather than using the diameter itself via the following equation.

$$q_m = \frac{m_2 - m_1}{t_2 - t_1} = \frac{A_{nt} * C'_d * C^* * p_0}{R_g * T_0} \quad (1)$$

where q_m – mass flow rate, kg/s; m_2 – mass final, kg; m_1 – mass initial, kg; t_2 – time final, s; t_1 – time initial, s; A_{nt} – hydraulic area, m²; C'_d - discharge coefficient; C^* - real critical flow function; p_0 – stagnation pressure, Pa; R_g – specific gas constant, J/kg-K; T_0 – stagnation temperature, K [16].

$$A_{nt} = \frac{\pi}{4} * d_{nt}^2 \quad (2)$$

where d_{nt} – hydraulic diameter of a circular orifice with similar flow characteristics, m.

$$C^* = \rho^* * a^* * \frac{\sqrt{R * T_0}}{p_0 * \sqrt{M_g}} \quad (3)$$

where ρ^* – density, kg/m^3 ; a^* - local sound speed, m/s ; R – universal gas constant, J/kmol-K ; T_0 – stagnation temperature, K ; p_0 – stagnation pressure; M_g – molecular mass of the fluid, kg/kmol ; superscript * indicates conditions at the nozzle throat [17].

2.2. LRQA System Calibration

System calibration has been completed with an orifice that has a throat diameter of 0.28 mm. This was a standard production orifice which was calibrated at the Colorado Engineering Experiment Station Incorporated (CEESI) on air. The left side of Fig. 2 shows the calculated equivalent orifice versus Reynold’s number obtained from system validation testing with the calibrated orifice. The right image in Fig. 2 shows the population distribution function of the calculated orifice vs the calculated orifice size. Data shown in Fig. 2 is from both deployment locations. The data matches well with the known orifice size with the mean of the calculated orifice being 0.25 mm compared to the known orifice size of 0.28 mm diameter. Agreement is also shown between the different types of gas, nitrogen, helium, and hydrogen. The discharge coefficient of the calibrated orifice was provided by CEESI along with the calibration documentation and was measured to be 0.883 ± 0.002 . To validate the assumption of using a discharge coefficient of 0.9 orifice data shown in Fig. 2 was calculated using the assumed discharge coefficient of 0.9.

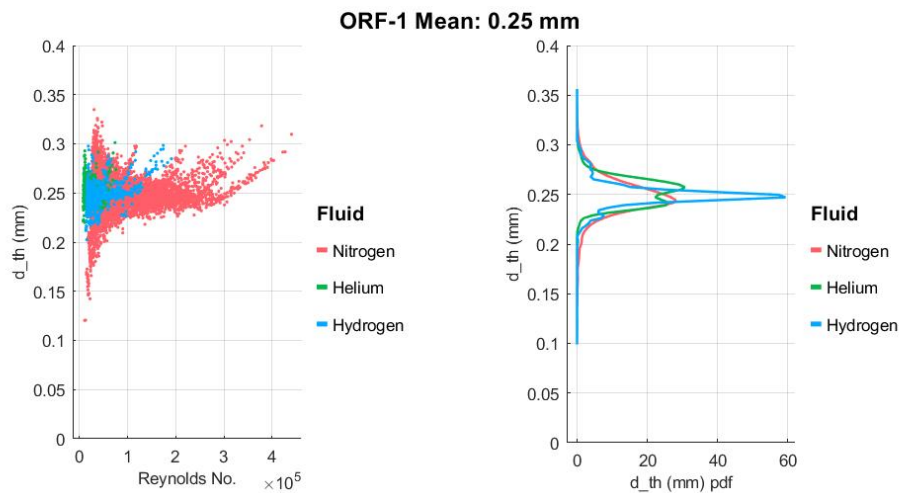


Figure 2. System validation data showing good agreement between the average calculated orifice size of 0.25 mm and the known calibrated orifice size of 0.28 mm throat diameter.

2.3. Results

The two subcategories of component failure modes that are being investigated are leak through and leak out. These two types of leaks create different risk scenarios. Leak through, captures leaks where hydrogen is not released to the atmosphere, remains in the tubing but flows past valves or other blocks (e.g., valve stem damage). These leaks lead to the presence of hydrogen gas in areas of the system where it is not expected. A leak out, is a failure mode where gas is released to the atmosphere (e.g., leak out of a weep hole due to a damaged O-ring). Depending on the leak location and system geometry a leak out has a higher risk due to ignition potential [9], [18]. Using the LRQA both types of leaks have been measured. A normally open (NO), air operated valve (AOV) was found to be leaking through when pneumatically closed even following valve stem adjustment. Results from this valve are shown in Fig. 3. This valve was found to have a mean orifice size of 0.08 mm with nitrogen and 0.09 mm with hydrogen.

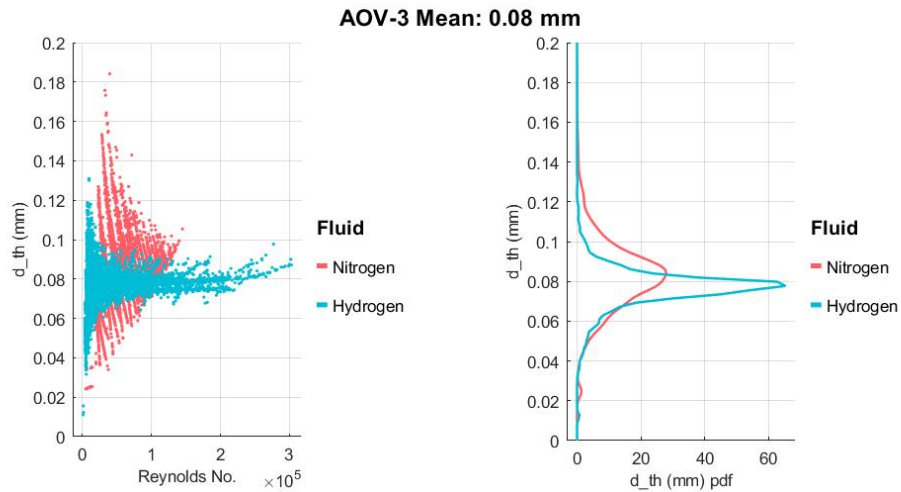


Figure 3. Data showing the equivalent orifice size of an AOV that is leaking through.

Another failed component, a soft seat check valve, was found to be leaking out of the weep hole on the component body when tested with helium. This leak could be due to failure or damage to the O-ring. Results from this check valve when deployed in the LRQA are shown in Fig. 4. The leak data behaved differently than the orifice and leak through data. Therefore, treatment of this leak as an ideal orifice does not accurately reflect observed behavior. Additional testing is needed on a larger dataset of failed components to determine if the behavior is repeatable. With an average calculated orifice diameter of 0.02 mm this leak was also much smaller than the other leak data shown. Furthermore, at pressures below approximately 31 MPa the leak stopped or the mass flow rate out of the system became negligible. Further indication that the leak behavior is being affected by other parameters such as pressure, flow, and temperature.

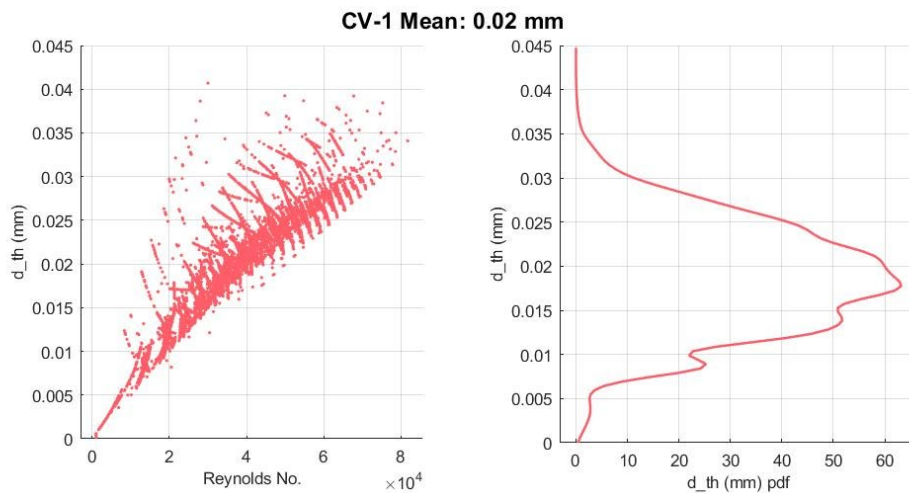


Figure 4. Helium leak data from a check valve leaking out of the weep hole, and for which the leak orifice is changing size with the Reynolds number.

2.4. LRQA Discussion

Beginning to characterize the size and behaviour of different leaks is a first step in the leak rate quantification research. Ultimately, if a significant number of failed components can be investigated this data can be utilized used to allow risk reduction credits through QRA in RCS. Models such as HyRAM are starting to be utilized for similar risk reduction credits for RCS based on scientific data [9], [10], [19]. Initial results clearly show different behaviour for different types of leaks. A larger dataset of failed components is needed to help determine the cause of this observed behaviour and

what methods should be used to accurately model different leaks. The knowledge that different types of leaks behave differently and that a leak potentially behaves significantly differently than a standard orifice is important. Potential causes of different behaviour could be related to the type of component, the type of seal (e.g., soft seat/O-ring), the type of leak (e.g., leak out), and the conditions of use or deployment life of the component. PHM and QRA work will take this failure information and begin to provide system level health and reliability information.

As previously mentioned, future work includes testing and obtaining leak rate data for a significant number of failed components. To do this there are two obvious challenges, 1) obtaining a significant number of diverse failed components and 2) obtaining known failed components to reliably leak upon redeployment in the LRQA. To address the first challenge NREL is requesting industry to send in failed components for testing. Obtaining failed components is challenging since many components are rebuilt by station operators for later redeployment and are not available for testing. There have also been challenges obtaining components that are leaking when deployed in the field to leak in the same way when deployed for testing in the LRQA. As shown by the data in Fig. 4 these leaks can be quite small and may not be detectable at low pressure. Depending on the type of leak, redeployment in the LRQA, including retorquing, could impact the size of the leak. One possible solution to this challenge would be in situ leak rate quantification testing. The LRQA has been designed to be a mobile measurement system but integrating into an operational hydrogen system comes with its own difficulties. NREL will continue to evaluate the possibility of in situ leak rate quantification testing.

3. EXPLORING KNOWLEDGE GAPS PHM AND QRA FOR HYDROGEN SYSTEMS

New approaches for data generation, collection and analysis are critical to close safety and reliability knowledge gaps regarding hydrogen infrastructure. The research team is exploring the use of QRA and PHM to fill these gaps. QRA is designed for system-level analysis, including contextual information. Incorporating real-time information collected from hydrogen systems through PHM can potentially deliver better estimates of the existing risks at the component or station-level and may improve passive security measures. Strengthening these passive measures under the established risk acceptance criteria may lead to the reduction or modification of other RCS requirements in the future. However, PHM has not been explored in this context.

To extend the use of QRA and PHM, a first step is to identify data needs for each framework. To do this, we start by using a case study consisting of a generic design of a hydrogen fueling station equipped with bulk liquid storage [20]. This generic station is used to exemplify the data requirements. A block diagram of the liquid storage section is presented in Fig. 5. The main components are identified as the liquid storage tank, which acts as a reservoir for the liquid hydrogen delivered to the station; the centrifugal cryogenic pump and the evaporator. The storage tank is equipped with a pressure relief device, the transport of the liquid hydrogen is controlled through a pressurized air-operated valve, and an isolation valve blocks the flow towards the evaporator. From this point onwards, the gaseous hydrogen continues into a compression stage, high-pressure gaseous storage cylinders, and the dispensing subsystem. In the next sections, both QRA and PHM are briefly introduced in the context of developing new hydrogen system risk assessment tools and the corresponding data requirements for these frameworks.

3.1. QRA in Hydrogen Systems

To date, most QRA efforts have focused on gaseous hydrogen systems and storage, while liquid hydrogen risks have been less explored. Hydrogen Risk Assessment Model (HyRAM) is a compendium QRA tool containing both probabilistic information and deterministic models to simulate hydrogen gas releases, thermal and pressure effects of deflagrations, detonations, and jet fires [9], [10]. Recently, the HyRAM tool was expanded to include deterministic physical models of liquid hydrogen behaviour [10].

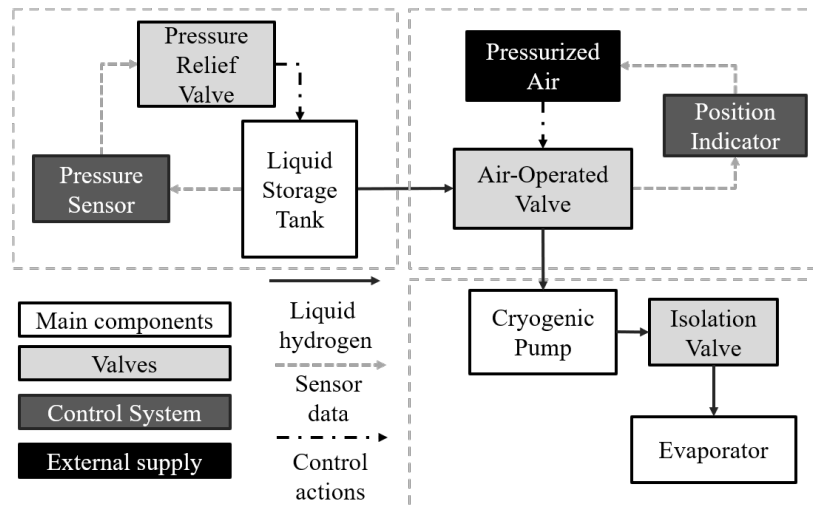


Figure 5: Liquid storage system case study block diagram.

Lack of cohesive databases of hydrogen-specific degradation, failure, and accident data is recognized as one of the biggest hindrances to credible QRAs [21]. To overcome this limitation, there is a need for systematic data collection of various types, such as the ones described in Fig. 6. While the collection of accident data [22], [23] aids the identification of relevant hazard and consequence characterization, hydrogen component reliability is scarce, hindering the estimation of hydrogen release event likelihood. There is a clear need for new probabilistic data to represent the new conditions present in liquid hydrogen systems, particularly regarding frequencies for liquid hydrogen-specific conditions. In addition, there is an opportunity to explore how new data types and techniques from reliability engineering can be further used within hydrogen RCS development.

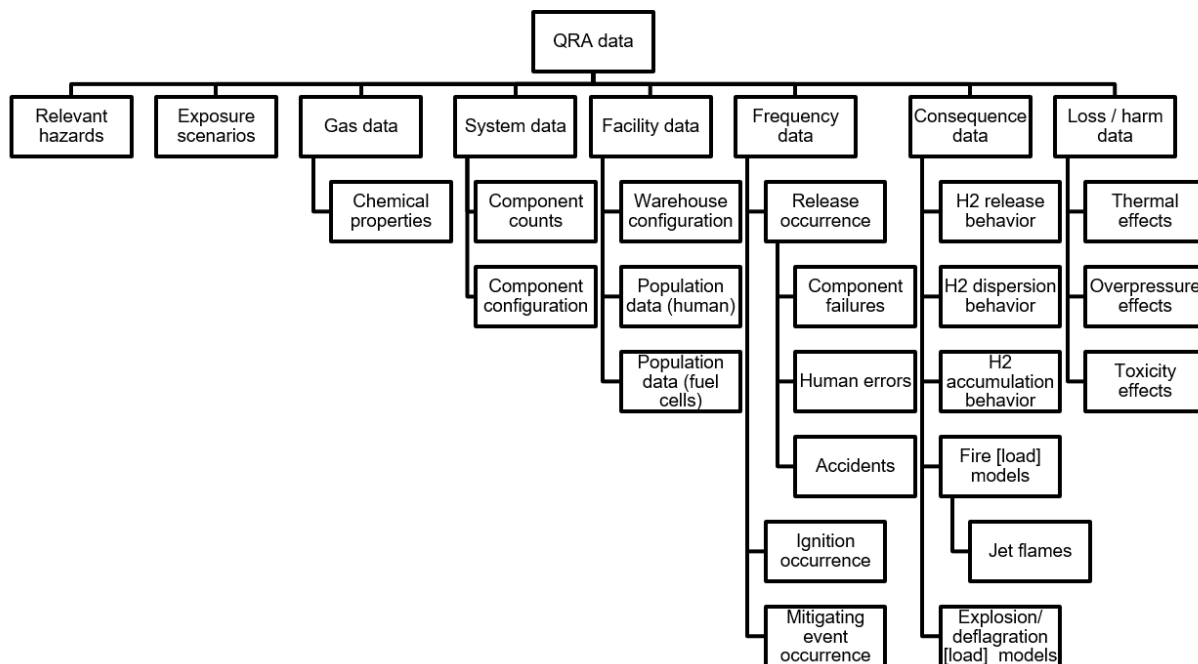


Figure 6: Types of data needed to perform QRA for a hydrogen system [21].

3.1.1. Data Requirements for QRA in Hydrogen Systems

This study is carried out through the analysis of a liquid storage system’s general design presented previously. Traditional QRA approaches are utilized to determine the system’s operation and failure

logic, as well as identifying critical failure modes and risk scenarios. Full results of this analysis are too long to present in this paper, but can be found in [24]. The failure scenarios that produce the highest risk of liquid hydrogen releases are a) malfunction due to cryogenic temperatures of the pressure relief valve system in the liquid storage tank; b) failure of the air-operated valve between the storage tank and the cryogenic pump; and c) rupture of the evaporator due to collision or external accident. These three high risk failure modes can lead to unintended release of gaseous and/or liquid hydrogen, depending on the pressure and temperature conditions of the release. Fig. 7 presents an event sequence diagram (ESD) created by extending the gaseous-focused ESD from HyRAM to include release events specifically related to liquid hydrogen.

To properly address the liquid hydrogen-related scenarios, the following aspects must be considered. For any risk scenario it is important to determine whether consequence analysis should distinguish different severity classes depending on the gaseous/liquid proportion of released hydrogen. For this, the development of physics models describing the evaporation, dispersion and ignition of liquid hydrogen releases is required. Detection, ignition, and dispersion behaviour probabilities may need to be updated, including new scenarios such as pooling or cryogenic plume described in Table 1.

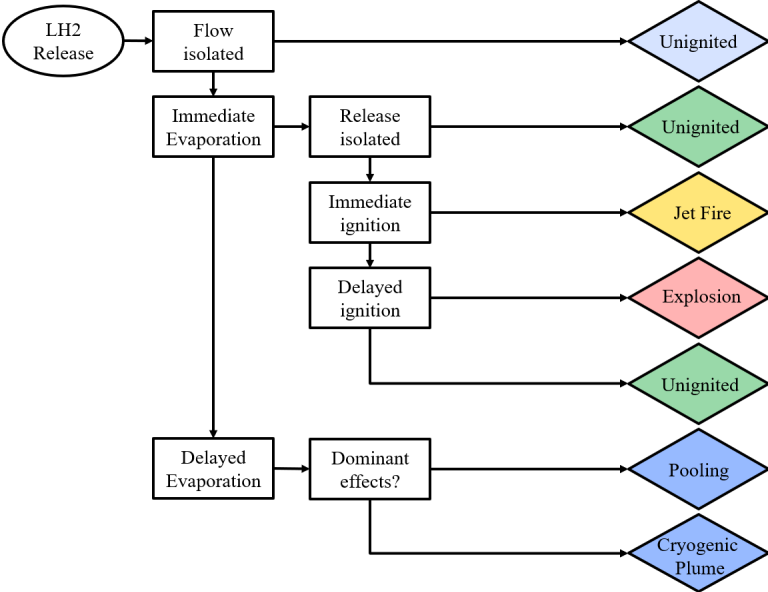


Figure 7: Proposed event sequence diagram for liquid hydrogen release events.

Table 1: Liquid hydrogen release events included in developed ESD.

Release events	Data Type
Component leak frequencies	Component reliability data and/or release frequencies per leak size.
Release Detection	A priori the same value for GH2 detection and isolation could be used. Depends on detection method.
Immediate Evaporation	Probability model. Possible dependency on physics-based model.
Delayed Evaporation leading to Pooling	Probability model. Possible dependency on physics-based model.
Delayed Evaporation leading to Cryogenic Plume	Probability model. Possible dependency on physics-based model.

Component reliability analysis is still an underdeveloped task regarding hydrogen infrastructure despite the potential application towards failure event frequency quantification and maintenance event scheduling. In this regard, leak frequencies need to be extended to represent liquid hydrogen conditions and components, particularly in those which have not been described previously in the gaseous hydrogen context (e.g., cryogenic pumps and evaporators; components in liquid service).

3.2. PHM in Hydrogen Systems

Recent advances in PHM may have benefits for hydrogen QRA. PHM is an important component in modern engineering systems, in which algorithms are designed and used to detect anomalies, diagnose faults, and predict future states of the system based on sensor measurement data. PHM combines various disciplines and data sources: sensor technology, physics of failure and degradation analysis, modern statistics, traditional reliability engineering, as well as novel applications of data-driven techniques. In the last two decades, data-driven health monitoring techniques have gained significant popularity due to the widespread deployment of low-cost sensors, high connectivity, and improvements in computational processing power [25]. Most PHM frameworks define similar stages from data acquisition to decision-making. For instance, Fig. 8 presents four distinct phases with subtasks corresponding to data acquisition, diagnostics, and prognostics assessments, which are then followed by a health management decision-making support stage [26].

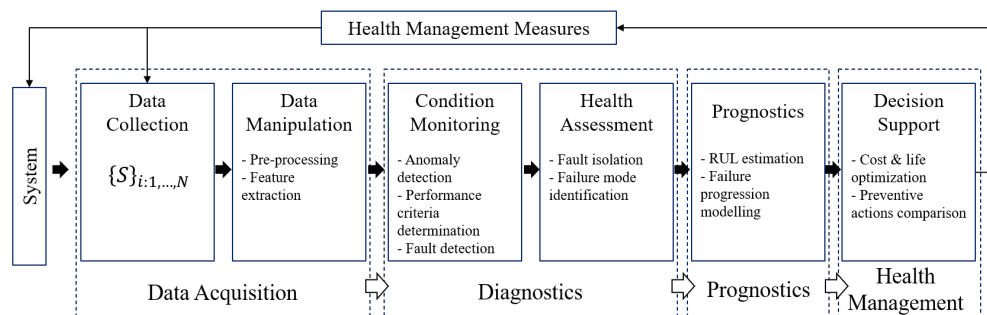


Figure 8: A holistic PHM Framework [26].

PHM could enable early leak failure detection capabilities in hydrogen systems, help identify what ambient, operational, or other conditions contribute to failure development and scheduling maintenance measures to prevent further degradation and unexpected component failure.

3.2.1. Data Requirements for PHM in Hydrogen Systems

Data acquisition is an initial and essential step of PHM frameworks, encompassing both sensor and event data. Condition-monitoring data are measurements collected via a variety of installed sensors in components whose performance is linked to the overall system's health state. Event data include the information on maintenance actions (component replacement, repairs, etc.) taken during such events (failure, breakdown, installation, etc.) that have occurred in the system. Both these data sources are employed to identify the relationship between anomalous sensor measurements and failure events. In this regard, applications of data-driven techniques could identify operational or ambient conditions that contribute to unexpected hydrogen releases. The opportunities for PHM applications in liquid hydrogen storage systems are summarized in Table 2. Some examples are described below.

Storage tanks and pipelines are the main components in the studied system. Previously, online monitoring systems have been applied for damage detection and localization in hydrogen vessels through piezoelectric sensor array and vibrations analysis [27]. Similarly, acoustic wave analysis has been implemented for leak detection in gas pipelines [28]. Vacuum conditions between double-walled component are monitored for safety reasons and could enable detection of thermal insulation loss or leakage from the inner tank [29]. Temperature and pressure anomalous variations could be employed as indicators for fault detection in these components. Another component of interest is the cryogenic pump. Given that its operation has known nominal operational conditions, the dynamic behaviours of its monitoring variables can be used to detect anomalies. For instance, centrifugal pump degradation

based on vibration measurements has been used to detect flow blockages and predict impending cavitation [30].

There are many fundamentally important variables for PHM applications in liquid hydrogen storage systems. A significant effort must be applied to develop data collection campaigns to explore data-driven reliability-focused applications in hydrogen systems. For diagnostic tasks, measurements such as vibrations and acoustic signals suggest promising results for damage detection and localization. While for prognostics, possible use sensor variables such as temperature and pressure fluctuations have potential to be employed.

Table 2: Opportunities for PHM applications in liquid hydrogen storage systems.

Component	Possible measurements	Possible Outputs
Centrifugal cryogenic pump	Discharge temperatures and flow rates, current consumption, vibrations and acoustic emissions.	Pump degradation and leak detection.
Storage tank, piping and pressure relief valves	Pressure in inner vessel/vacuum, temperature vacuum/outer jacket, and relative humidity in vent stacks, vibrations and acoustic emissions.	Leak detection and thermal insulation degradation.
System-level	Monitoring system layout, maintenance logs, fuel dispensing and delivery history.	Component failure rates and health-state prognosis

4. DISCUSSION AND FRAMEWORK INTEGRATION

NREL and UMD are working together to establish a scientific basis for risk and reliability analysis using hydrogen system data. Data collection, model development, and stakeholder engagement activities must progress in parallel to support each other and for the effort as a whole to succeed. Data collection and sharing with the LRQA at NREL and by industry stakeholders will enable the model development by providing data to test model assumptions against. These models will enable robust QRA and PHM, which need stakeholder engagement to apply these methods to hydrogen systems. NREL, as part of the National Laboratory system is positioned to reach and successfully engage industry on multiple fronts. Stakeholder engagement communication goes both ways enhancing model development and providing industry tools for risk and reliability analysis.

Both QRA and PHM can be valuable methods to allow flexible and technically based RCS. On the path toward technically based code development, station developers should be able to take credit for additional safety measures in a way which is comprehensive to the context of each individual system. QRA is fundamental to establish the technical, risk management framework, while PHM can be a way to extend QRA into a continuous process and giving the station designer's tools to face availability issues. The development of tools based on sensor monitoring data represents an opportunity for hydrogen station stakeholders to take credit for the inclusion of risk-informed barriers and mitigation measures for RCS compliance.

A united effort in the hydrogen community is the fastest way to push hydrogen systems forward toward wider adoption. The NREL and UMD collaboration will develop a framework and path for informed risk reduction which can be applied to improve both gaseous and liquid hydrogen systems. Hydrogen systems are highly instrumented and if appropriately used this instrumentation could lead to improved hydrogen system with reduced risk.

5. CONCLUSION

Ongoing challenges for hydrogen fueling stations include the use of risk informed RCS to design and permit the operation of these systems. Data collection and data analysis are key complementary aspects of overcoming these challenges. Development and use of the LRQA is providing new data on

hydrogen component leaks, while research into QRA and PHM algorithms provides insight into how to use this data to reduce risk for hydrogen systems. Quantifying the risks associated with hydrogen systems is of critical importance to address reliability and safety questions, further enabling the development of standards such as NFPA 2 and ISO 19880-1, and ultimately the widespread deployment of hydrogen infrastructure. This work constitutes an initial step in exploring hydrogen releases and data requirements which support the improvement of QRA frameworks and providing a pathway for using PHM to improve system safety.

6. ACKNOWLEDGEMENTS

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